Niobium Carbide ($NbC_{0.98}$) CRYSTAL $M_r = 104.6772$ Niobium Carbide ($NbC_{0.98}$) $C_{0.98}Nb_1(cr)$

$S°(298.15 K) = 34.966 \pm 0.4 J·K^{-1}·mol^{-1}$

$\Delta_f H°(0 K) = -138.061 \pm 2.5 kJ·mol^{-1}$

$\Delta_f H°(298.15 K) = -138.909 \pm 2.5 kJ·mol^{-1}$

Enthalpy of Formation

There are five oxygen bomb calorimetry studies on NbC reported in the literature[1-5] and one CO(g) equilibrium study.[6] The adopted $\Delta_f H°$(298.15 K) value is derived from the calorimetric study of Huber *et al.*[3] These authors studied the combustion of eight NbC_x samples where x covers the range 0.686 to 0.984. For each composition six to eight combustions were performed. Huber *et al.*[3] reported that the combustions varied from 98.78 to 100% of completion. Corrections of the order 0.51% or less were made to the enthalpy of combustion value to account for impurities in seven of the eight samples. The correction was 3.33% for the $x = 0.984$ sample. The calculated heats of formation were fitted to a quadratic equation by the least squares method by Huber *et al.*[3] Each value was weighted inversely proportional to the square of its uncertainty. Using the quadratic equation for $\Delta_f H°$(298.15 K) and correcting for the JANAF value of $\Delta_f H°(Nb_2O_5$, cr, 298.15 K),[7] we interpolate to $x = 0.98$, calculate and adopt $\Delta_f H°(298.15 K) = -33.20 \pm 0.6 kcal·mol^{-1}$. Due to the large error in the data points, a linear equation can be chosen to fit the data without making a statistically significant difference.[3]

Huber *et al.*[3] and Storms[8] have reanalyzed much of the calorimetric and equilibrium data[1-6] for NbC_x ($x = 0.686$ to 0.984). A graphical comparison of the results (i.e., $\Delta_f H°$(298.15 K) values vs. x) indicated that the quadratic equation suggested by Huber *et al.*[3] is a satisfactory representation of the various $\Delta_f H°$(298.15 K) results for NbC_x. The shortcomings of the various studies have been discussed by Huber *et al.*[3] and Storms.[8] For comparison, the oxygen combustion study by Mah and Boyle[1] leads to $\Delta_f H°(298.15 K) = -31.14 \pm 0.8 kcal·mol^{-1}$ for $NbC_{0.9445}$.

Heat Capacity and Entropy

There have been three low temperature heat capacity studies for NbC_x· Pankratz *et al.*[13] using a $NbC_{0.996}$ sample (52–296 K), Toth *et al.*[19] using five NbC_x samples where $x = 0.77$, 0.83, 0.86, 0.91, and 0.96 (1.5–18 K), and Sandernaw and Storms[14] using three NbC_x samples where $x = 0.702$, 0.825, and 0.980 (7.5–320 K). In addition there are numerous high temperature heat capacity and enthalpy studies on various NbC_x samples.[9-13, 15-18] The adopted heat capacity values are those suggested by Turchanin *et al.*[20] Their $C_p°$ values were represented by a five term equation for the range 0–3000 K and is a compromise of the reported data mentioned, all adjusted to the composition $NbC_{0.98}$.

Phase Data

NbC has a face centered cubic structure of the NaCl type.[8] The NbC phase exists, following the phase diagram of Storms,[8] from roughly $NbC_{0.70}$ to near $NbC_{0.99}$. At the NbC–C eutectic temperature of 3573 ± 50 K, the phase limit is $NbC_{0.97}$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J·K^{-1}mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0.98	0.98			1			
0	0.	0.	INFINITE	−5.422	−138.061	−138.061	INFINITE
100	14.426	7.983	56.725	−4.874	−138.352	−137.801	71.980
200	27.476	22.238	35.932	−2.739	−138.635	−137.103	35.808
298.15	36.233	34.966	34.966	0.	−138.909	−136.785	23.964
300	36.380	35.190	34.966	0.067	−138.903	−136.772	23.814
400	41.882	46.463	36.466	3.999	−138.481	−136.120	17.776
500	45.145	56.179	39.461	8.359	−137.986	−135.587	14.165
600	47.363	64 616	42.966	12.990	−137.514	−135.153	11.766
700	48.911	72.038	46.600	17.806	−137.091	−134 793	10.058
800	50.124	78.651	50.200	22.760	−136.718	−134.491	8.781
900	51.087	84.611	53.698	27.822	−136.389	−134.233	7.791
1000	51.923	90.038	57.065	32.973	−136.097	−134.009	7.000
1100	52.635	95.021	60.292	38.202	−135.839	−133.813	6.354
1200	53.304	99.630	63.380	43.499	−135.609	−133.640	5.817
1300	53.932	103.921	66.336	48.861	−135.398	−133.484	5.363
1400	54.504	107.939	69.165	54.283	−135.207	−133.344	4.975
1500	55.061	111.718	71.878	59.761	−135.038	−133.217	4.639
1600	55.605	115.289	74.480	65.295	−134.894	−133.101	4.345
1700	56.134	118.676	76.981	70.882	−134.781	−132.992	4.086
1800	56.651	121.900	79.388	76.521	−134.705	−132.889	3.856
1900	57.153	124.976	81.707	82.211	−134.671	−132.790	3.651
2000	57.656	127.920	83.944	87.952	−134.683	−132.691	3.466
2100	58.158	130.746	86.106	93.743	−134.745	−132.590	3.298
2200	58.660	133.463	88.197	99.583	−134.863	−132.484	3.146
2300	59.162	136.081	90.223	105.475	−135.042	−132.373	3.006
2400	59.664	138.610	92.187	111.416	−135.293	−132.251	2.878
2500	60.166	141.056	94.093	117.407	−135.630	−132.118	2.760
2600	60.668	143.425	95.945	123.449	−136.076	−131.969	2.651
2700	61.170	145.724	97.746	129.541	−136.669	−131.801	2.550
2800	61.672	147.958	99.500	135.683	−163.822	−131.122	2.446
2900	62.174	150.131	101.208	141.875	−163.565	−129.959	2.341
3000	62.676	152.247	102.874	148.118	−163.272	−128.805	2.243

PREVIOUS. CURRENT: December 1973

Niobium Carbide ($NbC_{0.98}$) $C_{0.98}Nb_1(cr)$

Carbon (C) (REFERENCE STATE – GRAPHITE, Spectroscopic–Grade Acheson) $M_r = 12.011$ Carbon (C) C_1(ref)

S°(298.15 K) = 5.74 0.21 J·K^{-1}·mol^{-1}

$\Delta_f H^\circ$(0 K) = 0 kJ·mol^{-1}
$\Delta_f H^\circ$(298.15 K) = 0 kJ·mol^{-1}

Enthalpy of Formation

$\Delta_f H^\circ$ is zero by definition for the adopted standard reference state of Achesson spectroscopic graphite, artificial graphite of spectroscopic grade which is graphitized near 2600°C in an Acheson–type elesctric furnace. This standard state was adopted by CODATA[1] in order to be more consistent with the samples used in determing $\Delta_f H^\circ$(298.15) of CO_2(g). CODATA[1] cites references which show the effects of various graphite samples on $\Delta_f H^\circ(CO_2)$. Their assigned uncertainty[1] of ±0.031 kcal·mol^{-1} for $\Delta_f H^\circ(CO_2)$ is a rough measure of the deviations of various high purity graphites from our standard state. Larger deviations occur in carbon samples which are impure or less completely graphitized or which have much disorder or high surface area. Gross deviations (up to several kcal·mol) have been found for other carbons; e.g., many "glassy" carbons appear to be more stable than graphite at elevated temperatures due to large $\Delta_f S$ values[2] which compensate for positive values of $\Delta_f H$.

Heat Capacity and Entropy

S°(298.15) and H°(298.15 K)–H°(0 K) are the values selected by CODATA[1] based on C_p° (13–301 K) of CS–grade Acheson graphite measured by DeSorbo and Tyler.[3] DeSorbo's later study[3] gave minor corrections to C_p° and more information on his sample. Due to differences in C_p° of various graphites, we increase the uncertainty of S°(298.15) from ±0.029[1] to ±0.05 cal·K^{-1}·mol^{-1}. The entropy extrapolation below 13 K was given[3] as 0.0041 cal·K^{-1}·mol^{-1}. Properties tabulated below 298.15 K are from our smoothing of the data.[3] C_p° above 298.15 K is based on enthalpy data of McDonald[4] and West and Ishihara[5] and on C_p° data of Cezairliyan *et al.*[6 7] Deviations of the enthalpy data from our table are −0.3 to +0.6%, (omitting 341 and 1037 K)[4] and 0.0 to −0.6%.[5] Deviations of the C_p° equations[6,7] from our table are much less than the estimated uncertainties of 3%[6] and 3 to 5%.[7] The selected studies[4-7] show reasonable agreement in their regions of overlap even though they involve different grades of graphite. Together, they yield mutually consistent data extending up to 3800 K.

Discrepancies in other C_p° data are of concern since no single type of graphite has been accurately measured over the whole temperature range. At all temperatures the many studies show unusually large differences, some of which are due to deviations of the graphite samples from our chosen standard state. For example, the C_p° of natural (Ceylon) graphite[3] was found to be approximately 9% lower from 200 to 300 K, yielding values of S°(298.15) and H°(298.15 K)–H°(0 K) which are lower by 0.08 cal·K^{-1}·mol^{-1} and 21 cal·mol^{-1}, respectively. Lutkov *et al.*[8] reported similar differences in C_p° among two graphites and one pyrolytic carbon. Discrepancies are even larger below 30 K[9 10] and above 3000 K.[6, 10-15] vaporization and melting. New studies of various graphites by laser flash[16] and differential scanning calorimetry[17] tend to confirm our C_p° at 350–950 K, where the largest deviations (−3%) are roughly equal to the experimental error. More controversial are C_p°[12] and enthalpy[13] studies which gave C_p° curves that rise very rapidly near 3500 K. Recent pulse–heating data,[7] however, gave a slowly rising C_p° which is linear up to 3800 K. Four C_p° studies[6,7,12,14] and an enthalpy study[15] agree satisfactorily below 3500 K, so the discrepancy must be due to temperature–dependent differences in experimental methods or graphite samples. This is a region where some graphites degrade rapidly with emission of particles, leading to possible bias in C_p° data. Moreover, Whittaker has proposed[18] that graphite is metastable in this region and slowly transforms to carbynes. If e this is the case, then very rapid measurements[7] should yield C_p° data which are different and more appropriate to graphite. Th rapidly rising enthalpy data[13] could be explained by Whittaker's proposal or by differences in the various graphite samples.[13]

Sublimation Data

See the tables for C(g), C_2(g), C_3(g), C_4(g), etc. The most abundant species is C_3. Recent analyses gave sublimation temperature values (corresponding to 1 atm total pressure of all carbon species) of 3895–4020 K[19] from carbon arc data, ≤4070 K[20] from mass–loss data at 0.1–11 atm, and approximately 3915 K[21] from extrapolation of mass–spectrometric data at low pressure. Earlier values for this controversial point (see below) were summarized by Palmer.[22]

Fusion Data and Phase Data

Controversy surrounds the solid–liquid–vapor triple point which recent studies place either at approximately 4000 K and approximately 1 atm (carbyne form)[18] or at 4130 ± 30 K and 120 ± 10 atm (pyrolytic graphite).[23] We doubt the latter triple point because the temperature is displaced by 400 to 800 kelvins from the sublimation curves (and ref. cited therein).[19-22] The nature of the observed phenomenon[22-24] has been questioned[18] as well as the measurement of temperature.[18 19,24] Also controversial is Whittaker's proposal[18] that several carbyne forms are more stable than graphite above 2600 K. Evidence includes X–ray data which were interpreted[18] to indicate slow forward transitions, graphite → carbynes, but rapid reverse transitions. These transitions might explain discrepancies observed in various C_p° curves but alternative explanations are possible. We retain graphite as the reference state at all temperatures; this arbitrary choice avoids the need to switch phases at the proposed transition point, sublimation point or melting point, all of which are subject to change.

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Continued on page 700

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−1.051	0.	0.	0.
100	1.674	0.952	10.867	−0.991	0.	0.	0.
200	5.006	3.082	6.407	−0.665	0.	0.	0.
250	6.816	4.394	5.871	−0.369	0.	0.	0.
298.15	8.517	5.740	5.740	0.	0.	0.	0.
300	8.581	5.793	5 741	0.016	0.	0.	0.
350	10.241	7.242	5.851	0.487	0.	0.	0.
400	11.817	8.713	6.117	1.039	0.	0.	0.
450	13.289	10.191	6.487	1.667	0.	0.	0.
500	14.623	11.662	6.932	2.365	0.	0.	0.
600	16.844	14.533	7.961	3.943	0.	0.	0.
700	18.537	17.263	9.097	5.716	0.	0.	0.
800	19.827	19.826	10.279	7.637	0.	0.	0.
900	20.824	22.221	11.475	9.672	0.	0.	0.
1000	21.610	24.457	12.662	11.795	0.	0.	0.
1100	22.244	26.548	13.831	13.989	0.	0.	0.
1200	22.766	28.506	14.973	16.240	0.	0.	0.
1300	23.204	30.346	16.085	18.539	0.	0.	0.
1400	23.578	32.080	17.167	20.879	0.	0.	0.
1500	23.904	33.718	18.216	23.253	0.	0.	0.
1600	24.191	35.270	19.234	25.658	0.	0.	0.
1700	24.448	36.744	20.221	28.090	0.	0.	0.
1800	24.681	38.149	21.178	30.547	0.	0.	0.
1900	24.895	39.489	22.107	33.026	0.	0.	0.
2000	25.094	40.771	23.008	35.525	0.	0.	0.
2100	25.278	42.000	23.883	38.044	0.	0.	0.
2200	25.453	43.180	24.734	40.581	0.	0.	0.
2300	25.618	44.315	25.561	43.134	0.	0.	0.
2400	25.775	45.408	26.365	45.704	0.	0.	0.
2500	25.926	46.464	27.148	48.289	0.	0.	0.
2600	26.071	47.483	27.911	50.889	0.	0.	0.
2700	26.212	48.470	28.654	53.503	0.	0.	0.
2800	26.348	49.426	29.379	56.131	0.	0.	0.
2900	26.481	50.353	30.086	58.773	0.	0.	0.
3000	26.611	51.253	30.777	61.427	0.	0.	0.
3100	26.738	52.127	31.451	64.095	0.	0.	0.
3200	26.863	52.978	32.111	66.775	0.	0.	0.
3300	26.986	53.807	32.756	69.467	0.	0.	0.
3400	27.106	54.614	33.387	72.172	0.	0.	0.
3500	27.225	55.401	34.005	74.889	0.	0.	0.
3600	27.342	56.170	34.610	77.617	0.	0.	0.
3700	27.459	56.921	35.203	80.357	0.	0.	0.
3800	27.574	57.655	35.784	83.109	0.	0.	0.
3900	27.688	58.372	36.354	85.872	0.	0.	0.
4000	27.801	59.075	36.913	88.646	0.	0.	0.
4100	27.913	59.763	37.462	91.432	0.	0.	0.
4200	28.024	60.437	38.001	94.229	0.	0.	0.
4300	28.134	61.097	38.531	97.037	0.	0.	0.
4400	28.245	61.745	39.051	99.856	0.	0.	0.
4500	28.354	62.381	39.562	102.685	0.	0.	0.
4600	28.462	63.006	40.065	105.526	0.	0.	0.
4700	28.570	63.619	40.560	108.378	0.	0.	0.
4800	28.678	64.222	41 047	111.240	0.	0.	0.
4900	28.785	64.814	41.526	114.114	0.	0.	0.
5000	28.893	65.397	41.997	116.997	0.	0.	0.
5100	28.999	65.970	42.462	119.892	0.	0.	0.
5200	29.106	66.534	42.919	122.797	0.	0.	0.
5300	29.211	67.089	43.370	125.713	0.	0.	0.
5400	29.317	67.636	43.814	128.640	0.	0.	0.
5500	29.422	68.175	44.252	131.577	0.	0.	0.
5600	29.528	68.706	44.684	134.524	0.	0.	0.
5700	29.632	69.230	45.110	137.482	0.	0.	0.
5800	29.737	69 746	45.531	140.451	0.	0.	0.
5900	29.842	70.255	45.945	143.429	0.	0.	0.
6000	29.946	70.758	46.355	146.419	0.	0.	0.

PREVIOUS· March 1978 (1 atm) CURRENT March 1983 (1 bar)

$IP(C, g) = 90820.42 \pm 0.1\ cm^{-1}$
$S°(298.15\ K) = 158.100 \pm 0.86\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 711.19 \pm 0.46\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 716.67 \pm 0.46\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights

ϵ_i, cm^{-1}	g_i
0.00	1
16.40	3
43.40	5
10192.63	5
21648.01	1
33735.20	5

Enthalpy of Formation

$\Delta_f H°(298.15\ K) = 171.29 \pm 0.11\ kcal \cdot mol^{-1}$ is the value selected by CODATA[1] based on $D_0°(CO) = 89595 \pm 30\ cm^{-1}$ ($256.165 \pm 0.086\ kcal \cdot mol^{-1}$) from Douglas and Moller.[2] The conversion factor used by CODATA[1] corresponds to the negligibly different value of 256.163 $kcal \cdot mol^{-1}$; this yields the adopted $\Delta_f H°$ when combined with $\Delta_f H°(CO, 0\ K) = -27.201 \pm 0.024\ kcal \cdot mol^{-1}$.[1,3] According to Krupenie[4] it is most likely that the atomic dissociation products are in their ground states as assumed in the adopted $D_0°(CO)$.

The enthalpy of sublimation, $\Delta_{sub}H° = \Delta_f H°$, is confirmed by Knudsen–effusion mass–spectrometric data of Wachi and Gilmartin[5] for graphite. They obtained absolute pressures from calibrations using gold and cobalt; pressures from the latter were higher by 8.74%. Our 3rd law analyses yield $\Delta_{sub}H°(298.15\ K) = 171.22 \pm 0.61$ and $170.78 \pm 0.61\ kcal \cdot mol^{-1}$ from gold and cobalt, respectively. 2nd law values are $\Delta_{sub}H°(298.15\ K) = 172.5 \pm 3.3\ kcal \cdot mol^{-1}$ and $\Delta_{sub}S°(\text{2nd law}) - \Delta_{sub}S°(\text{3rd law}) = 0.5 \pm 1.2$ (gold) and 0.7 ± 1.2 (cobalt) $cal \cdot K^{-1} \cdot mol^{-1}$). The data consisted of 14 points in the range 2509–2753 K. None of the other studies of C(g) over pure graphite included calibrations for conversion of ion intensities to absolute pressures.

Heat Capacity and Entropy

The atomic energy levels are from Moore.[6] $S°(298.15\ K)$ and $H°(0\ K) - H°(298.15\ K)$ are the same as the values selected by CODATA.[1] Observed and predicted levels above 60333 cm^{-1} are omitted since they do not change the thermodynamic functions at 6000 K. At 14000 K the BETHE–FILL cut–off method would yield a Gibbs energy function ~0.1 $cal \cdot K^{-1} \cdot mol^{-1}$ larger than either the present cut–off method (TEMPER).[7]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.536	711.185	711.185	INFINITE
100	21.271	135.180	176.684	−4.150	713.511	700.088	−365.689
200	20.904	149.768	160.007	−2.048	715.287	685.950	−179.152
250	20.861	154.427	158.443	−1.004	716.035	678.527	−141.770
298.15	20.838	158.100	158.100	0.	716.670	671.244	−117.599
300	20.838	158.228	158.100	0.039	716.693	670.962	−116.825
350	20.824	161.439	158.354	1.080	717.263	663.294	−98.991
400	20.815	164.219	158.917	2.121	717.752	655.550	−85.606
450	20.809	166.671	159.645	3.162	718.165	647.749	−75.189
500	20.804	168.863	160.459	4.202	718.507	639.906	−66.851
600	20.799	172.655	162.185	6.282	719.009	624.135	−54.336
700	20.795	175.861	163.916	8.362	719.315	608.296	−45.392
800	20.793	178.638	165.587	10.441	719.474	592.424	−38.681
900	20.792	181.087	167.175	12.520	719.519	576.539	−33.461
1000	20.791	183.278	168.678	14.600	719.475	560.654	−29.286
1100	20.791	185.259	170.097	16.679	719.360	544.777	−25.869
1200	20.793	187.068	171.437	18.758	719.188	528.913	−23.023
1300	20.796	188.733	172.704	20.837	718.968	513.066	−20.615
1400	20.803	190.274	173.905	22.917	718.709	497.237	−18.552
1500	20.814	191.710	175.044	24.998	718.415	481.427	−16.765
1600	20.829	193.053	176.128	27.080	718.092	465.639	−15.202
1700	20.850	194.317	177.162	29.164	717.744	449.871	−13.823
1800	20.878	195.509	178.148	31.250	717.373	434.124	−12.598
1900	20.912	196.639	179.092	33.340	716.984	418.399	−11.503
2000	20.952	197.713	179.996	35.433	716.577	402.694	−10.517
2100	20.999	198.736	180.864	37.530	716.156	387.010	−9.626
2200	21.052	199.714	181.699	39.633	715.722	371.347	−8.817
2300	21.110	200.651	182.503	41.741	715.277	355.703	−8.078
2400	21.174	201.551	183.278	43.855	714.821	340.079	−7.402
2500	21.241	202.417	184.026	45.976	714.357	324.474	−6.780
2600	21.313	203.251	184.750	48.103	713.884	308.888	−6.206
2700	21.387	204.057	185.450	50.238	713.405	293.321	−5.675
2800	21.464	204.836	186.129	52.381	712.920	277.771	−5.182
2900	21.542	205.591	186.787	54.531	712.429	262.239	−4.723
3000	21.621	206.322	187.426	56.689	711.932	246.723	−4.296
3100	21.701	207.032	188.047	58.856	711.431	231.224	−3.896
3200	21.780	207.723	188.651	61.030	710.925	215.742	−3.522
3300	21.859	208.394	189.239	63.212	710.414	200.275	−3.170
3400	21.936	209.048	189.812	65.401	709.899	184.824	−2.839
3500	22.012	209.685	190.371	67.599	709.380	169.389	−2.528
3600	22.087	210.306	190.916	69.804	708.857	153.968	−2.234
3700	22.159	210.912	191.448	72.016	708.329	138.561	−1.956
3800	22.230	211.504	191.968	74.235	707.797	123.169	−1.693
3900	22.298	212.082	192.477	76.462	707.260	107.791	−1.444
4000	22.363	212.648	192.974	78.695	706.719	92.427	−1.207
4100	22.426	213.201	193.461	80.934	706.173	77.077	−0.982
4200	22.487	213.742	193.937	83.180	705.621	61.740	−0.768
4300	22.544	214.272	194.404	85.432	705.065	46.416	−0.564
4400	22.600	214.791	194.861	87.689	704.503	31.105	−0.369
4500	22.652	215.299	195.310	89.951	703.936	15.807	−0.183
4600	22.702	215.797	195.750	92.219	703.363	0.521	−0.006
4700	22.750	216.286	196.182	94.492	702.784	−14.752	0.164
4800	22.795	216.766	196.605	96.769	702.199	−30.012	0.327
4900	22.838	217.236	197.022	99.051	701.607	−45.261	0.482
5000	22.878	217.698	197.431	101.337	701.009	−60.497	0.632
5100	22.917	218.151	197.832	103.626	700.404	−75.721	0.776
5200	22.953	218.597	198.227	105.920	699.793	−90.933	0.913
5300	22.987	219.034	198.616	108.217	699.174	−106.133	1.046
5400	23.020	219.464	198.998	110.517	698.548	−121.322	1.174
5500	23.051	219.887	199.374	112.821	697.914	−136.499	1.296
5600	23.080	220.302	199.744	115.127	697.273	−151.664	1.415
5700	23.107	220.711	200.108	117.437	696.625	−166.818	1.529
5800	23.133	221.113	200.467	119.749	695.968	−181.961	1.639
5900	23.157	221.509	200.820	122.063	695.304	−197.092	1.745
6000	23.181	221.898	201.168	124.380	694.631	−212.211	1.847

PREVIOUS: March 1978 (1 atm) CURRENT: March 1983 (1 bar)

Carbon, Ion (C^+) IDEAL GAS M_r = 12.01045 Carbon, Ion (C^+) $C_1^+(g)$

IP(C^+, g) = 196664.7 ± 0.5 cm^{-1}
$S°$(298.15 K) = 154.662 ± 0.02 $J·K^{-1}·mol^{-1}$

$\Delta_f H°$(0 K) = 1797.639 ± 0.46 $kJ·mol^{-1}$
$\Delta_f H°$(298.15 K) = [1809.435] $kJ·mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^2P_{1/2}$	0.0	2
$^2P_{3/2}$	63.42	4
$^4P_{1/2}$	43003.3	2
$^4P_{3/2}$	43025.3	4
$^4P_{5/2}$	43053.6	6

Enthalpy of Formation

$\Delta_f H°$(C^+, g, 0 K) is calculated from $\Delta_f H°$(C, g, 0 K)[1] using the spectroscopic value of IP(C) = 90820.42 ± 0.1 cm^{-1} (1086.454 ± 0.001 $kJ·mol^{-1}$) from Moore.[2] The ionization limit is converted from cm^{-1} to $kJ·mol^{-1}$ using the factor, 1 cm^{-1} = 0.01196266 $kJ·mol^{-1}$, which is derived from the 1973 CODATA fundamental constants.[3] Rosenstock *et al.*[4] and Levin and Lias[5] have summarized additional ionization and appearance potential data.

$\Delta_f H°$(C^+, g, 298.15 K) is calculated from $\Delta_f H°$(C, g, 0 K) by using IP(C) with JANAF[1] enthalpies, $H°(0\ K) - H°(298.15\ K)$, for C(g), C^+(g), and e^-(ref). $\Delta_f H°$($C \rightarrow C^+ + e^-$, 298.15 K) differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[4] $\Delta_f H°$(298.15 K) should be changed by −6.197 $kJ·mol^{-1}$ if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Moore,[2] is incomplete because many theoritically predicted levels that any reasonable method of filling in these missing levels and cutting off the summation in the partition function[6] has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of all levels other than the ground state and the first four excited states; the next excited state is 74930.1 cm^{-1} above the ground state. Since inclusion of these excited states has no effect on the thermodynamic functions (to 6000 K), we list only the ground state and the first four excited states. The reported uncertainty in $S°$(298.15 K) is due to uncertainties in the relative ionic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the excited states and use of different fill and cutoff procedures.[6]

References

[1] JANAF Thermochemical Tables: C (g), 3–31–83; e^-(ref), 3–31–82.
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[4] H. M. Rosenstock, K. Draxl *et al.*, J. Phys. Chem. Ref. Data 6, Supp. 1 (1977).
[5] R. D. Levin and S. G. Lias, U. S. Nat. Bur. Stand., NSRDS–NBS–71, (1982).
[6] J. R. Downey, Jr., The Dow Chemical Company, AFOSR–TR–0960, Contract No. F44620–75–1–0048, (1978).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J·K^{-1}mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.649	1797.639		
100	22.496	131.192	173.519	−4.233			
200	21.213	146.246	156.586	−2.068			
250	21.056	150.961	155.008	−1.012			
298.15	20.974	154.662	154.662	0.	1809.435	1758.779	−308.131
300	20.971	154.792	154.662	0.039	1809.496	1758.464	−306.176
350	20.921	158.020	154.918	1.086	1811.112	1749.830	−261.148
400	20.889	160.812	155.484	2.131	1812.644	1740.970	−227.347
450	20.867	163.271	156.215	3.175	1814.099	1731.923	−201.036
500	20.851	165.468	157.032	4.218	1815.483	1722.717	−179.971
600	20.831	169.268	158.765	6.302	1818.067	1703.917	−148.339
700	20.819	172.478	160.500	8.384	1820.455	1684.701	−125.714
800	20.811	175.257	162.175	10.466	1822.695	1665.154	−108.723
900	20.806	177.708	163.768	12.547	1824.819	1645.332	−95.493
1000	20.802	179.900	165.273	14.627	1826.855	1625.279	−84.896
1100	20.799	181.883	166.694	16.707	1828.820	1605.026	−76.216
1200	20.797	183.692	168.037	18.787	1830.727	1584.597	−68.976
1300	20.795	185.357	169.306	20.866	1832.586	1564.010	−62.843
1400	20.794	186.898	170.508	22.946	1834.405	1543.282	−57.581
1500	20.793	188.333	171.649	25.025	1836.188	1522.425	−53.016
1600	20.792	189.675	172.734	27.105	1837.941	1501.450	−49.017
1700	20.791	190.935	173.768	29.184	1839.667	1480.366	−45.486
1800	20.791	192.123	174.755	31.263	1841.368	1459.182	−42.344
1900	20.790	193.247	175.699	33.342	1843.047	1437.903	−39.531
2000	20.790	194.314	176.603	35.421	1844.705	1416.537	−36.996
2100	20.790	195.328	177.471	37.500	1846.344	1395.088	−34.701
2200	20.789	196.295	178.305	39.579	1847.964	1373.562	−32.613
2300	20.789	197.219	179.107	41.658	1849.568	1351.962	−30.704
2400	20.789	198.104	179.881	43.737	1851.156	1330.293	−28.953
2500	20.789	198.953	180.627	45.815	1852.729	1308.558	−27.341
2600	20.788	199.768	181.347	47.894	1854.286	1286.761	−25.851
2700	20.788	200.553	182.044	49.973	1855.829	1264.903	−24.471
2800	20.788	201.309	182.719	52.052	1857.359	1242.989	−23.188
2900	20.788	202.038	183.372	54.131	1858.875	1221.021	−21.993
3000	20.788	202.743	184.006	56.209	1860.377	1199.000	−20.876
3100	20.788	203.425	184.622	58.288	1861.867	1176.929	−19.831
3200	20.788	204.085	185.220	60.367	1863.345	1154.811	−18.850
3300	20.787	204.724	185.801	62.446	1864.809	1132.647	−17.928
3400	20.787	205.345	186.367	64.525	1866.262	1110.438	−17.060
3500	20.787	205.947	186.918	66.603	1867.703	1088.187	−16.240
3600	20.787	206.533	187.455	68.682	1869.132	1065.895	−15.466
3700	20.787	207.103	187.978	70.761	1870.549	1043.563	−14.732
3800	20.787	207.657	188.489	72.839	1871.955	1021.193	−14.037
3900	20.788	208.197	188.987	74.918	1873.349	998.787	−13.377
4000	20.788	208.723	189.474	76.997	1874.732	976.344	−12.750
4100	20.788	209.236	189.950	79.076	1876.104	953.868	−12.152
4200	20.788	209.737	190.415	81.155	1877.464	931.358	−11.583
4300	20.789	210.227	190.870	83.233	1878.814	908.815	−11.040
4400	20.789	210.705	191.315	85.312	1880.153	886.242	−10.521
4500	20.790	211.172	191.751	87.391	1881.480	863.638	−10.025
4600	20.791	211.629	192.179	89.470	1882.797	841.005	−9.550
4700	20.792	212.076	192.597	91.550	1884.103	818.343	−9.095
4800	20.794	212.514	193.008	93.629	1885.399	795.653	−8.658
4900	20.795	212.942	193.410	95.708	1886.683	772.937	−8.240
5000	20.797	213.362	193.805	97.788	1887.958	750.195	−7.837
5100	20.800	213.774	194.192	99.868	1889.222	727.427	−7.450
5200	20.803	214.178	194.573	101.948	1890.475	704.634	−7.078
5300	20.806	214.575	194.947	104.028	1891.718	681.818	−6.720
5400	20.810	214.964	195.314	106.109	1892.951	658.978	−6.374
5500	20.814	215.345	195.674	108.190	1894.174	636.115	−6.041
5600	20.819	215.720	196.029	110.272	1895.387	613.230	−5.720
5700	20.824	216.089	196.378	112.354	1896.590	590.324	−5.410
5800	20.831	216.451	196.721	114.437	1897.782	567.397	−5.110
5900	20.838	216.807	197.058	116.520	1898.965	544.449	−4.820
6000	20.845	217.158	197.390	118.604	1900.139	521.481	−4.540

PREVIOUS· March 1978 (1 atm) CURRENT: March 1983 (1 bar)

Carbon, Ion (C^+) $C_1^+(g)$

Carbon, Ion (C^-) IDEAL GAS $M_r = 12.01155$ Carbon, Ion (C^-) $C_1^-(g)$

EA(C, g) = 1.2629 ± 0.0003 eV
$S°(298.15\ K) = 151.384 \pm 0.003\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 589.33 \pm 2\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [588.284]\ kJ \cdot mol^{-1}$

Electonic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^4S_3$	0	4
^2D	9920	10

Enthalpy of Formation

$\Delta_f H°(C^-, g, 0\ K)$ is calculated from $\Delta_f H°(C, g, 0\ K)$[1] using the adopted electron affinity of EA(C) = 1.2629 + 0.0003 eV (121.850 ± 0.029 kJ·mol^{-1}). This value, recommended by Hotop and Lineberger,[2] is based on a laser photodetachment electron spectrometry study.[3] Additional information on $C^-(g)$ may be obtained in the critical discussions of Hotop and Lineberger,[2,4] Rosenstock *et al.*[5] and Massey.[6]

$\Delta_f H°(C^-, g, 298.15\ K)$ is obtained from $\Delta_f H°(C, g, 0\ K)$ by using EA(C) with JANAF[1] enthalpies, $H°(0\ K) - H°(298.15\ K)$, for $C^-(g)$, C(g), and e^-(ref). $\Delta_r H°(C^- \rightarrow C + e^-, 298.15\ K)$ differs from a room–temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[5] $\Delta_f H°(298.15\ K)$ should be changed by +6.197 kJ·mol^{-1} if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

Electronic energy levels are from the laser photodetachment study of Feldmann.[3] He found that the $C^-(^2D)$ state has a binding energy of 0.033 ± 0.001 eV (266 ± 8 cm^{-1}) relative to ground state $C(^3P_0)$. The electronic energy of 9920 cm^{-1} is the difference in binding energy between ground and excited states. Spin–orbit splitting of the ^2D state was not resolved[3] but has been estimated[2,4] to be 3 cm^{-1}. We neglect this splitting because its effect is negligible. $C^-(^2D)$ binding energies obtained by other mehtods[4,7] are in satisfactory agreement.

Note that we include the excited state even though its binding energy is only 266 cm^{-1}. If this state were omitted, the Gibbs energy function (J·K^{-1}·mol^{-1}) would change by −0.004 (1700 K), −0.176 (3000 K) and −1.732 (6000 K).

References

[1] JANAF Thermochemical Tables: C(g), 3–31–83; e^-(ref), 3–31–82.
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[7] V. A. Aparin *et al.*, Soviet Phys. – JETP 39, 989 (1974).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.197	589.335		
100	20.786	128.676	169.864	−4.119			
200	20.786	143.084	153.285	−2.040			
250	20.786	147.722	151.726	−1.001			
298.15	20.786	151.384	151.384	0.	588.284	551.115	−96.553
300	20.786	151.512	151.384	0.038	588.268	550.885	−95.918
350	20.786	154.716	151.637	1.078	587.797	544.690	−81.291
400	20.786	157.492	152.199	2.117	587.245	538.569	−70.330
450	20.786	159.940	152.926	3.156	586.617	532.521	−61.813
500	20.786	162.130	153.739	4.196	585.919	526.547	−55.008
600	20.786	165.920	155.463	6.274	584.340	514.817	−44.819
700	20.786	169.124	157.191	8.353	582.568	503.368	−37.562
800	20.786	171.900	158.860	10.431	580.647	492.183	−32.136
900	20.787	174.348	160.448	12.510	578.612	481.247	−27.931
1000	20.789	176.538	161.949	14.589	576.489	470.541	−24.579
1100	20.794	178.520	163.367	16.668	574.296	460.052	−21.846
1200	20.806	180.330	164.706	18.748	572.046	449.765	−19.578
1300	20.829	181.996	165.973	20.830	569.750	439.668	−17.666
1400	20.867	183.541	167.173	22.914	567.416	429.749	−16.034
1500	20.925	184.982	168.313	25.004	565.053	419.998	−14.626
1600	21.007	186.335	169.398	27.100	562.665	410.405	−13.398
1700	21.117	187.612	170.432	29.206	560.261	400.963	−12.320
1800	21.256	188.822	171.420	31.324	557.844	391.662	−11.366
1900	21.425	189.976	172.367	33.458	555.420	382.496	−10.516
2000	21.625	191.080	173.275	35.610	552.994	373.457	−9.754
2100	21.853	192.141	174.148	37.784	550.570	364.540	−9.067
2200	22.108	193.163	174.989	39.982	548.153	355.738	−8.446
2300	22.385	194.152	175.801	42.206	545.745	347.046	−7.882
2400	22.683	195.111	176.586	44.459	543.350	338.458	−7.366
2500	22.996	196.043	177.346	46.743	540.970	329.970	−6.894
2600	23.320	196.951	178.082	49.059	538.608	321.577	−6.461
2700	23.653	197.837	178.798	51.408	536.263	313.274	−6.061
2800	23.989	198.704	179.493	53.790	533.939	305.058	−5.691
2900	24.325	199.551	180.170	56.205	531.634	296.924	−5.348
3000	24.658	200.382	180.830	58.655	529.350	288.870	−5.030
3100	24.984	201.195	181.474	61.137	527.086	280.891	−4.733
3200	25.301	201.994	182.103	63.651	524.842	272.985	−4.456
3300	25.607	202.777	182.717	66.197	522.616	265.149	−4.197
3400	25.899	203.546	183.319	68.772	520.409	257.380	−3.954
3500	26.176	204.301	183.908	71.376	518.217	249.676	−3.726
3600	26.437	205.042	184.484	74.007	516.041	242.034	−3.512
3700	26.680	205.769	185.050	76.663	513.879	234.453	−3.310
3800	26.905	206.484	185.604	79.342	511.728	226.929	−3.119
3900	27.112	207.186	186.149	82.043	509.587	219.463	−2.939
4000	27.300	207.874	186.683	84.764	507.455	212.051	−2.769
4100	27.469	208.551	187.209	87.502	505.329	204.692	−2.608
4200	27.621	209.214	187.725	90.257	503.208	197.385	−2.455
4300	27.754	209.866	188.232	93.026	501.091	190.128	−2.310
4400	27.870	210.505	188.731	95.807	498.974	182.921	−2.172
4500	27.969	211.133	189.222	98.599	496.858	175.762	−2.040
4600	28.052	211.748	189.705	101.401	494.740	168.650	−1.915
4700	28.120	212.352	190.180	104.209	492.618	161.584	−1.796
4800	28.173	212.945	190.648	107.024	490.492	154.563	−1.682
4900	28.212	213.526	191.109	109.843	488.359	147.587	−1.573
5000	28.239	214.097	191.563	112.666	486.220	140.654	−1.469
5100	28.253	214.656	192.011	115.491	484.071	133.764	−1.370
5200	28.256	215.205	192.452	118.316	481.913	126.916	−1.275
5300	28.249	215.743	192.886	121.142	479.744	120.110	−1.184
5400	28.232	216.271	193.314	123.966	477.563	113.345	−1.096
5500	28.207	216.789	193.736	126.788	475.369	106.620	−1.013
5600	28.173	217.297	194.152	129.607	473.162	99.935	−0.932
5700	28.132	217.795	194.563	132.422	470.941	93.290	−0.855
5800	28.084	218.284	194.968	135.233	468.705	86.684	−0.781
5900	28.030	218.763	195.367	138.039	466.453	80.117	−0.709
6000	27.971	219.234	195.761	140.839	464.185	73.588	−0.641

PREVIOUS: March 1978 (1 atm) — CURRENT: March 1983 (1 bar)

Aluminum Carbide (AlC) IDEAL GAS $M_r = 38.99254$ Aluminum Carbide (AlC) $C_1Al_1(g)$

$S°(298.15 \text{ K}) = [223.4 \pm 4]\ \text{J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = [686.2 \pm 10]\ \text{kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = [689.5 \pm 10]\ \text{kJ·mol}^{-1}$

Electronic Level and Quantum Weight State	ϵ_i, cm^{-1}	g_i
$^2\Pi$	0	4

$\omega_e = [760]\ \text{cm}^{-1}$ $\omega_e x_e = [5.0]\ \text{cm}^{-1}$ $\sigma = 1$
$B_e = [0.650]\ \text{cm}^{-1}$ $\alpha_e = [0.006]\ \text{cm}^{-1}$ $r_e = [1.77]\ \text{Å}$

Enthalpy of Formation

$\Delta_f H°(0 \text{ K})$ was calculated from $D_0° = 83.0\ \text{kcal·mol}^{-1}$, estimated by Gordon.[1] The spectrum originally attributed to AlC(g)[2] was later shown to be due to $Al_2(g)$.[3,4]

Heat Capacity and Entropy

Molecular constants were estimated by Gordon.[1] The recent review by Huber and Herzberg[5] did not indicate any experimental data available for the vibrational–rotational constants for AlC(g).

References

[1] J. S. Gordon, Astrosystems, International, Livingston, N.J., personal communication, (1963).
[2] P. Zeeman, Can. J. Phys. 32, 9 (1954).
[3] D. S. Ginter, M. L. Ginter, and K. K. Innes, Astrophys. J. 139, 365 (1964).
[4] H. Wooley, U. S. Nat. Bur. Stand. Report 6928, (1960).
[5] K. P. Huber and G. Herzberg, "Constants of Diatomic Molecules," Van Nostrand Reinhold Company, New York, (1979).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−8.928	686.185	686.185	INFINITE
100	29.131	190.573	250.776	−6.020	688.550	670.287	−350.122
200	30.241	210.997	226.335	−3.067	689.375	651.620	−170.186
250	31.276	217.855	223.975	−1.530	689.503	642.164	−134.173
298.15	32.256	223.449	223.449	0.	689.523	633.044	−110.907
300	32.292	223.649	223.450	0.060	689.522	632.693	−110.162
350	33.178	228.695	223.846	1.697	689.454	623.226	−93.011
400	33.913	233.175	224.738	3.375	689.307	613.774	−80.151
450	34.513	237.205	225.903	5.086	689.086	604.345	−70.151
500	35.001	240.868	227.219	6.824	688.797	594.944	−62.153
600	35.729	247.318	230.046	10.363	688.022	576.242	−50.166
700	36.233	252.866	232.919	13.963	687.001	557.689	−41.615
800	36.598	257.729	235.722	17.605	685.742	539.299	−35.213
900	36.872	262.056	238.412	21.279	684.240	521.082	−30.243
1000	37.087	265.952	240.975	24.978	671.900	503.805	−26.316
1100	37.260	269.496	243.409	28.695	670.249	487.075	−23.129
1200	37.405	272.744	245.720	32.429	668.556	470.497	−20.480
1300	37.528	275.743	247.916	36.176	666.829	454.062	−18.244
1400	37.636	278.528	250.004	39.934	665.072	437.761	−16.333
1500	37.733	281.128	251.993	43.703	663.291	421.586	−14.681
1600	37.820	283.566	253.891	47.480	661.489	405.531	−13.239
1700	37.900	285.862	255.705	51.266	659.668	389.589	−11.971
1800	37.975	288.030	257.441	55.060	657.830	373.755	−10.846
1900	38.045	290.085	259.106	58.861	655.977	358.024	−9.843
2000	38.112	292.038	260.704	62.669	654.110	342.391	−8.942
2100	38.176	293.899	262.241	66.484	652.231	326.851	−8.130
2200	38.237	295.677	263.720	70.304	650.340	311.401	−7.394
2300	38.296	297.378	265.147	74.131	648.438	296.037	−6.723
2400	38.354	299.009	266.524	77.963	646.526	280.756	−6.110
2500	38.410	300.576	267.855	81.802	644.604	265.555	−5.548
2600	38.465	302.083	269.143	85.645	642.672	250.431	−5.031
2700	38.519	303.536	270.390	89.495	640.732	235.382	−4.554
2800	38.571	304.938	271.599	93.349	344.883	221.372	−4.130
2900	38.623	306.292	272.772	97.209	344.021	216.976	−3.908
3000	38.675	307.602	273.911	101.074	343.152	212.610	−3.702
3100	38.726	308.871	275.018	104.944	342.275	208.273	−3.509
3200	38.776	310.102	276.096	108.819	341.390	203.965	−3.329
3300	38.826	311.296	277.144	112.699	340.497	199.684	−3.161
3400	38.875	312.455	278.166	116.584	339.596	195.431	−3.002
3500	38.924	313.583	279.162	120.474	338.688	191.204	−2.854
3600	38.973	314.680	280.133	124.369	337.771	187.003	−2.713
3700	39.021	315.749	281.081	128.269	336.847	182.827	−2.581
3800	39.069	316.790	282.008	132.173	335.915	178.677	−2.456
3900	39.117	317.805	282.912	136.082	334.974	174.552	−2.338
4000	39.165	318.796	283.797	139.997	334.024	170.450	−2.226
4100	39.213	319.764	284.663	143.915	333.066	166.373	−2.120
4200	39.260	320.710	285.510	147.839	332.098	162.319	−2.019
4300	39.307	321.634	286.339	151.767	331.120	158.288	−1.923
4400	39.354	322.538	287.152	155.700	330.132	154.280	−1.832
4500	39.401	323.423	287.948	159.638	329.135	150.295	−1.745
4600	39.448	324.290	288.729	163.581	328.125	146.331	−1.662
4700	39.495	325.138	289.494	167.528	327.104	142.390	−1.582
4800	39.541	325.970	290.245	171.480	326.069	138.471	−1.507
4900	39.588	326.786	290.983	175.436	325.022	134.574	−1.435
5000	39.634	327.586	291.707	179.397	323.959	130.698	−1.365
5100	39.680	328.372	292.418	183.363	322.882	126.843	−1.299
5200	39.727	329.143	293.117	187.333	321.788	123.010	−1.236
5300	39.773	329.900	293.804	191.308	320.677	119.198	−1.175
5400	39.819	330.644	294.479	195.288	319.549	115.407	−1.116
5500	39.865	331.375	295.144	199.272	318.401	111.637	−1.060
5600	39.911	332.094	295.797	203.261	317.233	107.888	−1.006
5700	39.957	332.800	296.440	207.254	316.043	104.160	−0.955
5800	40.003	333.496	297.073	211.252	314.834	100.453	−0.905
5900	40.049	334.180	297.696	215.255	313.599	96.768	−0.857
6000	40.095	334.853	298.310	219.262	312.362	93.101	−0.811

PREVIOUS: June 1963 (1 atm) CURRENT: June 1963 (1 bar)

Aluminum Carbide (AlC) $C_1Al_1(g)$

$S°(298.15\ K) = [208.56]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 822.0 \pm 41\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 828.4 \pm 41\ kJ{\cdot}mol^{-1}$

Electronic Level and Quantum Weight		
State	ϵ_i, cm^{-1}	g_i
$^4\Sigma^-$	0	4

$\omega_e = [1350]\ cm^{-1}$
$B_e = [1.555]\ cm^{-1}$
$\omega_e x_e = [12.0]\ cm^{-1}$
$\alpha_e = [0.018]\ cm^{-1}$
$\sigma = 1$

Enthalpy of Formation

The enthalpy of formation at 298.15 K was calculated from $\Delta_f H°(0\ K) = 105 \pm 10\ kcal{\cdot}mol^{-1}$ for the reaction $BC(g) = B(g) + C(g)$ reported by Verhaegen *et al.*[1,2]

Heat Capacity and Entropy

All spectroscopic constants were obtained from Gordon.[3] Theoretical calculations by Kruba[4] predict a $^4\Sigma^-$ ground state. The recent review by Huber and Herzberg[5] did not indicate any experimental data available on the vibrational–rotational constants for BC(g).

References

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[2] D. G. Verhaegen, F. E. Stafford and J. Drowart, J. Chem. Phys. 40, 1622 (1964).
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[4] J. E. Kouba and V. Ohrn, J. Chem. Phys. 53, 3923 (1970).
[5] K. P. Huber and G. Herzberg, "Constants of Diatomic Molecules," Van Nostrand Reinhold Company, New York, (1979).

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−8.700	821.997	821.997	INFINITE
100	29.109	176.645	234.607	−5.796	824.817	807.279	−421.679
200	29.172	196.831	211.250	−2.884	827.070	788.804	−206.015
250	29.358	203.357	209.042	−1.421	827.866	779.141	−162.793
298.15	29.700	208.555	208.555	0.	828.432	769.702	−134.849
300	29.716	208.739	208.556	0.055	828.450	769.338	−133.954
350	30.212	213.355	208.919	1.553	828.850	759.452	−113.342
400	30.788	217.427	209.733	3.077	829.087	749.520	−97.877
450	31.388	221.088	210.795	4.632	829.186	739.567	−85.847
500	31.975	224.425	211.993	6.216	829.168	729.609	−76.222
600	33.032	230.351	214.571	9.468	828.861	709.720	−61.787
700	33.898	235.510	217.202	12.816	828.281	689.906	−51.481
800	34.589	240.084	219.782	16.242	827.503	670.190	−43.759
900	35.138	244.191	222.270	19.729	826.574	650.580	−37.759
1000	35.578	247.917	224.651	23.266	825.525	631.080	−32.964
1100	35.934	251.325	226.923	26.842	824.378	611.691	−29.047
1200	36.227	254.464	229.089	30.450	823.146	592.409	−25.787
1300	36.471	257.374	231.154	34.086	821.841	573.234	−23.033
1400	36.677	260.085	233.125	37.743	820.469	554.161	−20.676
1500	36.854	262.621	235.008	41.420	819.037	535.189	−18.637
1600	37.007	265.005	236.809	45.113	817.549	516.314	−16.856
1700	37.142	267.252	238.534	48.821	816.008	497.533	−15.287
1800	37.262	269.379	240.189	52.541	814.417	478.845	−13.896
1900	37.369	271.396	241.779	56.273	812.778	460.247	−12.653
2000	37.466	273.316	243.308	60.015	811.093	441.736	−11.537
2100	37.555	275.146	244.781	63.766	809.363	423.310	−10.529
2200	37.637	276.895	246.201	67.526	807.589	404.968	−9.615
2300	37.713	278.570	247.573	71.293	805.772	386.708	−8.782
2400	37.784	280.176	248.898	75.068	753.654	369.596	−8.044
2500	37.851	281.720	250.180	78.850	751.676	353.634	−7.389
2600	37.914	283.206	251.422	82.638	749.689	337.752	−6.786
2700	37.974	284.638	252.626	86.432	747.694	321.946	−6.228
2800	38.032	286.020	253.794	90.233	745.692	306.214	−5.712
2900	38.087	287.355	254.928	94.039	743.681	290.554	−5.233
3000	38.140	288.647	256.031	97.850	741.663	274.963	−4.788
3100	38.191	289.899	257.103	101.667	739.637	259.440	−4.372
3200	38.241	291.112	258.147	105.488	737.603	243.982	−3.983
3300	38.289	292.290	259.164	109.315	735.562	228.588	−3.618
3400	38.336	293.433	260.155	113.146	733.514	213.256	−3.276
3500	38.382	294.545	261.122	116.982	731.458	197.984	−2.955
3600	38.427	295.627	262.066	120.822	729.395	182.771	−2.652
3700	38.471	296.681	262.987	124.667	727.325	167.616	−2.366
3800	38.514	297.707	263.887	128.516	725.248	152.516	−2.096
3900	38.557	298.708	264.767	132.370	723.163	137.471	−1.841
4000	38.598	299.685	265.628	136.228	721.072	122.480	−1.599
4100	38.640	300.639	266.470	140.090	718.973	107.542	−1.370
4200	38.681	301.570	267.295	143.956	237.018	99.678	−1.240
4300	38.721	302.481	268.103	147.826	235.992	96.420	−1.171
4400	38.761	303.371	268.894	151.700	234.958	93.186	−1.106
4500	38.800	304.243	269.670	155.578	233.914	89.976	−1.044
4600	38.839	305.096	270.431	159.460	232.861	86.789	−0.986
4700	38.878	305.932	271.177	163.346	231.799	83.625	−0.929
4800	38.916	306.751	271.910	167.235	230.727	80.484	−0.876
4900	38.954	307.554	272.629	171.129	229.645	77.365	−0.825
5000	38.992	308.341	273.336	175.026	228.552	74.268	−0.776
5100	39.030	309.113	274.030	178.927	227.449	71.193	−0.729
5200	39.067	309.872	274.712	182.832	226.335	68.140	−0.684
5300	39.104	310.616	275.382	186.741	225.209	65.109	−0.642
5400	39.141	311.347	276.041	190.653	224.072	62.099	−0.601
5500	39.178	312.066	276.690	194.569	222.923	59.110	−0.561
5600	39.215	312.772	277.328	198.489	221.761	56.142	−0.524
5700	39.251	313.467	277.956	202.412	220.587	53.195	−0.487
5800	39.287	314.150	278.574	206.339	219.400	50.268	−0.453
5900	39.324	314.822	279.183	210.269	218.199	47.363	−0.419
6000	39.360	315.483	279.782	214.204	216.985	44.477	−0.387

PREVIOUS. June 1963 (1 atm)   CURRENT: June 1963 (1 bar)

Boron Carbide (B_4C) **CRYSTAL** **$M_r = 55.251$** **Boron Carbide (B_4C)** **$C_1B_4(cr)$**

$S°(298.15\ K) = 27.175 \pm 0.13\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{fus} = 2743 \pm 20\ K$

$\Delta_fH°(0\ K) = -62.40 \pm 6.28\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -62.68 \pm 6.28\ kJ{\cdot}mol^{-1}$
$\Delta_{fus}H° = [104.6 \pm 10]\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

Using a high temperature solution calorimetric technique, Hong and Kleppa[1] measured $\Delta_fH°(B_4C,\ cr,\ 1320\ K) = -15.98 \pm 0.84\ kcal{\cdot}mol^{-1}$. We adopt this value and correct to 298.15 K using tabulated enthalpy data[2] to obtain $\Delta_fH°(B_4C,\ cr,\ 298.15\ K) = -14.98 \pm 1.5\ kcal{\cdot}mol^{-1}$ which is a correction to that reported by Hong and Kleppa.[1] The uncertainty limit is that recommended by Hong and Kleppa.

Two additional experimental determinations of $\Delta_fH°(B_4C,\ cr,\ 298.15\ K)$ have been made. Smith *et al.*[3] measured a value of $\Delta_rH°(298.15\ K) = -683.2 \pm 2.2\ kcal{\cdot}mol^{-1}$ for the reaction $B_4C(cr) + 4\ O_2(g) \rightarrow 2\ B_2O_3(am) + CO_2(g)$. Due to the amorphous nature of the B_2O_3 product, a value of $\Delta_fH°(298.15\ K)$ derived from this reaction may be unreliable. Domalski and Armstrong[4] determined $\Delta_fH°(298.15\ K) = -17.1 \pm 2.7\ kcal{\cdot}mol^{-1}$ based on careful fluorine bomb calorimetry of the non– stoichiometric compound $B_{4.222}C(cr)$. The data were corrected to the stoichiometric $B_4C(cr)$ assuming the presence of excess free elemental boron. Note that the Hong and Kleppa[1] result lies within the stated uncertainty limits of the Domalski and Armstrong value.[4] In a review of similar data, Gurvich *et al.*[5] adopted a value for $\Delta_fH°(298.15\ K)$ of $-14.82 \pm 1.43\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

The low temperature heat capacities, 54–294 K, were taken from Kelley.[6] Above 298 K at least four enthalpy determinations have been made. The enthalpy data of King[7] in the range 298 to 1726 K were used to determine the equation: $C_p°/cal{\cdot}K^{-1}{\cdot}mol^{-1} = 22.99 + 5.40 \times 10^{-3}T - 10.72 \times 10^5T^{-2}$. Similar measurements of Ancey–Moret and Deniel[8] lead to the equation $C_p°/cal{\cdot}K^{-1}{\cdot}mol^{-1} = 23.077 + 5.24 \times 10^{-3}T - 10.75 \times 10^5T^{-2}$. Enthalpy measurements of Mathieu *et al.*[9] in the range 661–1014 K also support the latter two studies. We adopt the high temperature equation of King which joins smoothly at 298 K with the low temperature data of Kelley. The $S°(298.15\ K)$ is calculated based on the low temperature heat capacities of Kelley using $S°(53.1\ K) = 0.047\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$. The heat capacities adopted by Gurvich *et al.*[5] are in essential agreement with those adopted here up to 1500 K but are larger in the high temperature range (T>1500 K). This is due to the adoption (by Gurvich *et al.*) of the heat capacity results of Sheindlin *et al.*[10] which can be represented by the equation $C_p°/cal{\cdot}K^{-1}{\cdot}mol^{-1} = 22.65 + 5.27 \times 10^{-3}T - 12.82 \times 10^5T^{-2} + 6.45 \times 10^{13}T^{-2}\exp(-33 \times 10^3/T)$. Note the additional exponential term which causes the high temperature disparity. Due to the relatively high impurity content of the material used (5.6 mole%) and also the thermodynamic propensity and endothermicity of the reaction by $B_4C(cr) = 4\ B(cr) + C(cr)$ at temperatures greater than 1500 K, we are in doubt as to the exponential behavior of $C_p°$ as reported in the Sheindlin study.

Fusion Data

Of the several reported values of the fusion temperature, T_{fus}/K, [2623,[11,13] 2723,[12] 2713 ± 20,[10] 2633,[14] 2743 ± 20],[15] we adopt the value of Dolloff.[15] The value for $\Delta_{fus}H°$ is estimated. Note that $B_4C(cr)$ decomposes at moderate temperatures to form $B(cr,\ g) + C(cr)$.[2]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	$S°$ (J·K⁻¹mol⁻¹)	$-[G°-H°(T_r)]/T$ (J·K⁻¹mol⁻¹)	$H°-H°(T_r)$ (kJ·mol⁻¹)	$\Delta_fH°$ (kJ·mol⁻¹)	$\Delta_fG°$ (kJ·mol⁻¹)	log K_f
0	0.	0.	INFINITE	−5.635	−62.404	−62.404	INFINITE
100	5.071	1.634	56.731	−5.510	−62.435	−62.380	32.584
200	27.426	11.311	31.236	−3.985	−62.568	−62.279	16.266
298.15	53.764	27.175	27.175	0.	−62.676	−62.109	10.881
300	54.266	27.509	27.176	0.100	−62.676	−62.106	10.814
400	76.358	46.353	29.595	6.703	−62.546	−61.931	8.087
500	89.789	64.925	34.822	15.051	−62.448	−61.791	6.455
600	98.366	82.103	41.293	24.486	−62.517	−61.657	5.368
700	103.680	97.682	48.254	34.599	−62.796	−61.494	4.589
800	107.654	111.793	55.329	45.171	−63.277	−61.277	4.001
900	110.989	124.666	62.328	56.104	−63.906	−60.991	3.540
1000	114.299	136.533	69.163	67.370	−64.611	−60.630	3.167
1100	117.336	147.571	75.795	78.954	−65.341	−60.196	2.858
1200	120.190	157.904	82.211	90.831	−66.071	−59.696	2.599
1300	122.909	167.632	88.411	102.987	−66.781	−59.136	2.376
1400	125.533	176.837	94.402	115.410	−67.456	−58.522	2.183
1500	128.089	185.585	100.191	128.091	−68.086	−57.862	2.015
1600	130.587	193.932	105.791	141.025	−68.663	−57.161	1.866
1700	133.047	201.923	111.213	154.207	−69.178	−56.426	1.734
1800	135.474	209.596	116.467	167.633	−69.626	−55.663	1.615
1900	137.875	216.986	121.564	181.301	−70.004	−54.877	1.509
2000	140.256	224.118	126.514	195.208	−70.307	−54.072	1.412
2100	142.620	231.019	131.327	209.352	−70.532	−53.255	1.325
2200	144.971	237.708	136.012	223.731	−70.677	−52.428	1.245
2300	147.306	244.203	140.575	238.345	−70.739	−51.597	1.172
2400	149.637	250.522	145.025	253.193	−271.756	−46.490	1.012
2500	151.955	256.677	149.369	268.272	−271.961	−37.099	0.775
2600	154.268	262.682	153.612	283.583	−271.950	−27.704	0.557
2700	156.578	268.548	157.760	299.126	−271.722	−18.313	0.354
2743.000	157.569	271.030	159.517	305.880	--- CRYSTAL <--> LIQUID ---		
2800	158.887	274.284	161.820	314.899	−271.276	−8.935	0.167
2900	161.197	279.900	165.795	330.903	−270.614	0.423	−0.008
3000	163.507	285.403	169.691	347.138	−269.733	9.755	−0.170
3100	165.816	290.802	173.511	363.604	−268.635	19.054	−0.321
3200	168.126	296.103	177.259	380.301	−267.318	28.313	−0.462

PREVIOUS: December 1965 CURRENT: June 1983

Boron Carbide (B_4C) LIQUID $M_r = 55.251$ Boron Carbide (B_4C) $C_1B_4(l)$

$S°(298.15\ K) = [69.426]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$T_{fus} = 2743 \pm 20\ K$

$\Delta_fH°(298.15\ K) = [51.885]\ kJ{\cdot}mol^{-1}$

$\Delta_{fus}H° = [104.6 \pm 10]\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

$\Delta_fH°(B_4C, l, 298.15\ K)$ is calculated from $\Delta_fH°(B_4C, cr, 298.15\ K)$ by adding the enthalpy of fusion, $\Delta_{fus}H°$, and the difference in enthalpy, $H°(2743\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

A glass transition is assumed at 1750 K. The heat capacity below 1750 K is assumed to be that of the crystal. Above 1750 K the heat capacity is assumed constant and estimated as $135.98\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ or $27.196\ J{\cdot}K^{-1}\ g{\cdot}atom^{-1}$ ($6.5\ cal{\cdot}K^{-1}\ g{\cdot}atom^{-1}$).

The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Refer to the crystal table for details.

Enthalpy Reference Temperature = T_r = 298.15 K				Standard State Pressure = $p°$ = 0.1 MPa			
	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C°_p$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0							
100							
200							
298.15	53.764	69.426	69.426	0.	51.885	39.855	−6.982
300	54.266	69.760	69.427	0.100	51.885	39.780	−6.926
400	76.358	88.604	71.846	6.703	52.016	35.730	−4.666
500	89.789	107.176	77.074	15.051	52.113	31.645	−3.306
600	98.366	124.354	83.544	24.486	52.045	27.554	−2.399
700	103.680	139.933	90.506	34.599	51.765	23.491	−1.753
800	107.654	154.045	97.580	45.171	51.285	19.483	−1.272
900	110.989	166.917	104.580	56.104	50.656	15.544	−0.902
1000	114.299	178.785	111 414	67.370	49.950	11.681	−0.610
1100	117.336	189.822	118.046	78.954	49.220	7.889	−0.375
1200	120.190	200.155	124.463	90.831	48.491	4.164	−0.181
1300	122.909	209.884	130.663	102.987	47.781	0.499	−0.020
1400	125.533	219.089	136.653	115.410	47.105	−3.113	0.116
1500	128.089	227.837	142.443	128.091	46.475	−6.677	0.233
1600	130.587	236.184	148.043	141.025	45.899	−10.202	0.333
1700	133.047	244.174	153.464	154.207	45.384	−13.692	0.421
1750.000	134.265	248.049	156.112	160.890	GLASS <--> LIQUID TRANSITION		
1750.000	135.980	248.049	156.112	160.890			
1800	135.980	251.879	158.719	167.689	44.991	−17.155	0.498
1900	135.980	259.231	163.817	181.287	44.544	−20.596	0.566
2000	135.980	266.206	168.764	194.885	43.932	−24.009	0.627
2100	135.980	272.841	173.563	208.483	43.161	−27.388	0.681
2200	135.980	279.167	178.221	222.081	42.235	−30.726	0.730
2300	135.980	285.211	182.742	235.679	41.156	−34.019	0.773
2400	135.980	290.998	187.133	249.277	−161.109	−32.987	0.718
2500	135.980	296.549	191.399	262.875	−162.796	−27.614	0.577
2600	135.980	301.883	195.547	276.473	−164.498	−22.173	0.445
2700	135.980	307.014	199.581	290.071	−166.215	−16.666	0.322
2743.000	135.980	309.163	201.282	295.918	--- CRYSTAL <--> LIQUID ---		
2800	135.980	311.960	203.507	303.669	−167.945	−11.096	0.207
2900	135.980	316.731	207.329	317.267	−169.688	−5.463	0.098
3000	135.980	321.341	211.053	330.865	−171.445	0.230	−0.004
3100	135.980	325.800	214.683	344.463	−173.214	5.981	−0.101
3200	135.980	330.117	218.223	358.061	−174.996	11.790	−0.192
3300	135.980	334.302	221.678	371.659	−176.791	17.655	−0.279
3400	135.980	338.361	225.050	385.257	−178.597	23.574	−0.362
3500	135.980	342.303	228.344	398.855	−180.416	29.547	−0.441
3600	135.980	346.133	231.563	412.453	−182.246	35.572	−0.516
3700	135.980	349.859	234.710	426.051	−184.088	41.648	−0.588
3800	135.980	353.486	237.788	439.649	−185.942	47.773	−0.657
3900	135.980	357.018	240.801	453.247	−187.807	53.948	−0.723
4000	135.980	360.460	243.749	466.845	−189.684	60.171	−0.786
4100	135.980	363.818	246.637	480.443	−191.571	66.440	−0.846
4200	135.980	367.095	249.466	494.041	−2112.868	100.853	−1.254
4300	135.980	370.295	252.239	507.639	−2110.429	153.532	−1.865
4400	135.980	373.421	254.958	521.237	−2108.008	206.154	−2.447
4500	135.980	376.477	257.624	534.835	−2105.607	258.721	−3.003

PREVIOUS: December 1965 CURRENT: June 1983

Boron Carbide (B_4C) CRYSTAL–LIQUID

0 to 2743 K crystal
above 4500 K liquid

Refer to the individual tables for the details.

M_r = 55.251 Boron Carbide (B_4C) C_1B_4(cr,l)

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	Δ_fH°	Δ_fG°	log K_f
0	0.	0.	INFINITE	−5.635	−62.404	−62.404	INFINITE
100	5.071	1.634	56.731	−5.510	−62.435	−62.380	32.584
200	27.426	11.311	31.236	−3.985	−62.568	−62.279	16.266
298.15	53.764	27.175	27.175	0.	−62.676	−62.109	10.881
300	54.266	27.509	27.176	0.100	−62.676	−62.106	10.814
400	76.358	46.353	29.595	6.703	−62.546	−61.931	8.087
500	89.789	64.925	34.822	15.051	−62.448	−61.791	6.455
600	98.366	82.103	41.293	24.486	−62.517	−61.657	5.368
700	103.680	97.682	48.254	34.599	−62.796	−61.494	4.589
800	107.654	111.793	55.329	45.171	−63.277	−61.277	4.001
900	110.989	124.666	62.328	56.104	−63.906	−60.991	3.540
1000	114.299	136.533	69.163	67.370	−64.611	−60.630	3.167
1100	117.336	147.571	75.795	78.954	−65.341	−60.196	2.858
1200	120.190	157.904	82.211	90.831	−66.071	−59.696	2.599
1300	122.909	167.632	88.411	102.987	−66.781	−59.136	2.376
1400	125.533	176.837	94.402	115.410	−67.456	−58.522	2.183
1500	128.089	185.585	100.191	128.091	−68.086	−57.862	2.015
1600	130.587	193.932	105.791	141.025	−68.663	−57.161	1.866
1700	133.047	201.923	111.213	154.207	−69.178	−56.426	1.734
1800	135.474	209.596	116.467	167.633	−69.626	−55.663	1.615
1900	137.875	216.986	121.564	181.301	−70.004	−54.877	1.509
2000	140.256	224.118	126.514	195.208	−70.307	−54.072	1.412
2100	142.620	231.019	131.327	209.352	−70.532	−53.255	1.325
2200	144.971	237.708	136.012	223.731	−70.677	−52.428	1.245
2300	147.306	244.203	140.575	238.345	−70.739	−51.597	1.172
2400	149.637	250.522	145.025	253.193	−271.756	−46.490	1.012
2500	151.955	256.677	149.369	268.272	−271.961	−37.099	0.775
2600	154.268	262.682	153.612	283.583	−271.950	−27.704	0.557
2700	156.578	268.548	157.760	299.126	−271.722	−18.313	0.354
2743.000	157.569	271.030	159.517	305.880	CRYSTAL <--> LIQUID		
2743.000	135.980	309.163	159.517	410.480		TRANSITION	
2800	135.980	311.960	162.592	418.231	−167.945	−11.096	0.207
2900	135.980	316.731	167.825	431.829	−169.688	−5.463	0.098
3000	135.980	321.341	172.866	445.427	−171.445	0.230	−0.004
3100	135.980	325.800	177.728	459.025	−173.214	5.981	−0.101
3200	135.980	330.117	182.423	472.623	−174.996	11.790	−0.192
3300	135.980	334.302	186.962	486.221	−176.791	17.655	−0.279
3400	135.980	338.361	191.356	499.819	−178.597	23.574	−0.362
3500	135.980	342.303	195.612	513.417	−180.416	29.547	−0.441
3600	135.980	346.133	199.741	527.015	−182.246	35.572	−0.516
3700	135.980	349.859	203.748	540.613	−184.088	41.648	−0.588
3800	135.980	353.486	207.641	554.211	−185.942	47.773	−0.657
3900	135.980	357.018	211.426	567.809	−187.807	53.948	−0.723
4000	135.980	360.460	215.109	581.407	−189.684	60.171	−0.786
4100	135.980	363.818	218.695	595.005	−191.571	66.440	−0.846
4200	135.980	367.095	222.189	608.603	−2112.868	100.853	−1.254
4300	135.980	370.295	225.597	622.201	−2110.429	153.532	−1.865
4400	135.980	373.421	228.921	635.799	−2108.008	206.154	−2.447
4500	135.980	376.477	232.166	649.397	−2105.607	258.721	−3.003

PREVIOUS: CURRENT: June 1983

Boron Carbide (B_4C) C_1B_4(cr,l)

Beryllium Carbide (Be_2C) CRYSTAL M_r = 30.03536 Beryllium Carbide (Be_2C) $C_1Be_2(cr)$

$\Delta_f H°(0\ K)$ = Unknown

$S°(298.15\ K) = [16.3 \pm 4.2]\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = -90.79 \pm 10.5\ kJ \cdot mol^{-1}$

$T_{fus} = [2400]\ K$ $\Delta_{fus} H° = [75.312]\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The selected $\Delta_f H°(298.15\ K)$ was calculated by the 3rd law method using vapor pressures reported by Pollock.[1] Pressures for the reaction $Be_2C(cr) \rightarrow 2Be(g) + C(graphite)$ were measured by Pollock in the temperature range 1430–1669 K by Knudsen technique. Vapor pressure data for this decomposition reaction have also been reported by Baboin,[2] Quirk[3] and Muratov and Novoselova.[4] The calculated $\Delta_f H°(298.15\ K)$ values are summarized as follows:

Calc. Method	Number of Presentation	T/K	$\Delta_r H°(298.15\ K)$ kcal·mol^{-1}	$\Delta_f H°(298.15\ K)$ kcal·mol^{-1}	Source
3rd law	14	1430–1669	89.117	−21.7	Pollock[1]
2nd law	14	1430–1669	90.8	−25.1	Least squares fit of Pollock's v.p. to the equation: log P (atm) = 6.946–19,593/T
3rd law	6	1673–1953	71.411	+13.7	Muratov and Novoselova[4]
3rd law	8	1900–2600	81.278	− 6.1	Quirk[3]
3rd law	8	1600–2300	96.266	−36.0	Baboin[2]

Schick *et al.*[5] have listed the measured vapor pressures. The vapor pressures reported by Baboin[2] used in the 3rd law calculation were those listed by Schick *et al.*[5]

Heat Capacity and Entropy

The heat capacity values, from 298.15 to 1200 K, were derived from; the mean $C_p°$ data measured by Neely *et al.*[6] Neely *et al.* estimated an overall error of 15% in their mean heat capacity data. The powdered Be_2C material which was used analyzed 80 to 74% Be_2C. The impurities were mainly oxide and nitride of Be. No corrections were made for the effect of these impurities.

From 1200–2400 K the $C_p°$ was extrapolated so as to approach the value, 22 cal·K^{-1}·mol^{-1} calculated from Krikorian.[7] The $S°(298.15\ K) = 3.9$ cal·K^{-1}·mol^{-1}, was estimated by Krikorian.[7]

Fusion Data

Schick *et al.*,[5] have summarized the available melting data i.e.: Oishi and Hamona[8] have reported decomposition upon heating as low as 1873 K. Brewer *et al.*[9] and Gaev[10] reported melting or dissociation between 2373 and 2423 K.

The melting point is assumed to be 2400 K as estimated by Douglas and Victor[11] and Schick *et al.*[5] From the estimated melting point, 2400 K, and an estimated 2.5 cal·K^{-1}·g·atom^{-1} for the entropy of melting, the heat of melting was calculated.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	43.250	16.318	16.318	0.	−90.793	−88.317	15.473
300	43.329	16.585	16.318	0.080	−90.789	−88.302	15.375
400	47.614	29.689	18.076	4.645	−90.931	−87.468	11.422
500	49.752	40.543	21.516	9.513	−91.595	−86.535	9.040
600	51.890	49.706	25.469	14.542	−92.678	−85.426	7.437
700	60.434	58.401	29.552	20.194	−93.582	−84.139	6.279
800	64.706	66.750	33.686	26.451	−94.240	−82.744	5.403
900	68.977	74.617	37.801	33.135	−94.775	−81.273	4.717
1000	73.249	82.106	41.860	40.246	−95.153	−79.751	4.166
1100	77.525	89.288	45.847	47.785	−95.351	−78.200	3.713
1200	81.797	96.224	49.758	55.760	−95.343	−76.639	3.336
1300	85.011	102.905	53.591	64.108	−95.184	−75.087	3 017
1400	87.278	109.292	57.343	72.728	−94.968	−73.549	2.744
1500	88.881	115.371	61.011	81.540	−94.772	−72.026	2.508
1600	90.023	121.145	64.590	90.488	−123.720	−69.463	2.268
1700	90.843	126.629	68.080	99.534	−122.903	−66.096	2.031
1800	91.349	131.837	71.478	108.645	−122.087	−62.778	1.822
1900	91.621	136.784	74.786	117.795	−121.299	−59.505	1.636
2000	91.722	141.486	78.005	126.963	−120.556	−56.272	1.470
2100	91.797	145.963	81.135	136.139	−119.867	−53.075	1.320
2200	91.885	150.235	84.180	145.323	−119.231	−49.910	1.185
2300	91.964	154.322	87.141	154.515	−118.646	−46.772	1.062
2400	92.048	158.237	90.023	163.716	−118.113	−43.659	0.950
2400.000	92.048	158.237	90.023	163.716	--- CRYSTAL <--> LIQUID ---		
2500	92.153	161.997	92.827	172.926	−117.628	−40.567	0.848
2600	92.253	165.613	95.557	182.146	−117.191	−37.493	0.753
2700	92.350	169.097	98.217	191.376	−116.802	−34.435	0.666
2800	92.443	172.457	100.809	200.616	−698.373	−18.946	0.353
2900	92.534	175.703	103.335	209.865	−695.951	5.276	−0.095
3000	92.621	178.841	105.800	219.122	−693.543	29.416	−0.512
3100	92.705	181.879	108.206	228.389	−691.152	53.475	−0.901
3200	92.786	184.824	110.554	237.663	−688.781	77.457	−1.264
3300	92.864	187.680	112.848	246.946	−686.432	101.366	−1.604
3400	92.939	190.454	115.090	256.236	−684.110	125.203	−1.924
3500	93.010	193.149	117.282	265.534	−681.817	148.973	−2.223

PREVIOUS: March 1962 CURRENT: June 1963

Beryllium Carbide (Be$_2$C) LIQUID M_r = 30.03536

$S°$(298.15 K) = [47.467] J·K^{-1}·mol^{-1}

T_{fus} = [2400] K

$\Delta_f H°$(298.15 K) = [15.893] kJ·mol^{-1}

$\Delta_{fus}H°$ = [75.312] kJ·mol^{-1}

Enthalpy of Formation

$\Delta_f H°$(298.15 K) is calculated from that of the crystal by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°$(2400 K)–$H°$(298.15 K), between the crystal and liquid.

Heat Capacity and Entropy

The heat capacity is assumed constant and equal to the heat capacity of solid Be$_2$C at the estimated melting point. $S°$(298.15 K) is calculated in a manner similar to that used for the enthalpy of formation.

Fusion Data

The U. S. Nat. Bur. Stand.,[1] states that Be$_2$C seems to decompose easily only at temperatures above its reported melting point. For this reason they extended their Be$_2$C table into the liquid region. For detailed fusion data see the crystal table.

Reference

[1] U. S. Nat. Bur. Stand. Report 6645, (1960).

Beryllium Carbide (Be$_2$C) C$_1$Be$_2$(l)

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	43.250	47.467	47.467	0.	−15.893	−22.704	3.978
300	43.329	47.735	47.468	0.080	−15.889	−22.747	3.961
400	47.614	60.838	49.225	4.645	−16.031	−25.027	3.268
500	49.752	71.692	52.665	9.513	−16.694	−27.209	2.843
600	51.890	80.855	56.618	14.542	−17.778	−29.215	2.543
700	60.434	89.550	60.702	20.194	−18.682	−31.043	2.316
800	64.706	97.899	64.835	26.451	−19.340	−32.763	2.139
900	68.977	105.767	68.950	33.135	−19.875	−34.407	1.997
1000	73.249	113.255	73.009	40.246	−20.253	−36.000	1.880
1100	77.525	120.437	76.996	47.785	−20.450	−37.564	1.784
1200	81.797	127.374	80.907	55.760	−20.443	−39.118	1.703
1300	85.011	134.054	84.740	64.108	−20.284	−40.680	1.635
1400	87.278	140.441	88.492	72.728	−20.068	−42.257	1.577
1500	88.881	146.520	92.160	81.540	−19.872	−43.849	1.527
1600	90.023	152.295	95.739	90.489	−48.819	−44 401	1.450
1600.000	90.023	152.295	95.739	90.489	GLASS <--> LIQUID		
1600.000	92.048	152.295	95.739	90.489	TRANSITION		
1700	92.048	157.876	99.232	99.694	−47.843	−44.155	1.357
1800	92.048	163.137	102.638	108.899	−46.934	−43.965	1.276
1900	92.048	168.114	105.954	118.104	−46.090	−43.823	1.205
2000	92.048	172.835	109.181	127.308	−45.310	−43.724	1.142
2100	92.048	177.326	112.320	136.513	−44.592	−43.663	1.086
2200	92.048	181.608	115.373	145.718	−43.936	−43.634	1.036
2300	92.048	185.700	118.342	154.923	−43.339	−43.634	0.991
2400	92.048	189.617	121.231	164.128	−42.801	−43.659	0.950
2400.000	92.048	189.617	121.231	164.128	--- CRYSTAL <--> LIQUID ---		
2500	92.048	193.375	124.042	173.332	−42.321	−43.705	0.913
2600	92.048	196.985	126.779	182.537	−41.900	−43.769	0.879
2700	92.048	200.459	129.444	191.742	−41.535	−43.848	0.848
2800	92.048	203.807	132.040	200.947	−623.142	−31.494	0.588
2900	92.048	207.037	134.571	210.152	−620.764	−10.406	0.187
3000	92.048	210.157	137.039	219.356	−618.409	10.601	−0.185
3100	92.048	213.176	139.446	228.561	−616.080	31.529	−0.531
3200	92.048	216.098	141.796	237.766	−613.778	52.383	−0.855
3300	92.048	218.930	144.091	246.971	−611.507	73.166	−1.158
3400	92.048	221.678	146.333	256.176	−609.270	93.880	−1.442
3500	92.048	224.347	148.524	265.380	−607.070	114.528	−1.709

PREVIOUS. March 1962 CURRENT. June 1963

Beryllium Carbide (Be$_2$C) C$_1$Be$_2$(l)

Beryllium Carbide (Be_2C) CRYSTAL-LIQUID

0 to 2400 K crystal
above 2400 K liquid

Refer to the individual tables for details.

M_r = 30.03536 Beryllium Carbide (Be_2C) $C_1Be_2(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0							
100							
200							
298.15	43.250	16.318	16.318	0.	−90.793	−88.317	15.473
300	43.329	16.585	16.318	0.080	−90.789	−88.302	15.375
400	47.614	29.689	18.076	4.645	−90.931	−87.468	11.422
500	49.752	40.543	21.516	9.513	−91.595	−86.535	9.040
600	51.890	49.706	25.469	14.542	−92.678	−85.426	7.437
700	60.434	58.401	29.552	20.194	−93.582	−84.139	6.279
800	64.706	66.750	33.686	26.451	−94.240	−82.744	5.403
900	68.977	74.617	37.801	33.135	−94.775	−81.273	4.717
1000	73.249	82.106	41.860	40.246	−95.153	−79.751	4.166
1100	77.525	89.288	45.847	47.785	−95.351	−78.200	3.713
1200	81.797	96.224	49.758	55.760	−95.343	−76.639	3.336
1300	85.011	102.905	53.591	64.108	−95.184	−75.087	3.017
1400	87.278	109.292	57.343	72.728	−94.968	−73.549	2.744
1500	88.881	115.371	61.011	81.540	−94.772	−72.026	2.508
1600	90.023	121.145	64.590	90.488	−123.720	−69.463	2.268
1700	90.843	126.629	68.080	99.534	−122.903	−66.096	2.031
1800	91.349	131.837	71.478	108.645	−122.087	−62.778	1.822
1900	91.621	136.784	74.786	117.795	−121.299	−59.505	1.636
2000	91.722	141.486	78.005	126.963	−120.556	−56.272	1.470
2100	91.797	145.963	81.135	136.139	−119.867	−53.075	1.320
2200	91.885	150.235	84.180	145.323	−119.231	−49.910	1.185
2300	91.964	154.322	87.141	154.515	−118.646	−46.772	1.062
2400	92.048	158.237	90.023	163.716	−118.113	−43.659	0.950
2400.000	92.048	158.237	90.023	163.716	CRYSTAL <--> LIQUID		
2400.000	92.048	189.617	90.023	239.028		TRANSITION	
2500	92.048	193.375	94.082	248.233	−42.321	−43.705	0.913
2600	92.048	196.985	97.971	257.437	−41.900	−43.769	0.879
2700	92.048	200.459	101.703	266.642	−41.535	−43.848	0.848
2800	92.048	203.807	105.290	275.847	−623.142	−31.494	0.588
2900	92.048	207.037	108.743	285.052	−620.764	−10.406	0.187
3000	92.048	210.157	112.072	294.257	−618.409	10.601	−0.185
3100	92.048	213.176	115.285	303.461	−616.080	31.529	−0.531
3200	92.048	216 098	118.390	312.666	−613.778	52.383	−0.855
3300	92.048	218.930	121.394	321.871	−611.507	73.166	−1.158
3400	92.048	221.678	124.303	331.076	−609.270	93.880	−1.442
3500	92.048	224.347	127.124	340.281	−607.070	114.528	−1.709

PREVIOUS: CURRENT: June 1963

Beryllium Carbide (Be_2C) $C_1Be_2(cr,l)$

Bromomethylidyne (CBr) IDEAL GAS $M_r = 91.915$ Bromomethylidyne (CBr) $C_1Br_1(g)$

$S°(298.15\ K) = [233.45]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 514.3 \pm 63\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 510.4 \pm 63\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$X_2\ {}^2\Pi_{1/2}$	0	2
$X_1\ {}^2\Pi_{3/2}$	465	2
$A_1\ {}^2\Delta_{3/2}$	33163	2
$A_2\ {}^2\Delta_{5/2}$	33218	2
	[40000]	[2]

$\omega_e = [736]\ cm^{-1}$ $\omega_e x_e = [4.0]\ cm^{-1}$ $\sigma = 1$
$B_e = 0.4890\ cm^{-1}$ $\alpha_e = [0.0036]\ cm^{-1}$ $r_e = 1.8170$ Å

Enthalpy of Formation

Dixon and Kroto[1] have observed predissociation of CBr(g) which indicates that the dissociation energy D_0° is less than 94.7 kcal·mol^{-1}. They evaluated the kinetic data of Simons and Yarwood,[2] obtaining a value of $D_0^\circ = 97 \pm 5$ kcal·mol^{-1}, based on the enthalpy of formation of bromoform and the dissociation energy of HBr, and concluded that the true value of D_0° is very close to the upper limit of 94.7 kcal·mol^{-1}. Comparisons of C–X bond energies of CX_4 and CX compounds, however, indicate that this value is too high to be consistent with other carbon halides. Therefore the value of D_0° adopted is 75 ± 15 kcal·mol^{-1}. The corresponding $\Delta_f H°$(CBr, g, 298.15 K) is 122 ± 15 kcal·mol^{-1} (510.448 ± 63 kJ·mol^{-1}).

Heat Capacity and Entropy

The rotational structure of the near UV spectra of CBr(g) has been investigated by Dixon and Kroto[1] in the 3000 Å region. They assigned the above doublet electronic levels to the ground ($^2\Pi$) and first excited ($^2\Delta$) states and reported a value of $B_0 = 0.4872 \pm 0.0003$ cm^{-1} for the ground state. An additional electronic level ($^2\Sigma$) is expected to be close to the first excited state by analogy with CF(g) and CCl(g).

The fundamental vibrational frequency ω_e is estimated from Guggenheimer's relation for single bonded molecules.[3] The anharmonic vibrational term $\omega_e x_e$ is estimated by assuming $\omega_e x_e = \omega_e^2/(4D_0 + 2\omega_e)$. The value of α_e is calculated from the Morse potential function. The rotational constant B_e is calculated from $B_e = B_0 + \alpha_e/2$. The bond distance is calculated from B_e.

References

[1] R. N. Dixon and H. W. Kroto, Trans. Faraday Soc. 59, 1484 (1963).
[2] J. P. Simons and A. J. Yarwood, Trans. Faraday Soc. 57, 2167 (1961).
[3] K. M. Guggenheimer, Proc. Phys. Soc. (London) 58, 456 (1946).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−9.482	514.272	514.272	INFINITE
100	29.596	197.941	263.600	−6.566	515.732	498.725	−260.507
200	33.413	219.553	236.680	−3.425	516.095	481.543	−125.766
250	35.011	227.191	234.040	−1.712	516.105	472.901	−98.807
298.15	36.041	233.452	233.452	0.	510.448	465.246	−81.509
300	36.072	233.675	233.453	0.067	510.429	464.965	−80.958
350	36.733	239.290	233.895	1.888	495.454	458.199	−68.382
400	37.139	244.223	234.884	3.736	495.835	452.850	−59.136
450	37.388	248.613	236.170	5.599	496.150	447.457	−51.939
500	37.544	252.561	237.615	7.473	496.400	442.033	−46.179
600	37.708	259.423	240.695	11.237	496.726	431.125	−37.533
700	37.785	265.242	243.796	15.012	496.859	420.179	−31.354
800	37.829	270.291	246.800	18.793	496.842	409.224	−26.720
900	37.861	274.748	249.662	22.577	496.711	398.279	−23.115
1000	37.889	278.739	252.374	26.365	496.488	387.353	−20.233
1100	37.916	282.351	254.937	30.155	496.193	376.453	−17.876
1200	37.944	285.651	257.361	33.948	495.839	365.583	−15.913
1300	37.973	288.690	259.656	37.744	495.435	354.745	−14.254
1400	38.002	291.505	261.831	41.543	494.989	343.939	−12.833
1500	38.033	294.128	263.898	45.344	494.507	333.166	−11.602
1600	38.065	296.583	265.865	49.149	493.993	322.426	−10.526
1700	38.097	298.892	267.741	52.957	493.448	311.720	−9.578
1800	38.130	301.070	269.532	56.769	492.876	301.047	−8.736
1900	38.163	303.133	271.247	60.583	492.277	290.406	−7.984
2000	38.197	305.091	272.891	64.401	491.653	279.797	−7.308
2100	38.232	306.956	274.469	68.223	491.004	269.220	−6.696
2200	38.267	308.735	275.986	72.048	490.330	258.674	−6.142
2300	38.302	310.437	277.447	75.876	489.632	248.160	−5.636
2400	38.337	312.068	278.856	79.708	488.910	237.677	−5.173
2500	38.373	313.633	280.216	83.544	488.166	227.224	−4.748
2600	38.408	315.139	281.530	87.383	487.398	216.801	−4.356
2700	38.444	316.589	282.802	91.225	486.609	206.409	−3.993
2800	38.480	317.988	284.034	95.071	485.799	196.046	−3 657
2900	38.517	319.339	285.228	98.921	484.969	185.712	−3.345
3000	38.553	320.646	286.387	102.775	484.120	175.407	−3.054
3100	38.590	321.910	287.513	106.632	483.254	165.131	−2.782
3200	38.626	323.136	288.607	110.493	482.372	154.883	−2.528
3300	38.663	324.325	289.671	114.357	481.475	144.663	−2.290
3400	38.700	325.480	290.708	118.225	480.566	134.470	−2.066
3500	38.737	326.602	291.717	122.097	479.645	124.304	−1.855
3600	38.775	327.694	292.702	125.973	478.714	114.165	−1.656
3700	38.813	328.757	293.662	129.852	477.775	104.051	−1.469
3800	38.851	329.793	294.599	133.735	476.829	93.963	−1.292
3900	38.889	330.802	295.514	137.622	475.878	83.900	−1.124
4000	38.928	331.787	296.409	141.513	474.922	73.862	−0.965
4100	38.968	332.749	297.284	145.408	473.963	63.847	−0.813
4200	39.008	333.689	298.139	149.307	473.003	53.856	−0.670
4300	39.048	334.607	298.977	153.210	472.041	43.887	−0.533
4400	39.089	335.505	299.797	157.117	471.080	33.941	−0.403
4500	39.131	336.384	300.600	161.028	470.120	24.017	−0.279
4600	39.174	337.244	301.387	164.943	469.161	14.115	−0.160
4700	39.217	338.087	302.159	168.862	468.205	4.233	−0.047
4800	39.261	338.914	302.916	172.786	467.252	−5.629	0.061
4900	39.306	339.724	303.659	176.715	466.303	−15.471	0.165
5000	39.353	340.518	304.389	180.647	465.358	−25.293	0.264
5100	39.400	341.298	305.105	184.585	464.417	−35.097	0.359
5200	39.448	342.063	305.808	188.528	463.481	−44.882	0.451
5300	39.498	342.815	306.499	192.475	462.551	−54.650	0.539
5400	39.549	343.554	307.179	196.427	461.625	−64.399	0.623
5500	39.601	344.280	307.847	200.385	460.705	−74.132	0.704
5600	39.654	344.994	308.504	204.347	459.791	−83.848	0.782
5700	39.709	345.697	309.150	208.315	458.883	−93.548	0.857
5800	39.765	346.388	309.786	212.289	457.980	−103.232	0.930
5900	39.822	347.068	310.412	216.268	457.083	−112.900	1.000
6000	39.881	347.738	311.029	220.254	456.193	−122.554	1.067

PREVIOUS· June 1967 (1 atm) CURRENT. June 1967 (1 bar)

Bromotrifluoromethane ($CBrF_3$) IDEAL GAS $M_r = 148.910209$ Bromotrifluoromethane ($CBrF_3$) $C_1Br_1F_3(g)$

$S°(298.15\ K) = 297.83 \pm 0.50\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -636.9 \pm 2.9\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -648.9 \pm 2.9\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}
1086 (1)	1206 (2)
761 (1)	549 (2)
348 (1)	300 (2)

Ground State Quantum Weight: 1 $\sigma = 4$
Point Group: C_{3v}
Bond Distances: C–F = 1.328 Å; C–Br = 1.909 Å
Bond Angles: F–C–F = 108.6 ± 1°; F–C–Br = 110.33°
Product of the Moments of Inertia: $I_A I_B I_C = 2.340709 \times 10^{-113}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The selected value is obtained from least squares, *simultaneous adjustment of the enthalpies of formation* of CF_3, CF_3X (X = H, Cl, Br, I, CF_3) and C_2F_4. Details of the input data and the adjustment are given by Syverud.[1] Coomber and Whittle[2–4] have determined equilibrium data for $CClF_3(g) + BrCl(g) = CBrF_3(g) + Cl_2(g)$ and for $CF_3X(g) + Br_2(g) = CF_3Br(g) + BrX(g)$ where X = H, Cl, and CF. Equilibrium data for $CF_3I(g) + BrI(g) = CBrF_3(g) + I_2(g)$ were obtained by Lord *et al.*[5] These data link $CBrF_3$ with C_2F_6, CHF_3, $CClF_3$ and CF_3I.

Heat Capacity and Entropy

The molecular structure has been derived from electron–diffraction studies by Sharbaugh *et al.*,[6] Bowen,[7] and Anderson[8] and from microwave data by Sheridan and Gordy.[9] The adoped parameters are an average of those reported by.[8,9] Infrared spectra of the gas were observed by several investigators[10–12] and Raman spectra *of the liquid were obtained by Edgell and May.*[12] The vibrational assignments of McGee *et al.*[11] and Edgell and May[12] are in close agreement. These assignments are adopted but preference is given to frequencies observed for the gas. The value for ν_6 is taken as 300 cm^{-1} which is between the values of 305 and 297 ± 3 cm^{-1} derived from Raman spectra and IR (combination and overtone) spectra, respectively.

The thermodynamic functions of this table are essentially the same as those calculated by McGee *et al.*[11] Uncertainty in the entropy is *estimated to vary* from 0.12 to 0.5 cal/(K·mol^{-1}) over the range from 300 to 1000 K. Uncertainty in ν_6 and neglect of anharmonicity are the major sources of error. Discussions of the magnitude of anharmonic effects appear on the tables for $CClF_3(g)$ and $CF_4(g)$ The principal moments of inertia are: $I_A = 14.6768 \times 10^{-39}$ and $I_B = I_C = 39.9354 \times 10^{-39}\ g{\cdot}cm^2$.

References

[1] A. N. Syverud, Quarterly Tech. Report T–0009–2Q–69 under AFRPL contract NR F04611–67–C–0009, Dow Chemical Co., (July, 1969).
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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
0	0.	0.	INFINITE	−14.468	−636.863	−636.863	INFINITE
100	39.323	240.114	350.236	−11.012	−639.224	−634.892	331.634
200	56.420	272.770	303.778	−6.202	−641.584	−629.584	164.431
250	63.460	286.136	298.936	−3.200	−642.540	−626.472	130.894
298.15	69.330	297.827	297.827	0.	−648.938	−622.641	109.084
300	69.540	298.256	297.828	0.128	−648.983	−622.478	108.383
350	74.784	309.380	298.695	3.740	−664.551	−617.201	92.112
400	79.273	319.667	300.681	7.594	−664.608	−610.432	79.714
450	83.084	329.230	303.329	11.656	−664.596	−603.660	70.071
500	86.305	338.156	306.370	15.893	−664.531	−596.892	62.357
600	91.313	354.359	313.046	24.788	−664.284	−583.385	50.788
700	94.902	368.720	319.994	34.108	−663.933	−569.929	42.529
800	97.514	381.572	326.902	43.736	−663.517	−556.527	36.338
900	99.454	393.175	333.631	53.589	−663.062	−543.181	31.525
1000	100.923	403.733	340.122	63.611	−662.585	−529.886	27.678
1100	102.058	413.407	346.350	73.762	−662.099	−516.640	24.533
1200	102.949	422.327	352.315	84.014	−661.613	−503.437	21.914
1300	103.660	430.596	358.022	94.346	−661.134	−490.276	19.700
1400	104.236	438.300	363.485	104.742	−660.669	−477.150	17.803
1500	104.708	445.508	368.715	115.190	−660.220	−464.058	16.160
1600	105.100	452.279	373.728	125.681	−659.792	−450.994	14.723
1700	105.428	458.661	378.539	136.208	−659.386	−437.957	13.457
1800	105.705	464.695	383.159	146.765	−659.002	−424.943	12.332
1900	105.942	470.417	387.602	157.348	−658.640	−411.950	11.325
2000	106.145	475.856	391.880	167.952	−658.300	−398.974	10.420
2100	106.321	481.039	396.003	178.576	−657.978	−386.017	9.602
2200	106.475	485.989	399.982	189.216	−657.670	−373.073	8.858
2300	106.609	490.725	403.825	199.870	−657.375	−360.143	8.179
2400	106.727	495.265	407.541	210.537	−657.086	−347.227	7.557
2500	106.832	499.624	411.138	221.215	−656.800	−334.322	6.985
2600	106.925	503.816	414.622	231.903	−656.512	−321.428	6.458
2700	107.008	507.853	418.001	242.600	−656.217	−308.546	5.969
2800	107.083	511.746	421.280	253.304	−655.910	−295.675	5.516
2900	107.150	515.504	424.464	264.016	−655.587	−282.815	5.094
3000	107.211	519.138	427.560	274.734	−655.243	−269.966	4.701
3100	107.266	522.654	430.571	285.458	−654.874	−257.130	4.333
3200	107.316	526.061	433.502	296.187	−654.477	−244.306	3.988
3300	107.361	529.364	436.357	306.921	−654.048	−231.494	3.664
3400	107.403	532.569	439.140	317.659	−653.584	−218.697	3.360
3500	107.441	535.683	441.854	328.401	−653.082	−205.913	3.073
3600	107.476	538.711	444.503	339.147	−652.540	−193.144	2.802
3700	107.508	541.656	447.089	349.896	−651.956	−180.391	2.547
3800	107.538	544.523	449.616	360.649	−651.329	−167.655	2.305
3900	107.566	547.317	452.085	371.404	−650.657	−154.935	2.075
4000	107.591	550.041	454.500	382.162	−649.939	−142.233	1.857
4100	107.615	552.698	456.863	392.922	−649.175	−129.550	1.650
4200	107.637	555.291	459.176	403.685	−648.363	−116.886	1.454
4300	107.658	557.824	461.440	414.450	−647.505	−104.242	1.266
4400	107.677	560.299	463.659	425.216	−646.599	−91.618	1.088
4500	107.695	562.719	465.834	435.985	−645.647	−79.015	0.917
4600	107.712	565.087	467.966	446.755	−644.648	−66.435	0.754
4700	107.727	567.403	470.057	457.527	−643.603	−53.876	0.599
4800	107.742	569.671	472.109	468.301	−642.512	−41.340	0.450
4900	107.756	571.893	474.122	479.076	−641.377	−28.827	0.307
5000	107.769	574.070	476.100	489.852	−640.198	−16.338	0.171
5100	107.781	576.204	478.042	500.630	−638.976	−3.873	0.040
5200	107.793	578.297	479.950	511.408	−637.713	8.568	−0.086
5300	107.804	580.351	481.825	522.188	−636.408	20.984	−0.207
5400	107.814	582.366	483.668	532.969	−635.064	33.375	−0.323
5500	107.824	584.344	485.481	543.751	−633.681	45.741	−0.434
5600	107.833	586.287	487.263	554.534	−632.261	58.082	−0.542
5700	107.842	588.196	489.017	565.318	−630.804	70.396	−0.645
5800	107.851	590.072	490.744	576.102	−629.313	82.684	−0.745
5900	107.859	591.915	492.443	586.888	−627.787	94.948	−0.841
6000	107.866	593.728	494.116	597.674	−626.229	107.184	−0.933

PREVIOUS: June 1969 (1 atm) CURRENT: June 1969 (1 bar)

Cyanogen Bromide (BrCN) IDEAL GAS $M_r = 105.9217$ Cyanogen Bromide (BrCN) $C_1Br_1N_1(g)$

$\Delta_f H°(0\ K) = 192.75 \pm 6.3\ kJ{\cdot}mol^{-1}$

$S°(298.15\ K) = 248.363 \pm 0.040\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_f H°(298.15\ K) = 186.19 \pm 6.3\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
575 (1)
342.5 (2)
2200 (1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: $C_{\infty v}$
Bond Distances: C–Br = 1.789 Å; C–N = 1.158 Å
Bond Angle: Br–C–N = 180°
Rotational Constants: $B_0 = 0.137172\ cm^{-1}$; $D_0 = 2.929 \times 10^{-8}\ cm^{-1}$

Spectroscopic constants used in calculating corrections to rigid-rotator-harmonic oscillator approximation (cm^{-1}).

$\alpha_1 = 5.17 \times 10^{-4}$ $x_{11} = [-3.0]$ $x_{12} = [-4.0]$
$\alpha_2 = -3.84 \times 10^{-4}$ $x_{22} = -0.86$ $x_{23} = -6.19$
$\alpha_3 = 6.77 \times 10^{-4}$ $x_{33} = [-5.0]$ $x_{13} = [-3.0]$
$g_{22} = 1.14$

Enthalpy of Formation

The enthalpy of formation is calculated from $\Delta_f H°$(BrCN, cr, 298.15 K) = 33.58 kcal·mol^{-1}[1] and $\Delta_{sub}H°$ (298.15 K) = 10.92 ± 0.1 kcal·mol^{-1}. This latter is obtained from an anlysis of the vapor pressure data of Lord and Woof[2] and Baxter *et al.*[3]

The enthalpy of formation of the crystal is calculated from $\Delta_f H°$(298.15 K) = −56.0 kcal·mol^{-1} obtained by Lord and Woolf[2] for the reaction

$$BrCN(cr) + 2NaOH(56\ H_2O) = NaCNO(2800\ H_2O) + NaBr(2800\ H_2O) + H_2O(l).$$

The auxiliary data used were $\Delta_f H°$($NaOH{\cdot}56H_2O$, 298.15 K) = −112.26 kcal·mol^{-1},[1,4] $\Delta_f H$($NaCNO{\cdot}2800H_2O$, 298.15 K) = −92.25 kcal·mol^{-1},[1,4] and $\Delta_f H°$($NaBr{\cdot}2800H_2O$, 298.15 K) = −70.54 kcal·mol^{-1}.[1,4] The uncertainty in the final value reflects the uncertainty in $\Delta_r H$($NaCNO{\cdot}2800H_2O$) which was determined by Lord and Woolf[2] to be −93.6 kcal·mol^{-1} in excess $NaOH{\cdot}56H_2O$.

Heat Capacity and Entropy

Gordon[5] used the constants given above to calculate the adopted table, using the method of Pennington and Kobe[6] for anharmonicity, vibration rotation interaction, and centrifugal stretching corrections.

The bond lengths and angle were reported by Tyler and Sheridan.[7]

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−11.075	192.754	192.754	INFINITE
100	32.213	205.109	286.153	−8.104	192.817	183.084	−95.633
200	41.714	230.527	252.430	−4.381	192.308	173.560	−45.329
298.15	47.124	248.363	248.363	0.	186.188	165.104	−28.926
300	47.196	248.655	248.364	0.087	186.163	164.974	−28.724
400	50.137	262.658	250.253	4.962	171.316	160.993	−21.023
500	52.095	274.064	253.910	10.077	171.789	158.355	−16.543
600	53.664	283.704	258.092	15.367	172.149	155.632	−13.549
700	55.020	292.080	262.362	20.802	172.421	152.857	−11.406
800	56.204	299.506	266.550	26.365	172.631	150.047	−9.797
900	57.237	306.187	270.589	32.038	172.800	147.214	−8.544
1000	58.137	312.265	274.457	37.808	172.939	144.363	−7.541
1100	58.915	317.843	278.151	43.661	173.059	141.500	−6.719
1200	59.597	322.999	281.676	49.587	173.163	138.626	−6.034
1300	60.191	327.793	285.042	55.577	173.257	135.744	−5.454
1400	60.714	332.273	288.257	61.623	173.342	132.856	−4.957
1500	61.174	336.478	291.333	67.718	173.418	129.961	−4.526
1600	61.588	340.440	294.280	73.856	173.488	127.062	−4.148
1700	61.961	344.185	297.106	80.034	173.550	124.158	−3.815
1800	62.300	347.736	299.821	86.247	173.605	121.251	−3.519
1900	62.614	351.113	302.433	92.493	173.653	118.341	−3.253
2000	62.898	354.332	304.948	98.769	173.692	115.429	−3.015
2100	63.162	357.407	307.373	105.072	173.722	112.515	−2.799
2200	63.409	360.351	309.715	111.401	173.742	109.600	−2.602
2300	63.643	363.175	311.978	117.753	173.752	106.684	−2.423
2400	63.860	365.888	314.168	124.129	173.751	103.768	−2.258
2500	64.070	368.500	316.290	130.525	173.739	100.852	−2.107
2600	64.270	371.016	318.346	136.942	173.716	97.937	−1.968
2700	64.459	373.446	320.342	143.379	173.683	95.023	−1.838
2800	64.643	375.793	322.281	149.834	173.640	92.110	−1.718
2900	64.819	378.065	324.166	156.307	173.587	89.200	−1.607
3000	64.990	380.265	325.999	162.797	173.525	86.291	−1.502
3100	65.157	382.399	327.784	169.305	173.456	83.384	−1.405
3200	65.321	384.470	329.524	175.829	173.381	80.480	−1.314
3300	65.480	386.482	331.219	182.369	173.300	77.578	−1.228
3400	65.634	388.440	332.873	188.925	173.216	74.678	−1.147
3500	65.785	390.344	334.488	195.496	173.130	71.781	−1.071
3600	65.931	392.200	336.066	202.081	173.042	68.887	−1.000
3700	66.078	394.008	337.608	208.682	172.954	65.995	−0.932
3800	66.224	395.772	339.115	215.297	172.868	63.105	−0.867
3900	66.362	397.494	340.590	221.926	172.785	60.218	−0.807
4000	66.505	399.176	342.034	228.570	172.705	57.333	−0.749
4100	66.643	400.820	343.448	235.227	172.630	54.449	−0.694
4200	66.781	402.428	344.833	241.898	172.562	51.568	−0.641
4300	66.915	404.001	346.191	248.583	172.500	48.688	−0.591
4400	67.049	405.540	347.522	255.281	172.446	45.809	−0.544
4500	67.182	407.049	348.828	261.993	172.400	42.931	−0.498
4600	67.312	408.527	350.110	268.718	172.363	40.055	−0.455
4700	67.442	409.976	351.368	275.455	172.336	37.179	−0.413
4800	67.572	411.397	352.604	282.206	172.319	34.303	−0.373
4900	67.701	412.792	353.818	288.970	172.312	31.428	−0.335
5000	67.831	414.161	355.011	295.746	172.315	28.553	−0.298
5100	67.957	415.505	356.184	302.536	172.330	25.678	−0.263
5200	68.086	416.826	357.338	309.338	172.356	22.802	−0.229
5300	68.212	418.124	358.473	316.153	172.393	19.925	−0.196
5400	68.337	419.400	359.589	322.980	172.441	17.048	−0.165
5500	68.463	420.655	360.688	329.820	172.500	14.170	−0.135
5600	68.584	421.890	361.770	336.673	172.571	11.291	−0.105
5700	68.710	423.105	362.835	343.537	172.652	8.410	−0.077
5800	68.835	424.301	363.885	350.414	172.745	5.528	−0.050
5900	68.956	425.479	364.919	357.304	172.848	2.644	−0.023
6000	69.078	426.639	365.938	364.206	172.961	−0.242	0.002

PREVIOUS: June 1969 (1 atm) CURRENT. June 1969 (1 bar)

Tetrabromomethane (CBr$_4$) IDEAL GAS $M_r = 331.627$ Tetrabromomethane (CBr$_4$) C$_1$Br$_4$(g)

$S°(298.15\ K) = 358.095\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [79.890]\ kJ{\cdot}mol^{-1}$

$\Delta_f H°(298.15\ K) = [50.208]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	 ν, cm^{-1}
267.2(1)	670.7(3)
122.5(2)	182.5(3)

Ground State Quantum Weight: [1] $\sigma = 12$
Point Group: T$_d$
Bond Distance: C–Br = 1.942 Å
Bond Angle: Br–C–Br = 109° 28'
Product of the Moments of Inertia: $I_A I_B I_C = 2.376154 \times 10^{-111}\ g^3{\cdot}cm^6$

Enthalpy of Formation

$\Delta_f H°(298.15\ K)$ was calculated and reported by Rossini *et al.*[1]

Heat Capacity and Entropy

The molecular constants, bond distance, and bond angle were determined by electron diffraction by Finbak *et al.*[2,3] The constants reported by Finbak *et al.*[3] in 1943 were selected. These constants are listed in "Tables of Interatomic Distances and Configuration in Molecules and Ions," Special Publication No. 11, The Chemical Society (London), 1958. The principal moments of inertia calculated from these constants are: $I_A = I_B = I_C = 133.4417 \times 10^{-39}\ g{\cdot}cm^2$.

The vibrational frequencies used were assigned by Meister *et al.*[4] They measured the infrared and Raman spectrum, considered the previous literature, calculated force constants and made most probable value assignments for the frequencies. A more recent paper by Moszynska and Mathieu[5] made assignments from Raman and infrared spectra which agreed with all of Meister *et al.*'s[4] assignments except for ν_2 which they found was 126 cm^{-1} rather than 122 cm^{-1}.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−20.388	79.890	79.890	INFINITE
100	63.538	273.277	432.002	−15.873	78.759	62.296	−32.540
200	81.403	323.603	366.156	−8.511	75.992	46.857	−12.238
250	87.009	342.397	359.574	−4.294	74.282	39.763	−8.308
298.15	91.180	358.095	358.095	0.	50.208	35.914	−6.292
300	91.319	358.659	358.096	0.169	50.081	35.826	−6.238
350	94.594	372.993	359.221	4.820	−11.039	36.793	−5.491
400	97.081	385.795	361.757	9.615	−10.455	43.587	−5.692
450	98.987	397.344	365.080	14.519	−9.863	50.306	−5.839
500	100.464	407.853	368.840	19.507	−9.274	56.960	−5.951
600	102.548	426.368	376.926	29.665	−8.132	70.099	−6.103
700	103.902	442.285	385.153	39.992	−7.055	83.051	−6.197
800	104.823	456.223	393.184	50.431	−6.042	95.854	−6.259
900	105.475	468.609	400.889	60.948	−5.088	108.533	−6.299
1000	105.951	479.748	408.227	71.520	−4.187	121.108	−6.326
1100	106.310	489.864	415.196	82.134	−3.333	133.596	−6.344
1200	106.586	499.126	421.810	92.780	−2.523	146.008	−6.356
1300	106.802	507.666	428.090	103.449	−1.753	158.354	−6.363
1400	106.976	515.588	434.060	114.139	−1.022	170.642	−6.367
1500	107.116	522.973	439.744	124.844	−0.329	182.880	−6.368
1600	107.232	529.890	445.165	135.561	0.325	195.072	−6.368
1700	107.328	536.394	450.342	146.289	0.939	207.225	−6.367
1800	107.409	542.531	455.295	157.026	1.511	219.343	−6.365
1900	107.478	548.341	460.040	167.771	2.039	231.430	−6.362
2000	107.537	553.855	464.594	178.522	2.519	243.491	−6.359
2100	107.588	559.103	468.971	189.278	2.949	255.528	−6.356
2200	107.632	564.109	473.182	200.039	3.325	267.547	−6.352
2300	107.670	568.894	477.240	210.804	3.646	279.549	−6.349
2400	107.704	573.477	481.155	221.573	3.910	291.540	−6.345
2500	107.734	577.875	484.937	232.345	4.116	303.520	−6.342
2600	107.760	582.101	488.593	243.119	4.265	315.492	−6.338
2700	107.784	586.168	492.132	253.897	4.357	327.461	−6.335
2800	107.805	590.088	495.561	264.676	4.395	339.427	−6.332
2900	107.824	593.872	498.886	275.458	4.381	351.392	−6.329
3000	107.841	597.527	502.114	286.241	4.319	363.359	−6.327
3100	107.857	601.064	505.249	297.026	4.213	375.329	−6.324
3200	107.871	604.488	508.297	307.812	4.068	387.302	−6.322
3300	107.884	607.808	511.262	318.600	3.889	399.281	−6.320
3400	107.896	611.029	514.150	329.389	3.681	411.266	−6.318
3500	107.906	614.156	516.962	340.179	3.450	423.257	−6.317
3600	107.916	617.196	519.705	350.970	3.202	435.255	−6.315
3700	107.925	620.153	522.380	361.762	2.940	447.260	−6.314
3800	107.934	623.032	524.991	372.555	2.671	459.272	−6.313
3900	107.941	625.835	527.541	383.349	2.400	471.291	−6.312
4000	107.949	628.568	530.032	394.143	2.132	483.318	−6.311
4100	107.955	631.234	532.468	404.939	1.870	495.351	−6.311
4200	107.962	633.835	534.851	415.735	1.619	507.390	−6.310
4300	107.967	636.376	537.183	426.531	1.383	519.435	−6.310
4400	107.973	638.858	539.465	437.328	1.164	531.485	−6.310
4500	107.978	641.285	541.701	448.126	0.966	543.540	−6.309
4600	107.982	643.658	543.892	458.924	0.792	555.599	−6.309
4700	107.987	645.980	546.039	469.722	0.644	567.662	−6.309
4800	107.991	648.254	548.145	480.521	0.523	579.728	−6.309
4900	107.995	650.480	550.211	491.320	0.431	591.795	−6.309
5000	107.998	652.662	552.238	502.120	0.370	603.865	−6.309
5100	108.002	654.801	554.228	512.920	0.340	615.935	−6.308
5200	108.005	656.898	556.183	523.720	0.343	628.005	−6.308
5300	108.008	658.956	558.103	534.521	0.379	640.076	−6.308
5400	108.011	660.974	559.989	545.322	0.448	652.145	−6.308
5500	108.014	662.956	561.843	556.123	0.551	664.213	−6.308
5600	108.016	664.903	563.666	566.925	0.687	676.278	−6.308
5700	108.019	666.815	565.459	577.726	0.857	688.341	−6.308
5800	108.021	668.693	567.223	588.528	1.059	700.399	−6.308
5900	108.023	670.540	568.958	599.331	1.295	712.455	−6.308
6000	108.026	672.355	570.667	610.133	1.562	724.506	−6.307

PREVIOUS December 1963 (1 atm) CURRENT December 1963 (1 bar)

Chloromethylidyne (CCl) IDEAL GAS $M_r = 47.464$ Chloromethylidyne (CCl) $C_1Cl_1(g)$

$S°(298.15 \text{ K}) = 224.52 \pm 0.4 \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = 498.3 \pm 20 \text{ kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = 502.1 \pm 20 \text{ kJ·mol}^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$X^2\Pi_{1/2}$	0	2
$^2\Pi_{3/2}$	134.92	2
$[^4\Sigma]$	[20000]	[4]
$A^2\Delta$	36004	4

$\omega_e = 876.4 \text{ cm}^{-1}$ $\omega_e x_e = 6.15 \text{ cm}^{-1}$ $\sigma = 1$
$B_e = 0.69666 \text{ cm}^{-1}$ $\alpha_e = [0.0066] \text{ cm}^{-1}$ $r_e = 1.642$ Å

Enthalpy of Formation

The data of Miller and Palmer[1] provide a value of $D_0°(\text{CCl}) = 80 \pm 5$ kcal·mol^{-1}, which appears to be reasonably substantiated. They studied the chemiluminescence from flames of $CHCl_3$ and CCl_4 burning in potassium vapor. These flames exhibit C_2 Swan band radiation with major departures from vibrational and rotational equilibrium. The spectra are interpreted as due to the reaction $C + CCl \rightarrow C_2 + Cl$ where the carbon atom is either ^3D ground state or ^1D first excited state. The separation between the ground and first excited state of the carbon atom is matched closely by the difference in preferential population of the excited C_2 levels. The assumption is made that all the exothermicity of the reaction is retained as vibrational excitation of the C_2, thus the populated levels are measures of the heat of reaction In this manner we obtain a heat of reaction of 67 ± 2.5 kcal·mol^{-1} for the reaction $C + CCl \rightarrow C_2 + Cl$ which, using JANAF auxiliary data, gives $\Delta_f H°(\text{CCl, g}) = 124 \pm 2.5$ kcal·mol^{-1}; however, this represents the initial state of the CCl which in the flame is presumed to have about 4 kcal·mol^{-1} of vibrational energy at roughly 2000 K. Thus, we obtain $\Delta_f H°(\text{CCl, g}) = 120 \pm 5$ kcal·mol^{-1} (502.080 ± 20 kJ·mol^{-1}) which is adopted.

The enthalpy of formation can also be estimated from the dissociation energy calculated from the linear Birge–Sponer extrapolation of the ground state vibrational constants. This yields $D_0° = 89$ kcal·mol^{-1} or $\Delta_f H°(298.15 \text{ K}) = 111$ kcal·mol^{-1}. There are several indications that this dissociation energy is probably a maximum value, for example, Hildenbrand[5] has applied an ionic–covalent correction to the linear extrapolation which gives $D_0° = 72$ kcal·mol^{-1}. We would expect this enthalpy of formation to be a minimum value. A real minimum for the dissociation energy can be obtained from the knowledge that the first vibrational level of the $^2\Delta$ state is occupied and so the dissociation energy of this state must be greater than 850 cm^{-1}. This yields a minimum dissociation energy of the ground state of 76 kcal·mol^{-1}, assuming the dissociation products are $C(^1\Delta)$ and $Cl(^2P)$, and $\Delta_f H°(\text{CCl, g, 298.15 K}) = 124$ kcal·mol^{-1} which is the maximum value of the heat of formation.

Heat Capacity and Entropy

The rotational and electronic constants are those of Verma and Mulliken.[2] The vibrational constants are those derived by Ovcharenko *et al.*[3] from the data of Gordon and King.[4] The anharmonicities listed by Verma and Mulliken are not used, since these are based only on the 0,0 and 0,1 transitions. The $^4\Sigma$ level is estimated by analogy with CF(g). The value for α_e was obtained from the other constants assuming a Morse potential function.

References

[1] W. J. Miller and H. B. Palmer, J. Chem. Phys. 40, 3701 (1964).
[2] R. D. Verma and R. S. Mulliken, J. Mol. Spectrosc. 6, 419 (1961).
[3] I. E. Ovcharenko, Yu. Ya. Kuzyakov, and V. M. Tatievskii, Opt. Spectrosc. (Eng. Transl.) 19, 294 (1965).
[4] R. D. Gordon and G. W. King, Can. J. Phys. 39, 252 (1961).
[5] D. L. Hildenbrand, Douglas Advanced Research Laboratories, Huntington Beach, Calif., private communication, (December 30, 1969).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	$\Delta_f G°$ (kJ·mol^{-1})	log K_f
0	0.	0.	INFINITE	−9.395	498.327	498.327	INFINITE
100	32.553	189.824	252.667	−6.284	499.922	490.485	−256.203
200	31.329	211.872	227.428	−3.111	501.249	480.488	−125.491
250	31.663	218.890	225.043	−1.538	501.717	475.241	−99.296
298.15	32.254	224.516	224.516	0.	502.080	470.108	−82.361
300	32.279	224.715	224.516	0.060	502.092	469.909	−81.818
350	32.956	229.742	224.912	1.691	502.393	464.521	−69.326
400	33.594	234.185	225.799	3.355	502.630	459.093	−59.951
450	34.156	238.175	226.956	5.049	502.807	453.640	−52.657
500	34.637	241.799	228.262	6.769	502.932	448.170	−46.820
600	35.391	248.185	231.064	10.272	503.041	437.205	−38.062
700	35.934	253.684	233.912	13.840	503.000	426.233	−31.806
800	36.335	258.509	236.691	17.455	502.843	415.276	−27.115
900	36.639	262.807	239.359	21.104	502.598	404.344	−23.468
1000	36.877	266.680	241.900	24.780	502.283	393.443	−20.551
1100	37.068	270.204	244.316	28.478	501.911	382.577	−18.167
1200	37.226	273.437	246.610	32.193	501.494	371.747	−16.182
1300	37.360	276.422	248.789	35.922	501.038	360.953	−14.503
1400	37.476	279.195	250.863	39.664	500.550	350.195	−13.066
1500	37.577	281 784	252.839	43.417	500.033	339.473	−11.822
1600	37.668	284.212	254.725	47.179	499.490	328.787	−10.734
1700	37.751	286.498	256.528	50.950	498.925	318.135	−9.775
1800	37.827	288.658	258.253	54.729	498.338	307.517	−8.924
1900	37.898	290.705	259.908	58.515	497.732	296.932	−8.163
2000	37.965	292.651	261.497	62.309	497.107	286.380	−7.479
2100	38.029	294.505	263.025	66.108	496.464	275.859	−6.862
2200	38.090	296.275	264.496	69.914	495.803	265.370	−6.301
2300	38.149	297.970	265.915	73.726	495.124	254.911	−5.789
2400	38.207	299.595	267.285	77.544	494.428	244.481	−5.321
2500	38.264	301.155	268.608	81.367	493.714	234.082	−4.891
2600	38.321	302.657	269.889	85.197	492.982	223.711	−4.494
2700	38.378	304.105	271.130	89.032	492.233	213.368	−4.128
2800	38.436	305.501	272.333	92.872	491.466	203.054	−3.788
2900	38.494	306.851	273.500	96.719	490.682	192.767	−3.472
3000	38.555	308.157	274.633	100.571	489.881	182.508	−3.178
3100	38.616	309.422	275.735	104.430	489.063	172.276	−2.903
3200	38.680	310.649	276.807	108.295	488.230	162.070	−2.646
3300	38.746	311.841	277.851	112.166	487.382	151.891	−2.404
3400	38.814	312.998	278.868	116.044	486.520	141.737	−2.178
3500	38.885	314.124	279.859	119.929	485.646	131.609	−1.964
3600	38.959	315.221	280.826	123.821	484.760	121.506	−1.763
3700	39.035	316.289	281.770	127.721	483.865	111.428	−1.573
3800	39.114	317.331	282.692	131.628	482.961	101.374	−1.393
3900	39.196	318.348	283.594	135.543	482.051	91.344	−1.223
4000	39.281	319.342	284.475	139.467	481.135	81.338	−1.062
4100	39.369	320.313	285.337	143.400	480.217	71.355	−0.909
4200	39.459	321.263	286.181	147.341	479.296	61.393	−0.764
4300	39.553	322.192	287.008	151.292	478.376	51.454	−0.625
4400	39.649	323.103	287.818	155.252	477.458	41.536	−0.493
4500	39.748	323.995	288.612	159.222	476.543	31.639	−0.367
4600	39.849	324.870	289.391	163.201	475.632	21.763	−0.247
4700	39.953	325.728	290.155	167.192	474.728	11.906	−0.132
4800	40.059	326.570	290.905	171.192	473.831	2.068	−0.023
4900	40.167	327.397	291.641	175.203	472.943	−7.751	0.083
5000	40.277	328.210	292.364	179.226	472.065	−17.553	0.183
5100	40.390	329.008	293.075	183.259	471.197	−27.336	0.280
5200	40.503	329.794	293.774	187.304	470.342	−37.103	0.373
5300	40.619	330.566	294.461	191.360	469.500	−46.854	0.462
5400	40.736	331.327	295.136	195.427	468.671	−56.588	0.547
5500	40.854	332.075	295.801	199.507	467.857	−66.308	0.630
5600	40.974	332.812	296.456	203.598	467.057	−76.012	0.709
5700	41.095	333.539	297.100	207.702	466.273	−85.703	0.785
5800	41.216	334.254	297.734	211.817	465.505	−95.380	0.859
5900	41.338	334 960	298.359	215.945	464.753	−105.044	0.930
6000	41.462	335.656	298.975	220.085	464.018	−114.696	0.999

PREVIOUS: December 1969 (1 atm) CURRENT: December 1969 (1 bar)

Chloromethylidyne (CCl) $C_1Cl_1(g)$

Carbonic Chloride Fluoride (COClF) IDEAL GAS $M_r = 82.461803$ Carbonic Chloride Fluoride (COClF) $C_1Cl_1F_1O_1(g)$

$S°(298.15\ K) = [277.012]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = [-424.3 \pm 33]\ kJ{\cdot}mol^{-1}$

$\Delta_fH°(298.15\ K) = [-426.8 \pm 33]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	 ν, cm^{-1}
776(1)	1095(1)
1868(1)	415(1)
501(1)	667(1)

Ground State Quantum Weight: 1 $\sigma = 1$

Point Group. C_s

Product of the Moments of Inertia: $I_AI_BI_C = 2.7911 \times 10^{-114}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The enthalpies of formation of $COCl_2$ and COF_2 have been averaged to obtain that of COClF.

Heat Capacity and Entropy

The molecular constants are from Lovell *et al.*[1] The principle moments of inertia are: $I_A = 7.480 \times 10^{-39}$, $I_B = 16.008 \times 10^{-39}$, and $I_C = 23.31 \times 10^{-39}\ g{\cdot}cm^2$.

References

[1] R. J. Lovell, C. V. Stephenson and E. A. Jones, J. Chem Phys. 22, 1953 (1954).

Enthalpy Reference Temperature = T_r = 298.15 K | Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−11.904	−424.276	−424.276	INFINITE
100	34.405	231.656	317.256	−8.560	−425.354	−421.790	220.320
200	43.300	257.957	281.526	−4.714	−426.273	−417.838	109.128
250	48.207	268.154	277.852	−2.424	−426.569	−415.693	86.854
298.15	52.396	277.012	277.012	0.	−426.768	−413.579	72.457
300	52.545	277.337	277.013	0.097	−426.774	−413.497	71.996
350	56.256	285.723	277.667	2.820	−426.915	−411.272	61.379
400	59.407	293.446	279.163	5.713	−427.011	−409.031	53.414
450	62.091	300.602	281.152	8.753	−427.080	−406.779	47.218
500	64.390	307.266	283.434	11.916	−427.133	−404.520	42.260
600	68.086	319.349	288.434	18.549	−427.211	−399.990	34.822
700	70.879	330.064	293.631	25.503	−427.268	−395.448	29.509
800	73.020	339.674	298.796	32.703	−427.313	−390.899	25.523
900	74.684	348.375	303.829	40.091	−427.349	−386.345	22.423
1000	75.993	356.314	308.686	47.628	−427.380	−381.788	19.943
1100	77.036	363.608	313.352	55.281	−427.410	−377.227	17.913
1200	77.876	370.348	317.825	63.028	−427.442	−372.664	16.222
1300	78.561	376.610	322.109	70.851	−427.481	−368.097	14 790
1400	79.124	382.453	326.213	78.736	−427.528	−363.528	13.563
1500	79.593	387.928	330.146	86.673	−427.587	−358.954	12.500
1600	79.987	393.078	333.920	94.653	−427.660	−354.377	11.569
1700	80.320	397.938	337.544	102.668	−427.750	−349.794	10.748
1800	80.605	402.537	341.028	110.715	−427.856	−345.205	10.018
1900	80.849	406.902	344.382	118.788	−427.982	−340.610	9.364
2000	81.060	411.054	347.612	126.884	−428.126	−336.008	8.776
2100	81.244	415.014	350.728	134 999	−428.290	−331.398	8.243
2200	81.405	418.797	353.737	143.132	−428.473	−326.780	7 759
2300	81.546	422.419	356.645	151.279	−428.675	−322.153	7.316
2400	81.672	425.892	359.458	159.440	−428.897	−317 517	6.911
2500	81.783	429.228	362.183	167.613	−429.136	−312.871	6.537
2600	81.882	432.438	364.824	175.797	−429.393	−308.216	6.192
2700	81.971	435.530	367.385	183.989	−429.666	−303.550	5.873
2800	82.051	438.512	369.873	192.191	−429.955	−298.874	5.576
2900	82.123	441.393	372.290	200.399	−430.259	−294.187	5.299
3000	82.188	444.178	374.640	208.615	−430.576	−289.489	5.040
3100	82.247	446.874	376.927	216.837	−430.905	−284.781	4 799
3200	82.301	449.486	379.153	225.064	−431.245	−280.062	4.572
3300	82.350	452.019	381.323	233.297	−431.596	−275.332	4.358
3400	82.395	454 478	383.439	241.534	−431.954	−270.592	4.157
3500	82.437	456.867	385.503	249.776	−432.320	−265.841	3.967
3600	82.475	459.190	387.518	258.021	−432.691	−261.079	3.788
3700	82.510	461.451	389.485	266.271	−433.066	−256.307	3.618
3800	82.542	463.651	391.408	274.523	−433.444	−251.524	3.457
3900	82.572	465.796	393.288	282.779	−433.823	−246.731	3.305
4000	82.600	467.887	395.127	291.038	−434.203	−241.930	3.159
4100	82.626	469.927	396.927	299.299	−434.581	−237.118	3.021
4200	82.650	471.918	398.689	307.563	−434.956	−232.297	2.889
4300	82.672	473.863	400.415	315.829	−435.329	−227.468	2.763
4400	82.693	475.764	402.105	324.097	−435.696	−222.630	2.643
4500	82.713	477.623	403.763	332.368	−436.058	−217.783	2.528
4600	82.731	479.441	405.389	340.640	−436.414	−212.929	2.418
4700	82.748	481.220	406.983	348.914	−436.763	−208.067	2.312
4800	82.765	482.962	408.548	357.189	−437.104	−203.197	2.211
4900	82.780	484.669	410.084	365.467	−437.438	−198.320	2.114
5000	82.794	486.342	411.593	373.745	−437.763	−193.437	2.021
5100	82.808	487.981	413.074	382.025	−438.080	−188.547	1.931
5200	82.820	489.589	414.530	390.307	−438.388	−183.652	1.845
5300	82.832	491.167	415.962	398.589	−438.688	−178.750	1.762
5400	82.844	492.715	417.369	406.873	−438.979	−173.843	1.682
5500	82.854	494.236	418.752	415.158	−439.262	−168.931	1.604
5600	82.865	495.729	420.114	423.444	−439.538	−164.012	1.530
5700	82.874	497.195	421.453	431.731	−439.807	−159.090	1.458
5800	82.883	498.637	422.772	440.019	−440.068	−154.163	1.388
5900	82.892	500.054	424.069	448.308	−440.324	−149.232	1.321
6000	82.900	501 447	425.347	456.597	−440.575	−144.296	1.256

PREVIOUS: June1961 (1 atm) CURRENT: June 1961 (1 bar)

Carbonic Chloride Fluoride (COClF) $C_1Cl_1F_1O_1(g)$

$S°(298.15 \text{ K}) = 285.35 \pm 0.4 \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = -702.84 \pm 3.3 \text{ kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = -707.93 \pm 3.3 \text{ kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	 ν, cm^{-1}
1106(1)	1217(2)
782(1)	560(2)
474(1)	350(2)

Ground State Quantum Weight: 1 $\sigma = 3$
Point Group: C_{3v}
Bond Distances: C–F = 1.328 Å; C–Cl = 1.751 Å
Bond Angles. F–C–F = 108.6 ± 0.5°; F–C–Cl = 110.33°
Product of the Moments of Inertia: $I_A I_B I_C = 9.444771 \times 10^{-114}$ g^3·cm^6

Enthalpy Reference Temperature = T_r = 298.15 K						Standard State Pressure = $p°$ = 0.1 MPa	
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−13.782	−702.836	−702.836	INFINITE
100	36.815	231.109	335.022	−10.391	−705.321	−693.331	362.159
200	53.051	261 466	291.051	−5.917	−707.086	−680.571	177.747
250	60.573	274.131	286.420	−3.072	−707.600	−673.878	140.799
298.15	66.887	285.353	285.353	0.	−707.933	−667.351	116.917
300	67.112	285.767	285.354	0 124	−707.943	−667.099	116.152
350	72.738	296.546	286.192	3.624	−708.157	−660.274	98.540
400	77.534	306.581	288.121	7.384	−708.270	−653.424	85.328
450	81.595	315.954	290.699	11.365	−708.305	−646.566	75.051
500	85.019	324.733	293.668	15.533	−708.282	−639.707	66.830
600	90.333	340.731	300.206	24.315	−708.103	−626.006	54.499
700	94.135	354.958	307.030	33.549	−707.806	−612.345	45.694
800	96.901	367.718	313.833	43.108	−707.432	−598.733	39.093
900	98 953	379.255	320.471	52.906	−707.010	−585.170	33.962
1000	100.508	389 765	326.883	62.882	−706.560	−571.657	29.860
1100	101.709	399.403	333.044	72.996	−706.096	−558.189	26.506
1200	102.652	408.295	338.949	83.215	−705 627	−544.763	23.713
1300	103.404	416.542	344.604	93.520	−705.162	−531.377	21.351
1400	104.014	424.229	350.020	103.891	−704.706	−518.026	19.328
1500	104.513	431.422	355.210	114.319	−704.265	−504.707	17.575
1600	104.927	438 181	360.187	124.791	−703.840	−491 417	16.043
1700	105.274	444.553	364.964	135.302	−703.434	−478 153	14.692
1800	105.568	450.579	369.554	145.844	−703.047	−464.913	13.491
1900	105.818	456.294	373.970	156 414	−702.678	−451.694	12.418
2000	106.033	461.727	378.224	167.007	−702.325	−438.493	11.452
2100	106.219	466 905	382.324	177.620	−701.985	−425.310	10.579
2200	106.381	471.850	386.282	188.250	−701.656	−412.143	9.786
2300	106.523	476.582	390.106	198.895	−701.334	−398.990	9.061
2400	106.648	481.118	393 804	209.554	−701.014	−385.851	8.398
2500	106 759	485.474	397.384	220.224	−700.693	−372.726	7.788
2600	106.858	489 663	400.854	230.905	−700.367	−359.614	7.225
2700	106.946	493.698	404.218	241.596	−700.030	−346.514	6.704
2800	107.025	497.589	407.484	252.294	−699.680	−333 428	6.220
2900	107.096	501.346	410.656	263 000	−699.313	−320.353	5 770
3000	107.160	504.977	413.740	273.713	−698.926	−307.293	5.350
3100	107.218	508 492	416 740	284.432	−698.515	−294.245	4.958
3200	107.271	511.897	419.661	295.156	−698.078	−281.211	4.590
3300	107.319	515.199	422.506	305.886	−697.611	−268.191	4.245
3400	107.363	518.403	425.280	316.620	−697.113	−255.186	3.920
3500	107.404	521.516	427 985	327.359	−696.582	−242.195	3.615
3600	107 441	524.542	430.625	338.101	−696.015	−229.220	3.326
3700	107.475	527 486	433.203	348.847	−695.411	−216.262	3 053
3800	107.507	530.353	435.722	359.596	−694 769	−203.321	2.795
3900	107.536	533.146	438.185	370.348	−694.088	−190.397	2.550
4000	107.563	535.869	440.593	381.103	−693.365	−177.491	2.318
4100	107.588	538.525	442.949	391.860	−692.601	−164.603	2.097
4200	107.611	541.118	445.256	402.620	−691 795	−151 735	1 887
4300	107.633	543.650	447.515	413.382	−690.946	−138.887	1.687
4400	107 653	546.125	449.728	424 147	−690.053	−126.058	1.496
4500	107.672	548.544	451.897	434.913	−689.117	−113.250	1.315
4600	107.690	550.911	454.024	445.681	−688.136	−100 464	1.141
4700	107.707	553.227	456.110	456 451	−687.112	−87.700	0.975
4800	107.722	555.495	458 157	467.222	−686.045	−74.957	0.816
4900	107.737	557.716	460.166	477.995	−684.933	−62.238	0.663
5000	107.751	559.893	462.139	488.770	−683.778	−49.541	0.518
5100	107.764	562.027	464.077	499.546	−682.580	−36.868	0.378
5200	107.776	564.120	465.981	510.323	−681.340	−24.219	0.243
5300	107.788	566.173	467.852	521.101	−680.058	−11.594	0.114
5400	107.799	568.188	469.691	531.880	−678.734	1.006	−0.010
5500	107 809	570.166	471.500	542.660	−677.369	13.581	−0 129
5600	107.819	572.108	473.280	553.442	−675.964	26.131	−0.244
5700	107.828	574.017	475.030	564.224	−674.520	38.655	−0.354
5800	107.837	575.892	476.753	575.007	−673.037	51 154	−0 461
5900	107.845	577.736	478 449	585.792	−671.516	63.628	−0.563
6000	107 853	579.548	480.119	596.576	−669.959	76.074	−0.662

PREVIOUS June 1969 (1 atm) CURRENT June 1969 (1 bar)

Enthalpy of Formation

The selected value is obtained from least squares, simultaneous adjustment of the heats of formation of CF$_3$, CF$_3$X (X = H, Cl, Br, I, CF$_3$) and C$_2$F$_4$. Details of the input data and the adjustment are given by Syverud.[1] Coomber and Whittle[2] have determined equilibrium data for CClF$_3$(g) + BrX(g) = CBrF$_3$(g) + ClX(g) where X = Cl and Br. Lord *et al.*[3] studied the analogous equilibria CF$_3$I(g) + ClI(g) = CClF$_3$(g) + I$_2$(g). These data link CClF$_3$ with CBrF$_3$ and CF$_3$I.

Other data which were omitted from the adjustment include those of Baibuz,[4,5] Mears and Stahl,[6] Kolesov *et al.*,[7] Kirkbride and Davidson,[8] and von Wartenberg and Schiefer.[9] Baibuz[4,5] derived $\Delta_f H° = -166.2 \pm 2.2$ kcal·mol^{-1} by applying the method of explosion in a spherical bomb to mixtures of H$_2$, O$_2$ and CClF$_3$. By comparison with similar data for CF$_4$ and CCl$_4$, we estimate the bias in Baibuz' value to be about +2 kcal·mol^{-1}. Mears and Stahl[6] gave a preliminary report of values of $\Delta_r H$ at 300°C for reactions involving HF, HCl and CCl$_n$F$_{4-n}$(n = 1, 2, 3, 4). We derive $\Delta_f H° = -172$ and -173 kcal mol^{-1} from two different combinations of reactions, however, no detailed account of the data has been published. The other authors[7–9] measured $\Delta_r H$ for reaction of CClF$_3$ with an alkali metal (Na or K) to form amorphous carbon and mixtures of the fluoride and chloride. Discrepancies of many kcal·mol^{-1} exist in these studies, presumably due to inadequate characterization of the thermochemical reactions.

Heat Capacity and Entropy

The molecular structure has been derived from electron–diffraction studies by Bowen[10] and Bartell and Brockway [11] Results from Bartell and Brockway are adopted. These parameters are consistent with the microwave data of Coles and Hughes.[12] The principal moments of inertia are: $I_A = 14.6768 \times 10^{-39}$ and $I_B = I_C = 25\ 3677 \times 10^{-39}$ g·cm^2. Vibrational assignments are based on the work of Claassen[13] and the gas–phase Raman spectra observed by Holzer and Moser.[14]

The largest uncertainty in $C_p°$ and $S°$ probably results from the neglect of anharmonicity. Barho[15] and Albright *et al.*[16] have given estimates for the anharmonic contributions. These vary from 0.1 to 0.3 cal·K^{-1}·mol^{-1} in both $C_p°$ and $S°$ over the range from 300 to 1000 K, respectively. Somewhat larger contributions are possible based on the anharmonic functions calculated by McBride *et al* [17] for CF$_4$(g) We estimate the overall uncertainty in the entropy of this JANAF table to be 0.1 cal·K^{-1}·mol^{-1} at 300 K and 0.4 cal·K^{-1}·mol^{-1} at 1000 K $C_p°$ is consistent with $C_p°$ measured at 300 K by the wire–ribbon method.[18]

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Cyanogen Chloride (ClCN) IDEAL GAS $M_r = 61.4707$ Cyanogen Chloride (ClCN) $C_1Cl_1N_1(g)$

$S°(298.15 \text{ K}) = 236.334 \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = -137.24 \text{ kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = -137.95 \text{ kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
714.52 (1)
378.3 (2)
2215.5 (1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: $C_{\infty v}$
Bond Distances: Cl–C = 1.631 Å; C–N = 1 162 Å
Bond Angle: Cl–C–N = 180°
Rotational Constants: $B_o = 0.19817 \text{ cm}^{-1}$; $D_o = 5.503 \times 10^{-8} \text{ cm}^{-1}$

Spectroscopic constants used in calculating corrections to rigid rotator–harmonic oscillator approximation (cm^{-1}):

$\alpha_1 = 8.25 - 10^{-4}$ $x_{11} = [-4]$ $x_{12} = [-6.8]$ $g_{22} = 0.95$
$\alpha_2 = -5.46 - 10^{-4}$ $x_{22} = -0.65$ $x_{23} = -7.236$
$\alpha_3 = 1.06 - 10^{-3}$ $x_{33} = [-7]$ $x_{13} = -2.8$

Enthalpy of Formation

The enthalpy of formation was taken from U.S. NBS Tech. Note 270–1.[1]

Heat Capacity and Entropy

Gordon[2] has used the constants listed above to calculate $C_p°$ from 298.15 to 6000 K using the method of Pennington and Kobe[3] which takes anharmonicity, vibration–rotation interaction, and centrifugal stretching into account. The constants B_o and D_o were taken from Burrus and Gordy,[4] ω_1, x_1, x_3, x_{22}, x_{23}, x_{13}, and g_{22} were obtained by Laferty *et al.*,[5] α_2 has been taken from Townes *et al.*,[6] and x_{11}, x_{33} and x_{12} were estimated by Gordon.[2] The bond distances and bond angle were taken from Lafferty *et al.*[5]

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Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.686	137.237	137.237	INFINITE
100	31.246	195.017	272.421	−7.740	137.216	135.250	−70.648
200	39.643	219.305	240.225	−4.184	137.472	133.222	−34.794
298.15	45.271	236.334	236.334	0.	137.946	131.015	−22.953
300	45.346	236.614	236.335	0.084	137.956	130.972	−22.804
400	48.718	250.147	238.157	4.796	138.452	128.567	−16.789
500	51.024	261.275	241.701	9.787	138.861	126.046	−13.168
600	52.831	270 742	245.771	14.982	139.170	123.453	−10.748
700	54.354	279.003	249.941	20.343	139.401	120.814	−9.015
800	55.656	286.348	254.041	25.845	139.578	118.146	−7.714
900	56.781	292.970	258.005	31.469	139.718	115.459	−6.701
1000	57 748	299.003	261.807	37.196	139.834	112.757	−5.890
1100	58.504	304.543	265.444	43.009	139.929	110.044	−5.226
1200	59.204	309.664	268.918	48.895	140.009	107.324	−4.672
1300	59.847	314.429	272.238	54.848	140.079	104.597	−4.203
1400	60.432	318.886	275.412	60.862	140.147	101.865	−3.801
1500	60.961	323.073	278.452	66.932	140.213	99.129	−3.452
1600	61.365	327.021	281.365	73.049	140.275	96.388	−3.147
1700	61.745	330 752	284.161	79.205	140.331	93.643	−2.877
1800	62.103	334.292	286.849	85.397	140.384	90.895	−2.638
1900	62.437	337.659	289.435	91.624	140.433	88.144	−2.423
2000	62.747	340.869	291.927	97.884	140.480	85.391	−2.230
2100	63 010	343.937	294.331	104.172	140.523	82.636	−2.055
2200	63.262	346.874	296.653	110.485	140.560	79.878	−1.897
2300	63.503	349.692	298.899	116.824	140.591	77.119	−1.751
2400	63.733	352.399	301.072	123.186	140.616	74.359	−1.618
2500	63.952	355.005	303.177	129.570	140.635	71.598	−1.496
2600	64.150	357.518	305.219	135.975	140.646	68.836	−1.383
2700	64.342	359.942	307.201	142.400	140.648	66.074	−1.278
2800	64.529	362.286	309.127	148.844	140.642	63.312	−1.181
2900	64.710	364.553	310.999	155.306	140.628	60.551	−1.091
3000	64 885	366.750	312.821	161.785	140.604	57.790	−1.006
3100	65.050	368.880	314.596	168.282	140.572	55.030	−0.927
3200	65.212	370.948	316.324	174.795	140.530	52.271	−0.853
3300	65.371	372.957	318.010	181.325	140.481	49.514	−0 784
3400	65.527	374.911	319.655	187.870	140.424	46.758	−0.718
3500	65.680	376.813	321.261	194.430	140.360	44.004	−0.657
3600	65.828	378.665	322.830	201.005	140.290	41.252	−0.599
3700	65.973	380.471	324.364	207.595	140.215	38.502	−0.544
3800	66.117	382.232	325.864	214.200	140.137	35.754	−0.491
3900	66.259	383.951	327.331	220.819	140.055	33.008	−0.442
4000	66.400	385.631	328.768	227.452	139.973	30.264	−0.395
4100	66.536	387.272	330.175	234.099	139.890	27.523	−0.351
4200	66.670	388.877	331.553	240.759	139.808	24.783	−0.308
4300	66.804	390.447	332.905	247.433	139.729	22 045	−0.268
4400	66.937	391.984	334.230	254.120	139.653	19.309	−0.229
4500	67.070	393.490	335.530	260.820	139.582	16.575	−0.192
4600	67.201	394.966	336.806	267.534	139.518	13.842	−0.157
4700	67.331	396.412	338.059	274.260	139.460	11.111	−0.123
4800	67 461	397.831	339.290	281.000	139 411	8.380	−0.091
4900	67.590	399.224	340.499	287.752	139.372	5.651	−0.060
5000	67.718	400.590	341.687	294.518	139.342	2.922	−0.031
5100	67.845	401.933	342.855	301.296	139.323	0.194	−0.002
5200	67.972	403.251	344 004	308.087	139.316	−2.534	0.025
5300	68.097	404.547	345.134	314.890	139.321	−5.262	0.052
5400	68.222	405.821	346.246	321.706	139.339	−7.990	0.077
5500	68.346	407.074	347.341	328.535	139.370	−10.718	0.102
5600	68.469	408.307	348.418	335.375	139.415	−13.448	0.125
5700	68.591	409.520	349.480	342.228	139.474	−16.178	0.148
5800	68.712	410.714	350.525	349.093	139.547	−18.909	0.170
5900	68.833	411.889	351.555	355.971	139.634	−21.642	0.192
6000	68.952	413.047	352.571	362.860	139.735	−24.376	0.212

PREVIOUS· June 1966 (1 atm) CURRENT· June 1966 (1 bar)

Carbonyl Chloride (COCl) IDEAL GAS $M_r = 63.4634$ Carbonyl Chloride (COCl) $C_1Cl_1O_1(g)$

$S°(298.15\ K) = [265.965]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [-64.3 \pm 42]\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = [-62.8 \pm 42]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
570 (1)
281 (1)
1880 (1)

Ground State Quantum Weight: 2 $\sigma = 1$
Point Group: C_s
Bond Distances: C–Cl = [1.75] Å; C–O = [1.17] Å
Bond Angle: Cl–C–O = [120]°
Product of the Moments of Inertia: $I_AI_BI_C = [1.276664 \times 10^{-115}]\ g^3{\cdot}cm^6$

Enthaply of Formation

The enthalpy change ($\Delta_r H°$) for the reaction $COCl_2(g) = CO(g) + 2Cl(g)$ is calculated to be 82 kcal·mol^{-1}, which is the sum of two bond energies, i.e. D(Cl–COCl) + D(Cl–CO). By comparison with values, $D(H_3C–COCH_3)/D(H_3C–CO) = 72/18 = 4.0$ for CH_3COCH_3 (g) and $D(H_3C–COCl)/D(Cl–CO) = 4.3$ for $CH_3COCl(g)$, *the ratio of* D(Cl–COCl)/D(Cl–CO) *is estimated to be 4.0 for* $COCl_2(g)$. *Hence the enthalpy* change for the reaction $COCl_2(g) = COCl(g) + Cl(g)$ is calculated as $82 \times (4/5) = 65.6$ kcal·mol^{-1}. Using the $\Delta_r H°$ value obtained, the enthalpy of formation for COCl(g) is derived to be -15 ± 10 kcal·mol^{-1}.

Heat Capacity and Entropy

The vibrational frequencies were reported by Jacox and Milligan.[1] The bond distances and angle were estimated by Jacox and Milligan.[1] Due to the presence of one unpaired electron on C atom, the ground state quantum weight is calculated to be 2. The principal moments of inertia are: $I_A = 0.7159 \times 10^{-39}$, $I_B = 13.0005 \times 10^{-39}$, and $I_C = 13.7165 \times 10^{-39}\ g{\cdot}cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−11.551	−64.327	−64.327	INFINITE
100	35.882	221.891	303.521	−8.163	−63.908	−67.886	35.460
200	41.634	248.636	269.991	−4.271	−63.317	−72.083	18.826
250	43.627	258.152	266.699	−2.137	−63.016	−74.309	15.526
298.15	45.072	265.965	265.965	0	−62.760	−76.508	13.404
300	45.120	266.244	265.966	0.083	−62.751	−76.593	13.336
350	46.289	273.290	266.520	2.370	−62.533	−78.918	11.778
400	47.265	279.537	267.764	4.709	−62.369	−81.271	10.613
450	48.125	285.154	269.389	7.094	−62.258	−83.641	9.709
500	48.908	290.266	271.225	9.520	−62.199	−86.020	8.987
600	50.301	299.309	275.171	14.483	−62.211	−90.786	7.904
700	51.487	307.155	279.192	19.574	−62.356	−95.539	7.129
800	52.484	314.097	283.130	24.774	−62.595	−100.264	6.547
900	53.312	320.328	286.923	30.065	−62.901	−104.955	6.091
1000	53.996	325.981	290.550	35.431	−63.257	−109.609	5.725
1100	54.560	331.155	294.010	40.860	−63.652	−114.225	5.424
1200	55.028	335.923	297.306	46.340	−64.079	−118.804	5.171
1300	55.417	340.344	300.449	51.863	−64.533	−123.346	4.956
1400	55.743	344.463	303.447	57.421	−65.011	−127.852	4.770
1500	56.018	348.318	306.312	63.010	−65.513	−132.324	4.608
1600	56.251	351.941	309.051	68.624	−66.038	−136.761	4.465
1700	56.450	355.357	311.676	74.259	−66.585	−141.164	4.337
1800	56.621	358.589	314.193	79.913	−67.155	−145.535	4.223
1900	56.769	361.654	316.611	85.582	−67.748	−149.874	4.120
2000	56.898	364.570	318.937	91.266	−68.364	−154.180	4.027
2100	57.010	367.348	321.176	96.961	−69.004	−158.455	3.941
2200	57.109	370.003	323.336	102.667	−69.669	−162.699	3.863
2300	57.196	372.543	325.420	108.383	−70.359	−166.913	3.791
2400	57.274	374.979	327.435	114.106	−71.076	−171.096	3.724
2500	57.343	377.319	329.384	119.837	−71.820	−175.248	3.662
2600	57.405	379.569	331.271	125.575	−72.592	−179.370	3.604
2700	57.460	381.737	333.100	131.318	−73.391	−183.461	3.549
2800	57.510	383.827	334.875	137.066	−74.219	−187.523	3.498
2900	57.555	385.846	336.598	142.820	−75.075	−191.555	3.450
3000	57.596	387.798	338.272	148.577	−75.960	−195.556	3.405
3100	57.633	389.687	339.900	154.339	−76.872	−199.527	3.362
3200	57.667	391.517	341.485	160.104	−77.812	−203.469	3.321
3300	57.698	393.292	343.028	165.872	−78.779	−207.381	3.283
3400	57.726	395.015	344.532	171.643	−79.772	−211.263	3.246
3500	57.752	396.689	345.998	177.417	−80.789	−215.116	3.210
3600	57.776	398.316	347.429	183.193	−81.830	−218.939	3.177
3700	57.798	399.900	348.826	188.972	−82.893	−222.734	3.144
3800	57.818	401.441	350.190	194.753	−83.978	−226.498	3.113
3900	57.837	402.943	351.524	200.536	−85.082	−230.234	3.084
4000	57.855	404.408	352.828	206.320	−86.204	−233.942	3.055
4100	57.871	405.837	354.103	212.107	−87.343	−237.621	3.027
4200	57.887	407.231	355.352	217.895	−88.497	−241.273	3.001
4300	57.901	408.594	356.574	223.684	−89.666	−244.896	2.975
4400	57.914	409.925	357.772	229.475	−90.846	−248.493	2.950
4500	57.926	411.227	358.945	235.267	−92.038	−252.063	2.926
4600	57.938	412.500	360.095	241.060	−93.241	−255.606	2.902
4700	57.949	413.746	361.224	246.854	−94.452	−259.122	2.880
4800	57.959	414.966	362.331	252.650	−95.672	−262.613	2.858
4900	57.969	416.161	363.417	258.446	−96.899	−266.078	2.836
5000	57.978	417.333	364.484	264.244	−98.132	−269.518	2.816
5100	57.986	418.481	365.531	270.042	−99.372	−272.933	2.795
5200	57.994	419.607	366.560	275.841	−100.616	−276.325	2.776
5300	58.002	420.712	367.572	281.641	−101.867	−279.691	2.757
5400	58.009	421.796	368.566	287.441	−103.122	−283.035	2.738
5500	58.016	422.860	369.543	293.242	−104.381	−286.355	2.720
5600	58.023	423.906	370.505	299.044	−105.646	−289.652	2.702
5700	58.029	424.933	371.451	304.847	−106.915	−292.927	2.684
5800	58.035	425.942	372.382	310.650	−108.189	−296.179	2.667
5900	58.040	426.934	373.298	316.454	−109.469	−299.410	2.651
6000	58.045	427.910	374.200	322.258	−110.754	−302.618	2.635

PREVIOUS: December 1965 (1 atm) *CURRENT: December 1965 (1 bar)*

Dichloromethylene (CCl$_2$) IDEAL GAS M_r = 82.917 Dichloromethylene (CCl$_2$) C$_1$Cl$_2$(g)

$S°(298.15\ K) = [265.346]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 237.3 \pm 21\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 238.5 \pm 21\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights ϵ_i, cm^{-1}	g_i
0	1
[4000]	[3]
[17500]	[1]

Vibrational Frequencies and Degeneracies ν, cm^{-1}
721 (1)
[350] (1)
748 (1)

Point Group: C_{2v}
Bond Distance: C–Cl = [1.76] Å
Bond Angle: Cl–C–Cl = [100 ± 10]°
Product of the Moments of Inertia: $I_A I_B I_C = [1.101940 \times 10^{-114}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

Shapiro and Lossing[1] have measured mass–spectrometrically the appearance potentials 12.2 and 14.7 eV for the processes $CHCl_3(g) + e^- \rightarrow CCl_2^+(g) + HCl(g) + 2\bar{e}$ and $C_2Cl_4(g) + e^- \rightarrow CCl_2^+(g) + CCl_2(g) + 2\bar{e}$, respectively. The difference in these two processes gives $\Delta_r H° = 2.5$ eV (57.65 kcal·mol^{-1}), for the reaction $C_2Cl_4(g) + HCl(g) \rightarrow CCl_2(g) + CHCl_3(g)$ which leads to $\Delta_f H°(CCl_2, g, 298.15\ K) = 57.32$ kcal·mol^{-1}, using $\Delta_f H°(298.15\ K) = -2.97, -22.063$ and -24.7 kcal·mol^{-1} for $C_2Cl_4(g)$, HCl(g) and $CHCl_3(g)$, respectively. Since the authors claimed that the experimental error was probably 5 kcal·mol^{-1}, the value 57 ± 5 kcal·mol^{-1} (238.488 ± 21 kJ·mol^{-1}), is adopted for the enthalpy of formation.

Heat Capacity and Entropy

Milligan and Jacox[2] have found two stretching fundamentals (721 and 748 cm^{-1}) for the CCl$_2$ radical in the infrared and ultraviolet spectra by matrix–isolation, and proposed a bent molecular structure (the valence angle = 100 ± 10°) with a ground singlet state which was based on the analogy with the electronic absorption spectrum of CF$_2$. L. Andrews[3] has confirmed all these observations in his infrared spectrometric studies of dichlorocarbene in solid argon, and made vibrational assignment to the fundamentals and also eliminated the possibility of a linear molecular structure for CCl$_2$. The bending frequency (350 cm^{-1}) is estimated by the valence force method,[4] using the same ratio of bending over stretching force constants from CF$_2$(g).[5] The bond distance is estimated to be the same as that of CCl$_4$(g) measured by Bartell *et al*.[6] The principal moments of inertia are $I_A = 2.1829 \times 10^{-39}$, $I_B = 21.4029 \times 10^{-39}$, and $I_C = 23.5858 \times 10^{-39}\ g{\cdot}cm^2$.

The triplet low lying electronic level of 4000 cm^{-1} is estimated by analogy with that of CF$_2$(g). The other level of 17,5000 cm^{-1} is also estimated based on a weak band appearing between 4400 and 5600 Å in the spectra of CCl$_2$ observed by Milligan and Jacox.[2]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	$\Delta_f G°$ (kJ·mol^{-1})	log K$_f$
0	0.	0.	INFINITE	−11.388	237.332	237.332	INFINITE
100	34.695	222.225	302.564	−8.034	237.714	234.488	−122.484
200	40.669	248.013	269.408	−4.279	238.105	231.112	−60.360
250	43.720	257.422	266.094	−2.168	238.302	229.341	−47.918
298.15	46.249	265.346	265.346	0.	238.488	227.598	−39.874
300	46.337	265.632	265.347	0.086	238.495	227.530	−39.617
350	48.459	272.941	265.919	2.458	238.677	225.688	−33.682
400	50.142	279.526	267.215	4.924	238.841	223.821	−29.228
450	51.476	285.511	268.921	7.466	238.978	221.935	−25.762
500	52.546	290.992	270.858	10.067	239.086	220.035	−22.987
600	54.180	300.725	275.045	15.408	239.216	216.211	−18.823
700	55.475	309.176	279.330	20.892	239.256	212.373	−15.847
800	56.676	316.663	283.538	26.500	239.243	208.533	−13.616
900	57.888	323.408	287.599	32.228	239.216	204.696	−11.880
1000	59.129	329.571	291.492	38.079	239.207	200.861	−10.492
1100	60.369	335.265	295.216	44.054	239.238	197.025	−9.356
1200	61.560	340.569	298.777	50.151	239.322	193.184	−8.409
1300	62.656	345.541	302.185	56.362	239.462	189.334	−7.608
1400	63.622	350.220	305.451	62.677	239.656	185.471	−6.920
1500	64.437	354.638	308.584	69.082	239.895	181.593	−6.324
1600	65.093	358.819	311.594	75.559	240.168	177.697	−5.801
1700	65.593	362.781	314.490	82.095	240.463	173.784	−5.340
1800	65.948	366.541	317.278	88.673	240.767	169.853	−4.929
1900	66.173	370.113	319.965	95.280	241.068	165.905	−4.561
2000	66.286	373.510	322.558	101.904	241.354	161.941	−4.229
2100	66.306	376.745	325.062	108.534	241.618	157.964	−3.929
2200	66.250	379.829	327.482	115.163	241.849	153.975	−3.656
2300	66 134	382.771	329.823	121.782	242.040	149.976	−3.406
2400	65.971	385.583	332.088	128.388	242.187	145.970	−3.177
2500	65.776	388.272	334.282	134.976	242.285	141.959	−2.966
2600	65.556	390.848	336.408	141.542	242.330	137.945	−2.771
2700	65.321	393.317	338.470	148.086	242.320	133.930	−2.591
2800	65.078	395.688	340.472	154.606	242.253	129.917	−2.424
2900	64.831	397.968	342.415	161.102	242.129	125.907	−2.268
3000	64.585	400.161	344.304	167.572	241.947	121.902	−2.123
3100	64.343	402.275	346.140	174.019	241.709	117 904	−1.987
3200	64.107	404.314	347.926	180.441	241.415	113.915	−1.859
3300	63.879	406.283	349.665	186.840	241.068	109.936	−1.740
3400	63.660	408.187	351.359	193.217	240.670	105.968	−1.628
3500	63.451	410.030	353.009	199.573	240.223	102.013	−1.522
3600	63.253	411.814	354.618	205.908	239.731	98.071	−1.423
3700	63.064	413.545	356.187	212.224	239.197	94.143	−1.329
3800	62.886	415.224	357.719	218.521	238.624	90.230	−1.240
3900	62.718	416.855	359.214	224.801	238.015	86.333	−1.156
4000	62.560	418.441	360.675	231.065	237.375	82.452	−1.077
4100	62.411	419.984	362.103	237.314	236.707	78.587	−1.001
4200	62.272	421.486	363.499	243.548	236.015	74.739	−0.930
4300	62.141	422.950	364.865	249.768	235.302	70.907	−0.861
4400	62.018	424.377	366.201	255.976	234.572	67.092	−0.796
4500	61.903	425.770	367.509	262.172	233.827	63.294	−0.735
4600	61.795	427.129	368.791	268.357	233.072	59.513	−0.676
4700	61.694	428.457	370.046	274.531	232.309	55.748	−0.620
4800	61.599	429.755	371.277	280.696	231.542	52.000	−0.566
4900	61.510	431.024	372.483	286.851	230.771	48.267	−0.515
5000	61.427	432.266	373.666	292.998	230.001	44.550	−0.465
5100	61.348	433.482	374.827	299.137	229.234	40.849	−0.418
5200	61.275	434.672	375.967	305.268	228.470	37.162	−0.373
5300	61.206	435.839	377.085	311.392	227.713	33.491	−0.330
5400	61.141	436.982	378.184	317.509	226.964	29.833	−0.289
5500	61.080	438.103	379.263	323.620	226.224	26.190	−0.249
5600	61.022	439.203	380.324	329.725	225.495	22.559	−0.210
5700	60.968	440.283	381.366	335.825	224.778	18.942	−0.174
5800	60.916	441.343	382.391	341.919	224.073	15.337	−0.138
5900	60.868	442.384	383.399	348.008	223.382	11.744	−0.104
6000	60.822	443.406	384.391	354.093	222.705	8.162	−0.071

PREVIOUS: December 1968 (1 atm) CURRENT. December 1968 (1 bar)

Dichlorodifluoromethane (CCl_2F_2) IDEAL GAS M_r = 120.913806 Dichlorodifluoromethane (CCl_2F_2) $C_1Cl_2F_2(g)$

$\Delta_fH°(0\ K) = -487.4 \pm 8\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = 300.897 \pm 0.21\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_fH°(298.15\ K) = -491.6 \pm 8\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies		
ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
1099 (1)	457.5(1)	436(1)
261.5(1)	322 (1)	1162(1)
667.2(1)	922 (1)	446(1)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: C_{2v}
Bond Distances: C–Cl = 1.77 ± 0.02 Å; C–F = 1.33 ± 0.02 Å
Bond Angles: F–C–F = 109.5 ± 3°; Cl–C–Cl = 108.5 ± 2°
F–C–F plane perpendicular to Cl–C–Cl plane
Product of the Moments of Inertia: $I_AI_BI_C = 2.537004 \times 10^{113}\ g^3\ cm^6$

Enthalpy of Formation

Mears and Stahl[1] investigated several heats of reaction involving CF_4, CF_3Cl, CF_2Cl_2, $CFCl_3$, CCl_4, HF and HCl. Using JANAF values for all compounds except CF_2Cl_2 and $CFCl_3$ we obtain the following observations:

1. $\Delta_fH°(CCl_3F,\ g,\ 298.15\ K) = -70.12 \pm 1\ 1\ kcal \cdot mol^{-1}$
2. $\Delta_fH°(CCl_2F_2,\ g,\ 298\ 15\ K) = -116.53 \pm 1.5\ kcal \cdot mol^{-1}$
3. $\Delta_fH°(CCl_2F_2,\ g,\ 298\ 15\ K) - \Delta_fH°(CCl_3F,\ g,\ 298\ 15\ K) = -49\ 39 \pm 1.0\ kcal \cdot mol^{-1}$
4 $\Delta_fH°(CCl_2F_2,\ g,\ 298.15\ K) - 2\ \Delta_fH°(CCl_3F,\ g,\ 298.15\ K) = 20.34 \pm 1.0\ kcal\ mol^{-1}$
5. $\Delta_fH°(CCl_3F,\ g,\ 298.15\ K) - 2\ \Delta_fH°(CCl_2F_2,\ g,\ 298.15\ K) = 165.47 \pm 1.0\ kcal \cdot mol^{-1}$

The sum of the squares of the deviations is smallest when $\Delta_fH°(CCl_2F_2,\ g,\ 298.15\ K) = -117.5\ kcal \cdot mol^{-1}$ and $\Delta_fH°(CCl_3F,\ g,\ 298.15\ K) = -69\ kcal \cdot mol^{-1}$, and all the values are within their uncertainty ranges.

Peterson and Pitzer[8] obtained an approximate equilibrium constant for the reaction $2\ CClF_3(g) + CCl_4(g) = 3\ CCl_2F_2(g)$ of $\log K_{400} = -3.0$. This on 3rd law reaction gives $\Delta_rH°(298.15\ K) = 7.64\ kcal \cdot mol^{-1}$ and with $\Delta_fH°(CClF_3,\ g,\ 298.15\ K) = -169.2\ kcal\ mol^{-1}$ and $\Delta_fH°(CCl_4,\ g,\ 298.15\ K) = -22.94\ kcal \cdot mol^{-1}$ this yields $\Delta_fH°(CCl_2F_2,\ g,\ 298.15\ K) = -117\ 9\ kcal \cdot mol^{-1}$.

Kirkbride and Davidson[2] investigated the reaction of potassium with the chlorofluoromethanes and obtained $\Delta_fH°(CCl_2F_2,\ g,\ 298.15\ K) = -115.1 \pm 2\ kcal\ mol^{-1}$ and $\Delta_fH°(CCl_3F,\ g,\ 298.15\ K) = -72.9 \pm 4\ kcal \cdot mol^{-1}$ after correction with JANAF auxiliary data. Wartenberg and Schiefer[3] investigated the same reaction and we obtain, after correction with JANAF auxiliary data, $\Delta_fH°(CCl_2F_2,\ g,\ 298.15\ K) = -112.7\ kcal\ mol^{-1}$ and $\Delta_fH°(CCl_3F,\ g,\ 298.15\ K) = -63.1\ kcal \cdot mol^{-1}$. Kolesov *et al.*[4] have reported analogous data for the reaction with sodium which, after correction with JANAF auxiliary data, yields $\Delta_fH°(CCl_2F_2,\ g,\ 298.15\ K) = -114.4 \pm 3.5\ kcal \cdot mol^{-1}$.

We adopt the values calculated above from Mears and Stahl,[1] since they have a high degree of internal consistency and also lead to a realistic progression in the heats of atomization in going from CF_4 to CCl_4. With the adopted heats of formation, the successive replacement of F by Cl changes the atomization heats by 43.8, 41.6, 38.5, and 36.0 $kcal \cdot mol^{-1}$.

Heat Capacity and Entropy

Claassen[5] chose the frequencies given above from his own gas–phase Raman measurements and the infrared values of earlier investigators. The values are in good agreement with the assignment of Plyler and Benedict.[6] Masi[9] has measured the gas phase heat capacities at 243, 273, 318 and 363 K, within this range our adopted heat capacities are from 0 3 to 0 7% high. The entropies agree to within 0.05% and further adjustment to obtain better fits was not considered necessary. The molecular structure was determined from the microwave measurements of Long *et al.*[7] The principal moments of inertia are: $I_A = 21.0747 \times 10^{-39}$, $I_B = 31.7398 \times 10^{-39}$, and $I_C = 37.9277 \times 10^{-39}\ g\ cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−14.866	−487.429	−487.429	INFINITE
100	39.629	241.343	355.353	−11.401	−489.843	−477.944	249.652
200	58.584	274.768	307.109	−6.468	−491.203	−465.417	121.554
250	66.235	288.688	302.056	−3.342	−491.494	−458.933	95.889
298.15	72.404	300.897	300.897	0.	−491.620	−452.648	79.302
300	72.620	301.346	300.899	0.134	−491.622	−452.406	78.771
350	77.938	312.952	301.803	3.902	−491.633	−445.868	66.542
400	82.349	323.657	303.875	7.913	−491.556	−439.335	57.371
450	85.998	333.574	306.630	12.124	−491.416	−432.815	50.240
500	89.016	342.796	309.791	16.502	−491.230	−426.314	44.537
600	93.597	359.456	316.711	25.647	−490.769	−413.372	35.987
700	96.801	374.138	323.887	35.176	−490.236	−400.514	29.887
800	99.095	387.222	331.001	44.977	−489.666	−387.735	25.316
900	100.779	398.996	337.913	54.975	−489.077	−375.029	21.766
1000	102.044	409.683	344.564	65.119	−488.483	−362.389	18.929
1100	103.015	419.456	350.935	75.374	−487.891	−349.808	16.611
1200	103.773	428.453	357.025	85 715	−487.310	−337.281	14.681
1300	104.377	436.784	362.843	96.123	−486.741	−324 801	13.051
1400	104.864	444.538	368.405	106.586	−486.191	−312.365	11.654
1500	105.262	451.787	373.725	117.093	−485.659	−299.968	10.446
1600	105.592	458.591	378 819	127.636	−485.150	−287.605	9.389
1700	105.867	465.001	383 701	138.210	−484.663	−275.274	8.458
1800	106.100	471.059	388.388	148.808	−484.198	−262.970	7.631
1900	106.298	476.801	392.891	159 428	−483.756	−250.692	6.892
2000	106.469	482.258	397.224	170.067	−483.335	−238.436	6.227
2100	106.616	487.456	401.398	180 721	−482.935	−226.202	5 626
2200	106 744	492.419	405.424	191.390	−482.554	−213 985	5.081
2300	106.856	497 166	409.310	202.070	−482.190	−201.785	4.583
2400	106.955	501 716	413.066	212.760	−481.841	−189.602	4.127
2500	107.042	506.084	416 700	223.460	−481.505	−177.432	3.707
2600	107.120	510.284	420.219	234.169	−481.181	−165.275	3.320
2700	107.190	514.328	423.630	244.884	−480.866	−153.131	2.962
2800	107.252	518.228	426.940	255.606	−480.559	−140.998	2.630
2900	107.308	521.992	430.153	266.334	−480.256	−128.877	2.321
3000	107.358	525.631	433.275	277.068	−479.957	−116.765	2.033
3100	107 404	529.152	436.311	287.806	−479.658	−104.664	1.764
3200	107.446	532.563	439.266	298.548	−479.357	−92.572	1.511
3300	107.484	535.869	442.144	309.295	−479.053	−80.490	1.274
3400	107.518	539.079	444.948	320 045	−478.742	−68.417	1.051
3500	107.550	542.196	447.682	330.798	−478.422	−56.353	0.841
3600	107.579	545.226	450.350	341.555	−478.092	−44.298	0.643
3700	107.606	548.174	452.954	352.314	−477.747	−32.253	0.455
3800	107.631	551.044	455 498	363.076	−477.386	−20.218	0.278
3900	107.654	553.840	457.984	373.840	−477.007	−8.192	0.110
4000	107.675	556.566	460.414	384.607	−476.607	3.824	−0.050
4100	107.695	559.225	462.792	395.375	−476.183	15.830	−0.202
4200	107.713	561.820	465.119	406 146	−475 733	27.825	−0.346
4300	107 731	564.355	467.397	416.918	−475.256	39.808	−0.484
4400	107.746	566.832	469.629	427.692	−474.749	51.781	−0.615
4500	107.761	569.253	471.816	438.467	−474.211	63.742	−0.740
4600	107 775	571.622	473.960	449.244	−473.639	75.690	−0.859
4700	107 788	573.940	476.063	460.022	−473.032	87.625	−0.974
4800	107.801	576.210	478.126	470.802	−472.389	99.547	−1.083
4900	107.812	578.432	480.150	481.582	−471.709	111.456	−1.188
5000	107.823	580.611	482.138	492.364	−470.990	123.350	−1.289
5100	107 833	582.746	484.090	503.147	−470.232	135.229	−1.385
5200	107 843	584.840	486.007	513.931	−469.434	147.093	−1 478
5300	107.852	586.894	487.891	524.716	−468.595	158.942	−1.566
5400	107.861	588.910	489.743	535.501	−467.715	170.774	−1.652
5500	107.869	590.890	491.564	546.288	−466.794	182.589	−1.734
5600	107.877	592.833	493.356	557.075	−465.831	194.388	−1.813
5700	107 884	594.743	495.118	567.863	−464.827	206.168	−1.889
5800	107.891	596.619	496.851	578.652	−463.782	217.931	−1.963
5900	107.897	598 463	498.558	589.441	−462.695	229.676	−2.033
6000	107.904	600.277	500 238	600.231	−461.568	241.400	−2.102

PREVIOUS: June 1970 (1 atm) CURRENT June 1970 (1 bar)

Carbonic Dichloride ($COCl_2$) IDEAL GAS $M_r = 98.9164$ Carbonic Dichloride ($COCl_2$) $C_1Cl_2O_1(g)$

$S°(298.15\ K) = 283.796\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -218.371 \pm 3.3\ kJ\ mol^{-1}$
$\Delta_fH°(298.15\ K) = -220.08 \pm 3.3\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[570] (1)
1827 (1)
285 (1)
849 (1)
440 (1)
[585] (1)

Ground State Quantum Weight: 1
Point Group: C_{2v} $\sigma = 2$
Bond Distances: C–O = 1.166 ± 0.002 Å; Cl–O = 2.589 ± 0.001 Å;
Cl–Cl = 2.884 ± 0.001 Å; C–Cl = 1.746 ± 0.004 Å
Bond Angle: Cl–C–Cl = 111.3 ± 0.1°
Product of the Moments of Inertia: $I_AI_BI_C = 9.138289 \times 10^{-114}\ g^3{\cdot}cm^6$

Enthalpy of Formation

Thomsen[1] reports the enthaply of alkaline hydrolysis of $COCl_2$, from which $\Delta_fH°(298.15\ K)$ is calculated to be −54.4 ± 0.3 kcal mol^{-1}. From the enthalpy of combustion of $COCl_2$ in O_2 and H_2, reported by Thomsen,[2] $\Delta_fH°(298.15\ K)$ is calculated to be − 51.73 ± 0.43 kcal·mol^{-1}. Bodenstein and Plaut,[3] Christiansen,[4] and Bodenstein and Dunant[5] report 10 values of K_p from 647 to 876 K for the reaction $CO + Cl_2 = COCl_2$. These yield −25.91 ± 0.04 kcal for $\Delta_fH°(298.15\ K)$ for $COCl_2$ is −52.33 ± 0.62 kcal·mol^{-1}. The average of the 3 foregoing values of $\Delta_fH°(298.15\ K)$ weighted for the uncertainties, is adopted here. Values calculated from the degree of dissociation of $COCl_2$ from 374 to 778 K, reported by Atkinson *et al.*,[6] range from −47.06 to −53.11 kcal mol^{-1} and are ignored.

Heat Capacity and Entropy

The vibrational frequencies were assigned by Catalano and Pitzer,[7] on the basis of their own infra–red spectra and other data. The molecular dimensions listed above were deduced from microwave spectra by Robinson,[8] and are confirmed by electron–diffraction values compiled by Allen and Sutton.[9] The moments of inertia are weighted for the isotopes and were calculated from Robinson's dimensions by Giauque and Ott.[10] Giauque and Ott[10] determined $S°(298.15\ K)$ experimentally to be 67.81 cal·K^{-1}·mol^{-1}, with which the value calculated here agrees, i.e. 67.816 cal·K^{-1}·mol^{-1}. The principal moments of inertia are. $I_A = 10.6393 \times 10^{-39}$, $I_B = 24.4666 \times 10^{-39}$, and $I_C = 35.1059 \times 10^{-39}\ g{\cdot}cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−12.867	−218.372	−218.372	INFINITE
100	36.537	233.747	328.453	−9.471	−219.399	−215.113	112.363
200	48.362	262.618	288.800	−5.236	−219.985	−210.551	54.990
250	53.603	273.992	284.724	−2.683	−220.075	−208.180	43.497
298.15	57.695	283.796	283.796	0.	−220.078	−205.887	36.071
300	57.835	284.153	283.797	0.107	−220.077	−205.799	35.833
350	61.211	293.332	284.514	3.086	−220.026	−203.423	30.359
400	63.938	301.689	286.147	6.217	−219.945	−201.056	26.255
450	66.184	309.354	288.305	9.472	−219.853	−198.701	23.065
500	68.068	316.427	290.768	12.830	−219.760	−196.356	20.513
600	71.048	329.115	296.127	19.793	−219.587	−191.691	16.688
700	73.282	340.242	301.650	27.014	−219.438	−187.054	13.958
800	74.993	350.144	307.105	34.432	−219.309	−182.437	11.912
900	76.324	359.057	312.390	42.000	−219.198	−177.835	10.321
1000	77.373	367.155	317.468	49.687	−219.102	−173.244	9.049
1100	78.210	374.570	322.327	57.468	−219.020	−168.662	8.009
1200	78.886	381.406	326.969	65.324	−218.952	−164.087	7.143
1300	79.437	387.742	331.403	73.241	−218.898	−159.517	6.409
1400	79.891	393.646	335.641	81.208	−218.859	−154.951	5.781
1500	80.270	399.172	339.694	89.217	−218.836	−150.387	5.237
1600	80.588	404.363	343.575	97.260	−218.831	−145.824	4.761
1700	80.857	409.256	347.296	105.332	−218.845	−141.261	4.340
1800	81.086	413.885	350.868	113.430	−218.880	−136.697	3.967
1900	81.284	418.274	354.301	121.549	−218.937	−132.130	3.632
2000	81.455	422.448	357.605	129.686	−219.018	−127.559	3.331
2100	81.604	426.426	360.788	137.839	−219.125	−122.983	3.059
2200	81.734	430.225	363.859	146.006	−219.259	−118.402	2.811
2300	81.849	433.861	366.824	154.185	−219.423	−113.814	2.585
2400	81.950	437.347	369.690	162.375	−219.618	−109.218	2.377
2500	82.040	440.694	372.464	170.575	−219.846	−104.614	2.186
2600	82.120	443.913	375.150	178.783	−220.108	−99.999	2.009
2700	82.192	447.014	377.755	186.999	−220.405	−95.374	1.845
2800	82.257	450.004	380.282	195.221	−220.738	−90.737	1.693
2900	82.316	452.892	382.737	203.450	−221.108	−86.088	1.551
3000	82.368	455.683	385.122	211.684	−221.515	−81.425	1.418
3100	82.416	458.385	387.442	219.923	−221.958	−76.748	1.293
3200	82.460	461.002	389.700	228.167	−222.437	−72.057	1.176
3300	82.500	463.540	391.899	236.415	−222.951	−67.350	1.066
3400	82.537	466.004	394.043	244.667	−223.498	−62.626	0.962
3500	82.570	468.397	396.133	252.922	−224.076	−57.887	0.864
3600	82.601	470.723	398.173	261.181	−224.685	−53.130	0.771
3700	82.629	472.987	400.164	269.443	−225.320	−48.356	0.683
3800	82.656	475.191	402.110	277.707	−225.981	−43.564	0.599
3900	82.680	477.338	404.011	285.974	−226.664	−38.754	0.519
4000	82.703	479.432	405.871	294.243	−227.366	−33.927	0.443
4100	82.724	481.474	407.690	302.514	−228.085	−29.083	0.371
4200	82.743	483.468	409.471	310.787	−228.819	−24.220	0.301
4300	82.761	485.415	411.214	319.063	−229.564	−19.340	0.235
4400	82.778	487.318	412.922	327.340	−230.318	−14.442	0.171
4500	82.794	489.178	414.596	335.618	−231.079	−9.528	0.111
4600	82.809	490.998	416.237	343.898	−231.844	−4.596	0.052
4700	82.823	492.779	417.847	352.180	−232.611	0.352	−0.004
4800	82.836	494.523	419.426	360.463	−233.378	5.317	−0.058
4900	82.848	496.231	420.976	368.747	−234.143	10.299	−0.110
5000	82.860	497.905	422.498	377.033	−234.905	15.295	−0.160
5100	82.871	499.546	423.993	385.319	−235.662	20.306	−0.208
5200	82.881	501.155	425.462	393.607	−236.413	25.332	−0.254
5300	82.891	502.734	426.905	401.895	−237.157	30.373	−0.299
5400	82.900	504.284	428.323	410.185	−237.893	35.428	−0.343
5500	82.909	505.805	429.718	418.476	−238.620	40.496	−0.385
5600	82.917	507.299	431.090	426.767	−239.339	45.577	−0.425
5700	82.925	508.766	432.440	435.059	−240.048	50.671	−0.464
5800	82.932	510.209	433.769	443.352	−240.748	55.778	−0.502
5900	82.939	511.626	435.076	451.645	−241.438	60.896	−0.539
6000	82.946	513.020	436.364	459.940	−242.119	66.026	−0.575

PREVIOUS: June 1961 (1 atm) CURRENT: June 1961 (1 bar)

Trichloromethyl (CCl_3) **IDEAL GAS** **M_r = 118.370** **Trichloromethyl (CCl_3)** **$C_1Cl_3(g)$**

$S°(298.15\ K) = 296.83 \pm 6.3\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 80.1 \pm 8\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = 79.5 \pm 8\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[450] (1)
[460] (1)
898 (2)
[240] (2)

Ground State Quantum Weight: 2 $\sigma = 6$
Point Group: D_{3h}
Bond Distance: C–Cl = [1.74]Å
Bond Angle: Cl–C–Cl = [120]°
Product of the Moments of Inertia: $I_AI_BI_C = [3.822311 \times 10^{-113}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

Benson[1] has reanalysed the kinetic data of Sullivan and Davidson[2] for the reaction $Br_2(g) + CHCl_3(g) = HBr(g) + CBrCl_3(g)$ and has obtained from it the enthalpy of the initial step, $Br(g) + CHCl_3(g) \rightarrow CCl_3(g) + HBr(g)$, as 8.2 ± 1 kcal mol^{-1} Substituting this value and $\Delta_fH°(Br, g, 298.15\ K) = 26.74\ kcal{\cdot}mol^{-1}$, $\Delta_fH°(CHCl_3, g, 298.15\ K) = -24.66\ kcal{\cdot}mol^{-1}$ and $\Delta_fH°(HBr, g, 298\ 15\ K) = -8.71\ kcal{\cdot}mol^{-1}$, we obtain $\Delta_fH°(CCl_3, g, 298.15\ K) = 19 \pm 2\ kcal{\cdot}mol^{-1}$ ($79.496 \pm 8\ kJ{\cdot}mol^{-1}$), which is adopted here.

Heat Capacity and Entropy

Walsh[3] has predicted that CCl_3 is non–planar on the basis of his orbital correlation diagram. Andrews[4] indicates that his matrix infrared observations of the symmetric and antisymmetric stretches are consistent with a non–planar C_{3v} structure and a near tetrahedral angle. The antisymmetric stretch has been confirmed by Current and Burdett.[5] They rationalize the absence of the symmetric stretch and claim support of the C_{3v} structure. Rogers *et al.*[6] have made a thorough search for the symmetric stretch and did not find it in the region where is was reported by Andrews.[4] Thus, they conclude that since only the antisymmetric stretch has been confirmed, the possibility of a planar D_{3h} molecule cannot be excluded. Maget *et al.*[7] have observed the NMR spectrum of trapped CCl_3 and find it consistent with a planar molecule. The absence of the symmetric stretch strongly implies a planar configuration, and we adopt such a configuration until more definitive proof of the non–planarity can be obtained. The remaining vibrational frequencies are estimated by comparison with those of BCl_3 The bond length was estimated as 1.74 Å by Andrews[4] from a correlation with related molecules. The principal moments of inertia are $I_A = I_B = 26.7361 \times 10^{-39}$ and $I_C = 53.4723 \times 10^{-39}\ g{\cdot}cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−14.194	80.125	80.125	INFINITE
100	40.983	240.296	346.941	−10.665	79.226	83.643	−43.691
200	54.687	273.207	302.392	−5.837	79.171	88.135	−23.018
250	59.708	285.968	297.860	−2.973	79.311	90.361	−18.880
298.15	63.649	296.833	296.833	0.	79.496	92.473	−16.201
300	63.784	297.228	296.835	0.118	79.504	92.554	−16.115
350	67.068	307.316	297.624	3.392	79.729	94.711	−14.135
400	69.696	316.450	299.415	6.814	79.972	96.835	−12.645
450	71.799	324.785	301.778	10.353	80.219	98.928	−11.483
500	73.488	332.440	304.466	13.987	80.462	100.994	−10.551
600	75.965	346.073	310.293	21.468	80.916	105.057	−9.146
700	77.636	357.916	316.269	29.153	81.321	109.048	−8.137
800	78.803	368.364	322.141	36.978	81.676	112.984	−7.377
900	79.643	377.697	327.805	44.903	81.985	116.878	−6.783
1000	80.266	386.122	333.222	52.900	82.254	120.741	−6.307
1100	80.739	393.795	338.385	60.951	82.486	124.578	−5.916
1200	81.106	400.837	343.300	69.044	82.685	128.395	−5.589
1300	81.396	407.341	347.979	77.170	82.853	132.197	−5.312
1400	81.629	413.381	352.438	85.321	82.993	135.988	−5.074
1500	81.818	419.020	356.690	93.494	83.105	139.769	−4.867
1600	81.975	424.306	360.753	101.684	83.190	143.544	−4.686
1700	82.105	429.279	364.639	109.888	83.249	147.314	−4.526
1800	82.215	433.975	368.362	118.104	83.282	151.081	−4.384
1900	82.309	438.423	371.933	126.331	83.288	154.847	−4.257
2000	82.389	442.647	375.364	134.566	83.268	158.614	−4.143
2100	82.458	446.669	378.665	142.808	83.219	162.383	−4 039
2200	82.518	450.506	381.844	151.057	83.140	166.154	−3 945
2300	82.571	454.175	384.909	159.311	83.030	169.930	−3.859
2400	82.617	457.690	387.869	167.571	82.886	173.711	−3 781
2500	82.658	461.064	390.730	175.835	82.708	177.499	−3.709
2600	82.694	464.306	393.498	184.102	82.492	181.295	−3.642
2700	82.726	467.428	396.179	192.373	82.239	185 100	−3.581
2800	82.756	470.437	398.777	200.647	81.947	188.914	−3.524
2900	82.782	473.342	401.299	208.924	81.615	192.740	−3.472
3000	82.805	476.148	403.747	217.204	81.243	196.578	−3.423
3100	82.827	478.864	406.127	225.485	80.831	200.430	−3.377
3200	82.846	481.494	408.441	233.769	80.381	204.294	−3.335
3300	82.864	484.043	410.694	242.054	79.893	208.175	−3.295
3400	82.880	486.517	412.887	250.342	79.370	212.069	−3.258
3500	82.895	488.920	415.026	258.630	78.814	215.980	−3.223
3600	82.908	491.255	417.111	266.921	78.228	219.908	−3.191
3700	82.921	493.527	419 146	275.212	77.614	223.852	−3.160
3800	82.932	495.739	421.132	283.505	76.976	227.812	−3.131
3900	82.943	497.893	423.073	291.798	76.319	231.790	−3.104
4000	82.953	499.993	424.970	300.093	75.645	235.785	−3.079
4100	82.962	502.042	426.825	308.389	74.959	239.797	−3.055
4200	82.971	504.041	423.640	316.686	74.265	243.826	−3.032
4300	82.979	505.993	430.416	324.983	73.566	247.872	−3.011
4400	82.986	507.901	432.155	333.281	72.866	251.933	−2.991
4500	82.993	509.766	433.859	341.580	72.170	256.011	−2.972
4600	82.999	511.590	435.529	349.880	71.480	260.104	−2.954
4700	83.005	513.375	437.167	358.180	70.800	264.212	−2.936
4800	83.011	515.123	438.773	366.481	70.133	268.334	−2.920
4900	83.016	516.835	440.348	374.782	69.483	272.470	−2.905
5000	83.022	518.512	441.895	383.084	68.852	276.619	−2.890
5100	83.026	520.156	443.413	391.387	68.242	280.780	−2.876
5200	83.031	521.768	444.905	399.689	67.656	284.953	−2.862
5300	83.035	523.350	446.370	407.993	67.095	289.138	−2.850
5400	83.039	524.902	447.810	416.296	66.562	293.332	−2.837
5500	83.043	526.426	449.226	424.601	66.059	297.537	−2.826
5600	83.046	527.922	450.617	432.905	65.586	301.749	−2.815
5700	83.050	529.392	451.987	441.210	65.144	305.970	−2.804
5800	83.053	530.836	453.334	449.515	64.736	310.199	−2.794
5900	83.056	532.256	454.659	457.820	64.360	314.435	−2.784
6000	83.059	533.652	455.964	466.126	64.019	318.676	−2.774

PREVIOUS June 1970 (1 atm) CURRENT June 1970 (1 bar)

Trichloromethyl (CCl_3) **$C_1Cl_3(g)$**

Trichlorofluoromethane (CCl$_3$F) IDEAL GAS M_r = 137.368403 Trichlorofluoromethane (CCl$_3$F) C$_1$Cl$_3$F$_1$(g)

$S°(298.15\ K) = 309.735 \pm 0.21\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -285.52 \pm 6.3\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -288.70 \pm 6.3\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}
349.5(1)	241(2)
535.3(1)	398(2)
1085 (1)	847(2)

Ground State Quantum Weight: 1 $\sigma = 3$
Point Group: C_{3v}
Bond Distances: C–Cl = 1.76 Å; C–F = 1.33 Å
Bond Angles: Cl–C–Cl = 109°40′; F–C–Cl = 109°28′
Product of the Moments of Inertia: $I_A I_B I_C = 5.736023 \times 10^{-113}\ g^3{\cdot}cm^6$

Enthalpy of Formation

Mears and Stahl[1] investigated several enthalpiess of reaction involving CF$_4$, CF$_3$Cl, CF$_2$Cl$_2$, CFCl$_3$, CCl$_4$, HF and HCl Using JANAF values for all compounds except CF$_2$Cl$_2$ and CFCl$_3$, we obtain the following observations:

1. $\Delta_f H°(CCl_3F, g, 298.15\ K) = -70.12 \pm 1.1\ kcal{\cdot}mol^{-1}$
2. $\Delta_f H°(CCl_2F_2, g, 298.15\ K) = -116.53 \pm 1.5\ kcal{\cdot}mol^{-1}$
3. $\Delta_f H°(CCl_2F_2, g, 298.15\ K) - \Delta_f H°(CCl_3F, g, 298.15\ K) = -49.39 \pm 1.0\ kcal{\cdot}mol^{-1}$
4. $\Delta_f H°(CCl_2F_2, g, 298.15\ K) - 2\Delta_f H°(CCl_3F, g, 298.15\ K) = 20.34 \pm 1.0\ kcal{\cdot}mol^{-1}$
5. $\Delta_f H°(CCl_3F, g, 298.15\ K) - 2\Delta_f H°(CCl_2F_2, g, 298.15\ K) = 165.47 \pm 1.0\ kcal{\cdot}mol^{-1}$

The sum of the squares of the deviations is smallest when $\Delta_f H°(CCl_2F_2, g, 298.15\ K) = -117.5\ kcal{\cdot}mol^{-1}$ and $\Delta_f H°(CCl_3F, g, 298.15\ K) = -69\ kcal{\cdot}mol^{-1}$, and all the values are within their uncertainty ranges.

Petersen and Pitzer[9] obtained an approximate equilibrium constant for the reaction CClF$_3$(g) + 2CCl$_4$(g) = 3CCl$_3$F(g) of log $K_{400} = -4.5$. This on third law reduction gives $\Delta_r H°(298.15\ K) = 10.56\ kcal{\cdot}mol^{-1}$ and with $\Delta_f H°(CClF_3, g, 298.15\ K) = -169.2\ kcal{\cdot}mol^{-1}$ and $\Delta_f H°(CCl_4, g, 298.15\ K) = -22.94\ kcal{\cdot}mol^{-1}$ this yields $\Delta H°(CCl_3F, g, 298.15K) = -68.2\ kcal{\cdot}mol^{-1}$ Kirkbride and Davidson[2] investigated the reaction of potassium with the chlorofluoromethanes and obtained $\Delta_f H°(CCl_2F_2, g, 298.15\ K) = -115.1 \pm 2\ kcal{\cdot}mol^{-1}$ and $\Delta_f H°(CCl_3F, g, 298.15\ K) = -72.9 \pm 4\ kcal{\cdot}mol^{-1}$ after correction with JANAF auxiliary data. Wartenberg and Schiefer[3] investigated the same reaction and we obtain, after correction with JANAF auxiliary data, $\Delta_f H°(CCl_2F_2, g, 298.15\ K) = -112.7\ kcal{\cdot}mol^{-1}$ and $\Delta_f H°(CCl_3F, g, 298.15\ K) = -63.1\ kcal{\cdot}mol^{-1}$. Baibuz[4] has reported $\Delta_f H°(CCl_3F, g, 298.15\ K) = -66.4 \pm 2.1$ from heat of explosion measurements. A correlation of his other results would indicate that this value is not negative enough, possibly by as much as 3 kcal·mol^{-1}.

We adopt the values calculated above from Mears and Stahl,[1] since they have a high degree of internal consistency and also lead to a realistic progression in the heats of atomization in going from CF$_4$ to CCl$_4$. With the adopted enthalpies of formation, the successive replacement of F by Cl changes the atomization enthalpies by 43.8, 41.6, 38.5 and 36.0 kcal·mol^{-1}.

Heat Capacity and Entropy

Claassen[5] chose the frequencies given above from his own gas phase Raman measurements and the infrared values of earlier investigators. The values are in good agreement with the assignment of Plyler and Benedict,[6] and the matrix studies of King.[7] The molecular structure was determined from the microwave measurements of Long *et al.*[8] The principal moments of inertia are: $I_A = I_B = 34.3029 \times 10^{-39}$ and $I_C = 48.7471 \times 10^{-39}\ g{\cdot}cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−16.060	−285.522	−285.522	INFINITE
100	43.323	244.360	369.234	−12.487	−287.829	−275.301	143.802
200	64.411	281.288	316.474	−7.037	−288.727	−262.314	68.509
250	72.066	296.515	310.988	−3.618	−288.783	−255.700	53.426
298.15	78.018	309.735	309.735	0.	−288.696	−249.335	43.682
300	78.223	310.219	309.737	0.145	−288.691	−249.090	43.371
350	83.173	322.662	310.708	4.184	−288.494	−242.505	36.192
400	87.149	334.038	312.924	8.446	−288.227	−235.952	30.812
450	90.347	344.494	315.859	12.886	−287.912	−229.437	26.632
500	92.930	354.151	319.211	17.470	−287.569	−222.957	23.292
600	96.749	371.455	326.511	26.967	−286.835	−210.103	18.291
700	99.350	386.577	334 034	36.780	−286.079	−197.374	14.728
800	101.178	399.969	341.455	46.811	−285.322	−184.754	12.063
900	102.502	411.967	348.635	56.999	−284.577	−172.228	9.996
1000	103.488	422.820	355.520	67.300	−283.848	−159.784	8.346
1100	104.238	432.720	362.094	77.688	−283.139	−147.412	7.000
1200	104.822	441.816	368.364	88.143	−282.452	−135.104	5.881
1300	105.284	450.225	374.342	98.649	−281.788	−122.852	4.936
1400	105.655	458.042	380.044	109.196	−281.148	−110.650	4.128
1500	105.959	465.342	385.490	119.778	−280.533	−98.493	3.430
1600	106.209	472.189	390.697	130.386	−279.943	−86.377	2.820
1700	106.418	478.634	395.682	141.018	−279.379	−74.296	2.283
1800	106.594	484.722	400.461	151.669	−278.842	−62.248	1.806
1900	106.744	490.489	405.049	162.336	−278.330	−50.229	1.381
2000	106.872	495.968	409.459	173.017	−277.845	−38.237	0.999
2100	106.983	501.185	413.704	183.710	−277.387	−26.268	0.653
2200	107.080	506.164	417.794	194.413	−276.957	−14.320	0.340
2300	107.164	510.926	421.741	205.125	−276.553	−2.391	0.054
2400	107.239	515.488	425.552	215.846	−276.178	9.521	−0.207
2500	107.304	519.867	429.238	226.573	−275.830	21 418	−0.448
2600	107.363	524.077	432.805	237.306	−275.510	33.302	−0.669
2700	107.415	528.130	436.261	248.045	−275.219	45.174	−0.874
2800	107.462	532.037	439.612	258.789	−274.955	57.035	−1.064
2900	107.504	535.809	442.865	269.537	−274.719	68.888	−1.241
3000	107.542	539.454	446.024	280.290	−274.508	80.732	−1.406
3100	107.576	542.981	449 095	291.045	−274.323	92.571	−1.560
3200	107.607	546.397	452.083	301.805	−274.161	104.403	−1.704
3300	107.636	549.708	454.991	312.567	−274.020	116.231	−1.840
3400	107.662	552.922	457.824	323.332	−273.897	128.055	−1.967
3500	107.685	556.043	460.586	334.099	−273.791	139.875	−2.088
3600	107 707	559.077	463.280	344.869	−273.697	151.693	−2.201
3700	107.728	562.029	465.909	355.640	−273.613	163.509	−2.308
3800	107.746	564.902	468.477	366.414	−273.534	175.321	−2.410
3900	107.763	567.701	470.985	377.190	−273.458	187.132	−2.506
4000	107.779	570.429	473.437	387.967	−273.381	198.942	−2.598
4100	107 794	573.091	475.836	398.745	−273.298	210.749	−2.685
4200	107.808	575.688	478.182	409.526	−273.206	222.554	−2.768
4300	107.821	578.225	480.480	420.307	−273.102	234.356	−2.847
4400	107.832	580.704	482.729	431.090	−272.982	246.156	−2.922
4500	107.844	583.128	484.934	441.873	−272.842	257.953	−2.994
4600	107.854	585.498	487.094	452.658	−272.679	269.747	−3.063
4700	107.864	587.818	489.213	463.444	−272.490	281.537	−3.129
4800	107.873	590.089	491.291	474.231	−272.273	293.322	−3.192
4900	107.882	592.313	493.330	485.019	−272.024	305.103	−3.252
5000	107.890	594.493	495.331	495.807	−271.742	316.878	−3.310
5100	107.897	596.629	497.297	506.597	−271.424	328.648	−3.366
5200	107.905	598.724	499.227	517.387	−271.068	340.410	−3.419
5300	107.911	600.780	501.124	528.178	−270.674	352.166	−3.471
5400	107.918	602.797	502.988	538.969	−270.238	363.913	−3.520
5500	107.924	604.777	504.821	549.761	−269.761	375.653	−3.568
5600	107.930	606.722	506.623	560.554	−269.241	387.383	−3.613
5700	107.935	608.632	508.396	571.347	−268.678	399.103	−3.657
5800	107.940	610.510	510.140	582.141	−268.070	410.814	−3.700
5900	107.945	612.355	511.857	592.935	−267.418	422.513	−3.741
6000	107.950	614.169	513.547	603.730	−266.721	434.200	−3 780

PREVIOUS: June 1970 (1 atm) CURRENT: June 1970 (1 bar)

Tetrachloromethane (CCl_4) IDEAL GAS M_r = 153.823 Tetrachloromethane (CCl_4) $C_1Cl_4(g)$

$S°(298.15\ K) = 309.809 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -93.81 \pm 2.1\ kJ{\cdot}mol^{-1}$

$\Delta_fH°(298.15\ K) = -95.98 \pm 2.1\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
458 (1)
218 (2)
776 (3)
314 (3)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: T_d
Bond Distance: C–Cl = 1.760 Å
Bond Angle: Cl–C–Cl = 109.47°
Product of the Moments of Inertia: $I_AI_BI_C = 1.150034 \times 10^{-112}\ g^3{\cdot}cm^6$

Enthalpy of Formation

Hu and Sinke[1] have measured the enthalpy of combustion of $CCl_4(l)$ in the rotating platinum bomb calorimeter, using As_2O_3 solution as the reducing agent. They reported $\Delta_cH°(298.15\ K) = -86.02\ kcal{\cdot}mol^{-1}$ for $CCl_4(l) + 2H_2O(l) \rightarrow CO_2(g) + 4HCl\ (600\ H_2O, aq)$ which leads to $\Delta_fH°(CCl_4, l, 298.15\ K) = -30.69\ kcal{\cdot}mol^{-1}$, using $\Delta_fH°(298.15\ K) = -94.051$, -39.823 and $-68.315\ kcal\ mol^{-1}$ for $CO_2(g)$, $HCl(600\ H_2O, aq)$ and $H_2O(l)$, respectively.[2] The standard deviation of five combustion runs was ± 0.074 $kcal{\cdot}mol^{-1}$. Employing the enthalpy of vaporization of $CCl_4(l)$ at 298.15 K as 7.75 $kcal{\cdot}mol^{-1}$,[3] we obtain $\Delta_fH°(CCl_4, g, 298.15K) = -22.94\ kcal{\cdot}mol^{-1}$ which is adopted in the tabulation.

Smith *et al*.,[5] based on the combustion data of Eftring,[4] re–evaluated the enthalpy of combustion of carbon tetrachloride at 18.7°C as $\Delta_cE°/M = -567.5\ cal{\cdot}g^{-1}$ for $CCl_4(l) + 2\ H_2O(l) \rightarrow CO_2(g) + 4HCl(600H_2O, aq)$. This value needs to be further corrected for a change in the heat of oxidation of As_2O_3[6] and calculated to 25°C to give $\Delta_cE°(298.15\ K) = -88.105\ kcal{\cdot}mol^{-1}$ $\Delta_cH°(298.15\ K) = -87.513\ kcal{\cdot}mol^{-1}$, $\Delta_fH°(CCl_4, l, 298.15\ K) = -29.20\ kcal{\cdot}mol^{-1}$ and $\Delta_fH°(CCl_4, g, 298.15\ K) = -21.45\ kcal\ mol^{-1}$.

Neugebauer[7] has measured the enthalpy of reaction of CCl_4 with Mg in presence of hydrogen in the stationary bomb calorimeter and then derived the enthalpy of formation, $\Delta_fH°(CCl_4, l, 298.15\ K) = -32.3 \pm 2\ kcal{\cdot}mol^{-1}$ which yields $\Delta_fH°(CCl_4, g, 298.15\ K) = -24.55 \pm 2\ kcal{\cdot}mol^{-1}$. Baibuz,[8] using an explosion technique, obtained $\Delta_fH°(CCl_4, g, 298.15\ K) = -24.6 \pm 1\ 9\ kcal\ mol^{-1}$ Bodenstein and Gunther[9] have measured calorimetrically $\Delta_rH°(293\ K) = -62.57 \pm 0.35\ kcal{\cdot}mol^{-1}$ for $CCl_4(g) + 2H_2(g) \rightarrow C(cr) + 4HCl(g)$. They calibrated their calorimeter by means of the reaction $H_2(g) + Cl_2(g) \rightarrow 2HCl(g)$ for which they took $\Delta_fH°(293\ K) = -44\ kcal\ mol^{-1}$. Their data have been re–evaluated to give $\Delta_fH°(CCl_4, g, 298\ 15\ K) = -25.68\ kcal{\cdot}mol^{-1}$, but no correction is applied for the enthalpy of formation of carbon which was not the reference state "graphite" formed in the reaction. Domalski and Armstrong[10] reviewed several cases of active carbon formed in similar reactions and quoted a enthalpy of formation of carbon from +1.9 to +3.95 $kcal{\cdot}mol^{-1}$. If this correction is applied to the data of Bodenstein, their enthalpy of formation of $CCl_4(g)$ should be 2 to 4 $kcal{\cdot}mol^{-1}$ less negative than $-25.68\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

Bartell *et al*.[11] have measured the bond distance as 1.760 ± 0.004 Å by the electron diffrction measurement The assigned fundamental vibrational frequencies are obtained from Shimanouchi's selection[12] in which they are essentially the same as those frequencies determined from Raman and infrared spectra by Classen.[13] The principal moments of inertia are $I_A = I_B = I_C = 48.6299 \times 10^{-39}\ g{\cdot}cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	$S°$ (J·K⁻¹mol⁻¹)	$-[G°-H°(T_r)]/T$ (J·K⁻¹mol⁻¹)	$H°-H°(T_r)$ (kJ·mol⁻¹)	$\Delta_fH°$ (kJ·mol⁻¹)	$\Delta_fG°$ (kJ·mol⁻¹)	log K_f
0	0.	0.	INFINITE	−17.238	−93.806	−93.806	INFINITE
100	47.244	238.738	374.168	−13.543	−95.995	−81.972	42.818
200	69.995	279.142	317.054	−7.582	−96.436	−67.662	17.672
250	77.656	295.619	311.152	−3.883	−96.270	−60.485	12.638
298.15	83.401	309.809	309.809	0.	−95.981	−53.617	9.393
300	83.594	310.326	309.811	0.154	−95.968	−53.354	9.290
350	88.174	323.571	310.846	4.454	−95.577	−46.282	6.907
400	91.707	335.586	313.200	8.954	−95.131	−39.270	5.128
450	94.451	346.553	316.305	13.611	−94.654	−32.315	3.751
500	96.602	356.620	319.840	18.390	−94.165	−25.415	2.655
600	99.676	374.525	327.500	28.215	−93.182	−11.757	1.024
700	101.698	390.052	335.352	38.290	−92.223	1.737	−0.130
800	103.086	403.728	343.061	48.534	−91.300	15.096	−0.986
900	104 074	415.930	350.492	58.894	−90.415	28.342	−1.645
1000	104.800	426.935	357.595	69.340	−89.566	41.492	−2.167
1100	105.348	436.950	364.361	79.848	−88.751	54.558	−2.591
1200	105 771	446.135	370.798	90.405	−87.969	67.551	−2.940
1300	106.103	454.615	376.923	100.999	−87.219	80.481	−3.234
1400	106.370	462.488	382.757	111.624	−86.498	93.353	−3 483
1500	106.586	469.835	388.320	122.272	−85.806	106.175	−3.697
1600	106.765	476.720	393.632	132.940	−85.142	118.952	−3.883
1700	106.913	483.197	398.712	143.624	−84.508	131.689	−4.046
1800	107.038	489.311	403.577	154.321	−83.902	144.389	−4.190
1900	107.144	495.101	408.243	165.031	−83.326	157.055	−4.318
2000	107.235	500.600	412.725	175.750	−82.781	169.693	−4.432
2100	107.313	505.834	417 035	186.477	−82.270	182 304	−4.535
2200	107.381	510.827	421.186	197.212	−81.793	194.891	−4.627
2300	107.441	515.602	425.188	207.953	−81.354	207 458	−4.712
2400	107.493	520.176	429.051	218.700	−80.954	220.006	−4.788
2500	107.539	524.565	432.784	229.452	−80.597	232.539	−4.859
2600	107.580	528.783	436.396	240.208	−80.285	245.058	−4.923
2700	107.617	532.844	439.893	250.968	−80.019	257.566	−4.983
2800	107.650	536.759	443.283	261.731	−79.802	270.065	−5.038
2900	107.679	540.537	446.572	272.497	−79.633	282.557	−5.089
3000	107.706	544.188	449.765	283.267	−79.514	295.044	−5.137
3100	107.730	547.720	452.869	294.038	−79.444	307.528	−5.182
3200	107.752	551.140	455.886	304.813	−79.422	320.010	−5.224
3300	107.772	554.456	458.823	315.589	−79.446	332.493	−5.263
3400	107.790	557.674	461.684	326.367	−79.513	344.977	−5.300
3500	107.807	560.799	464.471	337.147	−79.621	357 464	−5.335
3600	107.822	563.836	467.189	347.928	−79.766	369.954	−5.368
3700	107.836	566.790	469.841	358.711	−79.943	382.448	−5.399
3800	107.849	569.666	472.431	369.495	−80.148	394.948	−5.429
3900	107.861	572.468	474.960	380.281	−80.377	407.453	−5.457
4000	107.872	575.199	477.432	391.067	−80.623	419.965	−5.484
4100	107.883	577.863	479.849	401.855	−80.883	432.483	−5.510
4200	107.892	580.462	482.214	412.644	−81.150	445.007	−5.534
4300	107.901	583.001	484.528	423.434	−81.419	457.538	−5.558
4400	107.909	585.482	486.795	434.224	−81.686	470.075	−5.581
4500	107.917	587.907	489.015	445.015	−81.946	482.618	−5.602
4600	107 925	590.279	491.191	455.808	−82.193	495.167	−5.623
4700	107.931	592.600	493.324	466.600	−82.423	507.720	−5.643
4800	107.938	594.873	495.416	477.394	−82.632	520.279	−5.662
4900	107.944	597.098	497.468	488.188	−82.815	532.842	−5.680
5000	107.949	599.279	499.483	498.983	−82.971	545.407	−5.698
5100	107.955	601.417	501.460	509.778	−83.094	557.977	−5.715
5200	107.960	603.513	503.403	520.574	−83.181	570.547	−5.731
5300	107.965	605.570	505.311	531.370	−83.231	583.119	−5 747
5400	107.969	607.588	507.187	542.166	−83.241	595.692	−5 762
5500	107.973	609.569	509.030	552.964	−83.209	608.265	−5.777
5600	107.977	611.515	510.843	563.761	−83.132	620.837	−5.791
5700	107.981	613.426	512.626	574.559	−83.010	633.406	−5.805
5800	107.985	615.304	514.380	585.357	−82.841	645.974	−5.818
5900	107.988	617.150	516.106	596.156	−82.624	658.538	−5.830
6000	107.992	618.965	517.806	606.955	−82.358	671.097	−5.842

PREVIOUS. December 1968 (1 atm) CURRENT December 1968 (1 bar)

Copper Cyanide (CuCN) CRYSTAL $M_r = 89.5637$ Copper Cyanide (CuCN) $C_1Cu_1N_1(cr)$

$\Delta_f H°(0\ K) = 93.32 \pm 2.1\ kJ \cdot mol^{-1}$
$S°(298.15\ K) = 90.002 \pm 0.25\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = 94.98 \pm 2.1\ kJ \cdot mol^{-1}$
$T_{fus} = 746\ K$ $\Delta_{fus} H° = 12 \pm 4\ kJ \cdot mol^{-1}$

Enthalpy of Formation

Taylor *et al.*[1] determined by solution calorimetry the enthalpy of reaction, $\Delta_r H°(298.15\ K) = -13.437 \pm 100\ cal \cdot K^{-1} \cdot mol^{-1}$ for $NaCN(cr) + 0.5\ Cu_2O(cr) + 0.5\ H_2O(l) \rightarrow CuCN(cr) + NaOH(128.5\ H_2O)$ This leads to $\Delta_f H°(CuCN, cr, 298.15\ K) = 22.70 \pm 0.5\ kcal \cdot mol^{-1}$ using the following auxiliary data. $\Delta_f H°(NaCN, cr, 298.15\ K) = -21.68 \pm 0.3\ kcal \cdot mol^{-1}$,[2] $\Delta_f H°(Cu_2O, cr, 298.15\ K) = -40.7 \pm 0.5\ kcal \cdot mol^{-1}$,[3] $\Delta_f H°(H_2O, l, 298.15\ K) = -68.315\ kcal \cdot mol^{-1}$ [4] and $\Delta_f H°(NaOH\ 128.5\ H_2O, aq, 298.15\ K) = -112.321\ kcal \cdot mol^{-1}$.[2,4]

Heat Capacity and Entropy

The heat capacity of CuCN(cr) has been measured adiabatically over the temperature range from 8 to 402 K by Taylor *et al.*[1] The smooth $C_p°$ values are adopted in the tabulation. The value of $S°(298\ 15\ K)$ is calculated from the $C_p°$ data and is based on an extrapolation of $S°(8\ K) = 0.104\ cal \cdot K^{-1} \cdot mol^{-1}$ They also found an anomaly in the heat capacity at 300 K which is considered as a second order phase transition. Heat capacities above 402 K are estimated by extrapolation of the measured $C_p°$ data.

Fusion Data

The melting point 746 K was determined by Truthe.[5] The heat of melting is calculated from the phase diagram studies of KCN–CuCN and NaCN–CuCN reported by Truthe.[5]

References

[1] A. R. Taylor, Jr., M. H. Brown and E. G. Taylor, U S. Bur. Mines RI 7499, (1971).
[2] JANAF Thermochemical Tables: NaCN(cr), 3–31–66; Cu₂O(cr), 6–30–66; NaOH(cr), 12–30–70.
[3] U. S. Nat. Bur. Stand. Tech. Note 270–3, (1968).
[4] JANAF NaOH(cr) table, dated December 30, 1970. Heat of dilution data is obtained from V. B. Parker, "Thermal Properties of Aqueous Uni–univalent Electrolytes," NSRDS–NBS2, (1965).
[5] W. Truthe, Z. Anorg. Chem. 76, 144 (1912).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
0	0.	0.	INFINITE	−12.052	93.317	93.317	INFINITE
100	35.238	36 869	137.842	−10.097	93.093	98.495	−51 449
200	52 484	67.308	95.337	−5.606	93.790	103.689	−27.081
298.15	61.024	90.002	90.002	0.	94.977	108.306	−18 975
300	62 195	90.383	90.003	0.114	95.003	108.389	−18.872
400	66.735	108.930	92.500	6.572	96.486	112.628	−14.708
500	70.249	124.212	97.358	13.427	97.978	116.491	−12.170
600	73.136	137.282	102.949	20.600	99.462	120.054	−10 452
700	75.689	148.753	108.689	28 045	100.938	123.370	−9.206
800	78.032	159.016	114.350	35.733	102.427	126.473	−8.258
900	80.249	168.337	119.838	43.649	103.943	129.388	−7.509
1000	82.341	176.900	125.122	51.778	105.495	132.132	−6.902

PREVIOUS. CURRENT December 1971

Fluoromethylidyne (CF) IDEAL GAS $M_r = 1.009403$ Fluoromethylidyne (CF) $C_1F_1(g)$

$\Delta_fH°(0\ K) = 251.6 \pm 8\ kJ{\cdot}mol^{-1}$

$S°(298.15\ K) = 213.03 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_fH°(298.15\ K) = 255.2 \pm 8\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^2\Pi_r$	0	2
	77.11	2
[$^4\Sigma$]	[25000]	[4]
	42705	2
	49452	2

$\omega_e = 1308.1\ cm^{-1}$ $\omega_ex_e = 11.10\ cm^{-1}$ $\sigma = 1$

$B_e = 1.4172\ cm^{-1}$ $\alpha_e = 0.0184\ cm^{-1}$ $r_e = 1.2667$ Å

Enthalpy of Formation

Faber *et al.*[1] have studied the weight change of graphite in CF_4 at high temperatures. Our reanalysis of their data use the equilibrium constants for CF_4, CF_3 and CF_2 from the JANAF Tables,[2] the only other C–F species considered is assumed to be CF. This treatment yields negative values for the CF pressure except at the highest temperature, where 3rd law analysis of the equilibrium constant yields $\Delta_fH°$(CF, g, 298 15 K) = 59.4 kcal·mol^{-1}. Farber *et al.*[1] also investigated mass–spectrometrically the vapor species present at equilibrium and followed the intensities of CF^+ and F^+ From a 2nd law treatment of the intensities they report $\Delta_fH°$(CF, g, 2300 K) = 62.0 kcal·mol^{-1}, or $\Delta_fH°$(CF, g, 298.15 K) = 64 kcal·mol^{-1}.

Porter *et al.*[3] have investigated the A–X band system under high dispersion. From an analytical extrapolation of the 10 observed levels they reported a dissociation energy of 126 9 ± 2.9 kcal·mol^{-1}, which yields $\Delta_fH°$(CF, g, 298 15 K) = 61.9 ± 2.9 kcal·mol^{-1}.

The predissociation limit of CF(g) has been reported by Thrush and Zwolenik[4] as <132 kcal mol^{-1}; Kuzyakov and Tatievsky[5] determined the same quantity as <133 kcal·mol^{-1}. These results yield $\Delta_fH°$(CF, g, 298.15 K) > 56 kcal·mol^{-1}. Thrush and Zwolenik[4] also report a predissociation limit for the reaction $CF_2 \rightarrow CF + F$ which is <120 kcal·mol^{-1}. This value has now been shown to be erroneous (see the CF_2(g) table for details).

Modica[6] has studied the equilibrium $CF_2 \rightarrow CF + F$ in a shock tube in the range 2680 to 3400 K. Since functions for CF_2, CF and F are well established, the data were analyzed using 2nd and 3rd law treatments. The 2nd law analysis gives $\Delta_rH°$(298.15 K) = 107.2 ± 7.6 kcal·mol^{-1}, in agreement with with value reported by Modica. The 3rd law analysis yields $\Delta_rH°$(298.15 K) = 134.9 ± 7.2 kcal·mol^{-1} and a drift of 9.7 ± 2.5 cal·K^{-1}·mol^{-1} The excessive drift indicates that the reported equilibrium constants do not represent the stated reaction.

Andrews and Barrow[7] report a dissociation energy of 114 kcal·mol^{-1} from an extrapolation of four B state levels. This extrapolation is considered unreliable by Porter *et al.*[3] since this state is formed from an avoided crossing and is likely to be perturbed.

The adopted value of $\Delta_fH°$(CF, g, 298.15 K) is 61 ± 2 kcal·mol^{-1} (255.224 ± 8 kJ·mol^{-1}), which is within the uncertainties and ranges of the acceptable investigations.

Heat Capacity and Entropy

The vibrational and rotational constants are from Porter *et al.*,[3] the higher electronic levels are those reported by Andrews and Barrow,[7] except that the B state is now considered to be $^2\Sigma$. The estimated level at 25000 cm^{-1} is proposed in order to explain the low bond dissociation energy of C_2F_2, by analogy with the reasoning used by Simons[8] for C_2F_4. This level would be a $^4\Sigma$ level and could correlate with the ground state atoms.

References

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[2] JANAF Thermochemical Tables CF_4(g), 6–30–69; CF_3(g), 6–30–69; CF_2(g), 7–30–70.
[3] T. L. Porter, D. E. Mann and N. Acquista, J. Mol. Spectrosc. 16, 228 (1965).
[4] B. A. Thrush and J. J. Zwolenik, Trans. Faraday Soc. 59, 582 (1963).
[5] Yu. Ya. Kuzyakov and V. M. Tatievsky, Opt. Spektrosk. 5, 699 (1958).
[6] A. P. Modica, J. Chem. Phys. 44, 1585 (1966).
[7] E. B. Andrews and R. F. Barrow, Proc. Phys. Soc. (London), 64A, 481 (1951).
[8] J. P. Simons, Nature 205, 1308 (1965).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−9.082	251.605	251.605	INFINITE
100	31.017	180.140	239.625	−5.948	253.226	243.826	−127.361
200	29.778	201.126	215.766	−2.928	254.455	233.912	−61.092
. 250	29.792	207.766	213.526	−1.440	254.896	228.723	−47.789
298.15	30.060	213.033	213.033	0.	255.224	223.650	−39.183
300	30 074	213.219	213.034	0.056	255.235	223.455	−38.907
350	30.537	217.888	213.402	1.570	255.484	218.137	−32.555
400	31.094	222.002	214.224	3.111	255.658	212.789	−27.787
450	31.681	225.698	215.297	4.680	255.765	207.423	−24.077
500	32.253	229.066	216.508	6.279	255.816	202.049	−21.108
600	33.280	235.040	219.111	9.557	255 779	191.296	−16.654
700	34.116	240.235	221.766	12.928	255.602	180.561	−13.474
800	34.780	244.836	224.368	16.374	255.322	169.859	−11.091
900	35.305	248.964	226 875	19.880	254.966	159.197	−9.240
1000	35 725	252.706	229.274	23.432	254.550	148.577	−7.761
1100	36.064	256.127	231.562	27.022	254 086	138.002	−6.553
1200	36.343	259.278	233 742	30.643	253.583	127.471	−5.549
1300	36.576	262.196	235.820	34.289	253.046	116.983	−4.700
1400	36.773	264.914	237.802	37.957	252.479	106.538	−3.975
1500	36.942	267.457	239.695	41.643	251.885	96.134	−3.348
1600	37.088	269.846	241.506	45.344	251.267	85.771	−2.800
1700	37.218	272.098	243.240	49.060	250.628	75.447	−2.318
1800	37.333	274.229	244.903	52.787	249.969	65.161	−1.891
1900	37.436	276.250	246.500	56.526	249.292	54.913	−1.510
2000	37.530	278.173	248.036	60.274	248.601	44.700	−1.167
2100	37.617	280.006	249.515	64.032	247.896	34.522	−0.859
2200	37.697	281.758	250.941	67.797	247.180	24.378	−0.579
2300	37 771	283.435	252.318	71.571	246.456	14.267	−0.324
2400	37 841	285.044	253.648	75.352	245.725	4.187	−0.091
2500	37.907	286.591	254.935	79.139	244.990	−5.861	0 122
2600	37 970	288.079	256.181	82.933	244.253	−15.881	0.319
2700	38.030	289.513	257.389	86.733	243.516	−25.872	0.501
2800	38.089	290.897	258.561	90.539	242.780	−35.836	0.669
2900	38.145	292.234	259.700	94.351	242.047	−45 774	0.824
3000	38.200	293.528	260.806	98.168	241.319	−55.686	0.970
3100	38 254	294.782	261.882	101.991	240.597	−65.574	1.105
3200	38.307	295.997	262.929	105.819	239.882	−75.439	1.231
3300	38.360	297.177	263 949	109.652	239.175	−85.282	1.350
3400	38.413	298.323	264 943	113 491	238.477	−95.104	1.461
3500	38.466	299.437	265.913	117.335	237.789	−104.905	1.566
3600	38.519	300.521	266.859	121.184	237 110	−114.686	1.664
3700	38.572	301.578	267.783	125.038	236.442	−124.449	1.757
3800	38.627	302.607	268.686	128.898	235.785	−134.195	1.845
3900	38.682	303.611	269.569	132.764	235.139	−143.922	1.928
4000	38.738	304.591	270.432	136.635	234.505	−153.634	2.006
4100	38.796	305.548	271.277	140.511	233.882	−163.330	2.081
4200	38.855	306 484	272.104	144.394	233.270	−173.010	2.152
4300	38.915	307.399	272.915	148.282	232.670	−182.676	2.219
4400	38.977	308.294	273 709	152.177	232.081	−192.329	2.283
4500	39.040	309.171	274.487	156.078	231.504	−201.968	2.344
4600	39.105	310.030	275.250	159.985	230.938	−211.594	2.403
4700	39.172	310.871	275.999	163.899	230.383	−221.209	2.458
4800	39.241	311.697	276.734	167.820	229.839	−230.811	2.512
4900	39.311	312.507	277.456	171.747	229.306	−240.403	2.563
5000	39.383	313.301	278.165	175.682	228.784	−249.983	2.612
5100	39.457	314.082	278.862	179.624	228.272	−259.553	2.658
5200	39.532	314.849	279.546	183.573	227.771	−269.114	2.703
5300	39.610	315.603	280.220	187.530	227.279	−278.664	2.746
5400	39.689	316.344	280.882	191.495	226.798	−288.206	2.788
5500	39.769	317.073	281.533	195.468	226.327	−297.739	2.828
5600	39.851	317.790	282.174	199.449	225.865	−307.263	2.866
5700	39.935	318.496	282.805	203.438	225.413	−316.779	2.903
5800	40.021	319.192	283.427	207.436	224.970	−326.288	2.939
5900	40 107	319.876	284.039	211.443	224.536	−335.788	2.973
6000	40.196	320.551	284 642	215.458	224.111	−345.282	3.006

PREVIOUS: June 1970 (1 atm) CURRENT June 1970 (1 bar)

Fluoromethylidyne, Ion (CF⁺) IDEAL GAS $M_r = 31.008854$ Fluoromethylidyne, Ion (CF⁺) $C_1F_1^+(g)$

$S°(298.15\ K) = 201.51 \pm 2.1\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 1140.0 \pm 5.0\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = 1149.4 \pm 5.0\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$X^1\Sigma$	0	1
$[a^3\Pi]$	[35000]	[6]

$\omega_e = [1380]\ cm^{-1}$ $\omega_e x_e = [11.6]\ cm^{-1}$ $\sigma = 1$
$B_e = [1.4361]\ cm^{-1}$ $\alpha_e = [0.0193]\ cm^{-1}$ $r_e = [1.263]\ Å$

Enthalpy of Formation

There have been no direct determinations of the ionization potential but Johns and Barrow[1] have calculated a value by assuming the $B^2\Sigma^+$ state of CF to be the first of a Rydberg series. They report IP = 8.91 eV (205.464 kcal mol^{-1}) which yields $\Delta_fH°(CF^+, g, 0\ K) = 265.6 \pm 10\ kcal{\cdot}mol^{-1}$. An identical value has been calculated by Carroll and Grennan[7] *who assumed the* $A^2\Sigma^+$ *state of CF to be the* start of a Rydberg series and estimated the termination by comparison with the same series in N_2, CO and NO.

Diebler and Liston[2] have measured the photoionization onset of the process $FCN + h\nu \rightarrow CF^+ + N + e^1$ ($\Delta H°(0\ K) = 377.03\ kcal{\cdot}mol^{-1}$). Using JANAF auxiliary data,[3] we obtain $\Delta_fH°(CF^+, g, 0\ K) = 273.0 \pm 4\ kcal{\cdot}mol^{-1}$.

Walter *et al.*[4] have observed the photoionization onset of the process $C_2F_4 + h\nu \rightarrow CF^+ + CF_3 + e^-$ ($\Delta H°(0\ K) = 317.306 \pm 0.23\ kcal{\cdot}mol^{-1}$). The JANAF values[3] for C_2F_4 and CF_3 are consistent since they are both derived from the same simultaneous solution, they yield $\Delta_fH°(CF^+, g, 0\ K) = 272.464 \pm 1.2\ kcal{\cdot}mol^{-1}$(1139.989 ± 5.0 kJ·mol^{-1}), which is adopted. This corresponds to an ionization potential of 212.328 kcal·mol^{-1} (9.21 eV).

Heat Capacity and Entropy

Spectra reported in the literature, Verma,[5] were later shown to belong to BF by Verma.[6] We estimated the molecular constants by *comparison with CF(g) and BF(g).*[3] *The* $^3\Pi$ *electronic level was estimated by comparison with AlCl(g).*[3] The enthalpy between 0 and 298.15 K is 2.072 kcal·mol^{-1}.

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−8.697	1139.985		
100	29.108	169.611	227.538	−5.793			
200	29.161	189.794	204.197	−2.881			
250	29.327	196.316	201.993	−1.419			
298.15	29.641	201.507	201.507	0.	1149.416	1115.024	−195.348
300	29.656	201.690	201.507	0.055	1149.464	1114.811	−194.106
350	30.125	206.295	201.870	1.549	1150.732	1108.934	−165.499
400	30.680	210.353	202.681	3.069	1151.925	1102.880	−144.021
450	31.266	214.001	203.740	4.617	1153.051	1096.682	−127.299
500	31.845	217.325	204.935	6.195	1154.120	1090.360	−113.909
600	32.900	223.227	207.504	9.434	1156.123	1077.418	−93.798
700	33.775	228.367	210.125	12.769	1157.988	1064.151	−79.408
800	34 477	232.924	212.695	16.183	1159.754	1050.624	−68.599
900	35.038	237.019	215.174	19.660	1161.448	1036.881	−60.179
1000	35.488	240.734	217.547	23.187	1163.086	1022.952	−53.434
1100	35.854	244.134	219.812	26.755	1164.678	1008.861	−47.907
1200	36.155	247.267	221.971	30.356	1166.234	994.627	−43.295
1300	36.405	250.172	224.030	33.984	1167.757	980.264	−39.388
1400	36 617	252.877	225.995	37.635	1169.252	965.785	−36.034
1500	36 798	255.410	227.873	41.306	1170.722	951.201	−33.124
1600	36.955	257.790	229.669	44.994	1172.169	936.519	−30.574
1700	37.093	260.035	231.390	48.697	1173.595	921.747	−28.322
1800	37.215	262.158	233.041	52.412	1175.003	906.891	−26.317
1900	37.325	264.174	234.627	56.139	1176.394	891.958	−24.522
2000	37 424	266.091	236.152	59.877	1177.770	876.952	−22.904
2100	37.514	267.919	237.622	63.624	1179.133	861.878	−21.438
2200	37.598	269.666	239.039	67.380	1180.486	846.739	−20.104
2300	37.675	271.339	240.407	71.143	1181.831	831.538	−18.885
2400	37 747	272.944	241.730	74.914	1183.169	816.279	−17.766
2500	37.814	274.486	243.009	78.693	1184.503	800.965	−16.735
2600	37.878	275.971	244.249	82.477	1185.836	785.597	−15.783
2700	37.939	277.401	245.450	86.268	1187.168	770.178	−14.900
2800	37.996	278.782	246.616	90.065	1188.501	754.710	−14.079
2900	38.052	280.116	247.748	93.867	1189.838	739.193	−13.314
3000	38.105	281.407	248.849	97.675	1191.179	723.631	−12.600
3100	38.157	282.658	249.919	101.488	1192.526	708.024	−11.930
3200	38.207	283.870	250.962	105.306	1193.880	692.373	−11.302
3300	38.256	285.046	251.977	109.130	1195.241	676.680	−10.711
3400	38.304	286.189	252.966	112.958	1196.611	660.946	−10.154
3500	38.352	287.300	253.931	116.790	1197.990	645.171	−9.629
3600	38.399	288.381	254.873	120.628	1199.379	629.356	−9.132
3700	38.446	289.434	255.793	124.470	1200.777	613.503	−8.661
3800	38.493	290.460	256.692	128.317	1202.186	597.612	−8.215
3900	38.540	291.460	257.571	132.169	1203.605	581.684	−7.791
4000	38.588	292.437	258.430	136.025	1205.034	565.719	−7.388
4100	38.637	293.390	259.271	139.886	1206.474	549.718	−7.003
4200	38.687	294.322	260.095	143.753	1207.925	533.682	−6.637
4300	38.738	295.233	260.901	147.624	1209.386	517.611	−6.288
4400	38.791	296.124	261.692	151.500	1210.858	501.507	−5.954
4500	38 846	296.996	262.467	155.382	1212.340	485.369	−5.634
4600	38.904	297.851	263.227	159.270	1213.833	469.197	−5.328
4700	38.964	298.688	263.972	163.163	1215.336	452.993	−5.034
4800	39.027	299.509	264.704	167.063	1216.849	436.757	−4.753
4900	39.094	300.314	265.423	170.969	1218.374	420.490	−4.482
5000	39.163	301.105	266.128	174.881	1219.908	404.191	−4.223
5100	39.237	301.881	266.822	178.801	1221.453	387.861	−3.973
5200	39.315	302.644	267.503	182.729	1223.008	371.501	−3.732
5300	39.396	303.393	268.174	186.665	1224.574	355.111	−3.500
5400	39.483	304.131	268.833	190.608	1226.150	338.691	−3.276
5500	39.574	304.856	269.481	194.561	1227.738	322.242	−3.060
5600	39.669	305.570	270.119	198.523	1229.336	305.764	−2.852
5700	39.770	306.273	270.747	202.495	1230.945	289.257	−2.651
5800	39.876	306.965	271.366	206.478	1232.565	272.722	−2.456
5900	39.988	307.648	271.975	210.471	1234.196	256.160	−2.268
6000	40.105	308.321	272.575	214.475	1235.839	239.569	−2.086

PREVIOUS December 1970 (1 atm) CURRENT. December 1970 (1 bar)

Cyanogen Fluoride (FCN) IDEAL GAS $M_r = 45.016103$ Cyanogen Fluoride (FCN) $C_1F_1N_1(g)$

$S°(298.15 \text{ K}) = 225.40 \pm 0.8 \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_fH°(0 \text{ K}) = 35.51 \pm 16.7 \text{ kJ·mol}^{-1}$
$\Delta_fH°(298.15 \text{ K}) = 35.98 \pm 16.7 \text{ kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
1077 (1)
[420] (2)
2290 (1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: $C_{\infty v}$
Bond Distances: C–F = 1.262 Å; C–N = 1.159 Å
Bond Angle: F–C–N = 180°
Rotational Constant: $B_0 = 0.353106 \text{ cm}^{-1}$

Enthalpy of Formation

Davis and Okabe[1] have determined the dissociation energy of FCN to F(g) and CN(g) by measuring the threshold energies of incident photon radiation to produce $B^2\Sigma^+$ CN which is monitored by its fluorescence. The dissociation energy determined by this technique is ≤111 kcal·mol^{-1} with an uncertainty of about 1 kcal in the determination of the limit.

Dibeler and Liston[2] have reported a dissociation energy of ≤115.6 kcal mol^{-1} from the threshold of the CN$^+$ ion as determined by photoionization.

We adopt a median value of 113.1 ± 2.5 kcal·mol^{-1} which leads to $\Delta_fH°$(FCN, g, 298.15 K) = 8.6 ± 4 kcal·mol^{-1} (35.982 ± 16.7 kJ·mol^{-1}) with auxiliary JANAF values for F(g) and CN(g).

Heat Capacity and Entropy

The molecular structure and bond lengths and angle were determined using microwave spectroscopy by Tyler and Sheridan.[3] The vibrational frequencies were reported by Aynsley *et al.*[4] from the infrared spectrum, except for the bending frequency which is estimated from the values for ClCN, BrCN and ICN, by comparison of bending force constants. The reasonable limits for this value as calculated from generous limits on the bending force constant are 405–450 cm^{-1}.

References

[1] D. D. Davis and H. Okabe, J. Chem Phys. 49, 5526 (1968).
[2] V. H. Dibeler and S. K. Liston, J. Chem. Phys. 47, 4548 (1967).
[3] J. K. Tyler and J. Sheridan, Trans. Faraday Soc. 59, 2661 (1963).
[4] E. E. Aynsley, R. E. Dodd, and R. Little, Proc. Chem. Soc. (London) 1959, 265.

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−10.272	35.509	35.509	INFINITE
100	30.550	186.140	259.533	−7.339	35.477	33.468	−17.482
200	37.491	209.468	229.132	−3.933	35.638	31.424	−8.207
250	40.199	218.136	226.088	−1.988	35.808	30.352	−6.342
298.15	42.312	225.403	225.403	0.	35.982	29.285	−5.131
300	42.385	225.665	225.404	0.078	35.989	29.243	−5.092
350	44.203	232.339	225.927	2.244	36.161	28.105	−4.194
400	45.750	238.345	227.110	4.494	36.314	26.944	−3.518
450	47.097	243.814	228.667	6.816	36.441	25.764	−2.991
500	48.291	248.839	230.436	9.201	36.542	24.573	−2.567
600	50.339	257.830	234.270	14.136	36.670	22.165	−1.930
700	52.041	265.722	238.211	19.258	36.721	19.743	−1.473
800	53.470	272.767	242.098	24.535	36.719	17.317	−1.131
900	54.669	279.136	245.865	29.944	36.677	14.894	−0.864
1000	55.674	284.950	249.487	35.463	36.608	12.477	−0.652
1100	56.518	290.297	252.957	41.073	36.516	10.068	−0.478
1200	57.227	295.246	256.278	46.762	36.406	7.668	−0.334
1300	57.826	299.851	259.454	52.515	36.279	5.279	−0.212
1400	58.333	304.155	262.495	58.324	36.136	2.899	−0.108
1500	58.765	308.195	265.408	64.179	35.977	0.531	−0.018
1600	59.135	311.999	268.203	70.075	35.804	−1.827	0.060
1700	59.453	315.594	270.886	76.005	35.616	−4.173	0.128
1800	59.729	319.000	273.465	81.964	35.415	−6.508	0.189
1900	59.969	322.236	275.947	87.949	35.200	−8.831	0.243
2000	60.178	325.318	278.339	93.957	34.973	−11.143	0.291
2100	60.362	328.258	280.647	99.984	34.736	−13.443	0.334
2200	60.524	331.070	282.876	106.028	34.489	−15.731	0.374
2300	60.668	333.764	285.030	112.088	34.234	−18.008	0.409
2400	60.796	336.349	287.115	118.162	33.974	−20.274	0.441
2500	60.910	338.833	289.134	124.247	33.708	−22.529	0.471
2600	61.013	341.224	291.092	130.343	33.440	−24.773	0.498
2700	61.105	343.528	292.992	136.449	33.171	−27.007	0.522
2800	61.188	345.752	294.836	142.564	32.902	−29.231	0.545
2900	61.264	347.901	296.629	148.687	32.634	−31.445	0.566
3000	61.332	349.979	298.373	154.816	32.369	−33.650	0.586
3100	61.394	351.991	300.071	160.953	32.107	−35.847	0.604
3200	61.451	353.941	301.724	167.095	31.850	−38.035	0.621
3300	61.503	355.833	303.335	173.243	31.598	−40.215	0.637
3400	61.551	357.669	304.906	179.395	31.352	−42.387	0.651
3500	61.595	359.454	306.439	185.553	31.112	−44.552	0.665
3600	61.635	361.190	307.936	191.714	30.878	−46.711	0.678
3700	61.672	362.879	309.398	197.880	30.652	−48.863	0.690
3800	61.707	364.524	310.827	204.049	30.432	−51.009	0.701
3900	61.739	366.128	312.225	210.221	30.218	−53.149	0.712
4000	61.769	367.691	313.592	216.396	30.012	−55.284	0.722
4100	61.796	369.217	314.930	222.575	29.812	−57.414	0.731
4200	61.822	370.706	316.241	228.756	29.618	−59.539	0.740
4300	61.846	372.161	317.524	234.939	29.430	−61.660	0.749
4400	61.869	373.583	318.782	241.125	29.248	−63.776	0.757
4500	61.890	374.974	320.015	247.313	29.072	−65.888	0.765
4600	61.909	376.334	321.225	253.503	28.901	−67.997	0.772
4700	61.928	377.666	322.412	259.695	28.735	−70.101	0.779
4800	61.945	378.970	323.577	265.888	28.572	−72.203	0.786
4900	61.962	380.247	324.720	272.084	28.414	−74.300	0.792
5000	61.977	381.499	325.843	278.281	28.259	−76.395	0.798
5100	61.992	382.727	326.947	284.479	28.108	−78.487	0.804
5200	62.005	383.931	328.031	290.679	27.959	−80.575	0.809
5300	62.018	385.112	329.097	296.880	27.812	−82.661	0.815
5400	62.031	386.271	330.145	303.083	27.667	−84.744	0.820
5500	62.042	387.410	331.176	309.286	27.523	−86.824	0.825
5600	62.053	388.528	332.190	315.491	27.380	−88.902	0.829
5700	62.064	389.626	333.188	321.697	27.238	−90.978	0.834
5800	62.074	390.706	334.170	327.904	27.095	−93.050	0.838
5900	62.083	391.767	335.138	334.112	26.952	−95.120	0.842
6000	62.092	392.810	336.090	340.320	26.808	−97.188	0.846

PREVIOUS June 1969 (1 atm) CURRENT. June 1969 (1 bar)

Carbonyl Fluoride (COF) IDEAL GAS $M_r = 47.008803$ Carbonyl Fluoride (COF) $C_1F_1O_1(g)$

$S°(298.15\ K) = [248.48]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = [-172.1 \pm 63]\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = [-171.5 \pm 63]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
1018(1)
626(1)
1855(1)

Ground State Quantum Weight: 2 $\sigma = 1$
Point Group: C_s
Bond Distances: C–F = [1.34] Å, C–O = [1.18] Å
Bond Angle: F–C–O = [135]°
Product of the Moments of Inertia: $I_AI_BI_C = [2.199751\text{–}10^{-116}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The enthalpy change $\Delta_rH°$ for the reaction $COF_2(g) = CO + 2F(g)$ was calculated as 160 5 kcal mol^{-1}. By analogy with $\Delta_{at}H°$(Cl–COCl, 0 K), $\Delta_{at}H°$(Cl–CO, 0 K), the value of $\Delta_{at}H°$(F–COF, 0 K), $\Delta_{at}H°$(F–CO, 0 K) was taken to be 4. Based on $\Delta_rH° = 160.5-(4/5) = 128.4$ kcal·mol^{-1} for the reaction $COF_2(g) = COF(g) + F(g)$, the enthalpy of formation of COF(g) was derived as -41 ± 15 kcal·mol^{-1}.

Heat Capacity and Entropy

The vibrational frequencies were reported by Milligan *et al* [1] The bond distances and bond angle were estimated by comparison with those for HFCO(g). Due to the presence of one unpaired electron on C atom, the ground state quantum weight is calculated to be 2. The principal moments of inertia are: $I_A = 0.3399 \times 10^{-39}$, $I_B = 7.8768 \times 10^{-39}$, and $I_C = 8.2167 \times 10^{-39}\ g{\cdot}cm^2$.

References

[1] D. E. Milligan, M. E. Jacox, M. A. Bass, J. J. Comeford and D. E. Mann, J. Chem. Phys. 42, 3187 (1965).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−10.393	−172.132	−172 132	INFINITE
100	33.341	210.080	280 740	−7.066	−171.770	−175.499	91.671
200	35.464	233.679	251.926	−3.649	−171.600	−179.306	46.830
250	37.207	241.777	249.110	−1.833	−171.560	−181.237	37.867
298.15	38.930	248 479	248.479	0.	−171.544	−183.103	32.079
300	38.995	248.720	248.479	0.072	−171.544	−183.175	31.894
350	40.702	254.860	248.960	2.065	−171.555	−185.113	27.627
400	42.284	260.400	250.050	4.140	−171.594	−187.048	24.426
450	43.733	265.465	251.485	6.291	−171.663	−188.975	21.936
500	45.051	270.142	253.120	8.511	−171.762	−190.894	19.943
600	47.318	278.564	256.674	13.134	−172.034	−194.696	16.950
700	49.151	286.001	260.343	17.960	−172.383	−198.447	14.808
800	50.621	292.663	263 974	22.952	−172.786	−202.143	13.199
900	51.799	298 696	267.502	28.075	−173.227	−205 787	11.944
1000	52.747	304.205	270.901	33.304	−173.697	−209.380	10.937
1100	53.514	309.269	274.162	38.618	−174.191	−212.924	10.111
1200	54.140	313.953	277.285	44.002	−174.706	−216.423	9.421
1300	54.655	318.308	280.275	49.443	−175.241	−219.877	8.835
1400	55.082	322.374	283.138	54.930	−175.795	−223.290	8.331
1500	55.440	326.187	285.883	60.457	−176.368	−226.663	7.893
1600	55.741	329.775	288.515	66.016	−176.962	−229.997	7.509
1700	55 997	333.162	291.042	71.603	−177.575	−233.293	7.168
1800	56.216	336.369	293.472	77.214	−178.209	−236.552	6.865
1900	56 405	339.414	295.811	82.846	−178.862	−239.776	6.592
2000	56.569	342.311	298.064	88.495	−179.535	−242.964	6.346
2100	56.711	345.075	300.237	94.159	−180.226	−246.119	6.122
2200	56 836	347.716	302.336	99.836	−180.934	−249.240	5 918
2300	56.947	350.245	304.364	105.526	−181.657	−252.329	5.731
2400	57 044	352.671	306.327	111.225	−182.396	−255.386	5.558
2500	57 131	355 001	308.228	116.934	−183.147	−258.412	5.399
2600	57 209	357.243	310.070	122.651	−183.909	−261.407	5.252
2700	57 278	359.404	311.857	128.375	−184 680	−264.373	5 115
2800	57.341	361 488	313.593	134 106	−185.460	−267.310	4.987
2900	57.397	363.501	315.279	139.843	−186.246	−270.220	4.867
3000	57 448	365.448	316.919	145.586	−187.038	−273.102	4.755
3100	57 495	367.332	318.515	151.333	−187.833	−275.958	4.650
3200	57.537	369 158	320.070	157.084	−188.631	−278.788	4.551
3300	57.576	370.930	321.584	162.840	−189.432	−281.593	4.457
3400	57.611	372.649	323.061	168.599	−190.233	−284.374	4.369
3500	57.643	374.319	324.502	174.362	−191.035	−287.131	4.285
3600	57.673	375.944	325.908	180.128	−191.836	−289 865	4.206
3700	57.701	377.524	327.282	185.897	−192.637	−292.577	4.130
3800	57.726	379 063	328.624	191 668	−193.436	−295.267	4.059
3900	57.750	380.563	329.937	197 442	−194.235	−297 936	3.990
4000	57.772	382.026	331.221	203.218	−195.032	−300.586	3.925
4100	57.792	383.452	332.478	208.996	−195.828	−303.215	3.863
4200	57.811	384.845	333 708	214.776	−196.623	−305 824	3.803
4300	57.829	386.206	334 913	220.558	−197.416	−308.415	3 746
4400	57.845	387.535	336.094	226.342	−198.209	−310 987	3.692
4500	57.861	388.835	337.252	232.127	−199.001	−313.541	3.639
4600	57.875	390.107	338.387	237.914	−199.792	−316.078	3.589
4700	57 889	391.352	339.501	243.702	−200.584	−318.597	3.541
4800	57 901	392.571	340.594	249.492	−201.377	−321.100	3 494
4900	57 913	393.765	341.667	255.283	−202.170	−323.586	3.449
5000	57 925	394.935	342.720	261.075	−202 966	−326.056	3.406
5100	57.935	396.082	343.755	266.868	−203.764	−328.509	3.365
5200	57 945	397.207	344.773	272.662	−204.565	−330.948	3.324
5300	57.955	398.311	345.772	278.457	−205.370	−333.370	3.286
5400	57.964	399.395	346.755	284.253	−206.179	−335.778	3.248
5500	57.972	400.458	347.722	290.049	−206.993	−338 171	3.212
5600	57.980	401.503	348.673	295.847	−207.814	−340.548	3.176
5700	57.988	402.529	349.609	301.645	−208.642	−342.911	3.142
5800	57.995	403.538	350.530	307.445	−209.477	−345.259	3.109
5900	58.002	404.529	351 437	313.244	−210.321	−347.594	3.077
6000	58.008	405.504	352.330	319.045	−211.175	−349.913	3.046

PREVIOUS December 1965 (1 atm) CURRENT. December 1965 (1 bar)

Difluoromethylene (CF$_2$) IDEAL GAS $M_r = 50.007806$ Difluoromethylene (CF$_2$) C$_1$F$_2$(g)

$S°(298.15\ K) = 240.833 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -182.48 \pm 6.3\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -182.00 \pm 6.3\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
X^{1}A$_1$	0	1
a^{3}B$_1$	[16000]	3
A^{1}B$_1$	37226	1

Vibrational Frequencies and Degeneracies

ν_1, cm^{-1}	ν_2, cm^{-1}	ν_3, cm^{-1}
1222 (1)	665 (1)	1110 (1)

Point Group: C$_{2v}$ $\sigma = 2$
Bond Distance C–F = 1.300 Å
Bond Angle F–C–F = 104.9°
Product of the Moments of Inertia: $I_AI_BI_C = 4.88015 \times 10^{-116}\ g^3{\cdot}cm^6$

Enthalpy of Formation

Thrush and Zwolenik[1] reported a predissociation limit for $CF_2 \rightarrow CF + F$, however, Marsigny *et al.*[2] have since observed in emission the assumed predissociated level, and others above it, which invalidates the reported limit.

Walter *et al.*[3] have obtained the photoionization threshold at 0 K for onset of the reaction $C_2F_4 + e^- \rightarrow CF_2^+ + CF_2 + 2\bar{e}$, as 14.63 ± 0.04 eV (337.37 kcal·mol^{-1}). The ionization potential of CF$_2$ has been reported as 11.7 eV,[4] 11.8 ± 0.3 eV[5] and 11.86 ± 0.1 eV.[6] Since these values were obtained by electron impact methods, there may be excess energy involved. Thus, adopting the lowest value as 11.7 ± 0.2 eV, we obtain $\Delta_fH°(CF_2, g, 298.15\ K) = -44.4 \pm 2.5$ kcal mol^{-1}.[7] All previous electron impact methods are considered superseded by this photoionization result.

Modica and LaGraff[8] determined equilibrium constants for the reaction (A) $C_2F_4 \rightarrow 2CF_2$ by use of a shock tube to achieve high temperatures and ultra violet absorption to detect the CF$_2$ concentration. Carlson[9] has studied the same reaction using a similar technique, and also Zmbov *et al*[5] have investigated this equilibrium in a mass spectrometer. A 2nd and 3rd law analysis of all three sets of data is given below along with our recalculated equilibrium data of Farber *et al.*[10] for the reaction (B) $C + 2F \rightarrow CF_2$ from weight loss experiments in the system C + CF$_4$.

Kinetic methods were used by Edwards and Small[11] to study the equilibrium (C) $CHF_2Cl(g) \rightleftarrows CF_2(g) + HCl(g)$. They analysed their data by assuming that the only other equilibrium occurring was $2CF_2(g) \rightleftarrows C_2F_4(g)$, and fit their kinetic data by trial and error. In this manner they obtained activation energies of the forward and back reaction (C) of 55.79 ± 0.49 and 6.21 ± 3.0 kcal mol^{-1}, thus $\Delta E_a = 49.6 \pm 3.0$ and $\Delta H(900\ K) = 51.4 \pm 3$ kcal·mol^{-1}, which yields $\Delta_fH(CF_2, 298.15\ K) = -42 \pm 4$ kcal·mol^{-1}.[7] They also obtained the activation energy of reaction (A) as 70.36 ± 1.3 kcal·mol^{-1}. Dalby[12] has reported the activation energy of the reverse of (A) as 1.2 ± 0.2 kcal·mol^{-1}, thus, $\Delta E_a = 69.2 \pm 1.3$ and $\Delta H(900\ K) = 71.0 \pm 1.3$ kcal·mol^{-1}, which yields $\Delta_fH(CF_2, 298.15\ K) = -42.6 \pm 1.0$ kcal·mol^{-1}.[7] Gozzo and Patrick[13] also investigated the kinetics of reaction C and obtained activation energies of 51.4 ± 2.5 and 14.4 ± 5 kcal·mol^{-1}, the latter value being corrected for the activation energy of CF$_2$ recombination.[12] Thus, we obtain $\Delta E_a = 37 \pm 7$ and $\Delta H(1000\ K) = 39 \pm 7$ kcal·mol^{-1}, which yields $\Delta_fH°(CF_2, 298.15\ K) = -54 \pm 9$ kcal mol^{-1}.[7]

Modica and LaGraff[14] investigated the kinetics of CHF$_3$ decomposition by a mass spectrometer coupled to a shock tube. They investigated the pressure dependence of the rate and concluded that at the hgh pressure limit $E_o = 58.4 \pm 2.2$ kcal·mol^{-1}. Taking this value as $\Delta H°(0\ K)$ for the reaction (D) $CHF_3(g) \rightarrow CF_2(g) + HF(g)$, we obtain $\Delta_fH°(CF_2, 298.15\ K) = -41.3 \pm 2.5$ kcal·mol^{-1}.[7] However, any activation energy of the reverse reaction (D) will make this value more negative. Since values of the reverse activation energy of analogous reaction (C) range from 6.2 to 14.4 kcal·mol^{-1}, it appears likely that reverse reaction (D) will have a significant activation enrgy; thus, $\Delta_fH(CF_2, 298.15\ K) < -41.3 \pm 2.5$ kcal·mol^{-1}. Tschiukow–Roux[15] has investigated the same reaction in a shock tube, but was unable to obtain sufficient variation of rate with pressure to calculate the high pressure limit.

Reference and Reaction		Points	T/R	Δ_rH(298.15 K) kcal·mol^{-1} 2nd law	3rd law	Drift eV	**Δ_fH(CF$_2$, g, 298.15 K) kcal·mol^{-1}
[8]	A	20*	1165-1620	70.89 ± 2.7	66.68 ± 2.28	−2.4 ± 2.1	−45.4 ± 2.0
[9]	A	35*	1240–1742	67.92 ± 0.7	68.40 ± 0.72	0.3 ± 0.5	−44.5 ± 0.7
[5]	A	11	1127–1244	77.3 ± 2.1	75.13 ± 0.5	−1.8 ± 1.8	−41.15 ± 1.5
[10]	B	8	2023–2474	−73.8 ± 1.4	−80.04 ± 1.0	−2.8 ± 0.6	−42.3 ± 1.0

*Points ommitted due to failure of a statistical test **Calculated from the 3rd law heat of reaction.

A median value of Δ_fH(CF$_2$, g, 298.15 K) covering the area of maximum probability is adopted as −43.5 ± 1.5 kcal·mol^{-1}.

Continued on page 700

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_fH°$ (kJ·mol^{-1})	$\Delta_fG°$ (kJ·mol^{-1})	log K$_f$
0	0.	0.	INFINITE	−10.354	−182.482	−182.482	INFINITE
100	33.311	202.633	272.908	−7.028	−182.122	−185.253	96.766
200	35.154	226.123	244.265	−3.628	−181.979	−188.456	49.220
250	36.964	234.154	241.463	−1.827	−181.975	−190.077	39.714
298.15	38.948	240.833	240.833	0.	−182.004	−191.635	33.574
300	39.026	241.074	240.834	0.072	−182.006	−191.695	33.377
350	41 119	247.248	241.316	2.076	−182.061	−193.306	28.849
400	43.097	252.869	242.414	4.182	−182.138	−194.907	25.452
450	44.887	258.051	243.867	6.383	−182.232	−196.498	22.809
500	46.465	262.864	245.529	8.667	−182.345	−198.077	20.693
600	49.020	271.573	249.160	13.448	−182.616	−201.199	17.516
700	50.913	279.279	252.923	18.449	−182.939	−204.271	15.243
800	52.319	286.173	256.656	23.614	−183.305	−207.294	13.535
900	53.376	292.400	260.287	28.901	−183.706	−210.269	12.204
1000	54 184	298.067	263.786	34.281	−184.139	−213.197	11.136
1100	54.812	303.262	267.142	39.732	−184.602	−216.081	10.261
1200	55.308	308.053	270.354	45.239	−185.092	−218.921	9.529
1300	55.705	312.497	273.427	50.791	−185.609	−221.719	8.909
1400	56.028	316.637	276.367	56.378	−186.152	−224.477	8.375
1500	56.293	320.512	279.182	61.994	−186.721	−227.195	7.912
1600	56.515	324.152	281.880	67.635	−187.314	−229.874	7.505
1700	56.702	327.584	284.469	73.296	−187.930	−232.515	7.144
1800	56.864	330.830	286.955	78.975	−188.568	−235.119	6.823
1900	57.006	333.908	289.346	84.668	−189.225	−237.688	6.534
2000	57 134	336.836	291.648	90.375	−189.899	−240.221	6.274
2100	57.252	339.626	293.867	96.095	−190.585	−242.721	6.037
2200	57.365	342.292	296.008	101.825	−191.280	−245.187	5.821
2300	57.475	344.844	298.076	107.567	−191.980	−247.621	5.624
2400	57.586	347.293	300.076	113.321	−192.680	−250.026	5.442
2500	57 700	349.646	302.012	119.085	−193.376	−252.401	5.274
2600	57.820	351.911	303.888	124.861	−194.062	−254.748	5.118
2700	57 947	354.096	305.707	130.649	−194 734	−257.069	4.973
2800	58 083	356.206	307.473	136.451	−195.388	−259.366	4.839
2900	58.229	358.246	309.189	142.266	−196.020	−261.640	4.713
3000	58.384	360.223	310.858	148.097	−196.625	−263.892	4.595
3100	58.551	362.140	312.481	153.943	−197.201	−266.125	4 484
3200	58.728	364.002	314.062	159.807	−197.743	−268.339	4.380
3300	58.916	365.812	315.603	165.689	−198.249	−270.538	4.282
3400	59 115	367.574	317.106	171.591	−198.716	−272.721	4.190
3500	59.323	369.290	318.572	177.513	−199.143	−274.891	4.103
3600	59.541	370.964	320.004	183.456	−199.527	−277.050	4.020
3700	59 768	372.599	321.404	189.421	−199.866	−279.199	3.942
3800	60.002	374.196	322.772	195.410	−200.160	−281.339	3.867
3900	60.242	375.758	324.111	201.422	−200.407	−283.472	3.797
4000	60 488	377.286	325.421	207.458	−200.607	−285.599	3.730
4100	60.739	378.783	326.705	213.520	−200.760	−287.722	3.666
4200	60.993	380.249	327.962	219.606	−200.865	−289.841	3.605
4300	61.250	381.687	329.195	225.718	−200.922	−291.959	3.547
4400	61.508	383.098	330.404	231.856	−200.932	−294.076	3.491
4500	61.766	384.484	331.590	238.020	−200.895	−296.193	3.438
4600	62.024	385.844	332.755	244.209	−200.811	−298.312	3.387
4700	62.280	387.181	333.899	250.425	−200.682	−300.433	3.339
4800	62.533	388.495	335.023	256.665	−200.508	−302.557	3.292
4900	62.783	389.786	336.127	262.931	−200.290	−304.685	3.248
5000	63.029	391.057	337.213	269.222	−200.029	−306.818	3.205
5100	63.270	392.308	338.281	275.537	−199.727	−308.957	3.164
5200	63.506	393.539	339.332	281.875	−199.385	−311.102	3.125
5300	63.735	394.751	340.366	288.238	−199.003	−313.254	3.087
5400	63.958	395.944	341.384	294.622	−198.584	−315.413	3.051
5500	64.174	397.120	342.387	301.029	−198.129	−317.581	3.016
5600	64.383	398.278	343.375	307.457	−197.639	−319.757	2.983
5700	64.584	399.419	344.348	313.905	−197.116	−321.943	2.950
5800	64.776	400.544	345.307	320.373	−196.561	−324.138	2.919
5900	64 961	401.653	346.253	326.860	−195.976	−326.342	2.889
6000	65.137	402.746	347.185	333.365	−195.361	−328.557	2.860

PREVIOUS June 1970 (1 atm) CURRENT June 1970 (1 bar)

Difluoromethylene, Ion (CF$_2^+$) IDEAL GAS M_r = 50.007257 Difluoromethylene, Ion (CF$_2^+$) C$_1$F$_2^+$(g)

$S°(298.15\ K) = [246.77 \pm 2.1]\ J\cdot K^{-1}\cdot mol^{-1}$

$\Delta_f H°(0\ K) = 935.12 \pm 12.6\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 941.79 \pm 12.6\ kJ\cdot mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^2A_1$	0	2
$^2B_1$	[15000]	2

Vibrational Frequencies and Degeneracies
ν, cm^{-1}

[1100] (1)
[650] (1)
[1400] (1)

Point Group: C_{2v}
Bond Distance: C–F = [1.32] Å
Bond Angle: F–C–F = [116 ± 10°]
Product of the Moments of inertia: $I_A I_B I_C = [5.07002 \times 10^{-116}]\ g^3\cdot cm^6$

Enthalpy of Formation

The ionization potential has been reported as 11.7 eV,[1] 11.8 eV,[2, 3] and 11.86 eV[4] from electron impact measurements. Since there may be excess energy involved we prefer the lowest value, 11.7 ± 0.2 eV. This leads to $\Delta_f H°(CF^+, g, 0\ K) = 226.2 \pm 6\ kcal\cdot mol^{-1}$ using the JANAF $\Delta_f H°(CF_2, g, 0\ K) = -43.61 \pm 1.5\ kcal\cdot mol^{-1}$.[5]

A more precise value is available from the photoionization measurements of Walter *et al.*,[6] who measured the photoionization threshold the process for:

$$C_2F_4 + h\nu \rightarrow CF_2^+ + CF_2 + e^- \qquad \Delta H°(0\ K) = 337.4 \pm 0.9\ kcal\cdot mol^{-1}$$

Employing JANAF auxiliary enthalpies[5] we obtain $\Delta_f H°(CF_2^+, g, 0\ K) = 223.5 \pm 3.0\ kcal\cdot mol^{-1}$ which is adopted.

Heat Capacity and Entropy

The configuration of CF$_2^+$ is predicted to be bent by Walsh,[7] since it has 17 electrons, thus, its ground state is $^2A_1$, a low lying electronic state is predicted by analogy with NO$_2$.[8] We estimate the angle to be 116 ± 10°, which is larger than CF$_2$ at 105°, this is expected from the Walsh correlations,[7] but smaller than isoelectronic CO$_2^-$ at 127° and NO$_2$ at 134°. The vibrational frequencies were estimated by comparison with those for CF$_2$, CO$_2^-$ and COF[7] as 1100 ± 150 cm^{-1}, 650 ± 50 cm^{-1} and 1400 ± 200 cm^{-1}.

The principal moments of interia are: $I_A = 0.7415 \times 10^{-39}$, $I_B = 7\ 9066 \times 10^{-39}$, and $I_C = 8.6481 \times 10^{-39}\ g\cdot cm^2$.

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[5] JANAF Thermochemical Tables: CF$_2$(g), 6–30–70; C$_2$F$_4$(g), 6–30–69; CO2$^-$(g), 12–31–66; COF(g), 12–31–65.
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Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.354	935.118		
100	33.321	208.556	278.829	−7.027			
200	35.209	232.075	250.193	−3.624			
250	36.922	240.111	247.397	−1.822			
298.15	38.754	246.769	246.769	0.	941.793	924.137	−161.905
300	38.826	247.009	246.770	0.072	941.830	924.028	−160.888
350	40.758	253.140	247.250	2.062	942.799	920.984	−137.449
400	42.608	258.704	248.339	4.146	943.741	917.803	−119.853
450	44.312	263.823	249 779	6.320	944.658	914.505	−106.153
500	45.841	268.572	251.423	8.574	945.555	911.106	−95.183
600	48.379	277.165	255.013	13.291	947.299	904.052	−78.705
700	50.311	284.774	258.731	18.230	948.992	896.710	−66.913
800	51.776	291.592	262.420	23.338	950.648	889.127	−58.054
900	52.895	297.758	266.010	28.574	952.274	881.339	−51.152
1000	53.761	303.378	269.470	33.908	953.874	873.372	−45.620
1100	54.440	308.535	272.790	39.320	955.450	865.245	−41.087
1200	54.980	313.296	275.970	44.792	957.003	856.976	−37.303
1300	55.415	317.715	279.013	50.312	958.534	848.578	−34.096
1400	55.770	321.835	281.926	55.872	960.043	840.063	−31.343
1500	56.063	325.693	284.717	61.464	961.528	831.441	−28.953
1600	56.308	329.319	287.392	67.083	962.992	822.721	−26.859
1700	56.515	332.739	289.960	72.724	964.435	813.910	−25.008
1800	56.692	335.974	292.427	78.385	965.857	805.014	−23.361
1900	56.846	339.044	294.801	84.062	967.262	796.040	−21.885
2000	56.982	341.963	297.086	89.754	968.652	786.993	−20.554
2100	57.103	344.746	299.290	95.458	970.029	777.876	−19.349
2200	57.214	347.405	301.417	101.174	971.397	768.693	−18.251
2300	57.317	349.951	303.472	106.901	972.761	759.449	−17.248
2400	57.414	352.392	305.460	112.637	974.123	750.145	−16.326
2500	57.507	354.738	307.385	118.383	975.488	740.785	−15.478
2600	57.598	356.995	309.250	124.138	976.859	731.370	−14.693
2700	57.688	359.171	311.059	129.903	978.242	721.902	−13.966
2800	57.778	361.270	312.815	135.676	979.638	712.382	−13.290
2900	57.869	363.299	314.521	141.458	981.052	702.813	−12.659
3000	57.961	365.263	316.180	147.250	982.486	693.194	−12.070
3100	58.054	367.165	317.794	153.051	983.943	683.526	−11.517
3200	58.150	369.010	319.366	158.861	985.426	673.812	−10.999
3300	58.247	370.800	320.897	164.681	986.936	664.051	−10.511
3400	58.346	372.541	322.391	170.510	988.476	654.243	−10.051
3500	58.446	374.233	323.848	176.350	990.045	644.390	−9.617
3600	58.549	375.881	325.270	182.200	991.647	634.492	−9.206
3700	58.653	377.487	326.660	188.060	993.281	624.549	−8.817
3800	58.758	379.053	328.018	193.930	994.948	614.560	−8.448
3900	58.864	380.580	329.346	199.811	996.648	604.528	−8.097
4000	58.970	382.072	330.646	205.703	998.381	594.452	−7.763
4100	59.077	383.529	331.918	211.605	1000.148	584.332	−7.444
4200	59.184	384.954	333.164	217.518	1001.949	574.168	−7.141
4300	59.291	386.348	334.385	223.442	1003.782	563.961	−6.851
4400	59.397	387.712	335.581	229.377	1005.647	553.711	−6.573
4500	59.503	389.048	336.755	235.322	1007.544	543.419	−6.308
4600	59.607	390.357	337.906	241.277	1009.472	533.084	−6.053
4700	59.710	391.640	339.035	247.243	1011.431	522.707	−5.809
4800	59.812	392.898	340.144	253.219	1013.419	512.287	−5.575
4900	59.912	394.133	341.234	259.205	1015.436	501.826	−5.350
5000	60.010	395.344	342.304	265.201	1017.481	491.324	−5.133
5100	60.105	396.533	343.356	271.207	1019.552	480.780	−4.924
5200	60.199	397.702	344.389	277.223	1021.650	470.196	−4.723
5300	60.290	398.849	345.406	283.247	1023.772	459.570	−4.529
5400	60.378	399.977	346.406	289.280	1025.918	448.905	−4.342
5500	60.464	401.086	347.391	295.323	1028.088	438.199	−4.162
5600	60.547	402.176	348.359	301.373	1030.279	427.455	−3.987
5700	60.628	403.248	349.313	307.432	1032.491	416.670	−3.818
5800	60.705	404.303	350.252	313.499	1034.723	405.846	−3.655
5900	60.780	405.342	351.177	319.573	1036.975	394.985	−3.497
6000	60.851	406.364	352.088	325.655	1039.244	384.084	−3.344

PREVIOUS: December 1970 (1 atm) — CURRENT: December 1970 (1 bar)

Carbonic Difluoride (COF_2) IDEAL GAS $M_r = 66.007206$ Carbonic Difluoride (COF_2) $C_1F_2O_1(g)$

$S°(298.15\ K) = 258.887 \pm 0.08\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -635.8 \pm 1.71\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -638.9 \pm 1.7\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}
965 (1)	1249 (1)
1928 (1)	584 (1)
626 (1)	774 (1)

Ground State Quantum Weight. 1 $\sigma = 2$
Point Group: C_{2v}
Bond Distances: C–F = 1.312 Å; C–O = 1.174 Å
Bond Angles: F–C–F = 108°; F–C–O = 126° 1'
Product of the Moments of Inertia. $I_AI_BI_C = 7.225667 \times 10^{-115}\ g^3{\cdot}cm^6$

Enthalpy Reference Temperature = T_r = 298.15 K				Standard State Pressure = $p°$ = 0.1 MPa			
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−11.119	−635.798	−635.798	INFINITE
100	33.489	217.322	295.224	−7.790	−636.888	−632.823	330.553
200	38.897	241 797	262.939	−4.228	−638.038	−628.302	164.096
250	43.168	250.931	259.642	−2.178	−638.514	−625.811	130 756
298.15	47.255	258.887	258.887	0.	−638.897	−623.329	109.205
300	47 407	259.180	258.888	0.088	−638.910	−623.232	108.514
350	51.305	266.786	259.480	2.557	−639.239	−620.592	92.618
400	54.778	273.868	260.841	5.211	−639.514	−617.909	80 691
450	57.831	280.500	262.661	8.028	−639.751	−615.194	71.410
500	60.502	286.735	264 759	10.988	−639.959	−612.454	63.983
600	64.875	298.170	269.393	17.266	−640.312	−606.918	52.837
700	68.225	308.434	274.250	23.929	−640.602	−601.329	44.872
800	70.811	317.720	279.112	30.886	−640.843	−595.701	38.895
900	72.827	326.181	283.879	38.072	−641.049	−590.046	34.245
1000	74.417	333.940	288.503	45.437	−641.228	−584.369	30.524
1100	75.686	341.094	292.963	52.945	−641.388	−578.676	27 479
1200	76 709	347.725	297.253	60.566	−641.538	−572.968	24.941
1300	77.544	353.899	301.376	68.280	−641.684	−567.247	22.792
1400	78.231	359.672	305.336	76.070	−641.831	−561.516	20.950
1500	78.804	365.089	309.141	83.923	−641.984	−555.774	19.354
1600	79 284	370.191	312.799	91.828	−642.147	−550.021	17.956
1700	79.691	375.010	316.318	99 777	−642.321	−544.258	16.723
1800	80.038	379.575	319.706	107.764	−642.508	−538.485	15.626
1900	80.337	383.911	322.973	115.783	−642.710	−532.700	14 645
2000	80.595	388.038	326.123	123.830	−642.925	−526.905	13.761
2100	80.820	391 976	329.166	131.901	−643.152	−521.098	12.962
2200	81.016	395.741	332.107	139.993	−643.390	−515.280	12.234
2300	81.189	399.346	334.953	148.103	−643.637	−509.452	11.570
2400	81.342	402.804	337.709	156.230	−643.890	−503.612	10.961
2500	81.478	406.128	340.379	164.371	−644.146	−497.762	10.400
2600	81.600	409.326	342.970	172.525	−644.402	−491.902	9.882
2700	81.708	412.408	345.485	180.691	−644.656	−486.031	9.403
2800	81.806	415.381	347.929	188.867	−644.904	−480.152	8.957
2900	81.894	418.253	350.304	197.052	−645.145	−474.264	8.542
3000	81.974	421.031	352.616	205.245	−645.376	−468.367	8.155
3100	82.046	423.720	354.866	213.446	−645.595	−462.463	7.792
3200	82.112	426.326	357.059	221.654	−645.800	−456.553	7 452
3300	82.173	428.854	359.196	229.869	−645.989	−450.636	7.133
3400	82.228	431.308	361.281	238.089	−646.162	−444.713	6.832
3500	82.278	433.692	363.316	246.314	−646.317	−438.786	6.549
3600	82.325	436.010	365.304	254.544	−646.453	−432.854	6.281
3700	82.368	438.267	367.245	262.779	−646.570	−426.920	6.027
3800	82.408	440 464	369.143	271.018	−646.668	−420.982	5.787
3900	82.444	442.605	371.000	279.260	−646.746	−415.041	5.559
4000	82.478	444.693	372.816	287.506	−646.804	−409.099	5.342
4100	82.510	446.730	374.594	295.756	−646.843	−403.156	5.136
4200	82.539	448.718	376.335	304.008	−646.863	−397.212	4 940
4300	82.567	450.661	378.041	312.264	−646.864	−391.268	4.753
4400	82.592	452.559	379.713	320.522	−646.846	−385.325	4.574
4500	82.616	454 415	381.353	328.782	−646.811	−379.381	4.404
4600	82.639	456.232	382.961	337.045	−646.760	−373.439	4.241
4700	82.660	458.009	384.539	345.310	−646.692	−367.498	4 084
4800	82.680	459.750	386.088	353.577	−646.609	−361.558	3.935
4900	82.698	461.455	387.608	361.846	−646.512	−355.621	3.791
5000	82.716	463.125	389.102	370.116	−646.402	−349.685	3.653
5100	82.732	464.764	390.570	378.389	−646.279	−343.752	3.521
5200	82.748	466.370	392.012	386.663	−646.146	−337.821	3.393
5300	82.762	467.947	393.430	394.938	−646.003	−331.893	3.271
5400	82.776	469.494	394.824	403.215	−645.851	−325.968	3.153
5500	82.789	471.013	396.196	411.493	−645.691	−320.047	3.040
5600	82.802	472.505	397.545	419.773	−645.525	−314.126	2.930
5700	82.814	473.970	398.873	428.054	−645.354	−308.211	2.824
5800	82.825	475.411	400.180	436.336	−645.179	−302.297	2.722
5900	82.836	476.827	401.467	444 619	−645.001	−296.387	2.624
6000	82.846	478.219	402.735	452.903	−644.822	−290.480	2.529

PREVIOUS December 1969 (1 atm) CURRENT. December 1969 (1 bar)

Enthalpy of Formation

Ruff and Li[1] measured equilibrium constants for the reaction

$$2COF_2(g) \rightleftarrows CO\ ({}_2g) + CF\ ({}_4g)$$

in the temperature range 573–1273 K. These equilibrium data were recently analyzed by Stull *et al.*[2] Their 3rd law analysis of the data clearly indicates that the three low temperature points are in error and should not be used in calculating Δ_fH(298.15 K). They reported Δ_fH(298.15 K) = −12 ± 3 kcal·mol^{-1} based upon an average of the five high temperature points. Combining this result with the enthalpy of formation of carbon dioxide and carbon tetrafluoride,[3] we derive,

$$\Delta_fH°(COF_2,\ g,\ 298.15\ K) = -152.5 \pm 3.3\ kcal{\cdot}mol^{-1}.$$

Wartenberg and Riteris[4] measured the enthalpy of hydrolysis of CF_2O. They reported $\Delta_rH = -26.7 \pm 0.2\ kcal{\cdot}mol^{-1}$ for the reaction

$$COF_2(g) + H_2O(l) \rightarrow CO_2(g) + 2HF{\cdot}300\ H_2O.$$

Combining this result with enthaply of formation data for carbon dioxide and HF($\Delta_fH°$(HF·300 H_2O, 298.15 K) = −76.84 kcal·mol^{-1}),[5] we derive

$$\Delta_fH°(COF_2,\ g,\ 298.15\ K) = -152.7 \pm 0.4\ kcal{\cdot}mol^{-1}.$$

Armstrong *et al.*[6] measured the enthalpies of combustion of CH_4 in O_2–F_2 mixtures and found $\Delta_fH°$(COF_2, g, 298.15 K) = −154.8 kcal·mol^{-1}. The value calculated from Wartenberg's data[4] is adopted here.

Heat Capacity nd Entropy

The vibrational frequencies are from the infrared studies of Hopper *et al.*[7] and are in good agreement with the results of Lovell *et al.*[8] and Nielsen *et al.*[9] The molecular constants are from the microwave studies of Laurie *et al.*[10] and are in reasonable agreement with the electron-diffraction work of Brown and Livingston.[11] The principal moments of inertia are: $I_A = 7.1086 \times 10^{-39}$, $I_B = 7.1359 \times 10^{-39}$, and $I_C = 14.2445 \times 10^{-39}\ g{\cdot}cm^2$.

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Carbonic Difluoride (COF_2) $C_1F_2O_1(g)$

Trifluoromethyl (CF_3) IDEAL GAS M_r = 69.006209 Trifluoromethyl (CF_3) $C_1F_3(g)$

$S°(298.15\ K) = 265.082 \pm 4.2\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -467.52 \pm 4.2\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -470.28 \pm 4.2\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}
1090 (1)	1259 (2)
701 (1)	[500] (2)

Ground State Quantum Weight: 2 $\sigma = 3$
Point Group: C_{3v}
Bond Distance: C–F = [1.33] Å
Bond Angle F–C–F = [112]°
Product of the Moments of Inertia: $I_AI_BI_C = [9.610547 \times 10^{-115}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The selected value is obtained from least squares, simultaneous adjustment of the enthalpies of formation of CF_3, CF_3X (X = H, Cl, Br, I, CF_3) and C_2F_4. Details of the input data and the adjustment are given by Syverud [1] Kinetic data provide the most consistent paths to $\Delta_fH°$ of $CF_3(g)$. Forward and reverse activation energies for the reactions $CHF_3(g) + X(g) \rightarrow CF_3(g) + HX(g)$ have been reported for X = Cl by Coomber and Whittle,[2] for X + Br by Amphlett and Whittle,[3] and for X = I by Goy *et al.*[4] Increases of about 0.3 $kcal{\cdot}mol^{-1}$ in the reverse activation energies for X = Cl and Br were proposed by Arthur and Gray[5] on the basis of additional data. Combining these values and reducing to 298.15 K, we get $\Delta_rH° = 2.93 \pm 0.7$ (X = Cl), 18.89 ± 0.7 (X = Br), and $35.5 \pm 3\ kcal{\cdot}mol^{-1}$ (X = I). Coomber and Whittle[2] reviewed data for the analogous reactions with X = CH_3 and CD_3; these yield $\Delta_rH° = 0.6 \pm 2\ kcal{\cdot}mol^{-1}$ at 298 15 K for X = CH_3. Activation energies have also been reported[6] for $CF_3I(g) + I(g) \rightarrow CF_3I(g) + I_2(g)$ from which we derive the average value $\Delta_rH° = 17.1 \pm 2\ kcal{\cdot}mol^{-1}$. The data of Tschuikow–Roux[7] for $C_2F_6(g) \rightarrow 2CF_3(g)$, recalculated as suggested by Coomber and Whittle[8] but with JANAF functions, yield $\Delta_rH° = 97.6 \pm 6\ kcal{\cdot}mol^{-1}$. Differences between the calculated and observed values of $\Delta_rH°$ are all less than half of the uncertainties assigned to the observed values.

The thorough discussion of photoionization data by Noutary[9] emphasized that CF_3^+ is formed with large amounts of excess energy both during ionization of CF_3 and during fragmentation of other fluorides. The amount of excess energy varies with the parent molecule. This may also be involved in electron–impact studies and could account for some of the discrepancies in bond– dissociation energies derived from appearance potentials and ionization potentials. Such data have been summarized by Coomber and Whittle.[10] Ionization data were omitted from the simultaneous adjustment due to uncertainty in the amounts of excess energy.

Also omitted was the mass–spectrometric study of $3C_2F_4(g) \rightarrow 4CF_3(g) + 2C(\text{graphite})$ by Ehlert[11] which gave $\Delta_fH° = -102 \pm 3\ kcal{\cdot}mol^{-1}$. The discrepancy of 10 $kcal{\cdot}mol^{-1}$ suggests that the data may not represent equilibrium for the above reaction. This reaction was one of many which resulted from heating MnF_3 in an effusion cell made of graphite.

Heat Capacity and Entropy

The bond length is assumed to be 1.33 Å by comparison with the molecules CF_3X, and the bond angle is estimated from molecular–orbital calculations of Morokuma *et al.*[12] and Beveridge *et al.*[13] The nonplanar structure is consistent with electron–spin–resonance spectra[14] of CF_3 in krypton and xenon matrices, with infrared spectra of CF_3 in various matrices[15] and in the gaseous phase,[16] and with photoionization spectra.[17] The principal moments of inertia are: $I_A = I_B = 7.9146 \times 10^{-39}$ and $I_C = 15.3421 \times 10^{-39}\ g\ cm.^2$ The observed vibrational fundamentals of Carlson and Pimentel[16] are confirmed by the matrix spectra of Milligan *et al* [15] The latter estimated ν_4 to be in the range of 500 to 600 cm^{-1}. We choose the lower value by comparison with CF_3H, SiF_3H and SiF_4.[18]

The uncertainty in ν_4 corresponds to an uncertainty in the entropy of 0.4 $cal{\cdot}K^{-1}\ mol^{-1}$ at 300 K and 0.7 $cal{\cdot}K^{-1}\ mol^{-1}$ at 1000 K Coomber and Whittle[2] and Amphlett and Whittle[19] used kinetic data to derive entropies of 63.2 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$ at 350 K and 71.5 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$ at 600 K. The calculated entropies from this table are higher by 2.0 and 1.7 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$, respectively These differences are only slightly larger than our estimate of the uncertainty in the kinetic results. We estimate the overall uncertainty in the calculated entropies as 1.0 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$ at 298.15 K and 1.6 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$ at 1000 K.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−11.525	−467.518	−467.518	INFINITE
100	33.941	221.531	303.427	−8.190	−468.603	−465.105	242.946
200	41.234	246.999	269.364	−4.473	−469.606	−461.194	120.452
250	45.682	256.679	265.879	−2.300	−469.982	−459.046	95.912
298.15	49.804	265.082	265.082	0.	−470.282	−456.912	80.049
300	49.957	265.390	265.082	0.092	−470.292	−456.829	79.541
350	53.911	273.393	265.705	2.691	−470.548	−454.564	67.840
400	57.467	280.828	267.136	5.477	−470.759	−452.266	59.060
450	60.598	287.782	269.048	8.430	−470.935	−449.943	52.228
500	63.315	294.311	271.251	11.530	−471.081	−447.602	46.761
600	67.663	306.259	276.110	18.090	−471.310	−442.884	38.556
700	70.862	316.942	281.193	25.024	−471.476	−438.132	32.694
800	73.232	326.567	286.274	32.235	−471.601	−433.360	28.296
900	75.013	335.300	291.243	39.651	−471.700	−428.574	24.874
1000	76.373	343.277	296.054	47.223	−471.786	−423.778	22.136
1100	77 431	350.608	300.684	54.915	−471.867	−418.973	19.895
1200	78.265	357.382	305.131	62.702	−471.951	−414.160	18.028
1300	78.934	363.674	309.395	70.563	−472.043	−409.341	16.448
1400	79.477	369.544	313.484	78.484	−472.147	−404.514	15.093
1500	79.923	375.043	317.407	86.455	−472.266	−399.679	13.918
1600	80.294	380.214	321.172	94.467	−472.403	−394.836	12.890
1700	80.605	385 091	324.790	102.512	−472.558	−389.983	11.983
1800	80.869	389.706	328.269	110.586	−472.730	−385.121	11.176
1900	81.094	394.085	331.619	118.685	−472.918	−380.249	10.454
2000	81.287	398.249	334.847	126.804	−473.120	−375.366	9.804
2100	81 455	402 219	337.962	134.941	−473.332	−370 473	9.215
2200	81.601	406.012	340.969	143.094	−473.550	−365.570	8.680
2300	81 729	409.642	343 877	151.261	−473.769	−360.657	8 191
2400	81.842	413.123	346.690	159.439	−473.985	−355.734	7.742
2500	81.942	416.466	349.415	167.629	−474.193	−350.803	7.330
2600	82.031	419.682	352.056	175.827	−474.388	−345.863	6.948
2700	82.110	422.779	354.618	184.034	−474.564	−340.917	6.595
2800	82.182	425.766	357.106	192.249	−474.719	−335.964	6.267
2900	82.246	428.651	359.524	200.470	−474.848	−331.006	5.962
3000	82.304	431.441	361.875	208.698	−474.947	−326.044	5.677
3100	82.356	434 140	364.163	216.931	−475.013	−321.080	5.410
3200	82.404	436 756	366.390	225.169	−475.044	−316.113	5.160
3300	82.448	439.292	368.561	233.412	−475.037	−311.147	4.925
3400	82.488	441 754	370.678	241.659	−474.992	−306.181	4.704
3500	82.524	444 146	372.743	249.909	−474.905	−301.217	4.495
3600	82.558	446.471	374.759	258.163	−474.777	−296.256	4.299
3700	82.589	448.733	376.728	266.421	−474.607	−291.299	4.112
3800	82.618	450.936	378.652	274.681	−474.394	−286.348	3.936
3900	82.644	453.083	380.533	282.944	−474.139	−281.403	3.769
4000	82.668	455.175	382.373	291.210	−473.841	−276.464	3.610
4100	82.691	457.217	384.174	299.478	−473.501	−271.534	3.459
4200	82.712	459.210	385.937	307.748	−473.120	−266.612	3.316
4300	82.732	461.156	387.663	316.020	−472.698	−261.701	3.179
4400	82.750	463 059	389.355	324.294	−472.236	−256.799	3.049
4500	82.768	464.918	391.014	332.570	−471.734	−251.908	2.924
4600	82.784	466.738	392.640	340.848	−471.195	−247.029	2.805
4700	82 799	468.518	394.236	349.127	−470.619	−242.162	2.691
4800	82.813	470.262	395.802	357.408	−470.007	−237.307	2.582
4900	82.826	471.969	397.339	365.690	−469.360	−232.466	2.478
5000	82.839	473.643	398.848	373.973	−468.680	−227.639	2.378
5100	82.851	475.283	400.331	382.257	−467.968	−222.825	2.282
5200	82.862	476.892	401.788	390.543	−467.224	−218.025	2.190
5300	82.872	478 471	403.220	398.830	−466.451	−213.240	2.102
5400	82.882	480 020	404.628	407.117	−465.648	−208.470	2.017
5500	82.892	481.541	406.012	415.406	−464.818	−203.716	1.935
5600	82.900	483.034	407.374	423.696	−463.962	−198.975	1.856
5700	82 909	484.502	408.715	431.986	−463.080	−194.252	1.780
5800	82.917	485.944	410.034	440.277	−462.174	−189.544	1.707
5900	82.924	487.361	411.332	448.569	−461.245	−184.850	1.637
6000	82.932	488 755	412.611	456.862	−460.294	−180 174	1.569

PREVIOUS. June 1969 (1 atm) CURRENT. June 1969 (1 bar)

Trifluoromethyl, Ion (CF_3^+) IDEAL GAS $M_r = 69.005660$ Trifluoromethyl, Ion (CF_3^+) $C_1F_3^+(g)$

$S°(298.15\ K) = 254.53 \pm 1.7\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 417.55 \pm 11.7\ kJ \cdot mol^{-1}$
$\Delta_f H°(298\ 15\ K) = 421.01 \pm 11.7\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[888] (1)
830 (1)
[1404] (2)
[480] (2)

Ground State Quantum Weight: 1
Point Group: D_{3h} $\sigma = 1$
Bond Distance: C–F = [1.33] Å
Bond Angle: F–C–F = [120]°
Product of the Moments of Inertia: $I_A I_B I_C = [1.173095 \times 10^{-114}]\ g^3 \cdot cm^6$

Enthalpy of Formation

The ionization potential of CF_3 has been carefully measured by Lifshitz and Chupka.[1] They used a photoionization technique on CF_3 radicals prepared by heating CF_3CH_2ONO. Because of the low ionization cross–section near the threshold it is very difficult to determine the value exactly. The authors conclude that it is improbable that the ionization potential differs from 9.25 eV by as much as 0.2 eV. They choose to accept a value of 9.25 ± 0.04 eV (213.3 ± 0.9 $kcal \cdot mol^{-1}$) based on their interpretation of the regular structure near the threshold. In a later paper, Walter *et al.*[9] use photodissociative ionization of CF_3I, CF_3Br and CF_3Cl to obtain an indirect ionization potential for CF_3 of 9.11 eV. We adopt a median value of 9.17 ± 0.08 eV (211.5 ± 1.8 $kcal \cdot mol^{-1}$), which with $\Delta_f H°(CF_3, g, 0\ K) = -111.7 \pm 1.0\ kcal \cdot mol^{-1}$ [2] gives $\Delta_f H°(CF_3^+, g, 0\ K) = 99.8 \pm 2.8\ kcal \cdot mol^{-1}$.

The above value supercedes all earlier values for the ionization potential of CF_3 which generally were obtained by electron impact methods, which do not have the energy resolution available in the photoionization technique. For further details of the older values see references.[3–7]

Heat Capacity and Entropy

The correlation rules proposed by Walsh[8] for AB_3 molecules indicate that molecules with less than 25 valence electrons are planar in their ground states. Since BF_3 is isoelectronic with CF_3^+, we estimate the vibrational frequencies by transferring the valence force field constants from BF_3 to CF_3^+. This gives 888, 674, 1404 and 480 cm^{-1}; however, Lifshitz and Chupka[1] conclude that the 674 cm^{-1} frequency is in fact at 830 cm^{-1}. This value is obtained from the spacings in the fine structure of the photoionization curve near threshold. They believe that the out–of–plane motion is most likely to be excited by the transition from pyramidal CF_3 to planar CF_3^+, thus, they ascribe the 830 cm^{-1} spacing to this motion. We adopt this one frequency in place of the calculated value. The bond lengths are assumed equal to those in CF_3. The principal moments of inertia are: $I_A = I_B = 8.3708 \times 10^{-39}$, and $I_C = 16.7416 \times 10^{-39}\ g \cdot cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
0	0.	0.	INFINITE	−11.543	417.554		
100	34.065	210.860	292.920	−8.206			
200	41.352	236.450	258.810	−4.472			
250	45.673	246.144	255.327	−2.296			
298.15	49.645	254.532	254.532	0.	421.007	431.267	−75.556
300	49.792	254.839	254.533	0.092	421.034	431.331	−75.101
350	53.582	262.804	255.153	2.678	421.805	432.987	−64.620
400	56.993	270.186	256.576	5.444	422.613	434.529	−56.744
450	60.013	277.077	258.475	8.371	423.450	435.969	−50.606
500	62.659	283.540	260.662	11.439	424.312	437.314	−45.686
600	66.955	295.363	265.479	17.930	426.093	439.748	−38.283
700	70.176	305.937	270.517	24.794	427.935	441.879	−32.973
800	72.600	315.474	275.551	31.939	429.823	443.742	−28.973
900	74.445	324.136	280.475	39.295	431.742	445.367	−25.848
1000	75.869	332.057	285.243	46.814	433.682	446.777	−23.337
1100	76.983	339.342	289.835	54.458	435.631	447.992	−21.273
1200	77.869	346.080	294.244	62.203	437.584	449.030	−19.546
1300	78.582	352.342	298.475	70.026	439.534	449.904	−18.077
1400	79.163	358.188	302.534	77.915	441.475	450.629	−16.813
1500	79.642	363.666	306.429	85.856	443.404	451.216	−15.713
1600	80.041	368.819	310.169	93.840	445.320	451.674	−14.746
1700	80.377	373.682	313.763	101.862	447.219	452.013	−13.889
1800	80.662	378.285	317.221	109.914	449.104	452.240	−13.124
1900	80.906	382.652	320.551	117.993	450.974	452.363	−12.436
2000	81.116	386.808	323.761	126.094	452.833	452.389	−11.815
2100	81.298	390.770	326.858	134.215	454.683	452.321	−11.251
2200	81.457	394.556	329.850	142.353	456.529	452.165	−10.736
2300	81.596	398.180	332.742	150.506	458.374	451.925	−10.264
2400	81.719	401.655	335.542	158.672	460.224	451.605	−9.829
2500	81.828	404.993	338.254	166.849	462.083	451.208	−9.427
2600	81.925	408.205	340.883	175.037	463.956	450.736	−9.055
2700	82.012	411.298	343.434	183.234	465.848	450.192	−8.709
2800	82.090	414.282	345.911	191.439	467.762	449.577	−8.387
2900	82.160	417.164	348.319	199.651	469.704	448.893	−8.085
3000	82.223	419.950	350.660	207.871	471.675	448.142	−7.803
3100	82.281	422.647	352.939	216.096	473.679	447.325	−7.537
3200	82.333	425.261	355.158	224.327	475.720	446.442	−7.287
3300	82.381	427.795	357.321	232.562	477.798	445.495	−7.052
3400	82.424	430.255	359.430	240.803	479.916	444.485	−6.829
3500	82.464	432.645	361.488	249.047	482.074	443.411	−6.618
3600	82.501	434.968	363.497	257.295	484.275	442.276	−6.417
3700	82.535	437.229	365.460	265.547	486.519	441.078	−6.227
3800	82.566	439.431	367.377	273.802	488.805	439.819	−6.046
3900	82.595	441.576	369.253	282.060	491.134	438.500	−5.873
4000	82.622	443.667	371.087	290.321	493.505	437.121	−5.708
4100	82.647	445.708	372.882	298.585	495.919	435.681	−5.551
4200	82.670	447.700	374.640	306.851	498.375	434.182	−5.400
4300	82.692	449.645	376.362	315.119	500.872	432.624	−5.255
4400	82.712	451.546	378.049	323.389	503.408	431.008	−5.117
4500	82.731	453.405	379.703	331.661	505.984	429.334	−4.984
4600	82.748	455.224	381.325	339.935	508.598	427.601	−4.856
4700	82.765	457.004	382.916	348.211	511.250	425.812	−4.732
4800	82.780	458.746	384.478	356.488	513.937	423.966	−4.614
4900	82.795	460.453	386.011	364.767	516.659	422.064	−4.499
5000	82.809	462.126	387.517	373.047	519.415	420.105	−4.389
5100	82.822	463.766	388.996	381.328	522.203	418.091	−4.282
5200	82.834	465.374	390.449	389.611	525.022	416.023	−4.179
5300	82.846	466.952	391.878	397.895	527.872	413.899	−4.079
5400	82.856	468.501	393.282	406.180	530.750	411.722	−3.983
5500	82.867	470.021	394.664	414 466	533.656	409.491	−3.889
5600	82.876	471.515	396.023	422.754	536.589	407.207	−3.798
5700	82.886	472.982	397.360	431.042	539.547	404.870	−3.710
5800	82.895	474.423	398.677	439.331	542.529	402.481	−3.625
5900	82.903	475.840	399.972	447.621	545.535	400.041	−3.542
6000	82.911	477.234	401.249	455.911	548.562	397.549	−3.461

PREVIOUS: December 1971 (1 atm) CURRENT. December 1971 (1 bar)

Trifluoroiodomethane (CF_3I) IDEAL GAS M_r = 195.910709 Trifluoriodomethane (ClF_3) $C_1F_3I_1(g)$

$\Delta_fH°(0\ K) = -583.23 \pm 3.3\ kJ\cdot mol^{-1}$

$S°(298.15\ K) = 307.629 \pm 0.63\ J\cdot K^{-1}\cdot mol^{-1}$ $\Delta_fH°(298.15\ K) = -589.11 \pm 3.3\ kJ\cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	 ν, cm^{-1}
1074 (1)	1185 (2)
742 (1)	539 (2)
284 (1)	260 (2)

Ground State Quantum Weight: 1 $\sigma = 3$

Point Group: C_{3v}

Bond Distances: C–F = 1.332 Å; C–I = 2.130 Å

Bond Angles: F–C–F = 108.3° ± 1°; F–C–I = 110.62°

Product of the Moments of Inertia: $I_AI_BI_C = 4.410587 \times 10^{-113}\ g^3\cdot cm^6$

Enthalpy of Formation

The selected value is obtained from least squares, simultaneous adjustment of the enthalpies of formation of CF_3, CF_3X (X = H, Cl, Br, I, CF_3) and C_2F_4. Details of the input data and the adjustment are given by Syverud.[1] Lord *et al.*[2,3] report equilibrium data for the reactions $CF_3X(g) + I_2(g) = CF_3I(g) + XI(g)$ where X = H, Cl, and Br. In addition to these prime links, there is a weak link to CF_3 through kinetic studies of $CF_3I(g) + I(g) \rightarrow CF_3(g) + I_2(g)$. Data for this reaction[3,12] yield the average value $\Delta_rH° = 17.1 \pm 2\ kcal\cdot mol^{-1}$ at 298.15 K.

Heat Capacity and Entropy

The molecular structure has been derived from electron–diffraction studies by Bowen,[4] Anderson,[5] and Wong and Schomaker.[6] Differences among the data are small. The results of Anderson are adopted since they are intermediate between the others. Microwave data[7] are consistent with the adopted parameters. Infrared spectra of the gas were observed by several investigators[8–10] and Raman spectra of the liquid were obtained by Edgell and May.[10] The vibrational assignments of[9,10] are in close agreement. These assignments are adopted but preference is given to frequencies observed for the gas. In particular, ν_6 is taken as 260 cm^{-1} (from overtone and combination bands of the gas) rather than 265 cm^{-1} (from the Raman spectra of the liquid). The approximate values of ν_2, ν_3 and ν_6 have been confirmed by analysis[11] of absorption spectra in the UV.

The thermodynamic functions of this table are essentially the same as those calculated by McGee *et al.*[9] Uncertainty in the entropy is estimated to vary from 0.15 to 0.6 cal·K^{-1}·mol^{-1} over the range from 300 to 1000 K. Uncertainty in ν_6 and neglect of anharmonicity are the major sources of error. Discussions of the magnitude of anharmonic effects appear on the tables for $CClF_3(g)$ and $CF_4(g)$. The principal moments of inertia are: $I_A = 14.7097 \times 10^{-39}$ and $I_B = I_C = 54.7578 \times 10^{-39}\ g\cdot cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
0	0.	0.	INFINITE	−15.008	−583.227	−583.227	INFINITE
100	41.917	247.280	361.949	−11.467	−585.632	−581.659	303.828
200	58.726	281.794	313.747	−6.391	−587.742	−576.793	150.643
250	65.362	295.629	308.766	−3.284	−588.499	−573.965	119.923
298.15	70.940	307.629	307.629	0.	−589.107	−571.109	100.056
300	71.139	308.068	307.630	0.131	−589.129	−570.997	99.419
350	76.154	319.420	308.515	3.817	−589.704	−567.930	84.759
400	80.462	329.878	310.541	7.735	−598.196	−564.510	73.717
450	84.124	339.573	313.234	11.852	−599.224	−560.237	65.031
500	87.220	348.601	316.325	16.138	−620.266	−553.952	57.871
600	92.033	364.953	323.096	25.114	−619.956	−540.717	47.074
700	95.478	379.413	330.129	34.499	−619.555	−527.541	39.366
800	97.982	392.335	337.111	44.179	−619.100	−514.427	33.589
900	99.840	403.988	343.905	54.074	−618.615	−501.372	29.099
1000	101.246	414.583	350.451	64.132	−618.117	−488.371	25.510
1100	102.331	424.286	356.729	74.313	−617.617	−475.421	22.576
1200	103.184	433.228	362.736	84.590	−617.126	−462.516	20.133
1300	103.863	441.515	368.481	94.944	−616.653	−449.651	18.067
1400	104.413	449.233	373.977	105.359	−616.208	−436.822	16.298
1500	104.864	456.452	379.237	115.823	−615.797	−424.023	14.766
1600	105.238	463.233	384.277	126.329	−615.428	−411.250	13.426
1700	105.551	469.622	389.111	136.869	−615.106	−398.499	12.244
1800	105.816	475.663	393.753	147.438	−614.834	−385.766	11.195
1900	106.042	481.390	398.216	158.031	−614.613	−373.046	10.256
2000	106.236	486.835	402.512	168.645	−614.440	−360.336	9.411
2100	106.403	492.022	406.652	179.277	−614.311	−347.635	8.647
2200	106.550	496.975	410.646	189.925	−614.220	−334.938	7.952
2300	106.678	501.715	414.503	200.586	−614.157	−322.245	7.318
2400	106.791	506.257	418.232	211.260	−614.113	−309.554	6.737
2500	106.890	510.619	421.841	221.944	−614.078	−296.865	6.203
2600	106.979	514.813	425.337	232.638	−614.041	−284.177	5.709
2700	107.059	518.852	428.726	243.339	−613.991	−271.491	5.252
2800	107.130	522.747	432.015	254.049	−613.919	−258.807	4.828
2900	107.194	526.507	435.209	264.765	−613.815	−246.126	4.433
3000	107.252	530.142	438.313	275.488	−613.671	−233.450	4.065
3100	107.304	533.660	441.332	286.215	−613.479	−220.779	3.720
3200	107.352	537.067	444.271	296.948	−613.233	−208.115	3.397
3300	107.395	540.371	447.133	307.686	−612.929	−195.459	3.094
3400	107.435	543.578	449.923	318.427	−612.561	−182.814	2.809
3500	107.471	546.693	452.643	329.172	−612.126	−170.181	2.540
3600	107.505	549.721	455.298	339.921	−611.622	−157.560	2.286
3700	107.536	552.667	457.890	350.673	−611.047	−144.955	2.046
3800	107.564	555.535	460.422	361.428	−610.400	−132.367	1.820
3900	107.590	558.329	462.897	372.186	−609.681	−119.796	1.604
4000	107.615	561.054	465.317	382.946	−608.890	−107.245	1.400
4100	107.637	563.711	467.685	393.709	−608.028	−94.715	1.207
4200	107.658	566.305	470.002	404.474	−607.094	−82.206	1.022
4300	107.678	568.839	472.271	415.241	−606.091	−69.721	0.847
4400	107.696	571.314	474.494	426.009	−605.021	−57.259	0.680
4500	107.713	573.735	476.673	436.780	−603.883	−44.822	0.520
4600	107.729	576.102	478.808	447.552	−602.681	−32.412	0.368
4700	107.744	578.419	480.903	458.326	−601.417	−20.028	0.223
4800	107.758	580.688	482.959	469.101	−600.091	−7.672	0.083
4900	107.772	582.910	484.976	479.877	−598.707	4.656	−0.050
5000	107.784	585.087	486.956	490.655	−597.265	16.955	−0.177
5100	107.796	587.222	488.901	501.434	−595.770	29.224	−0.299
5200	107.807	589.315	490.812	512.214	−594.221	41.465	−0.417
5300	107.817	591.369	492.690	522.995	−592.622	53.674	−0.529
5400	107.827	593.384	494.537	533.778	−590.974	65.853	−0.637
5500	107.837	595.363	496.352	544.561	−589.279	78.000	−0.741
5600	107.845	597.306	498.137	555.345	−587.540	90.118	−0.841
5700	107.854	599.215	499.894	566.130	−585.757	102.202	−0.937
5800	107.862	601.091	501.623	576.916	−583.934	114.255	−1.029
5900	107.869	602.935	503.324	587.702	−582.071	126.278	−1.118
6000	107 876	604.748	504.999	598.489	−580.170	138.268	−1.204

PREVIOUS. June 1969 (1 atm) CURRENT: June 1969 (1 bar)

Trifluoriodomethane (ClF_3) $C_1F_3I_1(g)$

Tetrafluoromethane (CF_4) **IDEAL GAS** **M_r = 88.004612** **Tetrafluoromethane (CF_4)** **$C_1F_4(g)$**

$S°(298.15 K) = 261.419 \pm 0.25 J·K^{-1}·mol^{-1}$

$\Delta_f H°(0 K) = -927.23 \pm 1.3 kJ·mol^{-1}$
$\Delta_f H°(298.15 K) = -933.20 \pm 1.3 kJ·mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}
908.5 (1)	1283.0 (3)
435.0 (2)	631.5 (3)

Ground State Quantum Weight: 1 $\sigma = 12$
Point Group: T_d
Bond Distance: C–F = 1.320 Å
Bond Angle: F–C–F = 109.4712°
Product of the Moments of Inertia: $I_A I_B I_C = 3.149690 \times 10^{-114} g^3·cm^6$

Enthalpy of Formation

The selected value is obtained from least squares, simultaneous adjustment of the enthaplies of formation of HF(g), HF(50 H_2O) and five closely related fluorides. Adjustment of 23 selected observations relating the 7 variables gives the following enthalpies of formation in kcal·mol^{-1} at 298.15 K: HF(g), −65.14 ± 0.2; HF(50 H_2O), −76.78 ± 0.1; NaF(cr), −137.52 ± 0.2; BF_3(g), −271.42 ± 0.4; CF_4(g), −223.04 ± 0.3; NF_3(g), −31.43 ± 0.3; and C_2F_4(polymer), −198.2 ± 0.7. The ± values are estimates of the overall uncertainty including systematic error. Further details of the simultaneous adjustment are given by Syverud.[1]

The selected value is essentially the same as that obtained by Greenberg and Hubbard[2] in their thorough calorimetric study of the combustion in fluorine of natural and synthetic graphite. Their results is confirmed by the data of Domalski and Armstrong[3] for combustion of graphite–Teflon mixtures. Reliable data[1] also link CF_4(g) with HF(n H_2O), NF_3(g) and C_2F_4(polymer). Armstrong[4,3] critically reviewed the more uncertain data which were omitted from the adjustment.

Heat Capacity and Entropy

The fundamental vibrations are those observed in the gas–phase Raman spectra by Monostori and Weber[5] and the gas–phase infrared spectra by Maki *et al.*[6] and Chalmers and McKean.[7] The frequencies are essentially the same as those selected by Shimanouchi[8] who also lists earlier spectral studies. Electron–diffraction studies of the gas were reported by Thornton[9] and Hoffman and Livingston.[10] The adopted bond length is the average of these two results which differ by only 0.006 Å. The principal moments of inertia are: $I_A = I_B = I_C = 14.6585 \times 10^{-39} g·cm^2$.

The most significant uncertainty in the calculated thermodynamic functions is due to neglect of anharmonic contributions. Estimates for these contributions were given by Barho[11] and Albright *et al.*,[12] and functions calculated with anharmonic terms were given by McBride *et al.*[13] Differences between McBride and this JANAF table vary from 0.1 to 0.75 cal·K^{-1}·mol^{-1} in $C_p°$ and 0.05 to 0.49 cal·K^{-1}·mol^{-1} in $S°$ over the range from 300 to 1000 K. Measurements[14] of C_v (303–473 K) suggest that anharmonic contributions are significant, but the data are not sufficiently accurate to test the calculations of McBride *et al.*[13] Heat capacity data[15] for the condensed phases were reviewed by Kelley and King[16] who derived $S°(298.15 K) = 62.8 \pm 0.5$ cal·K^{-1}·mol^{-1} for CF_4(g).

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
0	0.	0.	INFINITE	−12.731	−927.229	−927.229	INFINITE
100	34.745	212.363	306.188	−9.383	−929.755	−916.822	478.899
200	47.370	239.882	266.577	−5.339	−931.896	−902.995	235.838
250	54.623	251.239	262.389	−2.788	−932.645	−895.679	187.142
298.15	61.054	261.419	261 419	0.	−933.199	−888.507	155.663
300	61.288	261.798	261.420	0.113	−933.218	−888.229	154.654
350	67.217	271.700	262.189	3.329	−933.651	−880.695	131.437
400	72.400	281.022	263.966	6.822	−933.970	−873.107	114.016
450	76.875	289.815	266.354	10.557	−934.198	−865.485	100.463
500	80.712	298.118	269.120	14.499	−934.351	−857.841	89.618
600	86.781	313.399	275.249	22.890	−934.485	−842.523	73.348
700	91.209	327.127	281.697	31.801	−934.451	−827.197	61.726
800	94 476	339.530	288.164	41.093	−934.298	−811.884	53.011
900	96.927	350.806	294.507	50.669	−934.065	−796.596	46.233
1000	98.797	361.119	300 660	60.459	−933 778	−781.337	40.813
1100	100.249	370.607	306.593	70.415	−933.456	−766.108	36.379
1200	101.394	379.380	312.298	80 499	−933.115	−750.909	32.686
1300	102.312	387.534	317 776	90.686	−932.766	−735 739	29.562
1400	103.057	395.144	323.033	100.956	−932.417	−720.597	26.886
1500	103.669	402.276	328.081	111.293	−932.075	−705.479	24.567
1600	104.178	408.983	332.930	121.686	−931 744	−690.383	22.539
1700	104.605	415.312	337.591	132.126	−931.428	−675.308	20.750
1800	104.966	421.302	342.077	142.605	−931.125	−660.251	19.160
1900	105.275	426.986	346.398	153.117	−930.835	−645.210	17.738
2000	105.540	432.392	350.563	163.658	−930.556	−630.184	16.459
2100	105.770	437.547	354.584	174.224	−930.283	−615.173	15.302
2200	105.970	442.473	358.467	184.811	−930.011	−600.174	14.250
2300	106.146	447 187	362.223	195 417	−929.735	−585.187	13.290
2400	106.301	451.708	365.858	206.040	−929.449	−570.213	12.410
2500	106 438	456.050	369.379	216.677	−929.146	−555.251	11.601
2600	106.560	460.227	372.794	227.327	−928.821	−540.302	10.855
2700	106.669	464.251	376.107	237.988	−928.466	−525.365	10.164
2800	106.767	468.132	379.325	248.660	−928.077	−510.442	9.522
2900	106.855	471.880	382 452	259.342	−927.649	−495.534	8.926
3000	106.935	475.504	385 494	270.031	−927.177	−480.642	8.369
3100	107.007	479.012	388.454	280.728	−926.656	−465.766	7.848
3200	107.073	482.410	391.337	291.432	−926.084	−450.907	7.360
3300	107.132	485.706	394.147	302.143	−925.458	−436.068	6.902
3400	107.187	488.905	396.888	312.859	−924.775	−421.248	6.472
3500	107.237	492.013	399.561	323.580	−924.034	−406.449	6.066
3600	107.283	495.034	402.171	334.306	−923.233	−391.671	5.683
3700	107.326	497.974	404.721	345.036	−922.372	−376.918	5.321
3800	107.365	500.837	407 213	355 771	−921.450	−362.188	4.979
3900	107.401	503.626	409.650	366.509	−920.468	−347.483	4.654
4000	107.435	506.346	412.033	377.251	−919.425	−332.804	4.346
4100	107.466	508.999	414.366	387.996	−918.322	−318.153	4 053
4200	107 495	511.589	416.650	398.744	−917.160	−303.528	3.775
4300	107.522	514.119	418.887	409 495	−915.940	−288.932	3.510
4400	107.547	516.591	421.080	420.249	−914.663	−274.365	3.257
4500	107.571	519.008	423.229	431.005	−913.330	−259.827	3.016
4600	107.593	521.373	425.337	441.763	−911.943	−245.321	2.786
4700	107.614	523.687	427.405	452.523	−910.503	−230.844	2.566
4800	107.633	525.953	429.435	463.285	−909.011	−216.399	2.355
4900	107.651	528.172	431.427	474.050	−907.470	−201 986	2.153
5000	107.669	530.347	433.384	484.816	−905.880	−187.604	1.960
5100	107.685	532.480	435.306	495.583	−904.243	−173.255	1.774
5200	107.700	534.571	437.195	506.353	−902.562	−158.937	1.597
5300	107 714	536.622	439.052	517 123	−900.837	−144.653	1.426
5400	107.728	538.636	440.877	527.895	−899.069	−130.403	1.261
5500	107 741	540 613	442.673	538.669	−897.262	−116.185	1.103
5600	107.753	542.554	444 439	549 444	−895.416	−102.000	0.951
5700	107.765	544 461	446.177	560.219	−893.532	−87.849	0.805
5800	107.776	546.336	447.888	570.997	−891.613	−73.731	0.664
5900	107.786	548 178	449.572	581.775	−889.659	−59.645	0.528
6000	107 796	549.990	451.231	592.554	−887.672	−45.595	0.397

PREVIOUS: June 1969 (1 atm) CURRENT· June 1969 (1 bar)

Trifluoromethyl Hypofluorite (CF_3OF) IDEAL GAS M_r = 104.004012 Trifluoromethyl Hypofluorite (CF_3OF) $C_1F_4O_1(g)$

$S°(298.15\ K) = 322.53 \pm 2.9\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -756.4 \pm 13\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -764.8 \pm 13\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
1294.4 (1)	679.0 (1)	1223.2 (1)
1262.5 (1)	584.1 (1)	607.5 (1)
947.3 (1)	433.7 (1)	250.0 (1)
882.1 (1)	227.5 (1)	internal rotation

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: C_s
Bond Distances: C–F = [1.33] Å, F–O = [1.42] Å; C–O = [1.43] Å
Bond Angles: C–O–F = [103.2]°; F–C–F = [109.5]°
Product of the Moments of Inertia. $I_AI_BI_C = 1.151629 \times 10^{-113}\ g^3{\cdot}cm^6$

Enthalpy of Formation

Porter and Cady[1] measured equilibrium constants for the reaction $CF_3OF(g) = COF_2(g) + F_2(g)$ in the temperature range 630–750 K. Equilibrium constants were also determined with excess fluorine added to the system. 2nd and 3rd law analyses of these data yield the following enthalpy of reaction:

	$\Delta_rH°(298.15\ K)$, kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1} mol^{-1}
Set 1	27.65 ± 0.2	30.10	3.6 ± 0.3
Set added fluorine	25.11 ± 0.3	30.09	7.2 ± 0.5

The 3rd law analyses indicate significant trends within each set of equilibrium data. If the entire error is assigned to the Gibbs energy functions, then the drifts in the 3rd law analysis imply that the Gibbs energy functions for CF_3OF should be increased by 3.6 or 7.2 cal·K^{-1}·mol^{-1}. However, the real error in these Gibbs energy functions is probably no larger than 1 cal·K^{-1}·mol^{-1} in the temperature range of the experimental data. Apparently, the equilibrium reaction investigated by Porter and Cady[1] was affected by side reactions possibly involving perfluorodimethyl peroxide. However, since the only other approach to the enthalpy of formation of CF_3OF involves bond energies, we adopt the 3rd law value, $\Delta_rH° = 30.1$ kcal·mol^{-1}, and derive $\Delta_fH°(CF_3OF, g, 298.15\ K) = -182.8 \pm 3$ kcal·mol^{-1} with $\Delta_fH°(COF_2, g, 298.15\ K) = -152.7 \pm 0.4$ kcal·mol^{-1}.[2]

Czarnowski *et al.*[3] recently determined the O–F bond energy in CF_3OF from kinetic studies on the thermal decomposition of CF_3OF in the presence of SO_3. They reported the value $D_0°(O–F) = 43.5 \pm 0.5$ kcal·mol^{-1}. Combining this result with the following data,

$\Delta_fH°(C, g, 298.15\ K) = 170.89 \pm$ kcal·mol^{-1} [4]
$\Delta_fH°(F, g, 298.15\ K) = 18.86 \pm 0.40$ kcal·mol^{-1} [5]
$\Delta_fH°(O, g, 298.15\ K) = 59.559 \pm 0.03$ kcal·mol^{-1} [6]
$D_0°(C–F) = 117.4$ kcal·mol^{-1} (from $\Delta_fH°(CF_4, g, 298.15\ K) = -223.04 \pm 0.3$ kcal·mol^{-1} [7]
$D_0°(C–O) = 84$ kcal·mol^{-1} [8]

we derive $\Delta_fH°(CF_3OF, g, 298.15\ K) = -173.8$ kcal·mol^{-1}.

The value determined from Porter and Cady's equilibrium data[1] is adopted here.

Heat Capacity and Entropy

The vibrational frequencies are from the infrared and Raman studies of Wilt and Jones[9] and are in reasonable agreement with nine of the twelve expected fundamentals observed by Lagemann *et al.*[10] Bond lengths and angles are estimated quantities chosen by Wilt and Jones.[9] The principal moments of inertia are: $I_A = 14.8190 \times 10^{-39}$, $I_B = 27.8485 \times 10^{-39}$, and $I_C = 27.9057 \times 10^{-39}$ g cm^2. The contributions of hindered internal rotation to the thermodynamic properties of CF_3OF are from the tables of Pitzer and Gwinn.[11] The reduced moment of inertia, I_r, and the potential barrier, V_o, are from the work of Wilt and Jones[9] and are:

$I_r = 2.939 \times 10^{-39}$ g·cm^{-1} $V_o = 1130$ kcal·mol^{-1} ($\nu_{12} = 56$ cm^{-1})

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−14.644	−756.437	−756.437	INFINITE
100	50.170	253.856	383.560	−12.970	−762.089	−744.640	388.960
200	65.831	293.567	329.248	−7.136	−763.895	−726.383	189.712
298.15	79.354	322.533	322.533	0.	−764.835	−707.781	124.000
300	79.617	323.024	322.534	0 147	−764.847	−707.427	123.174
400	91.023	347.556	325.802	8.702	−765.239	−688.216	89.872
500	99.876	368.861	332.329	18.266	−765.263	−668.951	69.885
600	106.462	387.683	340.017	28.599	−765.034	−649.707	56.562
700	111.056	404.453	348.047	39.484	−764 652	−630.514	47.050
800	114.533	419.520	356.055	50.772	−764.174	−611.383	39.919
900	117 089	433.163	363.877	62.358	−763.633	−592.316	34.377
1000	119.039	445.604	371.437	74.167	−763.058	−573.312	29.947
1100	120.625	457.028	378.706	86.154	−762.459	−554.366	26.325
1200	121.779	467.574	385.678	98.275	−761.855	−535.475	23.309
1300	122.779	477.362	392.358	110.505	−761.254	−516.634	20.759
1400	123.591	486.492	398.760	122.825	−760.662	−497.840	18.575
1500	124.256	495.042	404.897	135.218	−760.085	−479.087	16.683
1600	124.805	503.080	410.784	147.672	−759.527	−460.372	15.030
1700	125.206	510.658	416.439	160.173	−758.995	−441.691	13.572
1800	125.599	517.826	421.874	172.714	−758.488	−423.041	12.276
1900	125.934	524.626	427.105	185.291	−758.004	−404.419	11.118
2000	126.219	531.093	432.144	197.899	−757.539	−385.821	10.077
2100	126.470	537.257	437.003	210.533	−757.090	−367.246	9.135
2200	126.687	543.146	441.695	223.192	−756.651	−348.692	8.279
2300	126.876	548 782	446.229	235.870	−756.218	−330.158	7.498
2400	127.043	554.185	450.616	248.566	−755.785	−311.644	6.783
2500	127 189	559.374	454.863	261.278	−755.345	−293.147	6.125
2600	127.261	564.364	458.979	274.001	−754.895	−274.668	5.518
2700	127.340	569.168	462.972	286.730	−754.431	−256.206	4.957
2800	127.445	573.801	466.848	299.470	−753.943	−237.762	4 436
2900	127.541	578.275	470.614	312.219	−753.425	−219.336	3.951
3000	127.629	582.601	474.275	324.978	−752.873	−200.929	3.498
3100	127.705	586.787	477.837	337.744	−752.280	−182.540	3.076
3200	127.775	590.842	481.305	350.518	−751.645	−164.172	2.680
3300	127.841	594.775	484.685	363.299	−750.964	−145.823	2.308
3400	127.901	598.593	487.979	376.086	−750.234	−127.497	1.959
3500	127.955	602.301	491.193	388.879	−749.453	−109.192	1.630
3600	128.005	605.906	494.329	401.677	−748.620	−90.910	1.319
3700	128 051	609.414	497.392	414.480	−747.734	−72.653	1.026
3800	128.093	612.830	500.386	427.287	−746.794	−54.420	0.748
3900	128.132	616.157	503.312	440.099	−745.799	−36.212	0.485
4000	128.168	619.402	506.173	452.914	−744.751	−18.031	0.235
4100	128.201	622.567	508.974	465.732	−743.649	0.123	−0.002
4200	128.231	625.657	511.715	478.554	−742.494	18.251	−0.227
4300	128.261	628.674	514.400	491.378	−741.287	36.349	−0.442
4400	128.289	631.623	517.031	504.206	−740.029	54.419	−0.646
4500	128.315	634.507	519.610	517.036	−738.721	72.461	−0.841
4600	128.340	637.327	522.138	529.869	−737.364	90.471	−1.027
4700	128.363	640 088	524.619	542.704	−735.961	108.453	−1.205
4800	128.384	642.790	527.053	555.541	−734.511	126.404	−1.376
4900	128.403	645.438	529.442	568.381	−733.019	144.325	−1.539
5000	128.420	648.032	531.788	581.222	−731.484	162.214	−1.695
5100	128.437	650.575	534 092	594.065	−729.909	180.073	−1.844
5200	128.454	653.069	536.356	606.909	−728.297	197.900	−1.988
5300	128 470	655.516	538.581	619.755	−726.647	215.696	−2.126
5400	128.485	657.918	540.769	632.603	−724.964	233.460	−2.258
5500	128.499	660.276	542.921	645.452	−723.248	251.192	−2.386
5600	128.512	662.591	545.037	658.303	−721.501	268.894	−2.508
5700	128.522	664.866	547.119	671.155	−719.727	286.563	−2.626
5800	128.533	667.101	549.169	684.007	−717.925	304.202	−2.740
5900	128.545	669.298	551.186	696.861	−716.099	321.810	−2.849
6000	128.558	671.459	553.173	709.716	−714.250	339.385	−2.955

PREVIOUS. December 1969 (1 atm) CURRENT· December 1969 (1 bar)

Continued on page 700

Pentafluoro(trifluoromethyl)sulfur (CF_3SF_5) IDEAL GAS $M_r = 196.058224$ Pentafluoro(Trifluoromethyl)Sulfur (CF_3SF_5) $C_1F_8S_1(g)$

$S°(298.15\ K) = [379.97 \pm 2.1]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = [-1700.4 \pm 63]\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = [-1717.1 \pm 63]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
1168(1)	Free Rotation	591(2)
883(1)	627(1)	558(2)
755(1)	319(1)	425(2)
692(1)	501(1)	290(2)
612(1)	1256(2)	220(2)
325(1)	903(2)	

Ground State Quantum Weight: 1 σ (overall) = 12
Point Group: C_{4v}
Bond Distances: C–F = [1.32] Å; S–F = [1.56] Å; C–S = 1.92 Å
Bond Angles: S–C–F = [109.5°]; F*–S–F* = 90°
F*–S–C = [90°]; F**–S–C = 180°
(* – equatorial ** – axial)
Product of Moments of Inertia: $I_AI_BI_C = [2.659738 \times 10^{-112}]\ g^3{\cdot}cm^6$
Reduced Moment of Inertia: $I_{red} = [9.9216 \times 10^{-39}]\ g{\cdot}cm^2$

Enthalpy of Formation

We adopt $D_0°(CF_3\text{–}SF_5) = 80 \pm 10\ kcal{\cdot}mol^{-1}$ from which $\Delta_fH°$ is calculated to be $-406.4 \pm 15\ kcal{\cdot}mol^{-1}$ at 0 K by combining $D_0°$ with $\Delta_fH°(CF_3, g) = -111.7 \pm 1.0\ kcal{\cdot}mol^{-1}$ and $\Delta_fH°(SF_5, g, 0\ K) = -214.7 \pm 3.6\ kcal{\cdot}mol^{-1}$[1] We estimate that the $D_0°$(C–S) in CF_3SF_5 of the C–C, S–S, and C–S bond lengths and the corresponding stretching frequencies for C_2F_6, S_2F_{10}, and CF_3SF_5 indicates that $D_0°$(C–S) should be intermediate between those for C–C and S–S. We calculate the heat of atomization ($\Delta_aH°$) and $\Delta_fH°$ value at 298.15 K as 788.6 ± 19 kcal·mol^{-1} and −410.385 ± 15 kcal·mol^{-1}, respectively.

Heat Capacity and Entropy

The microwave spectrum of CSF_8 observed by Kisliuk and Silvey[2] shows that the molecule is a symmetric rotor comprised of CF_3 and SF_5 groups joined by a C–S bond. The infrared,[3 4] and Raman[4] spectra obey the selection rules predicted for the point group C_{4v}. We estimate all structural data except for the C–S bond length by analogy with the CF_3 structure in C_2F_6 and the SF_5 structure in S_2F_{10}.[1] We select a value for the C–S bond length which when combined with the estimated data reproduces the experimentally determined amount of inertia ($I_A = I_B = 7.656 \times 10^{-38}\ g{\cdot}cm^2)^2$ within the experimental error. The principal moment of inertia about the symmetry axis is $I_C = 45.3692 \times 10^{-39}\ g{\cdot}cm^2$.

The vibrational frequencies are rounded values taken from the gas phase infrared and liquid phase Raman study of Griffiths.[4] The infrared data are supported by results obtained in an earlier study.[3] Griffiths[4] assigned the Raman band at 262 cm^{-1} to the b_1 SF_2 out-of-plane deformation mode (ν_9) by analogy with his assignment for $ClSF_5$ ($\nu_6 = 271$ cm^{-1}). More recent information[1] on $ClSF_5$ indicates that the 271 cm^{-1} Raman band is the low-frequency SF_5 rocking fundamental π_{11}. By analogy with this new assignment for $ClSF_5$, we assign the infrared band observed at 290 cm^{-1} by Griffiths[4] to the SF_5 rocking fundamental (π_{16}). The Raman band at 319 cm^{-1} is believed to be π_9 since it is close to the values (332 cm^{-1} and 317 cm^{-1}) predicted for the analogous deformation mode (π_6) in $ClSF_5$[1] by force field calculations. We assume that the internal rotation about the C–S bond is unrestricted based on spectroscopic evidence[3 4] which indicates that the barrier is very small Kisliuk and Silvey[2] have derived a potential barrier of 219 cm^{-1} (0.63 kcal mol^{-1}) from satellite lines observed in their microwave spectrum; however, these lines are probably due to the CF_3 rocking mode (π_{17}) rather than the torsional vibration (π_7), as indicated by Eggers *et al.*[3] The overall symmetry number is calculated as the product of the external (λ) and internal (x) symmetry numbers with x assumed equal to 12.

References

[1] JANAF Thermochemical Tables: $CF_3(g)$ and $C_2F_6(g)$, 6–30–69; $SF_5(g)$, $S_2F_{10}(g)$, and ClSF5(g),12–31–77.
[2] P. Kisliuk and G. A. Silvey, J. Chem. Phys. 20, 517 (1952).
[3] D. F. Eggers, Jr., H. E. Wright and D. W. Robinson, J. Chem. Phys. 35, 1045 (1961).
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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	4.157	0.	INFINITE	−24.084	−1700.372	−1700.372	INFINITE
100	55.764	278.734	477.625	−19.889	−1708.555	−1666.933	870.716
200	102.475	331.780	391.607	−11.965	−1714.316	−1622.806	423.833
250	122.790	356.890	382.170	−6.320	−1715.995	−1599.720	334.243
298.15	139.222	379.967	379.967	0.	−1717.051	−1577.222	276.323
300	139.794	380.830	379.969	0.258	−1717.082	−1576.354	274.468
350	153.755	403.463	381.725	7.609	−1717.724	−1552.844	231.749
400	165.138	424.764	385.787	15.591	−1720.246	−1529.177	199.690
450	174.415	444.768	391.241	24.087	−1720.972	−1505.256	174.726
500	181.997	463.550	397.543	33.004	−1721.551	−1481.253	154.745
600	193.374	497.804	411.456	51.808	−1721.803	−1433.155	124.767
700	201.250	528.240	426.007	71.563	−1721.375	−1385.073	103.355
800	206.857	555.499	440.520	91.983	−1720.525	−1337.084	87.303
900	210.958	580.112	454.685	112.884	−1772.531	−1288.138	74.762
1000	214.031	602.505	468.364	134.141	−1770.014	−1234.451	64.481
1100	216.384	623.020	481.505	155.667	−1767.433	−1181.020	56.082
1200	218.223	641.930	494 096	177.401	−1764.821	−1127.824	49.093
1300	219.683	659.457	506.150	199.299	−1762.201	−1074.847	43.188
1400	220.861	675.781	517.690	221.328	−1759.592	−1022.072	38.134
1500	221.824	691.053	528.744	243.464	−1757.006	−969.483	33.760
1600	222.621	705.396	539.341	265.687	−1754.451	−917.064	29.939
1700	223.287	718.913	549.510	287.984	−1751.931	−864.805	26.572
1800	223.850	731.692	559.280	310.341	−1749.446	−812.693	23.584
1900	224.329	743.808	568 676	332.751	−1746.992	−760.718	20.914
2000	224.740	755.325	577.723	355.205	−1744.564	−708.872	18.514
2100	225.095	766.299	586.443	377 697	−1742.151	−657.147	16.346
2200	225.405	776.778	594.859	400.222	−1739.742	−605.537	14.377
2300	225.676	786.803	602.988	422.777	−1737.327	−554.035	12.583
2400	225.914	796.413	610.848	445.356	−1734.891	−502.640	10.940
2500	226.125	805.640	618.457	467.958	−1732.421	−451.347	9.430
2600	226.313	814.512	625.828	490.581	−1729.903	−400.154	8.039
2700	226.480	823.057	632.975	513.220	−1727.325	−349.058	6.753
2800	226.630	831.296	639.912	535.876	−1724.676	−298.059	5.560
2900	226.765	839.251	646.649	558.546	−1721.944	−247.156	4.452
3000	226.888	846.941	653.198	581.229	−1719.119	−196.350	3.419
3100	226.998	854.382	659.569	603.923	−1716.194	−145.640	2.454
3200	227.099	861.591	665.770	626.628	−1713.161	−95.024	1.551
3300	227.190	868.581	671.810	649.342	−1710.014	−44.506	0.704
3400	227.274	875.364	677.698	672.066	−1706.748	5.915	−0.091
3500	227.351	881.953	683.440	694.797	−1703.361	56.239	−0.839
3600	227.421	888.359	689.044	717.536	−1699.849	106.465	−1.545
3700	227.486	894.591	694.515	740.281	−1696.212	156.590	−2.211
3800	227.546	900.658	699.860	763.033	−1692.447	206.615	−2.840
3900	227.601	906.570	705.085	785.790	−1688.555	256.540	−3.436
4000	227.652	912.333	710.195	808.553	−1684.538	306.364	−4.001
4100	227.700	917.955	715.194	831.320	−1680.395	356.085	−4.537
4200	227.744	923.442	720.087	854.093	−1676.130	405.704	−5.046
4300	227.786	928.802	724.879	876.869	−1671.743	455.219	−5.530
4400	227.824	934.039	729.573	899.650	−1667.238	504.632	−5.991
4500	227.860	939.159	734 174	922.434	−1662.617	553.942	−6.430
4600	227.894	944.168	738.685	945.222	−1657.883	603.146	−6.849
4700	227.925	949.069	743.109	968.013	−1653.040	652.247	−7.249
4800	227.955	953.868	747.450	990.807	−1648.090	701.244	−7.631
4900	227.983	958.569	751.711	1013.603	−1643.036	750.136	−7.997
5000	228.009	963.175	755.894	1036.403	−1637.883	798.924	−8.346
5100	228.034	967.690	760.003	1059.205	−1632.632	847.608	−8.681
5200	228.057	972.118	764.040	1082.010	−1627.289	896.189	−9.002
5300	228.079	976.463	768.007	1104.816	−1621.856	944.666	−9.310
5400	228.099	980.726	771.907	1127.625	−1616.336	993.039	−9.606
5500	228.119	984.912	775.741	1150.436	−1610.733	1041.308	−9.890
5600	228.138	989.022	779.513	1173.249	−1605.049	1089.477	−10.162
5700	228.155	993.060	783.225	1196.064	−1599.288	1137.541	−10.424
5800	228.172	997.028	786.877	1218.880	−1593.453	1185.504	−10.677
5900	228.188	1000.929	790.472	1241.698	−1587.547	1233.369	−10.919
6000	228.203	1004 764	794.011	1264.518	−1581.573	1281.129	−11.153

PREVIOUS: December 1977 (1 atm) CURRENT: December 1977 (1 bar)

$S°(298.15\ K) = 183.04 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 590.683 \pm 17.5\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = 594.128 \pm 17.5\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^2\Pi_r$	0	2
	17.9	2
$^4\Sigma^-$	[4500]	[4]
	23150	4
	25949	2
	31821	2

$\omega_e = 2861.39\ cm^{-1}$ $\omega_ex_e = 64.29\ cm^{-1}$ $\sigma = 1$
$B_e = 14.455\ cm^{-1}$ $\alpha_e = 0.5339\ cm^{-1}$ $r_e = 1.1198$ Å

Enthalpy of Formation

Herzberg[1] reanalyzed the rotational predissociation reported by Shidei[2] and concluded that $D_0^\circ = 80.0\ kcal{\cdot}mol^{-1}$ (3.47 eV). This yields $\Delta_fH°(CH, g, 298.15\ K) = 142.0\ kcal{\cdot}mol^{-1}(594.128 \pm 17.5\ kJ\ mol^{-1})$, and is the adopted value.

Brewer and Kester[3] have confirmed the value as 142 ± 5 kcal·mol^{-1}, from an equilibrium study of the temperature variation of the intensity of the $^2\Delta \rightarrow {}^2\Pi$ emission band.

Linevsky[4] determined the concentration of CH radicals in equilibrium with 1 atm. of hydrogen gas, by application of a high resolution spectro−photographic technique to three electronic transitions in absorption. A third law analysis, using the present functions, of 27 determinations in the temperature range 3065–3155 K yielded $\Delta_fH°(CH, g, 298.15\ K) = 142.01 \pm 1.28\ kcal\ mol^{-1}$ with a negligible drift. This value is in excellent agreement with the spectroscopic predissociation value.

Heat Capacity and Entropy

The vibrational and rotational constants and electronic levels are from Herzberg[1] with the exception of the estimated $^4\Sigma$ level. All the constants have been adjusted to the normal isotopic abundances for both carbon and hydrogen. The $^4\Sigma$ level is estimated from the ab initio calculations of Hurley[5] which include electron correlation effects. Earlier LCAO calculations had predicted the $^4\Sigma^-$ level to be the ground state, but Higuchi[6] used LCAO–SCF calculations and obtained the $^4\Sigma$ level at 800 cm^{-1}. Krauss and Wehner,[7] using essentially the same technique as Hurley,[5] obtained $^4\Sigma$ at 3000 cm^{-1}.

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−8.730	590.683	590.683	INFINITE
100	29.261	151.151	208.978	−5.783	592.071	582.087	−304.051
200	29.171	171.393	185.708	−2.863	593.317	571.596	−149.286
250	29.167	177.902	183.520	−1.404	593.782	566.110	−118.282
298.15	29.171	183.040	183.040	0.	594.128	560.747	−98.241
300	29.171	183.220	183.040	0.054	594.139	560.540	−97.599
350	29.187	187.718	183.395	1.513	594.403	554.918	−82.817
400	29.223	191.617	184.185	2.973	594.583	549.264	−71.727
450	29.291	195.063	185.206	4.436	594.687	543.592	−63.099
500	29.400	198.154	186.349	5.903	594.725	537.913	−56.195
600	29.757	203.543	188.778	8.859	594.638	526.555	−45.841
700	30.292	208.168	191.225	11.860	594.397	515.226	−38.447
800	30.967	212.256	193.603	14.922	594.062	503.937	−32.904
900	31.739	215.947	195.884	18.057	593.675	492.695	−28.595
1000	32.565	219.334	198.062	21.272	593.265	481.496	−25.151
1100	33 411	222.477	200.140	24.570	592.850	470.340	−22.335
1200	34.250	225.420	202.126	27.954	592.443	459.220	−19.989
1300	35.062	228.194	204.025	31.420	592.050	448.135	−18.006
1400	35.831	230.821	205.846	34.965	591.673	437.078	−16.308
1500	36.548	233.318	207.595	38.584	591.314	426.049	−14.836
1600	37.208	235.698	209.278	42.272	590.972	415.042	−13.550
1700	37.808	237.972	210.899	46.024	590.644	404.057	−12.415
1800	38.348	240.149	212.464	49.832	590.329	393.090	−11.407
1900	38.830	242.235	213.977	53.691	590.023	382.141	−10.506
2000	39.257	244.238	215.440	57.596	589.723	371.207	−9.695
2100	39.632	246.163	216.857	61.541	589.426	360.289	−8.962
2200	39.961	248.014	218.232	65.521	589.130	349.385	−8.295
2300	40.247	249.797	219.566	69.532	588.832	338.494	−7.687
2400	40.495	251.515	220.861	73.569	588.529	327.616	−7.130
2500	40.709	253.173	222.121	77.630	588.219	316.751	−6.618
2600	40.893	254.773	223.346	81.710	587.901	305.898	−6.146
2700	41 051	256.319	224.539	85.807	587.572	295.058	−5.708
2800	41.187	257.815	225.701	89.919	587.231	284.231	−5.302
2900	41.303	259.262	226.833	94.044	586.878	273.415	−4.925
3000	41.402	260.664	227.938	98.179	586.510	262.613	−4.572
3100	41.488	262.023	229.015	102.324	586.127	251.822	−4.243
3200	41.562	263.341	230.067	106.477	585.729	241.044	−3.935
3300	41.627	264.621	231.095	110.636	585.314	230.280	−3.645
3400	41.683	265.865	232.100	114.802	584.883	219.527	−3.373
3500	41 734	267.074	233.082	118.973	584.435	208.788	−3.116
3600	41.780	268.250	234.042	123.148	583.970	198.062	−2.874
3700	41.822	269.396	234.982	127.328	583.487	187.349	−2.645
3800	41.861	270.511	235.903	131.513	582.988	176.649	−2.428
3900	41.899	271.599	236.804	135.701	582.471	165.963	−2.223
4000	41.936	272.661	237.687	139.892	581.937	155.290	−2.028
4100	41.973	273.696	238.553	144.088	581.386	144.630	−1.843
4200	42.010	274.708	239.402	148.287	580.819	133.985	−1.666
4300	42.048	275.697	240.235	152.490	580.235	123.352	−1.498
4400	42.087	276.664	241.052	156.696	579.635	112.734	−1.338
4500	42.127	277.611	241.854	160.907	579.020	102.130	−1.185
4600	42.170	278.537	242.641	165.122	578.388	91.539	−1.039
4700	42.214	279.444	243.414	169.341	577.742	80.962	−0.900
4800	42.260	280.334	244.174	173.565	577.082	70.400	−0.766
4900	42.309	281.206	244.921	177.793	576.407	59.850	−0.638
5000	42.359	282.061	245.655	182.027	575.719	49.316	−0.515
5100	42.412	282.900	246.378	186.265	575.018	38.794	−0.397
5200	42.468	283.724	247.088	190.509	574.304	28.287	−0.284
5300	42.525	284.534	247.787	194.759	573.579	17.794	−0.175
5400	42.585	285.329	248.475	199.014	572.842	7.314	−0.071
5500	42.647	286.111	249.152	203.276	572.095	−3.152	0.030
5600	42.711	286.880	249.819	207.544	571.337	−13.604	0.127
5700	42.777	287.637	250.476	211.818	570.571	−24.043	0.220
5800	42.846	288.381	251.123	216.099	569.795	−34.468	0.310
5900	42.916	289.114	251.760	220.387	569.012	−44.879	0.397
6000	42.987	289.836	252.389	224.683	568.221	−55.278	0.481

PREVIOUS· December 1967 (1 atm) CURRENT· December 1967 (1 bar)

Methylidyne, Ion (CH$^+$) IDEAL GAS $M_r = 13.01839$ Methylidyne, Ion (CH$^+$) CH$^+$(g)

$S°(298.15\ K) = 171.67 \pm 0.21\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 1617.20 \pm 2.1\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 1626.74 \pm 2.1\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^1\Sigma^+$	0	1
$^1\Pi$	23596.94	2

$\omega_e = 2885.7\ cm^{-1}$ $\omega_e x_e = [73]\ cm^{-1}$ $\sigma = 1$
$B_e = 14.1776\ cm^{-1}$ $\alpha_e = 0.4917\ cm^{-1}$ $r_e = 1.3909$ Å

Enthalpy of Formation

Douglas and Herzberg[1] first observed the spectrum of CH$^+$ and concluded that $D_0^\circ(CH^+) = 3.61 \pm 0\ 22$ eV from a short extrapolation of the A state vibrational separations, this leads to IP = 11 13 ± 0.22 eV Later Douglas and Morton[2] showed that the basis for this extrapolation was incorrect and the value was thus invalidated. Herzberg and Johns[3] then reported a value of IP(CH) = 10 64 eV (245.36 kcal·mol^{-1}) which was obtained from the limit of the Rydberg states of CH (see also Herzberg) [4] This value in conjuntion with the JANAF value for $\Delta_f H°$(CH, g, 0 K) = 141.178 kcal·mol^{-1} leads to $\Delta_f H°$(CH$^+$, g, 0 K) = 386.5 ± 0.5 kcal·mol^{-1} (1617.116 ± 2.1 kJ mol^{-1}) and is adopted.

Heat Capacity and Entropy

The molecular constants are those reported by Douglas and Morton.[2] The value for ω_e is derived from the observed $\Delta G_{1/2}$ by adding $2\omega_e x_e$. The $\omega_e x_e$ value is that calculated by Moore *et al.*[5] from ab initio variational calculations of the $^1\Sigma$ and $^1\Pi$ states.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	.000	000	INFINITE	−8.628	1617.199		
100	29.124	139 844	197 578	−5.773			
200	29.135	160.035	174.337	−2.860			
250	29.143	166.537	172.151	−1.403			
298.15	29.153	171.671	171.671	.000	1626.739	1590.493	−278.648
300	29 154	171.851	171.671	.054	1626.789	1590.268	−276.890
350	29 173	176.346	172.026	1.512	1628.091	1584.077	−236.411
400	29.211	180.244	172.815	2.972	1629.310	1577.706	−206.027
450	29.279	183.688	173.836	4.434	1630.453	1571.186	−182.378
500	29.385	186.778	174.978	5.900	1631.529	1564.542	−163.447
600	29 723	192 163	177.406	8.854	1633.519	1550.955	−135.023
700	30.205	196.780	179.852	11.850	1635.351	1537.048	−114.696
800	30.778	200.850	182.227	14.898	1637.081	1522.885	−99.434
900	31.390	204.510	184.503	18.006	1638.746	1508.510	−87.552
1000	32.000	207.849	186.673	21.176	1640.369	1493.952	−78.036
1100	32.585	210.927	188.740	24.406	1641.964	1479.233	−70.243
1200	33.132	213.786	190.709	27.692	1643.538	1464.370	−63.742
1300	33.634	216.458	192.588	31.031	1645.096	1449.376	−58.237
1400	34 092	218.967	194.384	34.417	1646.640	1434.263	−53.513
1500	34.507	221.334	196.102	37.848	1648.170	1419.039	−49.415
1600	34.884	223.573	197 750	41.317	1649.688	1403.714	−45.827
1700	35.225	225.698	199.332	44.823	1651.194	1388.295	−42.657
1800	35.535	227.721	200.853	48.361	1652.687	1372.787	−39.837
1900	35 817	229.650	202.319	51.929	1654.168	1357.196	−37.312
2000	36 074	231 494	203.732	55.524	1655.637	1341.528	−35.037
2100	36.311	233.259	205 096	59 143	1657.093	1325.787	−32.977
2200	36.528	234.954	206 415	62.785	1658.538	1309.977	−31.103
2300	36 729	236.582	207.691	66.448	1659.970	1294.101	−29.390
2400	36.916	238 149	208.928	70.131	1661.391	1278.163	−27.818
2500	37.090	239.660	210.127	73.831	1662.800	1262.166	−26.372
2600	37.254	241.118	211.291	77.548	1664.197	1246.113	−25.035
2700	37.408	242.526	212.422	81.282	1665.583	1230.007	−23.796
2800	37.555	243.890	213.522	85.030	1666.957	1213.849	−22.645
2900	37 695	245.210	214.592	88.792	1668.319	1197.643	−21.572
3000	37.830	246 490	215.634	92.569	1669.671	1181.389	−20.570
3100	37.960	247.733	216 649	96.358	1671.012	1165.091	−19.632
3200	38.087	248.940	217 640	100.161	1672.342	1148.750	−18.751
3300	38.211	250.114	218.606	103.976	1673.661	1132.367	−17.924
3400	38.334	251.256	219.550	107.803	1674.970	1115.945	−17.144
3500	38.455	252.369	220.471	111.642	1676.269	1099.484	−16.409
3600	38.577	253 454	221.373	115 494	1677.559	1082.986	−15.714
3700	38.698	254.513	222.254	119.358	1678.839	1066.452	−15.056
3800	38.820	255.546	223.117	123.233	1680.109	1049.884	−14.432
3900	38.943	256.556	223.961	127.122	1681.371	1033.283	−13.839
4000	39.067	257.544	224.788	131.022	1682.625	1016.649	−13.276
4100	39 193	258.510	225.599	134.935	1683.870	999.985	−12.740
4200	39.322	259.456	226.394	138.861	1685.108	983.290	−12.229
4300	39.453	260.383	227.174	142.800	1686.339	966.565	−11.741
4400	39.586	261.291	227.939	146.751	1687.563	949.812	−11.276
4500	39.723	262.183	228.690	150.717	1688.780	933.031	−10.830
4600	39.862	263.057	229.428	154.696	1689.992	916.223	−10.404
4700	40.003	263.916	230.152	158.689	1691.199	899.389	−9.996
4800	40.148	264.760	230.865	162.697	1692.401	882.530	−9.604
4900	40.296	265.589	231.565	166.719	1693.598	865.645	−9.228
5000	40.446	266.405	232.253	170.756	1694.792	848.736	−8.867
5100	40.599	267.207	232.931	174.808	1695.983	831.803	−8.519
5200	40.755	267.997	233.598	178.876	1697.172	814.846	−8.185
5300	40.913	268.775	234.254	182.959	1698.359	797.867	−7.863
5400	41.074	269.541	234.900	187.059	1699.545	780.866	−7.553
5500	41.237	270.296	235.537	191.174	1700.730	763.842	−7.254
5600	41.402	271.041	236.165	195.306	1701.915	746.797	−6.966
5700	41.569	271.775	236.783	199.455	1703.101	729.731	−6.687
5800	41.738	272.499	237.392	203.620	1704.289	712.644	−6.418
5900	41.908	273.214	237.994	207.803	1705.478	695.536	−6.158
6000	42.080	273.920	238.586	212.002	1706.671	678.409	−5.906

PREVIOUS: December 1971 (1 atm) CURRENT: December 1971 (1 bar)

Methylidyne, Ion (CH$^+$) $C_1H_1^+$(g)

$S°(298.15\ K) = 234.91 \pm 0.21\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [334 \pm 42]\ kJ{\cdot}mol^{-1}$

$\Delta_f H°(298.15\ K) = [335 \pm 42]\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights ϵ_i, cm^{-1}	g_i
0	1
[3000]	3
12288	1

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[2800] (1)
1201 (1)
815 (1)

Ground State Quantum Weight: 1 $\sigma = 1$

Point Group: C_s

Bond Distances: C–H = 1.12 Å; C–Cl = 1.689 Å

Bond Angle: H–C–Cl = 103.4°

Product of the Moments of Inertia. $I_A I_B I_C = 3.9883 \times 10^{-117}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The enthalpy of formation can be estimated as the average of those of the CH_2 and CCl_2 radicals, which gives $\Delta_f H°(CHCl, g\ 298.15\ K) = 74.5 \pm 15\ kcal{\cdot}mol^{-1}$. A better value for the enthalpy of formation can be obtained by considering the reactions $CHCl \rightarrow CH + Cl$ and $CHCl \rightarrow CCl + H$. When $\Delta_f H°(CCl, g, 298.15\ K) = 74.5\ kcal{\cdot}mol^{-1}$ is substituted into the above equations it gives $D_0°(C\text{–}Cl) = 96\ kcal{\cdot}mol^{-1}$ and $D_0°(C\text{–}H) = 98\ kcal{\cdot}mol^{-1}$. Although these values are not unreasonable, the $D_0°(C\text{–}H)$ value appears to be too high compared to that in CFH. Thus, we adopt $\Delta_f H°(CHCl, g, 298.15\ K) = 80\ kcal{\cdot}mol^{-1}$ which gives $D_0°(C\text{–}Cl) = 91\ kcal{\cdot}mol^{-1}$ and $D_0°(C\text{–}H) = 92\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

The structure and electronic levels of the molecule have been established by Merer and Travis[1] from an analysis of the rotational structure of the visible absoorption bands. The estimated triplet state is based on the electronic levels of CCl_2 and CH_2 as given in these tables. The vibrational levels are from Jacox and Milligan[2] who investigated the infrared spectrum of matrix–isolated CHCl, and also estimated the missing frequency.

The principal moments of inertia are: $I_A = 0.1780 \times 10^{-39}$, $I_B = 4.6457 \times 10^{-39}$, and $I_C = 4.8237 \times 10^{-39}\ g{\cdot}cm^2$.

References

[1] A. J. Merer and D. N. Travis, Can. J. Phys. 44, 525 (1966).
[2] M. E. Jacox and D E. Milligan, J. Chem. Phys. 47, 1626 (1967).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.154	334.441	334 441	INFINITE
100	33.267	197.591	265.877	−6.829	334.751	329.574	−172.152
200	34.185	220.819	238.182	−3.473	334.915	324.305	−84.700
250	35.365	228.567	235.509	−1.735	334.849	321.659	−67.207
298.15	36.737	234.912	234.912	0.	334.720	319.129	−55.910
300	36.792	235.139	234.912	0.068	334.714	319.032	−55.548
350	38.276	240.922	235.366	1.945	334.536	316.432	−47.225
400	39.724	246.128	236.391	3.895	334.330	313.860	−40.986
450	41.113	250.888	237.741	5.916	334.105	311.315	−36.136
500	42.461	255.290	239.278	8.006	333.867	308.795	−32.260
600	45.130	263.267	242.625	12.385	333.388	303.826	−26.450
700	47.839	270 427	246.094	17.033	332.958	298.934	−22.307
800	50.542	276.992	249.551	21.953	332.631	294.097	−19.203
900	53.113	283.095	252.943	27.137	332.433	289.294	−16.790
1000	55.427	288.814	256.247	32.567	332.369	284.505	−14.861
1100	57.404	294.192	259 454	38.211	332.426	279.717	−13.283
1200	59.013	299.258	262.562	44.035	332.578	274.919	−11.967
1300	60.262	304.034	265.571	50.002	332.799	270.105	−10.853
1400	61.187	308.535	268.480	56.077	333.062	265.273	−9.897
1500	61.837	312.780	271.294	62.230	333.341	260.421	−9.069
1600	62.264	316.786	274.013	68.437	333.617	255.551	−8.343
1700	62.515	320.569	276.641	74 677	333.874	250.663	−7.702
1800	62.634	324.146	279.182	80.935	334.100	245.762	−7.132
1900	62.656	327.533	281.638	87.201	334.287	240.849	−6.621
2000	62.610	330.746	284 014	93.464	334.427	235.927	−6.162
2100	62.517	333.799	286.313	99.721	334.518	231.000	−5.746
2200	62.393	336.705	288.538	105.967	334.557	226.069	−5.368
2300	62.253	339.475	290.693	112.199	334.544	221.138	−5.022
2400	62.103	342.121	292.781	118.417	334.477	216.209	−4.706
2500	61.952	344.653	294.806	124.620	334.357	211.283	−4.415
2600	61.803	347.080	296.770	130.807	334.185	206.364	−4.146
2700	61.659	349 410	298.677	136.980	333.962	201.451	−3.897
2800	61.522	351.650	300.529	143.139	333.688	196.549	−3.667
2900	61.394	353.807	302.329	149.285	333.367	191.656	−3.452
3000	61.274	355.886	304.080	155.418	332.998	186.776	−3.252
3100	61 162	357.893	305.783	161.540	332.584	181 908	−3.065
3200	61.060	359.833	307.442	167.651	332.126	177.055	−2.890
3300	60.965	361.711	309.059	173.752	331.626	172.217	−2.726
3400	60.878	363.529	310.634	179.845	331.086	167.394	−2.572
3500	60.798	365.293	312.171	185.928	330.508	162.588	−2.426
3600	60.725	367.005	313.670	192.004	329.893	157.799	−2.290
3700	60 657	368.668	315.134	198.073	329.245	153.028	−2.160
3800	60.595	370.284	316.564	204.136	328.564	148.274	−2.038
3900	60.538	371.858	317.962	210.193	327.854	143.539	−1.922
4000	60.486	373.390	319.329	216.244	327.115	138.822	−1.813
4100	60.438	374.883	320.666	222.290	326.349	134.124	−1.709
4200	60.393	376.338	321.974	228.331	325.560	129.445	−1.610
4300	60.351	377.759	323.255	234.369	324.747	124.785	−1.516
4400	60.312	379 146	324.509	240.402	323.914	120.145	−1.426
4500	60.276	380.501	325.739	246.431	323.062	115.523	−1.341
4600	60.242	381.825	326.943	252.457	322.192	110.921	−1.260
4700	60.211	383.121	328.125	258.480	321.307	106.337	−1.182
4800	60.181	384.388	329.284	264 499	320.407	101.773	−1.108
4900	60.152	385.629	330.421	270.516	319.495	97.227	−1.036
5000	60.125	386.844	331.538	276.530	318.570	92.701	−0.968
5100	60.100	388.034	332.634	282.541	317.636	88.193	−0.903
5200	60.075	389.201	333.710	288.550	316.692	83.703	−0.841
5300	60.052	390.345	334.768	294.556	315.741	79.231	−0.781
5400	60.029	391.467	335.808	300.560	314.783	74.778	−0.723
5500	60.007	392.568	336.830	306.562	313.819	70.342	−0.668
5600	59.986	393.649	337.835	312.562	312.850	65.924	−0.615
5700	59.966	394.711	338.823	318.559	311.877	61.524	−0.564
5800	59.946	395.754	339.796	324.555	310.901	57.140	−0.515
5900	59.927	396.778	340.753	330.548	309.923	52.773	−0.467
6000	59.908	397.785	341.695	336.540	308.943	48.423	−0.422

PREVIOUS December 1969 (1 atm) CURRENT December 1969 (1 bar)

Chlorodifluoromethane (CHClF$_2$) IDEAL GAS M_r = 86.468746 Chlorodifluoromethane (CHClF$_2$) C$_1$H$_1$Cl$_1$F$_2$(g)

$S°$(298.15 K) = 280.97 ± 0.8 J·K^{-1}·mol^{-1}

$\Delta_f H°$(0 K) = −475.3 ± 13 kJ·mol^{-1}
$\Delta_f H°$(298.15 K) = −481.6 ± 13 kJ·mol^{-1}

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
3024(1)	812(1)	1350(1)
1312(1)	598(1)	1108(1)
836(1)	417(1)	400(1)

Ground State Quantum Weight: 1 σ = 1
Point Group: C_s
Bond Distances: C–H = 1.09 Å; C–Cl = 1.74 Å; C–F = 1.35 Å
Bond Angles: H–C–Cl = 107°; Cl–C–F = 110.5°; F–C–F = 107°
Product of the Moments of Inertia: $I_A I_B I_C$ = 3.435053−10^{-114} g^3·cm^6

Enthalpy of Formation

Edwards and Small[1] determined a single equilibrium constant at 600°C for the reaction 2CHClF$_2$(g) → C$_2$F$_4$(g) + 2HCl(g). The value was was obtained by extrapolation to eliminate the effects of side reactions. The equilibrium constant was used with JANAF free energy functions[2] to obtain $\Delta_r H°$(298.15 K) = 28.75 kcal·mol^{-1}, which yields $\Delta_f H°$(CHClF$_2$, g, 298.15 K) = −115.1 kcal·mol^{-1}. An uncertainty of ±3 kcal·mol^{-1} corresponds to an uncertainty of about ±500% in the equilibrium constant.

Heat Capacity and Entropy

The gas phase vibrational frequencies have been observed in the Raman by Holzer and Moser;[3] they do not see anything in the 1350 cm^{-1} region as reported in the liquid by Glockler and Edgell.[4] Plyler and Benedict[5] in their assignment replaced 831 cm^{-1} frequency by 1178 cm^{-1}. We essentially adopt Glockler and Edgell's assignment with updated gas phase values for the observed frequencies. The microwave spectrum gas been analyzed by McLay and Mann[6] and Beeson *et al.*,[7] who derive bond lengths and angles in excellent agreement with each other. The values given by Beeson *et al.* are adopted here.

Neilson and White[8] have measured the low temperature heat capacity and heat of vaporization and have reported an entropy in the gas phase at 232.5 K of 63.91 ± 0.28 cal·K^{-1}·mol^{-1} This compares with 63.959 cal·K^{-1}·mol^{-1} calculated from our adopted functions.

The principal moments of inertia are: I_A = 8.2033 × 10^{-39}, I_B = 17.4031 × 10^{-39}, and I_C = 24.0612 × 10^{-39} g cm^2.

References

[1] J. W. Edwards and P. A. Small, Ind. Eng. Chem. Fundamentals 4, 396 (1965).
[2] JANAF Thermochemical Tables: C$_2$F$_4$(g), 6–30–96; HCl(g), 9–30–64.
[3] W. Holzer and H. Moser, J. Mol. Spectrosc. 20, 185 (1966) and 25, 123 (1968).
[4] G. Glockler and W. F. Edgell, J. Chem. Phys. 9, 224 (1941).
[5] E. K. Plyler and W. S. Benedict, J. Res. Nat. Bur. Stand. 47, 202 (1951).
[6] D. B. McLay and C. R. Mann, Can J. Phys. 40, 61 (1962).
[7] E. L Beeson, T L. Weatherly and Q. Williams, J. Chem. Phys. 37, 2926 (1962).
[8] E. F Neilson and D. White, J. Amer. Chem Soc. 79, 5618 (1957).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−12.413	−475.292	−475.292	INFINITE
100	35.011	233.244	323.826	−9.058	−477.859	−469.564	245.275
200	45.732	260.548	285.833	−5.057	−479.979	−460.404	120.245
250	51.680	271.395	281.879	−2.621	−480.848	−455.407	95.152
298.15	57.126	280.968	280.968	0.	−481.578	−450.439	78.915
300	57.328	281.322	280.969	0.106	−481.604	−450.246	78.395
350	62.496	290.554	281.687	3.104	−482.250	−444.967	66.408
400	67 107	299.207	283.342	6.346	−482.794	−439.603	57 406
450	71.156	307.350	285.561	9.805	−483.249	−434.176	50.398
500	74.683	315.034	288.128	13.453	−483.626	−428.702	44.786
600	80.420	329.181	293.813	21.221	−484.191	−417.660	36.361
700	84.813	341.923	299.791	29.492	−484.549	−406.541	30.336
800	88.253	353.481	305.791	38.152	−484.745	−395.382	25.816
900	91.004	364.041	311.685	47.120	−484.814	−384.206	22.299
1000	93.244	373.749	317.412	56.336	−484.781	−373 029	19.485
1100	95.093	382.725	322.947	65.756	−484.670	−361.858	17.183
1200	96.636	391.067	328.280	75.345	−484.498	−350.701	15.266
1300	97.935	398.855	333.413	85.075	−484.282	−339.560	13.644
1400	99.038	406.154	338.351	94.925	−484.036	−328.436	12.254
1500	99.979	413.020	343.102	104.877	−483.768	−317.331	11.050
1600	100.788	419 499	347.676	114.917	−483.488	−306.245	9.998
1700	101.488	425.631	352.083	125.031	−483.202	−295.176	9 070
1800	102.096	431.450	356.332	135.211	−482.914	−284 123	8.245
1900	102.627	436.984	360.433	145.448	−482.628	−273.088	7.508
2000	103.093	442.260	364.393	155.734	−482.346	−262.066	6.844
2100	103.505	447.300	368.222	166.065	−482.068	−251.059	6.245
2200	103.869	452.124	371.927	176.434	−481 795	−240.065	5.700
2300	104.192	456.748	375.515	186.837	−481.526	−229.083	5.203
2400	104.481	461.189	378.993	197.271	−481.260	−218.113	4.747
2500	104 740	465.460	382.367	207.732	−480.996	−207.154	4.328
2600	104.972	469.572	385.642	218.218	−480.732	−196.206	3 942
2700	105.182	473.538	388.824	228.726	−480.467	−185.268	3.584
2800	105.372	477.367	391.919	239.254	−480.199	−174.339	3.252
2900	105.544	481.067	394.929	249.800	−479.926	−163.420	2.944
3000	105.700	484.648	397.861	260.362	−479.647	−152.511	2.655
3100	105.843	488.116	400.716	270.939	−479.361	−141.612	2.386
3200	105.974	491.479	403.500	281.530	−479.065	−130.721	2.134
3300	106 093	494.742	406.216	292.134	−478.758	−119.840	1.897
3400	106.203	497.910	408.867	302.749	−478.440	−108.968	1.674
3500	106.305	500.990	411.455	313.374	−478.108	−98.106	1.464
3600	106.398	503.986	413.984	324.009	−477.761	−87.254	1.266
3700	106.484	506.903	416.456	334.654	−477.399	−76.411	1.079
3800	106.564	509.744	418.874	345.306	−477.021	−65.579	0.901
3900	106.639	512.513	421.239	355.966	−476.624	−54.757	0.733
4000	106.708	515.213	423.555	366.634	−476.209	−43.945	0.574
4100	106.772	517.849	425.823	377.308	−475.775	−33.144	0.422
4200	106.832	520.423	428.045	387.988	−475.321	−22.353	0.278
4300	106.888	522.937	430.222	398.674	−474.846	−11.574	0.141
4400	106.940	525.395	432.358	409.365	−474.349	−0.806	0.010
4500	106.989	527.799	434.452	420.062	−473.831	9.951	−0.116
4600	107.035	530.151	436.507	430.763	−473.291	20.696	−0.235
4700	107.078	532.453	438.524	441.468	−472.727	31 428	−0.349
4800	107.119	534.708	440.504	452.178	−472.141	42.149	−0.459
4900	107.157	536.917	442.449	462.892	−471.531	52.857	−0.563
5000	107.193	539.082	444.361	473.610	−470.898	63.553	−0.664
5100	107.227	541.206	446.239	484.331	−470.241	74.235	−0.760
5200	107.259	543.288	448.085	495.055	−469.560	84.905	−0.853
5300	107.289	545.331	449.901	505.782	−468.855	95.561	−0.942
5400	107.318	547.337	451.687	516.513	−468.126	106.203	−1.027
5500	107.345	549.307	453.444	527.246	−467.373	116.832	−1.110
5600	107.371	551.241	455.173	537.982	−466.596	127.447	−1.189
5700	107.395	553.142	456.875	548.720	−465.796	138.048	−1.265
5800	107.418	555.010	458.551	559.461	−464.971	148.634	−1.339
5900	107.441	556.846	460.201	570.204	−464.123	159.207	−1.410
6000	107.462	558.652	461.827	580.949	−463.251	169.764	−1.478

PREVIOUS June 1970 (1 atm) CURRENT: June 1970 (1 bar)

Chlorodifluoromethane (CHClF$_2$) C$_1$H$_1$Cl$_1$F$_2$(g)

$S°(298.15\ K) = 293.260 \pm 0.8\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [-277.7 \pm 13]\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = [-283.3 \pm 13]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
3023(1)	741(1)	1242(1)
1313(1)	455(1)	806(1)
1079(1)	270(1)	368(1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: C_s
Bond Distances. C–H = 1.09 Å; C–Cl = 1.75 Å; C–F = 1.367 Å
Bond Angles: Cl–C–Cl = 112°12'; F–C–Cl = 109°; H–C–Cl = 109°45'
Product of the Moments of Inertia: $I_A I_B I_C = 1.110094\text{–}10^{-113}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The change in enthalpy of atomization by successive replacement of F by Cl in the CF$_4$ to CCl$_4$ series follows a regular pattern (see CCl$_2$F$_2$ table). A similar pattern is to be expected in the CHF$_3$ to CHCl$_3$ series. The first replacement of the series is, in fact, 4 kcal·mol^{-1} higher than the mean versus 3.8 kcal·mol^{-1} higher in the CF$_4$–CCl$_4$ series. Thus, we have selected the atomization energy of the second and third replacements to continue this pattern. In this manner we have selected the atomization energy of CHCl$_2$F as 367.4 kcal·mol^{-1} which corresponds to $\Delta_f H°$(CHCl$_2$F, g, 298.15 K) = −67.7 kcal mol^{-1}. With this adopted value, the successive replacement of F by Cl changes the enthalpy of atomization by 41.4, 37.3 and 33.0 kcal·mol^{-1}.

Heat Capacity and Entropy

Holzer[1] has reported the gas phase Raman spectra which is in excellent agreement with the assignments of Plyler and Benedict.[2] The only discrepancy is in ν_7, which Plyler and Benedict assign at 1242 cm^{-1}, and Holzer[1] does not report a band in this region. Holzer does, however, report a band at 728 cm^{-1} which has not been reported in the earlier liquid studies. There is strong evidence from correlations with CHCl$_3$ and CHF$_3$ that two frequencies should occur between 1220 and 1376 cm^{-1}. On this basis we adopt the assignment of Plyler and Benedict for ν_7, while accepting the gas phase values of Holzer for the other frequencies. The extra band at 728 cm^{-1} is not used. It is probable that the bands at 741 and 728 cm^{-1} are due to the Fermi resonance of ν_4 with $2\nu_9$; the unperturbed level would lie at 735 cm^{-1}. The symmetry classes of ν_4 and $2\nu_9$ are identical and thus Fermi resonance is allowed.

McLay[3] has reported the molecular structure from his microwave investigations. The principle moments of inertia are: $I_A = 12.028 \times 10^{-39}$, $I_B = 25.7010 \times 10^{-39}$, and $I_C = 35.9855 \times 10^{-39}\ g{\cdot}cm^2$.

References

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[2] E. K. Plyler and W. S. Benedict, J. Res. Nat. Bur. Stand. 47, 202 (1951).
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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−13.293	−277.672	−277.672	INFINITE
100	37.673	241.161	339.849	−9.869	−280.172	−271.738	141.941
200	50.180	271.154	298.501	−5.469	−281.948	−262.564	68.575
250	55.897	282.973	294.236	−2.816	−282.659	−257.633	53.830
298.15	60.995	293.260	293.260	0.	−283.257	−252.758	44.282
300	61.182	293.638	293.261	0.113	−283.278	−252.569	43.976
350	65.973	303.436	294.024	3.294	−283.806	−247.407	36.924
400	70.228	312.529	295 776	6.701	−284.245	−242.177	31.625
450	73.950	321.021	298.114	10.308	−284.606	−236.896	27.498
500	77.184	328.983	300.807	14.088	−284.900	−231.578	24.193
600	82.432	343.542	306.740	22.081	−285.319	−220.871	19.229
700	86.446	356.563	312.944	30.534	−285.556	−210.108	15.678
800	89.594	368.320	319.143	39.342	−285.650	−199.322	13.014
900	92.119	379.024	325.211	48.432	−285.629	−188.532	10.942
1000	94.182	388.840	331.090	57.750	−285.517	−177 748	9.285
1100	95.891	397.899	336.757	67.256	−285.334	−166.980	7.929
1200	97.322	406.306	342.206	76.919	−285 097	−156.230	6.801
1300	98.530	414.145	347.442	86.713	−284.819	−145.502	5.846
1400	99.558	421.485	352.471	96.619	−284.512	−134.797	5.029
1500	100.438	428.385	357.305	106.620	−284.186	−124.115	4.322
1600	101.195	434.891	361.952	116.702	−283.848	−113.454	3.704
1700	101.851	441.047	366.426	126.856	−283.505	−102.815	3.159
1800	102.422	446.885	370.735	137.070	−283.162	−92.196	2.675
1900	102.922	452.436	374.890	147.338	−282.822	−81.596	2.243
2000	103.361	457.727	378.901	157.652	−282.490	−71.014	1.855
2100	103.748	462.779	382.775	168.008	−282.168	−60 448	1.504
2200	104.091	467.614	386.523	178.400	−281.857	−49.898	1.185
2300	104.397	472.248	390.150	188.825	−281.560	−39.361	0.894
2400	104.669	476.697	393.664	199.279	−281.277	−28.836	0.628
2500	104.914	480.974	397.071	209.758	−281.010	−18.324	0.383
2600	105.134	485.094	400.378	220.261	−280.759	−7.821	0 157
2700	105.332	489.065	403.590	230.784	−280.525	2.672	−0.052
2800	105.511	492.899	406.711	241.326	−280.308	13.157	−0.245
2900	105.674	496.605	409.747	251.886	−280.108	23.634	−0.426
3000	105.822	500.190	412.703	262.461	−279.925	34.105	−0.594
3100	105.958	503.662	415.581	273.050	−279.758	44.570	−0.751
3200	106.081	507.028	418.387	283.652	−279.606	55.029	−0.898
3300	106.195	510.294	421.122	294.266	−279.468	65.485	−1.037
3400	106.299	513.466	423.792	304.890	−279.343	75.936	−1.167
3500	106.395	516.548	426.398	315.525	−279.228	86.383	−1.289
3600	106.483	519.547	428.944	326.169	−279.123	96.828	−1.405
3700	106.565	522.465	431.433	336.822	−279.026	107.270	−1.514
3800	106.641	525.308	433.866	347.482	−278.933	117.709	−1 618
3900	106.711	528.079	436.246	358.150	−278.844	128.146	−1.716
4000	106.777	530.782	438.576	368.824	−278.755	138.580	−1.810
4100	106.838	533.419	440.857	379.505	−278.666	149.013	−1.898
4200	106.895	535.994	443.092	390.191	−278.572	159.443	−1.983
4300	106.948	538.510	445.282	400.884	−278.473	169.870	−2.064
4400	106.997	540.970	447.429	411.581	−278.366	180.296	−2.140
4500	107.044	543.375	449.534	422.283	−278.249	190.719	−2.214
4600	107.087	545.728	451.600	432.990	−278.120	201.139	−2.284
4700	107.128	548.031	453.627	443.700	−277.978	211.556	−2.351
4800	107.167	550.287	455.617	454.415	−277.819	221.970	−2.416
4900	107.203	552.497	457.572	465.134	−277.643	232.380	−2.477
5000	107.237	554.663	459.492	475.856	−277.449	242.787	−2.536
5100	107.269	556.787	461.379	486.581	−277.234	253.190	−2.593
5200	107.300	558.871	463.234	497.310	−276.998	263.588	−2.648
5300	107.329	560.915	465.058	508.041	−276.739	273.981	−2.700
5400	107.356	562.921	466.852	518.775	−276.457	284.370	−2.751
5500	107.382	564.891	468.616	529.512	−276.150	294.752	−2.799
5600	107.406	566.826	470.353	540.252	−275.818	305.130	−2.846
5700	107.430	568.728	472.062	550.993	−275.460	315.500	−2.891
5800	107.452	570.596	473.745	561.737	−275.075	325.865	−2.935
5900	107.473	572.433	475.402	572.484	−274.662	336.222	−2.977
6000	107.493	574.240	477.034	583.232	−274.222	346.572	−3.017

PREVIOUS: June 1970 (1 atm) CURRENT June 1970 (1 bar)

Trichloromethane (CHCl$_3$) IDEAL GAS M_r = 119.37794 Trichloromethane (CHCl$_3$) C$_1$H$_1$Cl$_3$(g)

$S°(298.15\text{ K}) = 295.620 \pm 0.04\ \text{J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0\text{ K}) = -98.27 \pm 1.3\ \text{kJ·mol}^{-1}$
$\Delta_f H°(298.15\text{ K}) = -103.18 \pm 1.3\ \text{kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}
3034(1)	1220
680(1)	774
363(1)	261

Ground State Quantum Weight: 1 $\sigma = 3$
Point Group: C_{3v}
Bond Distances: C–H = 1.100 Å; C–Cl = 1.758 Å
Bond Angles Cl–C–Cl = 111°18', H–C–Cl = 107°34'
Product of the Moments of Inertia. $I_A I_B I_C = 3.282103 \times 10^{-113}\ \text{g}^3\text{·cm}^6$

Enthalpy of Formation

Hu and Sinke[1] have measured the enthalpy of combustion of CHCl$_3$(l) in the rotating bomb calorimeter, using As$_2$O$_3$ solution as the reducing agent. The reported $\Delta_c H°(298.15\text{ K}) = -113.10\ \text{kcal·mol}^{-1}$ for $\text{CHCl}_3(\text{l}) + 0.5\text{O}_2(\text{g}) + \text{H}_2\text{O(l)} \rightarrow \text{CO}_2(\text{g}) + 3\text{HCl(aq, }600\text{H}_2\text{O)}$ which leads to $\Delta_f H°(\text{CHCl}_3\text{, l, }298.15\text{ K}) = -32.10\ \text{kcal mol}^{-1}$, using $\Delta_f H°(298.15\text{ K}) = -94.051, -39.823, -68.315\ \text{kcal·mol}^{-1}$ for CO$_2$(g), HCl(aq, 600H$_2$O) and H$_2$O(l), respectively.[2] The standard deviation of six combustion runs was 0.09 kcal·mol^{-1}. Employing the heat of vaporization of chloroform at 298.15 K as 7.44 kcal·mol^{-1},[3] we obtain $\Delta_f H°(\text{CHCl}_3\text{, g, }298.15\text{ K}) = -24.66\ \text{kcal·mol}^{-1}$ (-103.177 ± 1.3 kJ·mol^{-1}) which is adopted in the tabulation.

Simth *et al.*,[4] based on the combustion data of Eftring,[5] re-evaluated the enthalpy of combustion of chloroform at 18.7°C as $\Delta_c E/M° = -947.7\ \text{cal K}^{-1}\text{·mol}^{-1}$ for $\text{CHCl}_3(\text{l}) + 0.5\text{O}_2(\text{g}) + \text{H}_2\text{O(l)} \rightarrow \text{CO}_2(\text{g}) + 3\text{HCl(aq, }600\text{H}_2\text{O)}$. This value needs to be further corrected for a change in the enthalpy of oxidation of As$_2$O$_3$[6] and calculated to 25°C to give $\Delta_c H°(298.15\text{ K}) = -113.44\ \text{kcal·mol}^{-1}$, $\Delta_f H°(\text{CHCl}_3\text{, l, }298.15\text{ K}) = -31.76\ \text{kcal·mol}^{-1}$ and $\Delta_f H°(\text{CHCl}_3\text{, g, }298.15\text{ K}) = -24.32\ \text{kcal·mol}^{-1}$.

Heat Capacity and Entropy

The assigned fundamental vibrational frequencies are obtained from Shimanouchi's selection,[7] based on the infrared and Raman spectra measured by Nielson and Ward,[8] Madigan and Cleveland,[9] Gibian and McKinney,[10] and Stanevich and Yaroslaviskii.[11]

The bond distances and angles were obtained from the microwave spectra by Jen and Lide.[12] The principle moments of inertia are: $I_A = I_B = 25.7217 \times 10^{-39}$ and $I_C = 49.6081 \times 10^{-39}\ \text{g·cm}^2$.

References

[1] A. T. Hu and G. C. Sinke, presented at the 23rd Calorimetry Conference, Midland, MI (1968).
[2] U. S. Nat. Bur. Stand. Tech. Note 270-3 (1968).
[3] J. H. Mathews, J. Am. Chem. Soc. 48, 562 (1926).
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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0	0.	INFINITE	-14.153	-98.275	-98.275	INFINITE
100	40.321	239.353	345.889	-10.654	-100.702	-91.155	47.614
200	54.302	271.795	301.259	-5.893	-102.171	-80.983	21.151
250	60.243	284.561	296.668	-3.027	-102.727	-75.620	15.800
298.15	65.383	295.620	295.620	0	-103.177	-70.357	12.326
300	65.568	296.025	295.621	0.121	-103.193	-70.154	12.215
350	70.235	306.492	296.437	3.519	-103.569	-64.616	9.643
400	74.255	316.139	298.305	7.134	-103.861	-59.031	7.709
450	77.685	325.089	300.790	10.935	-104.083	-53.413	6.200
500	80.609	333.429	303.641	14.894	-104.246	-47.774	4.991
600	85.262	348.558	309.893	23.199	-104.432	-36.459	3.174
700	88.772	361.977	316.394	31.908	-104.472	-25.125	1.875
800	91.513	374.017	322.857	40.928	-104.399	-13.794	0.901
900	93.716	384.927	329.157	50.193	-104.236	-2.477	0.144
1000	95.524	394.898	335.240	59.658	-104.001	8.817	-0.461
1100	97.031	404.075	341.086	69.288	-103.710	20.085	-0.954
1200	98.299	412.574	346.693	79.056	-103.375	31.325	-1.364
1300	99.376	420.485	352.069	88.941	-103.007	42.535	-1.709
1400	100.296	427.884	357.223	98.926	-102.617	53.717	-2.004
1500	101.086	434.832	362.168	108.996	-102.212	64.869	-2.259
1600	101.770	441.378	366.916	119.140	-101.798	75.994	-2.481
1700	102.363	447.566	371.479	129.347	-101.383	87.094	-2.676
1800	102.881	453.432	375.871	139.610	-100.970	98.169	-2.849
1900	103.336	459.007	380.101	149.921	-100.565	109.221	-3.003
2000	103.735	464.318	384.180	160.275	-100.172	120.252	-3.141
2100	104.089	469.388	388.118	170.667	-99.794	131.264	-3.265
2200	104.402	474.237	391.923	181.092	-99.436	142.258	-3.378
2300	104.682	478.885	395.604	191.546	-99.102	153.236	-3.480
2400	104.932	483.345	399.167	202.027	-98.795	164.201	-3.574
2500	105.156	487.633	402.621	212.532	-98.518	175.153	-3.660
2600	105.358	491.762	405.970	223.058	-98.273	186.095	-3.739
2700	105.540	495.741	409.222	233.603	-98.065	197.029	-3.812
2800	105.705	499.583	412.381	244.165	-97.893	207.955	-3.879
2900	105.855	503.295	415.452	254.743	-97.761	218.875	-3.942
3000	105.991	506.886	418.440	265.336	-97.669	229.792	-4.001
3100	106.116	510.363	421.350	275.941	-97.616	240.706	-4.056
3200	106.230	513.734	424.184	286.559	-97.604	251.620	-4.107
3300	106.335	517.004	426.948	297.187	-97.630	262.534	-4.156
3400	106.431	520.180	429.643	307.825	-97.695	273.448	-4.201
3500	106.519	523.267	432.275	318.473	-97.794	284.366	-4.244
3600	106.601	526.269	434.844	329.129	-97.927	295.286	-4.284
3700	106.677	529.190	437.355	339.793	-98.091	306.211	-4.323
3800	106.747	532.036	439.809	350.464	-98.282	317.140	-4.359
3900	106.812	534.810	442.209	361.142	-98.497	328.075	-4.394
4000	106.872	537.515	444.558	371.826	-98.732	339.016	-4.427
4100	106.929	540.155	446.858	382.516	-98.984	349.963	-4.459
4200	106.981	542.732	449.110	393.212	-99.249	360.916	-4.489
4300	107.030	545.250	451.317	403.913	-99.524	371.876	-4.517
4400	107.076	547.711	453.480	414.618	-99.804	382.842	-4.545
4500	107.119	550.118	455.601	425.328	-100.086	393.814	-4.571
4600	107.160	552.473	457.681	436.042	-100.367	404.793	-4.597
4700	107.198	554.778	459.722	446.760	-100.643	415.777	-4.621
4800	107.233	557.035	461.726	457.481	-100.910	426.768	-4.644
4900	107.267	559.246	463.694	468.206	-101.167	437.764	-4.667
5000	107.299	561.414	465.627	478.935	-101.410	448.765	-4.688
5100	107.328	563.539	467.526	489.666	-101.636	459.771	-4.709
5200	107.357	565.623	469.392	500.400	-101.843	470.781	-4.729
5300	107.383	567.668	471.227	511.137	-102.029	481.795	-4.748
5400	107.409	569.676	473.032	521.877	-102.191	492.812	-4.767
5500	107.433	571.647	474.807	532.619	-102.329	503.832	-4.785
5600	107.455	573.583	476.554	543.363	-102.440	514.854	-4.802
5700	107.477	575.485	478.273	554.110	-102.523	525.878	-4.819
5800	107.497	577.354	479.965	564.859	-102.576	536.903	-4.835
5900	107.517	579.192	481.631	575.609	-102.598	547.929	-4.851
6000	107.535	580.999	483.272	586.362	-102.590	558.954	-4.866

PREVIOUS: December 1968 (1 atm) CURRENT December 1968 (1 bar)

Fluoromethylene (CHF) IDEAL GAS $M_r = 32.017343$

$S°(298.15\ K) = 223.35 \pm 0.21\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = [125.2 \pm 29]\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [125.5 \pm 29]\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights ν_i, cm^{-1}	g_i
0	1
[10000]	3
17287	1

Vibrational Frequencies and Degeneracies ν, cm^{-1}
714.52(1)
378.3 (2)
2215.5 (1)

Point Group: C_s $\sigma = 1$
Bond Distances. C–H = 1.121 Å; C–F = 1.314 Å
Bond Angle: H–C–F = 101.6°
Product of the Moments of Inertia: $I_A I_B I_C = 1.0217 \times 10^{-117}\ g^3 \cdot cm^6$

Enthalpy of Formation

The enthalpy of formation can be estimated as the average of the CH_2 and CF_2 radicals, which gives $\Delta_f H°(CHF, g, 298.15\ K) = 25 \pm 20$ kcal·mol^{-1}. A better value for the enthalpy of formation can be obtained by considering bond energies $CHF \rightarrow CH + F \rightarrow CF + H$. When $\Delta_f H°(CHF, g, 298.15\ K) = 25$ kcal·mol^{-1} is substituted into the above equation it gives $D_0°(CF) = 136$ kcal·mol^{-1} and $D_0°(CH) = 86$ kcal·mol^{-1}. These are not unreasonable values but are probably close to the upper and lower limits respectively. A value of $\Delta_f H°(CHF, g, 298.15\ K) = 30$ kcal·mol^{-1} gives $D_0°(CF) = 131$ kcal·mol^{-1} and $D_0°(CH) = 81$ kcal·mol^{-1} which are more probable since both fall within the bonds of normal bond strengths. The strongest established C–F bond is 135 kcal·mol^{-1} in CF_3 and the weakest established C–H bond is 80 kcal·mol^{-1} in CH. We adopt $\Delta_f H°(CHF, g, 298.15\ K) = 30 \pm 7$ kcal·mol^{-1} (125.520 kJ·mol^{-1}).

Heat Capacity and Entropy

The structure and electronic levels of the molecule have been established by Merer and Travis[1] from an analysis of the rotational structure of the visible absorption basis. The estimated triplet state is based on the electronic levels of CF_2 and CH_2 as given in these tables. The vibrational levels are from Merer and Travis[1] and Jacox and Milligan,[2] the latter investigated the infrared spectrum of matrix-isolated HCF and also estimated the missing frequency.

The principal moments of inertia are: $I_A = 0.1795 \times 10^{-39}$, $I_B = 2.2980 \times 10^{-39}$, and $I_C = 2.4774 \times 10^{-39} g \cdot cm^2$.

References

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Fluoromethylene (CHF) $C_1H_1F_1(g)$

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−9.982	125.235	125.235	INFINITE
100	33.258	186.756	253.322	−6.657	125.548	120.522	−62.954
200	33.415	209.828	226.465	−3.327	125.739	115.396	−30.138
250	33.855	217.325	223.913	−1.647	125.675	112.816	−23.572
298.15	34.604	223.348	223.348	0.	125.520	110.352	−19.333
300	34.639	223.562	223.349	0.064	125.513	110.258	−19.198
350	35.681	228.978	223.774	1.821	125.280	107.733	−16.078
400	36.860	233.818	224.732	3.634	124.998	105.245	−13.744
450	38.079	238.230	225.990	5.508	124.679	102.795	−11.932
500	39.277	242.304	227.421	7.442	124.334	100.382	−10.487
600	41.503	249.666	230.528	11.483	123.596	95.660	−8.328
700	43.461	256.214	233.738	15.733	122.829	91.064	−6.795
800	45.165	262.132	236.923	20.167	122.060	86.579	−5.653
900	46.649	267.539	240.029	24.759	121.303	82.190	−4.770
1000	47.940	272.522	243.032	29.490	120.564	77.883	−4.068
1100	49.066	277.146	245.926	34.342	119.843	73.650	−3.497
1200	50.052	281.458	248.709	39.299	119.136	69.482	−3.024
1300	50.922	285.499	251.385	44.348	118.442	65.373	−2.627
1400	51.701	289.302	253.959	49.480	117.757	61.316	−2.288
1500	52.408	292.894	256.436	54.686	117.079	57.308	−1.996
1600	53.063	296.297	258.822	59.960	116.408	53.345	−1.742
1700	53.680	299.533	261.122	65.297	115.744	49.425	−1.519
1800	54.273	302.618	263.343	70.695	115.088	45.542	−1.322
1900	54.851	305.568	265.488	76.151	114.443	41.696	−1.146
2000	55.422	308.396	267.563	81.665	113.811	37.884	−0.989
2100	55.990	311.113	269.573	87.235	113.197	34.103	−0.848
2200	56.557	313.731	271.521	92.863	112.604	30.350	−0.721
2300	57.126	316.258	273.411	98.547	112.035	26.624	−0.605
2400	57.696	318.701	275.248	104.288	111.494	22.923	−0.499
2500	58.265	321.068	277.033	110.086	110.984	19.243	−0.402
2600	58.832	323.364	278.771	115.941	110.509	15.583	−0.313
2700	59.394	325.595	280.465	121.852	110.071	11.940	−0.231
2800	59.949	327.765	282.115	127.820	109.672	8.313	−0.155
2900	60.494	329.878	283.726	133.842	109.313	4.700	−0.085
3000	61.027	331.938	285.299	139.918	108.995	1.098	−0.019
3100	61.544	333.948	286.836	146.047	108.719	−2.494	0.042
3200	62.043	335.910	288.339	152.226	108.485	−6.078	0.099
3300	62.523	337.826	289.810	158.455	108.291	−9.655	0.153
3400	62.982	339.700	291.250	164.730	108.138	−13.227	0.203
3500	63.417	341.532	292.660	171.050	108.023	−16.794	0.251
3600	63.828	343.324	294.043	177.413	107.945	−20.359	0.295
3700	64.214	345.078	295.398	183.815	107.903	−23.923	0.338
3800	64.575	346.795	296.728	190.255	107.894	−27.486	0.378
3900	64.909	348.477	298.034	196.729	107.915	−31.048	0.416
4000	65.218	350.124	299.316	203.236	107.965	−34.612	0.452
4100	65.500	351.738	300.574	209.772	108.041	−38.177	0.486
4200	65.757	353.320	301.812	216.335	108.140	−41.745	0.519
4300	65.989	354.870	303.028	222.923	108.260	−45.315	0.550
4400	66.196	356.389	304.223	229.532	108.399	−48.888	0.580
4500	66.380	357.879	305.399	236.161	108.553	−52.464	0.609
4600	66.541	359.340	306.556	242.807	108.721	−56.044	0.636
4700	66.681	360.773	307.694	249.469	108.900	−59.628	0.663
4800	66.799	362.178	308.815	256.143	109.087	−63.216	0.688
4900	66.898	363.556	309.918	262.828	109.282	−66.807	0.712
5000	66.979	364.908	311.004	269.522	109.481	−70.403	0.735
5100	67.042	366.235	312.074	276.223	109.684	−74.003	0.758
5200	67.089	367.538	313.128	282.930	109.887	−77.606	0.780
5300	67.120	368.816	314.167	289.640	110.090	−81.214	0.800
5400	67.138	370.071	315.191	296.353	110.291	−84.825	0.821
5500	67.142	371.303	316.200	303.067	110.489	−88.441	0.840
5600	67.134	372.513	317.194	309.781	110.683	−92.059	0.859
5700	67.115	373.701	318.175	316.494	110.871	−95.681	0.877
5800	67.085	374.868	319.143	323.204	111.052	−99.307	0.894
5900	67.047	376.014	320.097	329.910	111.226	−102.935	0.911
6000	67.000	377.141	321.038	336.613	111.392	−106.566	0.928

PREVIOUS: December 1969 (1 atm)   CURRENT· December 1969 (1 bar)

Formyl Fluoride (HCOF) **IDEAL GAS** $M_r = 48.016743$ **Formyl Fluoride (HCOF)** $C_1H_1F_1O_1(g)$

$S°(298.15\ K) = 246.520 \pm 0.8\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [-372.964]\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = [-376.560]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}
2981 (1)	1064.8(1)
1836.9(1)	662.5(1)
1342.5(1)	[1030] (1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: C_1
Bond Distances: C–F = 1.31 ± 0.02 Å; C–O = 1.183 ± 0.003 Å; C–H = 1.10 ± 0.02 Å
Bond Angles: F–C–O = 122.7 ± 0.05°; H–C–F = 108.3 ± 3°; H–C–O = 129 ± 3°
Product of the Moments of Inertia: $I_A I_B I_C = 4.96336 \times 10^{-116}\ g^3{\cdot}cm^6$

Enthalpy of Formation

$\Delta_f H°$ for III was estimated to be the average of the $\Delta_r H$'s of I and II.
(I) $CH_2O(g) = CO(g) + 2\ H(g)$ 106 kcal·mol^{-1}
(II) $CF_2O(g) = CO(g) + 2\ F(g)$ 162 kcal·mol^{-1}
(III) $CHFO(g) = CO(g) + F(g) + H(g)$ [134] kcal·mol^{-1}

The auxiliary $\Delta_f H°(298.15\ K)$ of $CH_2O = -28$, H = 52, F = 19, CO = −26, $CF_2O = -150$ kcal·mol^{-1} was used. See the respective sheets for details. The estimated enthalpy of formation is consistent with the instability of CHFO(g) at room temperature.

Heat Capacities and Entropies

The molecular structural parameters were obtained by LeBlanc *et al.*[1] from combining the results of microwave measurements with those of electron diffraction determined by Jones *et al.*[2] Agreement within the assigned uncertainties was obtained by Stratton and Nielsen[3] on the basis of infrared measurements.

Five of the fundamentals were observed by Stratton and Nielsen[3] in agreement with those obtained by Morgan *et al.*[4] The estimated frequency was based upon the observed value of 857.4 cm^{-1} for the fundamental in the infrared spectrum of the deuterated compound and the application of the Teller–Redlich isotope rule. The principal moments of inertia are:

$$I_A = 0.9081 \times 10^{-39},\ I_B = 6.9527 \times 10^{-39},\ \text{and}\ I_C = 7.8608 \times 10^{-39}\ g{\cdot}cm^2.$$

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	$S°$ (J·K⁻¹mol⁻¹)	$-[G°-H°(T_r)]/T$ (J·K⁻¹mol⁻¹)	$H°-H°(T_r)$ (kJ·mol⁻¹)	$\Delta_f H°$ (kJ·mol⁻¹)	$\Delta_f G°$ (kJ·mol⁻¹)	log K_f
0	0.	0.	INFINITE	−10.443	−372.964	−372.964	INFINITE
100	33.314	207.960	279.124	−7.116	−374.103	−372.583	194.617
200	35.452	231.500	250.043	−3.709	−375.288	−370.617	96.795
250	37.759	239.647	247.170	−1.881	−375.934	−369.375	77.177
298.15	40.414	246.520	246.520	0.	−376.560	−368.054	64.482
300	40.521	246.771	246.521	0.075	−376.584	−368.002	64.075
350	43.451	253.236	247.025	2.174	−377.213	−366.521	54.700
400	46.351	259.229	248.180	4.419	−377.810	−364.952	47.658
450	49.110	264.849	249.723	6.807	−378.373	−363.311	42.172
500	51.678	270.158	251.504	9.327	−378.903	−361.609	37.777
600	56.197	279.992	255.446	14.728	−379.861	−358.058	31 172
700	59.958	288.946	259.601	20.541	−380.693	−354.356	26.442
800	63.083	297.163	263.790	26.698	−381.406	−350.544	22.888
900	65.689	304.748	267.925	33 141	−382.016	−346.649	20.119
1000	67.874	311.785	271.963	39.822	−382.535	−342.690	17.900
1100	69 714	318.343	275.885	46.704	−382.981	−338.684	16.083
1200	71.270	324.478	279.682	53.755	−383.367	−334.639	14.566
1300	72.594	330.236	283.351	60.950	−383.708	−330.564	13.282
1400	73.724	335 658	286.896	68.268	−384.014	−326.465	12.181
1500	74.694	340.779	290.319	75.690	−384.297	−322.344	11.225
1600	75.531	345.627	293.625	83.202	−384.563	−318.205	10.388
1700	76.256	350.228	296.821	90.792	−384.820	−314 050	9.650
1800	76.888	354.605	299.910	98.450	−385.074	−309.880	8.992
1900	77.441	358.777	302.900	106.167	−385.328	−305.696	8.404
2000	77.926	362.762	305.794	113.936	−385.585	−301.498	7.874
2100	78.355	366.575	308.598	121.751	−385.848	−297.287	7.395
2200	78.734	370.229	311.317	129.605	−386.118	−293.063	6.958
2300	79.072	373.736	313.955	137.496	−386.396	−288.827	6.559
2400	79.374	377.108	316.517	145.419	−386.682	−284.579	6.194
2500	79 644	380.354	319.006	153.370	−386.976	−280.319	5.857
2600	79.887	383.482	321.426	161.347	−387.277	−276.047	5.546
2700	80.106	386.501	323.781	169.346	−387.585	−271.763	5.258
2800	80.304	389.418	326.073	177.367	−387.900	−267.467	4.990
2900	80.484	392.239	328.306	185 407	−388.220	−263.161	4.740
3000	80.648	394.971	330.483	193.463	−388.546	−258.842	4.507
3100	80.797	397.618	332.606	201.536	−388.876	−254.513	4.289
3200	80.934	400.185	334.678	209.622	−389.211	−250.174	4.084
3300	81.059	402.678	336.701	217.722	−389.549	−245.824	3.891
3400	81.174	405.099	338.677	225.834	−389.890	−241.463	3.710
3500	81.280	407.454	340.609	233.957	−390.234	−237.093	3.538
3600	81.377	409.745	342.498	242.089	−390.580	−232.713	3.377
3700	81.468	411.976	344.345	250.232	−390.930	−228.323	3.223
3800	81.551	414.149	346.154	258.383	−391.282	−223.923	3.078
3900	81.629	416.269	347.925	266.542	−391.637	−219.514	2.940
4000	81.701	418.336	349.659	274.708	−391.995	−215.096	2.809
4100	81.768	420.355	351.359	282.882	−392.356	−210.669	2.684
4200	81.831	422.326	353.025	291.062	−392.721	−206.233	2.565
4300	81.889	424.252	354.659	299.248	−393.089	−201.789	2.451
4400	81.944	426.135	356.263	307.440	−393.461	−197.336	2.343
4500	81.995	427.977	357.836	315.637	−393.838	−192.875	2.239
4600	82.043	429.780	359.380	323.838	−394.219	−188.405	2.139
4700	82.088	431.545	360.897	332.045	−394.606	−183.926	2.044
4800	82.131	433.274	362.387	340.256	−394.999	−179.439	1.953
4900	82.171	434.968	363.851	348.471	−395.399	−174.944	1.865
5000	82.208	436.628	365.290	356.690	−395.805	−170.441	1.781
5100	82.244	438.256	366.705	364.913	−396.218	−165.929	1.699
5200	82.278	439.854	368.096	373.139	−396.639	−161.410	1.621
5300	82.309	441.421	369.465	381.368	−397.069	−156.882	1.546
5400	82.339	442.960	370.812	389.601	−397.508	−152.346	1.474
5500	82.368	444.471	372.137	397.836	−397.956	−147.803	1.404
5600	82.395	445.955	373.442	406.074	−398.413	−143.250	1.336
5700	82.420	447.414	374.727	414.315	−398.882	−138.690	1.271
5800	82.445	448.848	375.993	422.558	−399.361	−134.120	1.208
5900	82.468	450.257	377.240	430.804	−399.852	−129.544	1.147
6000	82.490	451.643	378.468	439.052	−400.355	−124.958	1.088

PREVIOUS. June 1961 (1 atm) CURRENT June 1961 (1 bar)

Formyl Fluoride (HCOF) $C_1H_1F_1O_1(g)$

$S°(298.15\ K) = 259.657 \pm 0.34\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = [-690.10 \pm 3.3\ kJ{\cdot}mol^{-1}$

$\Delta_fH°(298.15\ K) = -697.05 \pm 3.3\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}
3035(1)	1376(2)
1137(1)	1152(2)
700(1)	508(2)

Ground State Quantum Weight: 1 $\sigma = 3$

Point Group: C_{3v}

Bond Distances: C–F = 1.333 Å; C–H = 1.098 Å

Bond Angles: F–C–F = 108.6 ± 0.5°; F–C–H = 110.33°

Product of the Moments of Inertia: $I_AI_BI_C = 9.722739 \times 10^{-115}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The selected value is obtained from least squares, simultaneous adjustment of the enthalpies of formation of CF$_3$, CF$_3$X (X=H,Cl,Br,I,CF$_3$) and C$_2$F$_4$. Details of the input data and the adjustment are given in Syverud's study.[1] Trifluoromethane is linked to HF(aq, 21.5 H$_2$O) by calorimetric data, to CBrF$_3$(g) and CF$_3$I(g) by equilibrium data, and to CF$_3$(g) by kinetic data. Neugebauer and Margrave[2] reported calorimetric data for $CHF_3(g) + 0.5\ O_2(g) + H_2O(l) = CO_2(g) + 3HF(aq, 21.5\ H_2O)$, where CF$_4$ was also formed in a competing reaction. Recalculation of the original data with $\Delta_fH°(CF_4, g, 298.15\ K) = -223.0\ kcal\ mol^{-1}$ yields the mean value $\Delta_fH°(298.15\ K) = -90.35 \pm 0.7\ kcal{\cdot}mol^{-1}$, but the individual values of $\Delta_rH°$ show a disturbing trend with the amount of competing reaction. Possible causes for the trend include corrosion and error in the analysis of the reaction products. Calibration was done in the presence of HF in an attempt to eliminate the heat due to corrosion. Because of this unexplained trend, we increase the uncertainty to ± 1.0 kcal·mol^{-1}. Goy *et al.*[3] and Coomber and Whittle[4] determined equilibrium data for $CHF_3(g) + X_2(g) = CF_3X(g) + HX(g)$ where X = I and Br. Kinetic data pertinent to CHF$_3$ are noted on the table for CF$_3$(g).

Heat Capacity and Entropy

The molecular strcuture has been derived from electron–diffraction data by Thorton[5] and from microwave data by Ghosh *et al.*[6] The results are in close agreement with and average values are adopted. Vibrational frequencies are from the assignment of Long *et al.*[7] who reviewed the spectral data and gave force–constant calculations. Preferences have been given to the gas–phase spectra, particularly the Raman data of Claassesn and Nielsen.[8] Shimanouchi[9] assigned $\nu_2 = 1117$ rather than 1137 cm^{-1}, but he apparently did not consider previous gas–phase data.[8,10] The principal moments of inertia are: $I_A = I_B = 8.1086 \times 10^{-39}$ and $I_C = 14.7875 \times 10^{-39}\ g{\cdot}cm^2$.

Valentine *et al.*[11] used low–temperature calorimetric data to derive the ideal gas entropy at the normal boiling point of 190.97 K. The experimental value of 57.18 cal·K^{-1}·mol^{-1} is in good agreement with 57.216 cal·K^{-1}·mol^{-1} obtained from this table. Schwing[12] measured $C_p°$ for CHF$_3$ vapor (25–100°C) and confirmed that the vibrational assignment is adequate. Uncertainty in the $C_p°$ and $S°$ increases at higher temperatures due to neglect of anharmonicity in the calculations. Discussions of anharmonic contributions are given on the tables for CF$_4$(g) and CClF$_3$(g). The error probably does not exceed 0.3 cal·K^{-1}·mol^{-1}in $S°$ at 1000 K. $C_p°$ is consistent with $C_p°$ measured at 300 K by the wire–ribbon method.[13]

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Enthalpy Reference Temperature = T_r = 298.15 K						Standard State Pressure = $p°$ = 0.1 MPa	
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−11.564	−690.096	−690.096	INFINITE
100	33.889	215.987	298.282	−8.230	−692.682	−683.593	357.072
200	41.227	241.391	264.002	−4.522	−695.041	−673.566	175.917
250	46.139	251.112	260.470	−2.339	−696.106	−668.072	139.586
298.15	51.040	259.657	259.657	0.	−697.054	−662.586	116.082
300	51.228	259.973	259.658	0.095	−697.089	−662.372	115.329
350	56.250	268.250	260.300	2.782	−697.980	−656.514	97.979
400	61.000	276.075	261.787	5.715	−698.773	−650.535	84.951
450	65.358	283.515	263.791	8.876	−699.472	−644.462	74.807
500	69.278	290.608	266.121	12.244	−700.081	−638.317	66.685
600	75.849	303.844	271.322	19.513	−701.065	−625.867	54.487
700	80.998	315.939	276.845	27.366	−701.781	−613.274	45.763
800	85.065	327.031	282.435	35.677	−702.282	−600.593	39.215
900	88.323	337.245	287.965	44.352	−702.610	−587.861	34.119
1000	90.969	346.692	293.371	53.321	−702.801	−575.100	30.040
1100	93.146	355.468	298.622	62.530	−702.885	−562.325	26.703
1200	94.954	363.652	303.704	71.938	−702.886	−549.546	23.921
1300	96.470	371.314	308.613	81.511	−702.826	−536.770	21.568
1400	97.751	378.512	313.352	91.224	−702.721	−524.000	19.551
1500	98.842	385.294	317.924	101.055	−702.584	−511.239	17.803
1600	99.777	391.704	322.337	110.987	−702.426	−498.488	16.274
1700	100.583	397.778	326.597	121.006	−702.253	−485.747	14.925
1800	101.282	403.547	330 713	131.100	−702.073	−473.016	13.727
1900	101.891	409.040	334.693	141.260	−701.887	−460.296	12.654
2000	102.425	414.280	338.542	151.476	−701.696	−447.585	11.690
2100	102.895	419.289	342.269	161.742	−701.502	−434.885	10.817
2200	103.310	424.085	345.879	172.053	−701.302	−422.193	10.024
2300	103.679	428.686	349.380	182.403	−701.093	−409.511	9.300
2400	104.008	433.106	352.777	192.788	−700.874	−396.838	8.637
2500	104.302	437.357	356.076	203.203	−700.640	−384 175	8.027
2600	104.567	441.453	359.282	213.647	−700.389	−371.521	7.464
2700	104.805	445.404	362.399	224.116	−700.116	−358.877	6.943
2800	105.020	449.220	365.432	234.607	−699.818	−346.244	6.459
2900	105.215	452.909	368.385	245.119	−699.493	−333.622	6.009
3000	105.393	456.479	371.262	255.650	−699.138	−321.012	5.589
3100	105.555	459.937	374.067	266.197	−698.750	−308.415	5.197
3200	105.703	463.291	376.803	276.760	−698.327	−295.830	4.829
3300	105.838	466.545	379.474	287.337	−697.868	−283.258	4.484
3400	105.962	469.707	382.081	297.928	−697.371	−270.702	4.159
3500	106.077	472.780	384.629	308.530	−696.835	−258.161	3.853
3600	106.183	475.770	387.119	319.143	−696.261	−245.635	3.564
3700	106.280	478.681	389.555	329.766	−695.647	−233.126	3.291
3800	106.371	481.516	391.938	340.398	−694.994	−220.634	3.033
3900	106.454	484.280	394.270	351.040	−694.302	−208.160	2.788
4000	106.532	486.976	396.554	361.689	−693.572	−195.704	2.556
4100	106.605	489.608	398.792	372.346	−692.803	−183.267	2.335
4200	106.673	492.178	400.985	383.010	−691.998	−170.848	2.125
4300	106.736	494.688	403.135	393.680	−691.156	−158.450	1.925
4400	106.795	497.143	405.244	404.357	−690.279	−146.072	1.734
4500	106.850	499.544	407.313	415.039	−689.368	−133.713	1.552
4600	106.902	501.893	409.343	425.727	−688.424	−121.376	1.378
4700	106.951	504.192	411.337	436.419	−687.448	−109.059	1.212
4800	106.996	506.444	413.295	447.117	−686.441	−96.763	1.053
4900	107.039	508.651	415.219	457.819	−685.405	−84.489	0.901
5000	107.080	510.814	417.109	468.525	−684.340	−72.236	0.755
5100	107.118	512.935	418.967	479.235	−683.247	−60.005	0.615
5200	107.154	515.015	420.794	489.948	−682.127	−47.795	0.480
5300	107.189	517.057	422.591	500.665	−680.983	−35.608	0.351
5400	107.221	519.060	424.359	511.386	−679.813	−23.442	0.227
5500	107.252	521.028	426.099	522.110	−678.620	−11.298	0.107
5600	107.281	522.961	427.812	532.836	−677.405	0.825	−0.008
5700	107.308	524.860	429.498	543.566	−676.167	12.924	−0.118
5800	107.334	526.726	431.158	554.298	−674.908	25.003	−0.225
5900	107.359	528.561	432.793	565.033	−673.629	37.060	−0.328
6000	107.383	530.366	434.404	575.770	−672.330	49.094	−0.427

PREVIOUS. June 1969 (1 atm) CURRENT: June 1969 (1 bar)

Hydrogen Cyanide (HCN) IDEAL GAS $M_r = 27.02564$ Hydrogen Cyanide (HCN) $C_1H_1N_1(g)$

$\Delta_fH°(0\ K) = 135.53 \pm 8.4\ kJ\cdot mol^{-1}$

$S°(298.15\ K) = 201.828 \pm 0.04\ J\cdot K^{-1}\cdot mol^{-1}$ $\Delta_fH°(298.15\ K) = 135.14 \pm 8.4\ kJ\cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
2096.3(1)
713.5(2)
3311.5(1)

Ground State Quantum Weights: 1 $\sigma = 1$
Point Group: $C_{\infty v}$
Bond Distances: C–H = 1.066 Å; C–N = 1.153 Å
Bond Angle: H–C–N = 180°
Rotational Constant: $B_0 = 1.484360\ cm^{-1}$

Spectroscopic constants used in calculating corrections to the rigid–rotator harmonic oscillator approximation (cm^{-1}):

$\alpha_1 = 10.10 \times 10^{-3}$ $-x_{11} = 7.07$ $-x_{12} = 2.53$ $g_{22} = 5.16$
$\alpha_2 = -3.61 \times 10^{-3}$ $-x_{22} = 2.65$ $-x_{23} = 19.01$
$\alpha_3 = 10.42 \times 10^{-3}$ $-x_{33} = 52.49$ $-x_{13} = 10.44$

Enthalpy of Formation

The value adopted is from NBS.[1] The data of Thomsen[2] who measured both C_2N_2 and HCN and Berthelot[3] were used in conjunction with the well established value for C_2N_2 to derive the adopted value.[4]

Badger[5] studied the equilibrium $NH_3(g) + C(cr) = HCN(g) + H_2(g)$ from both sides, we obtain a 3rd law $\Delta_rH°(298.15\ K) = 46 \pm 0.9$ $kcal\cdot mol^{-1}$ and a 2nd law $\Delta_rH°(298.15\ K) = 34.5 \pm 19\ kcal\cdot mol^{-1}$, the 3rd law drift is $14 \pm 24\ cal\cdot K^{-1}\cdot mol^{-1}$. The 3rd law value leads to $\Delta_fH°(HCN, g, 298.15\ K) = 35 \pm 1\ kcal\cdot mol^{-1}$.

Horiuchi *et al.*[6] studied the equilibrium $2\ CO(g) + NH_3(g) = HCN(g) + CO_2(g) + H_2(g)$. We obtain $\Delta_rH°(298.15\ K) = 1.1 \pm 0.5\ kcal\cdot mol^{-1}$ from a 3rd law analysis with a drift of $-2 \pm 3\ cal\cdot K^{-1}\cdot mol^{-1}$, and a 2nd law value of $2.9 \pm 2.6\ kcal\cdot mol^{-1}$. The 3rd law value leads to $\Delta_fH°(HCN, g, 298.15\ K) = 31.35 \pm 0.6\ kcal\cdot mol^{-1}$. The two sets of equilibrium data are self-consistent but disagree with each other and the direct combustions. We adopt an uncertainty of $2.0\ kcal\cdot mol^{-1}$ to draw attention to this unsatisfactory situation.

Heat Capacity and Entropy

McBride *et al.*[7] used the constants listed above to calculate the adopted table which includes first and second corrections for anharmonicity, vibration–rotation interaction and centrifugal stretching. The bond lengths and molecular constants are those listed by Rank *et al.*[8] A more extensive set of anharmonic constants has recently been determined by Nakagawa and Morino,[9] they are in generally good agreement with the values used.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J\cdot K^{-1}mol^{-1}$			$kJ\cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−9.234	135.529	135.529	INFINITE
100	29.167	167.608	230.911	−6.330	135.422	131.784	−68.837
200	31.719	188.377	204.966	−3.318	135.306	128.187	−33.479
298.15	35.857	201.828	201.828	0.	135.143	124.725	−21.851
300	35.928	202.050	201.829	0.066	135.140	124.660	−21.705
400	39.229	212.863	203.281	3.833	134.972	121.192	−15.826
500	41.731	221.894	206.125	7.885	134.766	117.769	−12.303
600	43.806	229.690	209.417	12.164	134.511	114.393	−9.959
700	45.643	236.583	212.815	16.638	134.222	111.063	−8.288
800	47.317	242.788	216.180	21.287	133.919	107.775	−7.037
900	48.844	248.451	219.456	26.096	133.618	104.525	−6.066
1000	50.229	253.670	222.619	31.051	133.328	101.308	−5.292
1100	51.484	258.517	225.665	36.137	133.052	98.120	−4.659
1200	52.610	263.046	228.594	41.343	132.793	94.955	−4.133
1300	53.618	267.298	231.409	46.655	132.549	91.812	−3.689
1400	54.522	271.305	234.117	52.063	132.318	88.687	−3.309
1500	55.329	275.095	236.724	57.556	132.099	85.579	−2.980
1600	56.049	278.689	239.235	63.126	131.889	82.484	−2.693
1700	56.697	282.107	241.657	68.764	131.685	79.403	−2.440
1800	57.275	285.364	243.996	74.463	131.486	76.333	−2.215
1900	57.794	288.475	246.255	80.217	131.289	73.274	−2.014
2000	58.262	291.451	248 441	86.020	131.094	70.226	−1.834
2100	58.689	294.304	250.558	91.868	130.898	67.187	−1.671
2200	59.070	297.043	252.609	97.756	130.700	64.158	−1.523
2300	59 421	299.677	254.598	103.681	130.499	61.138	−1.388
2400	59.739	302.213	256.530	109.639	130.294	58.127	−1.265
2500	60.028	304.657	258.406	115.628	130.085	55.124	−1.152
2600	60.296	307.017	260.231	121.644	129.869	52.130	−1.047
2700	60.542	309.297	262.006	127.686	129.647	49.144	−0.951
2800	60.764	311.503	263.735	133.752	129.417	46.167	−0.861
2900	60.973	313.639	265.419	139.838	129.180	43.198	−0.778
3000	61.170	315.710	267.061	145.946	128.934	40.237	−0.701
3100	61.347	317.718	268.663	152.072	128.679	37.284	−0.628
3200	61.513	319.669	270.226	158.215	128.415	34.340	−0.561
3300	61.669	321.564	271 754	164.374	128.141	31.405	−0.497
3400	61.814	323.407	273.246	170.548	127.856	28.478	−0.438
3500	61 948	325.201	274.705	176.736	127.560	25.559	−0.381
3600	62.074	326.948	276.132	182.938	127.253	22.649	−0.329
3700	62.190	328.650	277.528	189.151	126.934	19.748	−0.279
3800	62.300	330.310	278.896	195.376	126.603	16.855	−0.232
3900	62.401	331.930	280.235	201.611	126.259	13.971	−0.187
4000	62.496	333.511	281.547	207.855	125.902	11.097	−0.145
4100	62.587	335.055	282.833	214.110	125.532	8.231	−0.105
4200	62.672	336.564	284 095	220.373	125.148	5.375	−0.067
4300	62.750	338.040	285.332	226.644	124.750	2.528	−0.031
4400	62.823	339.483	286.546	232.923	124.338	−0.310	0.004
4500	62.890	340.896	287.739	239.208	123.911	−3.138	0.036
4600	62.952	342.279	288.909	245.500	123.469	−5 957	0.068
4700	63.011	343.633	290.059	251.799	123.013	−8.765	0.097
4800	63.065	344.961	291.189	258.102	122.541	−11.564	0.126
4900	63.115	346.261	292.300	264.412	122.054	−14.353	0.153
5000	63.162	347.537	293.392	270.725	121.552	−17.131	0.179
5100	63.206	348.788	294.466	277.044	121.034	−19.900	0.204
5200	63.245	350.016	295.522	283.366	120.501	−22.658	0.228
5300	63.278	351.221	296.562	289.693	119.952	−25.406	0.250
5400	63.308	352.404	297.585	296.022	119.388	−28.143	0.272
5500	63.335	353.566	298.593	302.354	118.808	−30.870	0.293
5600	63.358	354.707	299.584	308.689	118.212	−33.586	0.313
5700	63.378	355.829	300.561	315.026	117.601	−36.292	0.333
5800	63.395	356.931	301.524	321.364	116.975	−38.986	0.351
5900	63.407	358.015	302.472	327.705	116.333	−41.670	0.369
6000	63.417	359.081	303.407	334.046	115.675	−44.342	0.386

PREVIOUS· December 1969 (1 atm) CURRENT December 1969 (1 bar)

$S°(298.15\ K) = 238.228 \pm 0.4\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -98.7 \pm 8\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -101.7 \pm 8\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies	
ν, cm^{-1}	ν, cm^{-1}
3531(1)	659.8(1)
2274(1)	577.5(1)
1327(1)	777.1(1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: C_s
Bond Distances: H–N = 0.987 Å; N–C = 1.207 Å; C–O = 1.171 Å
Bong Angles: H–N–C = 128.1°; N–C–O = 180°
Product of the Moments of Inertia: $I_AI_BI_C = 5.3166 \times 10^{-117}\ g^3{\cdot}cm^6$

Enthalpy of Formation

Okabe[1] has measured the onset of photodissociation for the process $HNCO(g) \rightarrow NH(c'\ \Pi) + CO(g)$ as 8.79 ± 0.03 eV (202.7 ± 0.7 kcal·mol^{-1}). Okabe and Lenzi[2] have also reported the onset of photodissociation for the process $NH_3(g) \rightarrow NH(c'\Pi) + H_2(g)$ as 9.35 ± 0.06 eV (215.6 ± 1.4 kcal·mol^{-1}). Elimination of the NH(c'Π) gives

$$NH_3(g) + CO(g) \rightarrow NHCO(g) + H_2(g) \quad \Delta_fH°(0\ K) = 12.9 \pm 2\ kcal{\cdot}mol^{-1}$$

which with JANAF auxiliary data[3] yields $\Delta_fH°$(HNCO, g, 0 K) = -23.6 ± 2 kcal·mol^{-1}, or $\Delta_fH°$(HNCO, g, 298.15 K) = -24.3 ± 2 kcal·mol^{-1}.

The heat of formation of ionized cyanic acid in aqueous solution is -34.9 kcal·mol^{-1}.[4] Since the ions from cyanic acid and isocyanic acid are identical in solution we can use this value for aqueous isocyanic acid. Assuming the heat of solution is -3 ± 3 kcal·mol^{-1}, a value covering the range of heats of solution of most organic liquids,[4] we obtain $\Delta_fH°$(HNCO, l, 298.15 K) = -32 ± 3 kcal·mol^{-1}. Using $\Delta_{vap}H° = 7.2$ kcal·mol^{-1} [5] we obtain $\Delta_fH°$(HNCO, g, 298.15 K) = -25 ± 3 kcal·mol^{-1}. If we assume that $\Delta_fH°$(HNCO, g, 298.15 K)–$\Delta_fH°$(HNCO, ionized aq, 298.15 K) = $\Delta_fH°$(HNCS, g, 298.15 K)–$\Delta_fH°$(HCNS, ionized aq, 298.15 K) then we obtain $\Delta_fH°$(HNCO, g, 298.15 K) = -23 kcal·mol^{-1} employing values from U.S. Nat. Bur. Stand. Tech. Note 270-3.[4] We adopt the value $\Delta_fH°$(HNCO, g, 298.15 K) = -24.3 ± 2 kcal·mol^{-1} (-101.671 ± 8 kJ·mol^{-1}).

Heat Capacity and Entropy

The vibrational frequency determinations have been summarized by Herzberg and Reid.[6] Ashby and Werner[7] have remeasured the three lower fundamentals under much higher resolution. They reverse the assignments of ν_5 and ν_6 of Herzberg and Reid. Dixon and Kirby[8] have discussed the corrections due to Coriolis interaction made by Ashby and Werner and conclude they are in the wrong direction. On this basis they reverse the ν_4 and ν_6 assignments of Herzberg and Reid.

The bond distances and angles are from the microwave measurements of Jones *et al.*[9] which give rotational constants in good agreement with the later microwave work of Kewley.[10] The principal moments are: $I_A = 0.0912 \times 10^{-39}$, $I_B = 7.5910 \times 10^{-39}$, and $I_C = 7.6822 \times 10^{-39}$ g·cm^2.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0	0.	INFINITE	−10.961	−98.671	−98.671	INFINITE
100	33.470	197.325	273.654	−7.633	−99.805	−97.750	51.060
200	38.269	221.663	242.134	−4.094	−100.851	−95.279	24.884
250	41.813	230.583	238.952	−2.092	−101.299	−93.833	19.605
298.15	45.043	238.228	238.228	0.	−101.671	−92.360	16.181
300	45.160	238.507	238.229	0.083	−101.684	−92.302	16.071
350	48.133	245.697	238.790	2.417	−102.013	−90.712	13.538
400	50.729	252.297	240.071	4.890	−102.297	−89.077	11.632
450	53.001	258.407	241.773	7.485	−102.553	−87.409	10.146
500	55.007	264 097	243.724	10.186	−102.789	−85.714	8.954
600	58.410	274.437	247.999	15.863	−103.226	−82.257	7.161
700	61.228	283.659	252.446	21.849	−103.631	−78.730	5.875
800	63.627	291.995	256.877	28.094	−104.006	−75.147	4.907
900	65.704	299.612	261.208	34.563	−104.349	−71.519	4.151
1000	67.516	306.631	265.404	41.226	−104.662	−67.854	3.544
1100	69.104	313.142	269.452	48.059	−104.946	−64.159	3.047
1200	70.498	319.216	273.348	55.041	−105.204	−60.439	2.631
1300	71.724	324.908	277.098	62.153	−105.439	−56.699	2.278
1400	72.802	330.264	280.706	69.381	−105.657	−52.941	1.975
1500	73.752	335.320	284.180	76.709	−105.862	−49.169	1.712
1600	74.591	340.107	287.527	84.127	−106.057	−45.383	1.482
1700	75.333	344.652	290.755	91.624	−106.248	−41.585	1.278
1800	75.990	348.976	293.870	99.191	−106.437	−37.776	1.096
1900	76.575	353.101	296.880	106.820	−106.628	−33.956	0.934
2000	77.095	357.042	299.790	114.504	−106.824	−30.126	0.787
2100	77.560	360.815	302.607	122.237	−107.028	−26.287	0.654
2200	77.977	364.433	305.336	130.014	−107.241	−22.437	0.533
2300	78.351	367.908	307.981	137.831	−107.465	−18.577	0.422
2400	78.688	371.250	310.548	145.683	−107.702	−14.707	0.320
2500	78.992	374.468	313.041	153.568	−107.954	−10.828	0.226
2600	79.268	377.572	315.464	161.481	−108.220	−6.937	0.139
2700	79.518	380.568	317.820	169.420	−108.504	−3.036	0.059
2800	79.745	383.464	320.113	177.384	−108.804	0.875	−0.016
2900	79.953	386.266	322.346	185.369	−109.122	4.798	−0.086
3000	80.143	388.980	324.522	193.374	−109.459	8.732	−0.152
3100	80.316	391.611	326.644	201.397	−109.814	12.678	−0.214
3200	80.476	394.163	328.714	209.437	−110.189	16.635	−0.272
3300	80.623	396.642	330.735	217.492	−110.583	20.604	−0.326
3400	80.758	399.051	332.709	225.561	−110.997	24.585	−0.378
3500	80.883	401.393	334.638	233.643	−111.430	28.579	−0.427
3600	80.999	403.674	336.524	241.737	−111.884	32.586	−0.473
3700	81.106	405.894	338.369	249.842	−112.358	36.605	−0.517
3800	81.205	408.059	340.175	257.958	−112.852	40.638	−0.559
3900	81.298	410.169	341.943	266.083	−113.367	44 684	−0.598
4000	81.384	412.229	343.674	274.217	−113.903	48.744	−0.637
4100	81.464	414.239	345.371	282.360	−114.459	52.817	−0.673
4200	81.539	416.203	347.034	290.510	−115.037	56.904	−0.708
4300	81.610	418.123	348.665	298.667	−115.635	61.005	−0.741
4400	81.675	420.000	350.265	306.832	−116.255	65.119	−0.773
4500	81.737	421.836	351.835	315.002	−116.895	69.248	−0.804
4600	81 795	423.633	353.377	323.179	−117.558	73.392	−0.833
4700	81.850	425.393	354.890	331.361	−118.241	77.551	−0.862
4800	81.901	427.116	356.377	339.549	−118.947	81.724	−0.889
4900	81.949	428.806	357.838	347.741	−119.674	85.912	−0.916
5000	81.995	430.462	359.274	355.939	−120.424	90.116	−0.941
5100	82.038	432.086	360.686	364.140	−121.196	94.334	−0.966
5200	82.079	433.679	362.074	372.346	−121.990	98.567	−0.990
5300	82.117	435.243	363.440	380.556	−122.806	102.817	−1.013
5400	82.154	436.778	364.784	388.770	−123.646	107.082	−1.036
5500	82.188	438.286	366.107	396.987	−124.508	111.362	−1.058
5600	82.221	439.767	367.409	405.207	−125.393	115.659	−1.079
5700	82.252	441.223	368.691	413.431	−126.302	119.971	−1.099
5800	82.282	442.654	369.954	421.658	−127.234	124.300	−1.119
5900	82.310	444.060	371.198	429.887	−128.190	128.644	−1.139
6000	82.337	445.444	372.424	438.120	−129.170	133.006	−1.158

PREVIOUS: December 1970 (1 atm) CURRENT· December 1970 (1 bar)

$\Delta_f H°(0\ K) = 43.2 \pm 8\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = 224.649 \pm 0.04\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = 43.5 \pm 8\ kJ \cdot mol^{-1}$

			Electronic Levels and Molecular Constants				
State	ϵ_i, cm^{-1}	g_i	ν_1, cm^{-1}	ν_2, cm^{-1}	ν_3, cm^{-1}	B_0, cm^{-1}	$I_AI_BI_C$ g^3·cm^6
X^2A'	0	2	2488 (1)	1083 (1)	1820 (1)	—	0.4655×10^{-117}
$\tilde{A}^2\Sigma^-$	9294	2	3316.2 (1)	802.3 (2)	1813.4(1)	1.333284	—
$\tilde{B}^2A'$	38691	2	[2488] (1)	[1083] (1)	[1820] (1)	—	1.0087×10^{-117}
$\tilde{C}^2A''$	41270	2	[2488] (1)	[1083] (1)	[1820] (1)	—	$[0.4655] \times 10^{-117}$

Point Group: C_s $\sigma = 1$

Bond Distance (X^2A'). C–H = 1.16 Å; C–O = 1.17 Å

Bond Angle (X^2A'): H–C–O = 123.8°

Enthalpy of Formation

The adopted $\Delta_f H°$(HCO, g, 298.15 K) = 10.4 ± 2 kcal·mol^{-1} is calculated from $\Delta_a H°$(OHC–CHO, g) = 71.5 ± 2 kcal·mol^{-1} and $\Delta_f H°$(glyoxal, g, 298.15 K) = −50.66 ± 0.2 kcal·mol^{-1}. The C–C bond dissociation energy in glyoxal was determined from chemiluminescent recombination of formyl radicals by Hartley.[1] The heat of formation of glyoxal was determined from flame combustion calorimetry by Fletcher and Pilcher.[2]

The other route to derive the enthalpy of formation of formyl radical was from $\Delta_a H°$(H–CHO) which has been studied by many investigators listed below. There are several conflicting values between 77 to 91 kcal·mol^{-1} for $\Delta_a H°$(H–CHO). Based on the adopted $\Delta_f H°$(HCO, g, 298.15 K) = 10.4 ± 2 kcal·mol^{-1}, we have derived $\Delta_a H°$(H–CHO) = 89.3 ± 2 kcal·mol^{-1} which is in essential agreement with the high values of $\Delta_a H°$(H–CHO). The low values were probably not reliable as pointed out by Calvert,[3] Walsh and Benson,[5] Haney and Franklin.[9]

Source	Method	$\Delta_a H°$(H–CHO) kcal·mol^{-1}	
Calvert[3]	Kinetic	91	
Klein and Schoen[4]	Kinetic	77	
Walsh and Benson[5]	Kinetic	87	±1
Brand and Reed[6]	Spectroscopic	<82.3	
Reed and Brand[7]	Electron Impact	75	±2.3
Shannon and Harrison[8]	Electron Impact	79	±3
Haney and Franklin[9]	Electron Impact	87	±3

Heat Capacity and Entropy

The thermodynamic functions were calculated by summing over the individual partition functions for the separate states. The observed molecular constants and electronic levels were taken from Herzberg and Ramsay[10–12] and Dixon.[13] The vibrational frequency (ν_1 = 2488 cm^{-1}) was observed using the matrix isolation infrared technique by Milligan and Jacox.[14] Using the same technique, Ewing *et al.*[15] found ν_2 = 1091 cm^{-1} and ν_3 = 1860 cm^{-1} which are in good agreement with the values adopted.[10] These small differences are probably due to matrix shifts. The bond lengths and angle were calculated from the normal coordinate analyses by Shirk and Pimentel.[16] These values are a better fit than those calculated by Johns *et al.*[12] who assumed a normal CH bond length of 1.08 Å.

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Enthalpy Reference Temperature = T_r = 298.15 K						Standard State Pressure = $p°$ = 0.1 MPa	
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−9.989	43.151	43.151	INFINITE
100	33.258	188.025	254.660	−6.664	43.465	38.459	−20.089
200	33.469	211.108	227.769	−3.332	43.667	33.352	−8.711
250	33.921	218.619	225.214	−1.649	43.628	30.776	−6.430
298.15	34.597	224.649	224.649	0.	43.514	28.309	−4.960
300	34.627	224.863	224.650	0.064	43.508	28.215	−4.913
350	35.518	230.266	225.074	1.817	43.327	25.680	−3.833
400	36.530	235.074	226.029	3.618	43.100	23.174	−3.026
450	37.614	239.438	227.280	5.471	42.837	20.698	−2.403
500	38.733	243.459	228.699	7.380	42.545	18.254	−1.907
600	40.965	250.719	231.777	11.365	41.908	13.455	−1.171
700	43.068	257.194	234.954	15.568	41.242	8.765	−0.654
800	44.962	263.071	238.106	19.972	40.580	4.171	−0.272
900	46.623	268.465	241.184	24.553	39.936	−0.341	0.020
1000	48.056	273.454	244.165	29.289	39.316	−4.783	0.250
1100	49.282	278.093	247.041	34.157	38.717	−9.164	0.435
1200	50.329	282.427	249.811	39.139	38.134	−13.491	0.587
1300	51.224	286.492	252.478	44.218	37.562	−17.770	0.714
1400	51.991	290.317	255.045	49.380	36.995	−22.004	0.821
1500	52.651	293.927	257.518	54.613	36.429	−26.199	0.912
1600	53.223	297.343	259.901	59.907	35.859	−30.356	0.991
1700	53.722	300.585	262.200	65.255	35.282	−34.477	1.059
1800	54.161	303.669	264.419	70.650	34.695	−38.563	1.119
1900	54.549	306.608	266.563	76.085	34.096	−42.617	1.172
2000	54.896	309.415	268.636	81.558	33.483	−46.638	1.218
2100	55.206	312.101	270.642	87.063	32.854	−50.629	1.259
2200	55.488	314.675	272.585	92.598	32.209	−54.589	1.296
2300	55.744	317.148	274.469	98.160	31.546	−58.520	1.329
2400	55.978	319.525	276.298	103.746	30.866	−62.422	1.359
2500	56.195	321.815	278.073	109.355	30.167	−66.294	1.385
2600	56.395	324.023	279.798	114.985	29.450	−70.139	1.409
2700	56.581	326.155	281.475	120.634	28.713	−73.955	1.431
2800	56.755	328.215	283.108	126.300	27.959	−77.744	1.450
2900	56.918	330.210	284.698	131.984	27.185	−81.505	1.468
3000	57.071	332.142	286.248	137.684	26.393	−85.240	1.484
3100	57.216	334.016	287.758	143.398	25.582	−88.947	1.499
3200	57.353	335.835	289.233	149.127	24.753	−92.629	1.512
3300	57.483	337.601	290.672	154.868	23.905	−96.284	1.524
3400	57.606	339.319	292.077	160.623	23.039	−99.913	1.535
3500	57.723	340.991	293.451	166.389	22.154	−103.517	1.545
3600	57.835	342.619	294.794	172.167	21.252	−107.094	1.554
3700	57.942	344.205	296.108	177.956	20.331	−110.647	1.562
3800	58.044	345.751	297.395	183.756	19.393	−114.174	1.569
3900	58.141	347.260	298.654	189.565	18.436	−117.676	1.576
4000	58.235	348.733	299.888	195.384	17.462	−121.154	1.582
4100	58.324	350.172	301.096	201.212	16.469	−124.607	1.588
4200	58.410	351.579	302.282	207.048	15.459	−128.036	1.592
4300	58.493	352.954	303.444	212.894	14.430	−131.440	1.597
4400	58.573	354.300	304.585	218.747	13.384	−134.821	1.601
4500	58.650	355.617	305.704	224.608	12.320	−138.178	1.604
4600	58.724	356.907	306.803	230.477	11.238	−141.510	1.607
4700	58.796	358.171	307.883	236.353	10.137	−144.819	1.609
4800	58.866	359.409	308.944	242.236	9.018	−148.104	1.612
4900	58.933	360.624	309.986	248.126	7.881	−151.365	1.614
5000	58.999	361.815	311.011	254.022	6.726	−154.603	1.615
5100	59.063	362.984	312.018	259.926	5.552	−157.818	1.616
5200	59.126	364.132	313.009	265.835	4.360	−161.010	1.617
5300	59.187	365.258	313.985	271.751	3.149	−164.179	1.618
5400	59.248	366.365	314.945	277.673	1.919	−167.325	1.619
5500	59.307	367.453	315.889	283.600	0.671	−170.448	1.619
5600	59.365	368.522	316.820	289.534	−0.596	−173.547	1.619
5700	59.423	369.573	317.736	295.473	−1.882	−176.624	1.619
5800	59.480	370.607	318.639	301.418	−3.188	−179.678	1.618
5900	59.536	371.625	319.528	307.369	−4.512	−182.711	1.618
6000	59.593	372.626	320.405	313.326	−5.855	−185.719	1.617

PREVIOUS December 1970 (1 atm) CURRENT: December 1970 (1 bar)

Formyl, Ion (HCO^+) IDEAL GAS $M_r = 29.01779$ Formyl, Ion (HCO^+) $C_1H_1O_1^+(g)$

$\Delta_f H°(0\ K) = 827.2 \pm 8\ kJ{\cdot}mol^{-1}$

$S°(298.15\ K) = [203.417 \pm 4]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_f H°(298.15\ K) = 833.0 \pm 8\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[3223](1)
[707](2)
[2088](1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: $[C_{\infty v}]$
Bond Distances: C–H = [1.07] Å; C–O = [1.17] Å
Bond Angles: H–C–O = [180]°
Rotational Constant: $B_0 = [1.367073]\ cm^{-1}$

Enthalpy of Formation

Using the photoionization technique, Matthews and Warneck[1] measured the appearance potentials of $HCO^+(g)$ from formaldehyde, formic acid and acetaldehyde as 11.95, 12.79 and 11.79 eV, respectively, whose average yields $\Delta_f H°(CHCO^+, g, 0\ K) = 197.7 \pm 1.5\ kcal{\cdot}mol^{-1}$, based on the following $\Delta_f H°(0\ K)$ data (in units of $kcal{\cdot}mol^{-1}$): 51.63 for H(g), 9.35 for OH(g), 35.62 for $CH_3(g)$, −26.78 for $H_2CO(g)$,[2] −88.74 for HCOOH(g)[3] and −37.14 for CH_3CHO.[4] The appearance potentials obtained from photoionization are several tenths to 1 eV lower than the recent electron impact data.[5-9] The appearance potentials determined by the electron impact method tend to be high because the fundamental nature of the process does not lead to a sharp onset in contrast to the step-function behavior of photoionization onset.

Heat Capacity and Entropy

The molecular configuration is assumed to be linear based on two reasons: (1) the molecule $HCO^+(g)$ is isoelectronic with HCN(g) which is linear; (2) Walsh[10] predicted that "HAB" molecules with 10 or less valence electrons will be linear in their ground state. $HCO^+(g)$ has 10 valence electrons.

The bond distances HC and CO were estimated to be the same as those in HCN and HCO molecules, respectively. The vibrational frequencies were calculated by the valence force method from the estimated stretching and bending force constants which were obtained from HCN(g).

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−9.249	827.215		
100	29.166	169.137	232.573	−6.344			
200	31.793	189.930	206.575	−3.329			
250	33.980	197.259	203.998	−1.685			
298.15	35.963	203.417	203.417	0.	833.034	817.906	−143.294
300	36.035	203.639	203.417	0.067	833.070	817.812	−142.394
350	37.811	209.331	203.863	1.914	834.023	815.193	−121.661
400	39.328	214.482	204.873	3.843	834.964	812.439	−106.094
450	40.645	219.192	206.206	5.843	835.886	809.568	−93.972
500	41.819	223.536	207.725	7.905	836.787	806.595	−84.264
600	43.892	231.348	211.025	12.194	838.531	800.392	−69.680
700	45.727	238.254	214.431	16.676	840.223	793.901	−59.242
800	47.389	244.471	217.804	21.333	841.893	787.169	−51.397
900	48.895	250.141	221.087	26.149	843.563	780.229	−45.283
1000	50.251	255.364	224.256	31.107	845.244	773.102	−40.383
1100	51.463	260.211	227.307	36.194	846.942	765.805	−36.365
1200	52.541	264.736	230.240	41.395	848.657	758.354	−33.010
1300	53.496	268.980	233.058	46.698	850.387	750.759	−30.166
1400	54.339	272.976	235.768	52.091	852.130	743.029	−27.723
1500	55.084	276.751	238.376	57.563	853.881	735.175	−25.601
1600	55.741	280.327	240.887	63.105	855.638	727.204	−23.741
1700	56.322	283.725	243.308	68.708	857.395	719.124	−22.096
1800	56.837	286.959	245.644	74.367	859.151	710.939	−20.631
1900	57.293	290.044	247.900	80.074	860.901	702.657	−19.317
2000	57.700	292.993	250.082	85.824	862.644	694.284	−18.133
2100	58.062	295.818	252.193	91.612	864.377	685.823	−17.059
2200	58.386	298.526	254.238	97.435	866.098	677.280	−16.081
2300	58.677	301.128	256.220	103.288	867.806	668.659	−15.186
2400	58.939	303.631	258.144	109.169	869.499	659.964	−14.364
2500	59.175	306.042	260.012	115.075	871.175	651.199	−13.606
2600	59.388	308.367	261.827	121.004	872.835	642.367	−12.905
2700	59.581	310.612	263.593	126.952	874.478	633.472	−12.255
2800	59.757	312.782	265.311	132.919	876.102	624.516	−11.650
2900	59.917	314.882	266.984	138.903	877.707	615.502	−11.086
3000	60.063	316.916	268.615	144.902	879.293	606.434	−10.559
3100	60 197	318.887	270.205	150.915	880.859	597.313	−10.065
3200	60.320	320.800	271.756	156.941	882.406	588.141	−9.600
3300	60.433	322.658	273.271	162.979	883.933	578.921	−9.164
3400	60.537	324.464	274.750	169.028	885.439	569.656	−8.752
3500	60.633	326.220	276.196	175.086	886.925	560.347	−8.363
3600	60.722	327.930	277.609	181.154	888.391	550.995	−7.995
3700	60.804	329.594	278.992	187.230	889.837	541.603	−7.646
3800	60.880	331.217	280.345	193.314	891.262	532.172	−7.315
3900	60.951	332.799	281.670	199.406	892.666	522.705	−7.001
4000	61.017	334.343	282.967	205.504	894.050	513.200	−6.702
4100	61.078	335.851	284.239	211.609	895.413	503.662	−6.417
4200	61.136	337.323	285.485	217.720	896.755	494.091	−6.145
4300	61.190	338.762	286.707	223.836	898.077	484.488	−5.885
4400	61.240	340.170	287.907	229.958	899.377	474.855	−5.637
4500	61.287	341.546	289.083	236.084	900.657	465.192	−5.400
4600	61.331	342.894	290.239	242.215	901.915	455.501	−5.172
4700	61.373	344.213	291.373	248.350	903.152	445.783	−4.954
4800	61.412	345.506	292.487	254.490	904.368	436.039	−4.745
4900	61.449	346.773	293.582	260.633	905.563	426.270	−4.544
5000	61.484	348.014	294.659	266.779	906.736	416.476	−4.351
5100	61.517	349.232	295.717	272.929	907.888	406.660	−4.165
5200	61.548	350.427	296.757	279.083	909.018	396.820	−3.986
5300	61.577	351.600	297.781	285.239	910.127	386.960	−3.814
5400	61.605	352.751	298.788	291.398	911.213	377.079	−3.648
5500	61.632	353.882	299.780	297.560	912.277	367.177	−3.487
5600	61.657	354.992	300.756	303.724	913.319	357.257	−3.332
5700	61.680	356.084	301.717	309.891	914.339	347.318	−3.183
5800	61.703	357.157	302.664	316.060	915.337	337.362	−3.038
5900	61.724	358.212	303.596	322.232	916.312	327.388	−2.898
6000	61.745	359.249	304.515	328.405	917.264	317.398	−2.763

PREVIOUS: December 1970 (1 atm) CURRENT. December 1970 (1 bar)

Methinophosphide (CHP) IDEAL GAS $M_r = 43.99270$ Methinophosphide (CHP) $C_1H_1P_1(g)$

$S°(298.15\ K) = 215.06 \pm 0.04\ J\ K^{-1}\cdot mol^{-1}$

$\Delta_f H°(0\ K) = [151.2 \pm 63]\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [149.9 \pm 63]\ kJ\cdot mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$X^1\Sigma^+$	0	1
$a^3\Sigma^+$	24440	3
$b^3\Sigma^+$	30430	6
$c^3\Sigma^-$	31024	3
A^1A-	34746	1
$B^1\pi$	35927	2
$d^3\pi$	35976	6
C^1A-	40248	1

Vibrational Frequencies and Degeneracies

ν, cm^{-1}
3216.9(1)
674.7(2)
1278.4(1)

Spectroscopic constants used in calculating corrections to rigid rotator–harmonic oscillator approximation (cm^{-1}):

$\alpha_1 = 3.4 \times 10^{-3}$ $-x_{11} = [3.7]$ $-x_{12} = [1.9]$
$\alpha_2 = -3.4 \times 10^{-4}$ $-x_{22} = [2.4]$ $-x_{23} = [18.0]$
$\alpha_3 = 3.1 \times 10^{-3}$ $-x_{33} = [51.0]$ $-x_{13} = [8.0]$

Point Group: $C_{\infty v}$ $\sigma = 1$
Bond Distances: C–H = 1.0667 Å, C–P = 1.5421 Å
Bond Angle: H–C–P = 180°
Rotational Constant. $B_0 = 0.667545\ cm^{-1}$

Enthalpy of Formation

The bonding in HCP and HCN is very similar, as evidenced by the bond lengths and vibrational frequencies. We assume that the C–H bond strength is thus the same in these two molecules. For the reactions $HCN \rightarrow H + CN$ we derive $\Delta_r H° = 128\ kcal\cdot mol^{-1}$ from $\Delta_f H°$(HCN, 2981.5 K) = 32.3, $\Delta_f H°$(H, 298.15 K) = 52.1 and $\Delta_f H°$(C, 2981.5 K) = 104 kcal·mol^{-1}. Applying this to the reaction $HCP \rightarrow H + CP$, we obtain $\Delta_f H°$(HCP, g, 2981.5 K) = 40 ± 15 kcal·mol^{-1}, from $\Delta_f H°$(CP, 2981.5 K) = 111.7 kcal·mol^{-1}.

Heat Capacity and Entropy

The molecular configuration was first obtained by Gier,[1] and later the bond lengths were determined by Tyler[2] using microwave spectroscopy. The vibrational frequencies and electronic levels were obtained from an analysis of the ultraviolet spectrum by Johns *et al.*[3] Since the first excited state is above 24000 cm^{-1} and the first nonlinear state at 34000 cm^{-1}, there is negligible error introduced by assuming ground state molecular constants for all excited states. The anharmonic constants were estimated from those of Hcn by Gordon[4] and the adopted table includes these corrections and the electronic contributions.

References

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[2] J. K. Tyler, J. Chem. Phys. 40, 1170 (1964).
[3] J. W. C. Johns, H. F. Shurvell and J. K. Tyler, Can J. Phys. 47, 893 (1969).
[4] J. S. Gordon, Atlantic Research Corp., Alexandria, VA, personal communication, (January 12, 1970).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−9.353	151.192	151.192	INFINITE
100	29.196	180.303	244.749	−6.445	151.654	140.524	−73.402
200	32.275	201.236	218.271	−3.407	150.755	129.490	−33.819
298.15	37.166	215.062	215.062	0.	149.900	119.219	−20.887
300	37.254	215.293	215.063	0.069	149.882	119.029	−20.725
400	41.430	226.606	216.577	4.011	148.097	109.082	−14.245
500	44.593	236.205	219.567	8.319	146.984	99.458	−10.390
600	47.011	244.556	223.051	12.903	145.893	90.055	−7.840
700	48.936	251.951	226.661	17.703	144.819	80.834	−6.032
800	50.551	258.594	230.245	22.679	143.765	71.766	−4.686
900	51.944	264.630	233.735	27.806	142.737	62.828	−3.646
1000	53.166	270.167	237.105	33.062	141.736	54.003	−2.821
1100	54.254	275.287	240.346	38.434	140.762	45.277	−2.150
1200	55.225	280.050	243.459	43.909	76.242	37.717	−1.642
1300	56.095	284.505	246 447	49.476	76.091	34.513	−1.387
1400	56.869	288.691	249.316	55.125	75.956	31.319	−1.169
1500	57.568	292.639	252.074	60.847	75.833	28.136	−0.980
1600	58.195	296.374	254.727	66.636	75.721	24.959	−0.815
1700	58.764	299.920	257.282	72.484	75.617	21.790	−0.670
1800	59.279	303.293	259.745	78.387	75.519	18.627	−0.541
1900	59.743	306.511	262.123	84.338	75.426	15.468	−0.425
2000	60.170	309.586	264 419	90.334	75.337	12.315	−0.322
2100	60.563	312.532	266 641	96.371	75.249	9.166	−0.228
2200	60.923	315.358	268.791	102.445	75.162	6.021	−0.143
2300	61.254	318.073	270.876	108.554	75.074	2.881	−0.065
2400	61.568	320.687	272.897	114.696	74.986	−0.256	0.006
2500	61.852	323.206	274.859	120.867	74.896	−3.389	0.071
2600	62.128	325.637	276.766	127.066	74.804	−6.519	0.131
2700	62.383	327.987	278.619	133.292	74.709	−9.645	0.187
2800	62.626	330.260	280.423	139.542	74.611	−12.768	0.238
2900	62.856	332.462	282.180	145.816	74.510	−15.887	0.286
3000	63.078	334.596	283.892	152.113	74.405	−19.002	0.331
3100	63.300	336.668	285.561	158.432	74.296	−22.114	0.373
3200	63.509	338.681	287.190	164.773	74.184	−25.222	0.412
3300	63.718	340.639	288.780	171.134	74.068	−28.326	0.448
3400	63.923	342.544	290.333	177.516	73.949	−31.428	0.483
3500	64.132	344.400	291.852	183.919	73.827	−34.525	0.515
3600	64.337	346.209	293.337	190.342	73.703	−37.619	0.546
3700	64.551	347.975	294.790	196.787	73.577	−40.710	0.575
3800	64.772	349.700	296.212	203.253	73.450	−43.797	0.602
3900	64.990	351.385	297.605	209.741	73.322	−46.881	0.628
4000	65.220	353.033	298.970	216.251	73.195	−49.961	0.652
4100	65.471	354 647	300.309	222.786	73.070	−53.038	0.676
4200	65.714	356.227	301.621	229.345	72.948	−56.113	0.698
4300	65 977	357.777	302.909	235.929	72.830	−59.184	0.719
4400	66.258	359.297	304.174	242.541	72.718	−62.253	0.739
4500	66.547	360.789	305.415	249.181	72.613	−65.319	0.758
4600	66.852	362.255	306.635	255.851	72.518	−68.384	0.777
4700	67.178	363.696	307.834	262.552	72.433	−71.446	0.794
4800	67.513	365.114	309.012	269.287	72.361	−74.506	0.811
4900	67.873	366.509	310.172	276.056	72.304	−77.565	0.827
5000	68.249	367.884	311.312	282.862	72.265	−80.623	0.842
5100	68.647	369.240	312.435	289.706	72.244	−83.681	0.857
5200	69.065	370.577	313.540	296.592	72.245	−86.738	0.871
5300	69.496	371.896	314.629	303.520	72.270	−89.796	0.885
5400	69.948	373.200	315.701	310.492	72.321	−92.854	0.898
5500	70.425	374.487	316.758	317.510	72.401	−95.914	0.911
5600	70.919	375.761	317.801	324.577	72.511	−98.975	0.923
5700	71.433	377.021	318.829	331.695	72.655	−102.038	0.935
5800	71.965	378.268	319.843	338.865	72.834	−105.104	0.947
5900	72.521	379.502	320.843	346.089	73.052	−108.174	0.958
6000	73.090	380.726	321.831	353.369	73.311	−111.248	0.969

PREVIOUS December 1969 (1 atm) CURRENT December 1969 (1 bar)

Methylene (CH_2) **IDEAL GAS** **M_r = 14.02688 Methylene (CH_2)** **$C_1H_2(g)$**

$S°(298.15\ K) = 193.93 \pm 0.5\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 385.92 \pm 4.2\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 386.39 \pm 4.2\ kJ{\cdot}mol^{-1}$

Electronic Levels, Quantum Weights and Molecular Constants

State	ϵ_i, cm^{-1}	g_i	ν, cm^{-1}	C–H Distance, Å	H–C–H Angle, °	$I_A I_B I_C$ g^3·cm^6
X $^3B_1$	0	3	[2954](1) [1056(1) [3123](1)	1.029	136	4.506×10^{-120}
a $^1A_1$	[2600]	1	[3026](1) [1398](1) [3074](1)	1.11	102.4	13.53×10^{-120}
b $^1B_1$	7100 + [2600]	1	[2931](1) [761](1) [3110](1)	1.05	140	4.373×10^{-120}
c $^1A_1$	27700 + [2600]	1	[2954](1) [1056](1) [3123](1)	[1.029]	[136]	4.506×10^{-120}
			Point Group = C_{2v}			

Enthalpy of Formation

The electron impact data of Langer *et al.*[1] was reanalyzed by Prophet[2] to give $\Delta_f H°(CH_2, g, 298.15\ K) = 95 \pm 5\ kcal{\cdot}mol^{-1}$ Dibeler and Liston[3] reported the photoionization threshold for the process $CH_3CN \rightarrow CH_2^+ + HCN$ as 14.94 eV (344.55 kcal·mol^{-1}). Using auxiliary data from[4] and,[5] we obtain $\Delta_f H°(CH_2, g, 0\ K) = 95\ kcal{\cdot}mol^{-1}$, which is a maximum value as the process is likely to occur with excess energy. $\Delta_f H°(CH_2, g, 0\ K)$ values of 95.5 kcal·mol^{-1} (a maximum) and 86.8 ± 6.0 kcal·mol^{-1} have been obtained by Chupka *et al.*[6] from the appearance threshold of CH_2^+ from $C_2H_4(g)$ by photoionization,[6] and from chemical equilibria measured in a mass spectrometer,[7] respectively. Chupka[8] and Dibeler *et al.*[9] have determined the photoionization threshold for the production of CH_2^+ from CH_4. If the latter value is corrected for rotational energy effects as suggested by Chupka,[8] then both studies yield $\Delta_f H°(CH_2, g, 0\ K) = 94.6\ kcal{\cdot}mol^{-1}$. Chupka[8] indicates that this is a maximum value since the process of H_2 elimation is likely to occur with excess energy in the products at the threshold.

Chupka and Lifshitz[10] have obtained the photoionization threshold for CH_2^+ from CH_3 as 15.09 ± 0.03 eV. Combining this with the spectroscopic IP,[4] they report $\Delta_a H°(CH_2{-}H) = 4.694 \pm 0.033$ eV (108.25 ± 0.77 kcal·mol^{-1}). Using $\Delta_f H°(CH_3, g, 0\ K) = 35.64\ kcal{\cdot}mol^{-1}$ and $\Delta_f H°(H, g, 0\ K) = 51.63\ kcal{\cdot}mol^{-1}$ from these tables yields $\Delta_f H°(CH_2, g, 0\ K) = 92.24 \pm 1.0\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

Bernheim *et al.*,[11] in examining the EPR spectra of CH_2 which was produced by the photolysis of diazirine and trapped in xenon at 4 K, concluded that the ground state of CH_2 is a triplet state and it is bent. In similar followup work, they deduced a bond angle of 137.7 ± 0.6 for CD_2 from a measurement of the isotropic component of the ^{13}C hyperfine interaction. Wasserman *et al.*,[12] observing the EPR spectra on photolysis of diazomethane and diazirine at 4K, concluded that CH_2 has a triplet ground state with a probable bond angle of 136 ± 8. Waserman *et al.*[13] also reported that their investigation of the EPR spectra of CD_2 and CHD supported their earlier conclusions.[12] In these latter two works,[12, 13] the bond angle was determined from the zero–field parameter. In more recent work by Wasserman *et al.*,[14] the ^{13}C hyperfine structure was observed in the EPR spectrum of ground state $^{13}CD_2$ at 4 K. The authors conclude that ground state CH_2, by analogy, has an angle of 137–143°.

Herzberg and Johns[15] state that the electronic spectra of CH_2 and its isotopic derivatives is not only compatible with a linear ground state but it is also consistent with a bond angle of 136° if an ad hoc assumption of a heterogeneous predissociation of the excited state is made. Recent theoretical calculations indicate a bent ground state.[16, 17] We adopt the triplet ground state, X $^3B_1$, as bent with an angle of 136 ± 5° on the basis of the previously mentioned experimental work and weighted by the remarks of Herzberg and Johns.[15] The bond length is 1.029 Å as reported by Herzberg.[4] The bond lengths and angles for the a $^1A_1$ and b $^1B_1$ states are also from Herzberg and Johns.[18]

The singlet electronic levels are firmly established.[19] The unobserved singlet–triplet separation is likely to be less then 8000 cm^{-1}, as suggested by Herzberg.[19] Many theoretical arguments yield energy separations within 10% of this value.[16, 17, 20] Goldberg and Riter[24] estimate a value of 2600 ± 2000 cm^{-1} by calculations which allow for correlation energy effects in different states, all assumed to be linear, however. Foner and Hudson[21] suggest a "small" separation due to the absence of resolved structure in the CH_2 ionization curve. Carr *et al.*[22] via ketone photolysis deduced an energy gap of roughly 350–700 cm^{-1} Halberstadt and McNesby[23] suggest 880 cm^{-1} based on ketone photolysis in the presence of methane and propane. The value chosen for the singlet–triplet energy separation is 2600 ± 2000 cm^{-1}. This value is intermediate between the experimental and theoretical suggestions.

The vibrational frequencies for the three lower lying states were calculated via the valence force field method using the force constants calculated by O'Neil *et al.*[17] The geometry and vibrational levels for the c $^1A_1$ state were estimated. The uncertainty in the entropy mainly reflects the uncertain position of the low lying electronic levels.

References

[1] A. Langer, J. A. Hipple, and D. P. Stevenson, J. Chem. Phys. 22, 1836 (1954).
[2] H. Prophet, J. Chem. Phys. 38, 2345 (1963).
[3] V. H. Dibeler and S. K. Liston, J. Chem. Phys. 48, 4765 (1968).
[4] G. Herzberg, Proc. Roy. Soc. (London) A262, 291 (1961).
[5] U. S. Nat. Bur. Stand. Tech. Note 270-3, (1968).
[6] W. A. Chupka, J. Berkowitz, and K. M. A Rafaey, J. Chem. Phys. 50, 1938 (1969).

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Enthalpy Reference Temperature = T_r = 298.15 K; Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	$\Delta_f G°$ (kJ·mol^{-1})	log K_f
0	0.	0.	INFINITE	−9.994	385.917	385.917	INFINITE
100	33.258	157.288	223.967	−6.668	386.184	380.623	−198.817
200	33.499	180.376	197.055	−3.336	386.496	374.920	−97.919
298.15	34 600	193.931	193.931	0.	386.392	369.245	−64.690
300	34.627	194.146	193.932	0.064	386.387	369.139	−64.273
400	36.142	204.313	195.308	3.602	385.996	363.443	−47.461
500	37.663	212.541	197.957	7.292	385 437	357.866	−37.386
600	39.206	219.544	200.985	11.135	384.773	352.413	−30.680
700	40.808	225.707	204.085	15.135	384.063	347.076	−25.899
800	42.442	231.263	207 140	19.298	383.351	341.841	−22.320
900	44 048	236.355	210.107	23.623	382.667	336.693	−19.541
1000	45.571	241.075	212 971	28.105	382.022	331.620	−17.322
1100	46.976	245.486	215.728	32.733	381.418	326.609	−15.509
1200	48.247	249.629	218.382	37.495	380.850	321.652	−14.001
1300	49.379	253.536	220.938	42.378	380.313	316.741	−12.727
1400	50.381	257.233	223.399	47.367	379.799	311.870	−11.636
1500	51.264	260.740	225.773	52.450	379.299	307.036	−10.692
1600	52.040	264.073	228.063	57.616	378.809	302.234	−9.867
1700	52.724	267.249	230.276	62.855	378.323	297.463	−9 140
1800	53.327	270.280	232.415	68.158	377.835	292.721	−8.495
1900	53.861	273.178	234.484	73.518	377.343	288.005	−7.918
2000	54.336	275.953	236.489	78.928	376.844	283.316	−7.399
2100	54 760	278.615	238.432	84.384	376.335	278.652	−6.931
2200	55.142	281.171	240.317	89.879	375.815	274.013	−6.506
2300	55 485	283.630	242.147	95.411	375.282	269.398	−6.118
2400	55.797	285 998	243.925	100.975	374.736	264.806	−5.763
2500	56.080	288.282	245.654	106.569	374.174	260.237	−5.437
2600	56.338	290.486	247.336	112.190	373.598	255.690	−5.137
2700	56.575	292.617	248.974	117.836	373.005	251 167	−4.859
2800	56.792	294.678	250.570	123.505	372.396	246.665	−4.602
2900	56.993	296 675	252.125	129.194	371.770	242.186	−4.362
3000	57.177	298.610	253.643	134.903	371.127	237.728	−4.139
3100	57.348	300.488	255.124	140.629	370.466	233.292	−3.931
3200	57.506	302.311	256.570	146.372	369.787	228.878	−3.736
3300	57.652	304.083	257.983	152.130	369.089	224.486	−3.553
3400	57.787	305.806	259.364	157.902	368.372	220.115	−3.382
3500	57.913	307.483	260.715	163.687	367.636	215.765	−3.220
3600	58.030	309.116	262.037	169.484	366.880	211.436	−3.068
3700	58.139	310.708	263.331	175.293	366.103	207.129	−2.924
3800	58.240	312.259	264.598	181.112	365.307	202.843	−2.788
3900	58.334	313.773	265.840	186.940	364.489	198.578	−2.660
4000	58.421	315.251	267.057	192.778	363.650	194.335	−2.538
4100	58.502	316.695	268.250	198.624	362.790	190.113	−2.422
4200	58.577	318.106	269.420	204.478	361.908	185.912	−2.312
4300	58 647	319.485	270.569	210.339	361.003	181.732	−2.208
4400	58.713	320.834	271.696	216.207	360.077	177.573	−2.108
4500	58.773	322.154	272.802	222.082	359.129	173.436	−2.013
4600	58.830	323.446	273.889	227.962	358.158	169.320	−1.923
4700	58.882	324.712	274.957	233.848	357.164	165.226	−1.836
4800	58.931	325.952	276.007	239.738	356.149	161.153	−1.754
4900	58.976	327.168	277.039	245.634	355.111	157.101	−1.675
5000	59.018	328.360	278.053	251.533	354.052	153.071	−1.599
5100	59.058	329.529	279.051	257.437	352.971	149.062	−1.527
5200	59.094	330.676	280.033	263.345	351.868	145.074	−1.457
5300	59.128	331.802	280.999	269.256	350.745	141.108	−1.391
5400	59.160	332.908	281.950	275.170	349.602	137.164	−1.327
5500	59.189	333.993	282.886	281.088	348.438	133.240	−1.265
5600	59.217	335.060	283.809	287.008	347.256	129.338	−1.206
5700	59 242	336.108	284.717	292.931	346.054	125.457	−1.150
5800	59.266	337.139	285.612	298.857	344.835	121.598	−1.095
5900	59.288	338.152	286.494	304.784	343.599	117.759	−1.043
6000	59.309	339.149	287.363	310.714	342.347	113.942	−0.992

PREVIOUS. December 1972 (1 atm) CURRENT: December 1972 (1 bar)

Chlorofluoromethane (CH_2ClF) IDEAL GAS M_r = 68.478283 Chlorofluoromethane (CH_2ClF) $C_1H_2Cl_1F_1(g)$

$S°(298.15\ K) = 264.421 \pm 0.4\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = [-254.649 \pm 13]\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [-261.918\ \ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies		
ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
2993 (1)	1068 (1)	3048 (1)
1470 (1)	760 (1)	1236 (1)
1351 (1)	385 (1)	1004 (1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: C_s
Bond Distances: C–H = 1.078 ± 0.005 Å; C–Cl = 1.759 Å; C–F = 1.378 Å
Bond Angles: H–C–H = 111°54′; F–C–Cl = 110°; H–C–Cl = 109°06′
Product of the Moments of Inertia: $I_A I_B I_C = 4.818560 \times 10^{-115}\ g^3 \cdot cm^6$

Enthalpy of Formation

The change in enthalpy of atomization by successive replacement of F by Cl, in the CF_4 CCl_4 series and CHF_3 to $CHCl_3$ series, follows a regular pattern (see CCl_2F_2 and $CHCl_2F$ tables). We make the assumption that this same regular variation occurs also in the CH_2F_2 to CH_2Cl_2 series. Thus, the difference between the atomization energies of HC_2F_2 andf CH_2Cl_2 is divided into two unequal parts which fall into the patter n established in the CF_4 and CHF_2 sequences. We adopt an enthalpy of atomization of 385.5 kcal which corresponds to a $\Delta_f H°(CH_2ClF, g, 298.15\ K) = -62.6\ kcal \cdot mol^{-1}$. The changes in kcal, in the enthalpy of atomization by successive replacement of F by Cl are tabulated, below for all three series.

CF_4		
43.8		
CF_3Cl	CHF_3	
41.6	41.4	
CF_2Cl_2	CHF_2Cl	CH_2F_2
38.5	37.3	35.0
$CFCl_3$	$CHFCl_2$	CH_2FCl
36.0	33.0	29.7
CCl_4	$CHCl_3$	CH_2Cl_2

Heat Capacity and Entropy

Plyler and Benedict[1] assigned the vibrational frequencies from the infrared and Raman data for the liquid. The molecular structure was obtained from the microwave measurements of Muller.[2] The principal moments of inertia are: $I_A = 2.0097 \times 10^{-39}$, $I_B = 14.7640 \times 10^{-39}$, and $I_C = 16.2396 \times 10^{-39}\ g \cdot cm^2$.

References

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[2] N. Muller, J. Amer. Chem. Soc. 75, 800 (1953).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−11.251	−254.649	−254.649	INFINITE
100	34.287	222.046	301.119	−7.907	−257.273	−251.341	131.287
200	39.571	247.291	268.467	−4.235	−259.604	−244.502	63.857
250	43 143	256.493	265.173	−2.170	−260.791	−240.589	50.268
298.15	47.037	264.421	264.421	0.	−261.918	−236.595	41.451
300	47.192	264.712	264.422	0.087	−261.961	−236.438	41.168
350	51.421	272.304	265.012	2.552	−263.069	−232.096	34.638
400	55.568	279.443	266.374	5.228	−264.093	−227.600	29.722
450	59.472	286.216	268.205	8.105	−265.026	−222.981	25.883
500	63.064	292.671	270.331	11.170	−265.869	−218.264	22.802
600	69.292	304.738	275.075	17.798	−267.301	−208.603	18.160
700	74.417	315.817	280.115	24.991	−268.430	−198.726	14.829
800	78.676	326.041	285.225	32.652	−269.297	−188.707	12.321
900	82.258	335.520	290.293	40.704	−269.942	−178.592	10.365
1000	85.296	344.348	295.262	49 086	−270.401	−168.416	8.797
1100	87.887	352.603	300.104	57.748	−270.706	−158.201	7.512
1200	90.108	360.347	304.805	66.651	−270.887	−147.965	6.441
1300	92.019	367.637	309.361	75.760	−270.968	−137.717	5.534
1400	93.668	374.518	313.771	85.046	−270.972	−127.467	4.756
1500	95.097	381.031	318.040	94.486	−270.915	−117.218	4.082
1600	96.340	387.209	322.172	104.059	−270.812	−106.975	3.492
1700	97.425	393.083	326.172	113.749	−270.675	−96.739	2.972
1800	98.376	398.679	330.046	123.540	−270.514	−86.512	2.511
1900	99.212	404.021	333.799	133.420	−270.335	−76.295	2.097
2000	99 950	409.129	337.439	143.379	−270.145	−66.087	1.726
2100	100.604	414 021	340.970	153.407	−269.948	−55.889	1.390
2200	101.186	418.715	344.398	163.497	−269.749	−45.700	1.085
2300	101.705	423.225	347.728	173.642	−269.549	−35.521	0.807
2400	102.170	427.563	350.965	183.837	−269.352	−25.350	0.552
2500	102.587	431.743	354.113	194.075	−269.159	−15 187	0.317
2600	102.964	435.774	357.176	204.353	−268.971	−5.032	0.101
2700	103.304	439.666	360.160	214.666	−268.789	5.116	−0.099
2800	103 612	443.429	363.067	225.012	−268.614	15.258	−0.285
2900	103.892	447.069	365.901	235.388	−268.445	25.393	−0.457
3000	104.147	450.596	368.666	245.790	−268.285	35.523	−0.619
3100	104.381	454.015	371.364	256.216	−268.131	45.647	−0.769
3200	104.594	457.332	373.999	266.665	−267.985	55.766	−0.910
3300	104.790	460.554	376.573	277.135	−267.847	65.882	−1.043
3400	104.970	463.685	379.090	287.623	−267.715	75.992	−1.167
3500	105 136	466.730	381.550	298.128	−267.590	86.100	−1.285
3600	105.290	469.694	383.958	308.650	−267.470	96.203	−1.396
3700	105.432	472.581	386.314	319.186	−267.356	106.304	−1.501
3800	105.563	475.394	388.622	329.736	−267.247	116.401	−1.600
3900	105.686	478.138	390.882	340.298	−267.142	126.496	−1.694
4000	105.799	480.815	393.097	350.873	−267.040	136.588	−1.784
4100	105.905	483.429	395.268	361.458	−266.941	146.677	−1.869
4200	106.004	485.982	397.398	372.053	−266.843	156.765	−1.950
4300	106.096	488.477	399.487	382.658	−266.747	166.849	−2.027
4400	106.183	490.918	401.537	393.272	−266.652	176.932	−2.100
4500	106.263	493.305	403.550	403.895	−266.556	187.012	−2.171
4600	106.339	495.641	405.527	414.525	−266.459	197.090	−2.238
4700	106.411	497.929	407.469	425.162	−266.360	207.166	−2.302
4800	106.478	500.170	409.377	435.807	−266.259	217.241	−2.364
4900	106.541	502.366	411.252	446.458	−266.154	227.312	−2.423
5000	106.601	504.519	413.096	457.115	−266.046	237.382	−2.480
5100	106.657	506.631	414.909	467.778	−265.933	247.449	−2.534
5200	106.710	508.702	416.693	478.446	−265.814	257.514	−2.587
5300	106.760	510.735	418.448	489.120	−265.690	267.577	−2.637
5400	106.808	512.731	420.176	499.798	−265.560	277.638	−2.686
5500	106.853	514.692	421.877	510.481	−265.422	287.695	−2.732
5600	106.896	516.617	423.551	521.169	−265.276	297.751	−2.777
5700	106.936	518.510	425.201	531.860	−265.121	307.804	−2.821
5800	106.975	520.370	426.826	542.556	−264.958	317.854	−2.863
5900	107.011	522.199	428.427	553.255	−264.784	327.900	−2.903
6000	107.046	523.998	430.005	563.958	−264.600	337.944	−2.942

PREVIOUS: June 1970 (1 atm) CURRENT June 1970 (1 bar)

Chlorofluoromethane (CH_2ClF) $C_1H_2Cl_1F_1(g)$

Dichloromethane (CH_2Cl_2) IDEAL GAS $M_r = 84.93288$ Dichloromethane (CH_2Cl_2) $C_1H_2Cl_2(g)$

$S°(298.15 \text{ K}) = 270.293 \pm 0.04 \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = -88.663 \pm 1.3 \text{ kJ·mol}^{-1}$

$\Delta_f H°(298.15 \text{ K}) = -95.521 \pm 1.3 \text{ kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	 ν, cm^{-1}	 ν, cm^{-1}
2999 (1)	282 (1)	898 (1)
1467 (1)	1153 (1)	1268 (1)
717 (1)	3040 (1)	758 (1)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: C_{2v}
Bond Distances: C–H = 1.068 Å; C–Cl = 1.7724 Å
Bond Angles: H–C–H = 112°; Cl–C–Cl = 111.8°
Product of the Moments of Inertia: $I_A I_B I_C = 1.869359 \times 10^{-114} \text{ g}^3\text{·cm}^6$

Enthalpy of Formation

Hu and Sinke[1] have measured the enthalpy of combustion of $CH_2Cl_2(l)$ in the rotating bomb calorimeter, using As_2O_3 solution as the reducing agent. They reported $\Delta_c H°(298.15 \text{ K}) = -144.00 \text{ kcal·mol}^{-1}$ for $CH_2Cl_2(l) + CO_2(g) + 2 \text{ HCl(aq, 600 } H_2O)$ which leads $\Delta_f H°(CH_2Cl_2,(l), 298.15 \text{ K}) = -29.70 \text{ kcal·mol}^{-1}$, using $\Delta_f H°(298.15 \text{ K}) = -94.051$ and $-39.823 \text{ kcal·mol}^{-1}$ for $CO_2(g)$ and HCl(aq, 600 H_2O), respectively.[2] The standard deviation of five combustion runs was 0.12 kcal·mol^{-1}. Employing the heat of vaporization of $CH_2Cl_2(l)$ at 298.15 K as 6.87 kcal·mol^{-1},[3] we obtain $\Delta_f H°(CH_2Cl_2, g, 298.15 \text{ K}) = -22.83 \text{ kcal·mol}^{-1}$ (-95.521 ± 1.3 kJ·mol^{-1} *which is adopted in* the tabulation.

Smith *et al.*,[4] based on the combustion data of Eftring,[5] re-evaluated the enthalpy of combustion of dichloromethane at 18.7°C as $\Delta E°/M = -1701.4 \text{ cal·g}^{-1}$ for $CH_2Cl_2(l) + O_2(g) + CO_2(g) + 2 \text{ HCl(aq, 600 } H_2O)$. This value needs to be further corrected for a change in the enthalpy of oxidation of As_2O_3[6] and calculated to 25°C to give $\Delta_c E°(298.15 \text{ K}) = \Delta_c H°(298.15 \text{ K}) = -144.89 \text{ kcal mol}^{-1}$, $\Delta_f H°(CH_2Cl_2, l, 298.15 \text{ K}) = -28.80 \text{ kcal·mol}^{-1}$ and $\Delta_f H°(CH_2Cl_2, g, 298.15 \text{ K}) = -21.93 \text{ kcal·mol}^{-1}$.

Lacher *et al.*[7] have measured the enthalpy of hydrogenation of dichloromethane to methane and hydrogen chloride at 250°C as −40.07 kcal·mol^{-1}. Correction to 298.15 K gives $\Delta_f H°(CH_2Cl_2, g\ 298.15 \text{ K}) = -23.05 \text{ kcal·mol}^{-1}$ which is in good agreement with the value adopted.

Heat Capacity and Entropy

The bond distances and angles have been determined from the microwave spectra by Meyers and Gwinn.[8] The principal moments of inertia are: $I_A = 2.6307 \times 10^{-39}$, $I_B = 25.6246 \times 10^{-39}$, and $I_C = 27.7305 \times 10^{-39} \text{ g·cm}^2$.

The assigned fundamental vibrational frequencies are obtained from Shimanouchi's selection,[9] based on infrared and Raman spectra by Shimanouchi and Syzuki,[10] Welsh *et al.*,[12] and Palma *et al.*[11]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−11.842	−88.663	−88.663	INFINITE
100	35 760	225.132	309.694	−8.456	−91.248	−84 693	44.239
200	42.366	251.822	274.664	−4.568	−93.419	−77.291	20.186
250	46.584	261.721	271.107	−2.347	−94.507	−73.133	15.280
298.15	50.896	270.293	270.293	0.	−95.521	−68.924	12.075
300	51.062	270.609	270.294	0.094	−95.558	−68.759	11.972
350	55 459	278.813	270.932	2.758	−96.533	−64.214	9.583
400	59.570	286 490	272.402	5.635	−97.416	−59.536	7.775
450	63.309	293.726	274.373	8.709	−98.207	−54.752	6.355
500	66.667	300.574	276.654	11.960	−98.912	−49.885	5.211
600	72.367	313.251	281.715	18.922	−100.090	−39.964	3.479
700	76.997	324.766	287.055	26.398	−100.996	−29.868	2.229
800	80.838	335.306	292.437	34.295	−101.672	−19.658	1.284
900	84.079	345.020	297.747	42.545	−102.151	−9.376	0.544
1000	86.842	354.025	302.930	51.095	−102.465	0.951	−0.050
1100	89.211	362.416	307.961	59.901	−102.643	11.302	−0.537
1200	91.252	370.268	312.829	68.926	−102.708	21.664	−0.943
1300	93.014	377.643	317.534	78.142	−102.685	32.028	−1.287
1400	94.542	384.593	322.078	87.521	−102.591	42.387	−1.581
1500	95.869	391.163	326.467	97.043	−102.442	52.738	−1.836
1600	97 026	397.388	330.707	106.690	−102.252	63.077	−2.059
1700	98.039	403.301	334.804	116.444	−102.032	73.404	−2.255
1800	98.927	408.930	338.767	126.293	−101.791	83.717	−2.429
1900	99.710	414.300	342.603	136.226	−101.537	94.016	−2.585
2000	100.403	419.433	346.317	146.232	−101.278	104.301	−2.724
2100	101.017	424.347	349.916	156.304	−101.019	114.574	−2.850
2200	101.564	429.059	353 407	166.433	−100.765	124.834	−2.964
2300	102.052	433.584	356.796	176 615	−100.523	135.083	−3.068
2400	102.490	437.937	360.086	186.842	−100.295	145.322	−3.163
2500	102.883	442.129	363.285	197.111	−100.086	155.552	−3.250
2600	103.238	446 171	366.395	207.417	−99.899	165.773	−3.330
2700	103.559	450.074	369.423	217.757	−99.738	175.988	−3.405
2800	103.849	453.845	372.371	228.128	−99.603	186.198	−3.474
2900	104 114	457.494	375.244	238.526	−99.499	196.403	−3.538
3000	104.355	461.028	378.044	248.950	−99.425	206.605	−3.597
3100	104.575	464.453	380.777	259.397	−99.383	216.806	−3.653
3200	104.777	467.777	383.444	269.864	−99.373	227.005	−3.705
3300	104 962	471.004	386.049	280.352	−99.395	237.205	−3.755
3400	105.133	474.140	388.594	290.856	−99.450	247.405	−3.801
3500	105.290	477 189	391.082	301.378	−99.536	257.608	−3.845
3600	105.435	480.158	393.515	311.914	−99.651	267.814	−3.886
3700	105.570	483.048	395.896	322.464	−99.796	278.023	−3.925
3800	105.694	485.865	398.226	333.028	−99.967	288.237	−3.962
3900	105.810	488.612	400.509	343.603	−100.164	298.455	−3.997
4000	105.917	491.293	402.745	354.189	−100.383	308.679	−4.031
4100	106.018	493.909	404.937	364.786	−100.624	318.908	−4.063
4200	106.111	496 465	407.086	375.393	−100.883	329.144	−4.094
4300	106.199	498.963	409.194	386.008	−101.159	339.386	−4.123
4400	106.280	501.405	411.262	396.632	−101.448	349.634	−4.151
4500	106.357	503.795	413.292	407.264	−101.750	359.889	−4.177
4600	106.429	506.133	415.284	417.903	−102.061	370.152	−4.203
4700	106.497	508.423	417.242	428.550	−102.379	380.420	−4.228
4800	106.560	510.665	419.165	439.203	−102.702	390.697	−4.252
4900	106.620	512.863	421.055	449.862	−103.028	400.979	−4.274
5000	106.677	515.018	422.913	460.527	−103.355	411.268	−4.296
5100	106.730	517.131	424.739	471.197	−103.682	421.564	−4.318
5200	106.780	519.204	426.536	481.872	−104.005	431.866	−4.338
5300	106.828	521.238	428.304	492.553	−104.325	442.174	−4.358
5400	106.873	523.236	430.043	503.238	−104.637	452.488	−4.377
5500	106.916	525 197	431.756	513.927	−104.943	462.808	−4.395
5600	106.956	527.124	433.441	524.621	−105.239	473.134	−4.413
5700	106.995	529.017	435.102	535.319	−105.524	483.464	−4.430
5800	107.031	530.878	436.737	546.020	−105.798	493.800	−4.447
5900	107.066	532.708	438.348	556.725	−106.058	504.140	−4.463
6000	107.099	534.508	439.936	567.433	−106.304	514.484	−4.479

PREVIOUS: December 1968 (1 atm) CURRENT: December 1968 (1 bar)

Difluoromethane (CH_2F_2) IDEAL GAS $M_r = 52.023686$

$\Delta_fH^\circ(0\ K) = -443.005 \pm 1.7\ kJ{\cdot}mol^{-1}$

$S^\circ(298.15\ K) = 246.698 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_fH^\circ(298.15\ K) = -450.659 \pm 1.7\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
2949 (1)	530 (1)	1176 (1)
1508 (1)	1262 (1)	1435 (1)
1116 (1)	3013 (1)	1090 (1)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: C_{2v}
Bond Distances: C–F = 1.358 ± 0.001 Å; C–H = 1.092 ± 0.003 Å
Bond Angles: F–C–F = 108° 17' ± 6'; H–C–H = 111° 52' ± 25'
Product of the Moments of Inertia: $I_AI_BI_C = 1.22816 \times 10^{-115}\ g^3{\cdot}cm^6$

Enthalpy of Formation

Neugebauer and Margrave[1] measured the enthalpy of combustion of CH_2F_2. Their result for the combustion reaction

$$CH_2F_2(g) + O_2(g) \rightarrow CO_2(g) + 2HF{\cdot}21.5\ H_2O$$

was $\Delta_fH(298.15\ K) = -139.84 \pm 0.22\ kcal{\cdot}mol^{-1}$. Using $\Delta_fH^\circ(HF{\cdot}21.5\ H_2O, 298.15\ K) = -76.75 \pm 0.1\ kcal{\cdot}mol^{-1}$,[2] obtained with dilution data compiled by Parker,[3] we derive, $\Delta_fH^\circ(CH_2F_2, g, 298.15\ K) = -107.7 \pm 0.4\ kcal{\cdot}mol^{-1}$ ($-450.659 \pm 1.7\ kJ{\cdot}mol^{-1}$) from Neugebauer and Margrave's data.

Heat Capacity and Entropy

The vibrational frequencies are average values from the infrared studies of Stewart and Nielsen[4] and Plyler and Benedict.[5] Pricipal moments of inertia are calculated from the rotational constants reported by Lide[6] with the result $I_A = 1.7088 \times 10^{-39}$, $I_B = 7.9171 \times 10^{-39}$, and $I_C = 9.0781 \times 10^{-39}\ g{\cdot}cm^2$. The molecular structure data are from the microwave studies of Lide[6] and are in excellent agreement with electron-diffraction studies of Brockway, Thornton, and Bartell whose results are reported in the Annual review of Physical Chemistry.[7]

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Difluoromethane (CH_2F_2) $C_1H_2F_2(g)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	Δ_fH°	Δ_fG°	log K_f
0	0.	0.	INFINITE	-10.690	-443.005	-443.005	INFINITE
100	33.494	206.992	280.603	-7.361	-445.642	-439.137	229.381
200	36.678	230.995	250.396	-3.880	-448.111	-431.680	112.743
250	39.472	239.465	247.384	-1.980	-449.405	-427.424	89.305
298.15	42.859	246.698	246.698	0.	-450.659	-423.076	74.121
300	43.000	246.964	246.699	0.079	-450.706	-422.905	73.634
350	46.984	253.888	247.237	2.328	-451.967	-418.171	62.409
400	51 113	260.431	248.481	4.780	-453.153	-413.261	53.966
450	55 154	266.686	250.158	7.438	-454.252	-408.208	47.384
500	58.973	272.697	252.114	10.292	-455.257	-403.037	42.105
600	65.767	284.068	256.503	16.539	-456.991	-392.424	34.164
700	71.458	294.646	261.206	23.408	-458.383	-381.549	28.472
800	76.212	304.508	266.009	30.799	-459.476	-370.494	24.191
900	80.205	313 722	270.804	38.625	-460.313	-359.319	20.854
1000	83.577	322.352	275.532	46.819	-460.936	-348 062	18.181
1100	86.438	330.455	280.161	55.324	-461.384	-336.752	15.991
1200	88.876	338.083	284.673	64.093	-461.691	-325.407	14.165
1300	90.962	345.282	289.061	73.087	-461.885	-314.042	12.618
1400	92.754	352.090	293.322	82.275	-461.991	-302.665	11.293
1500	94.301	358.543	297.457	91.630	-462.030	-291.282	10.143
1600	95.641	364.673	301.468	101.129	-462.016	-279.900	9.138
1700	96.807	370.507	305.359	110.752	-461.963	-268.519	8.251
1800	97.825	376.070	309.134	120.485	-461.881	-257 142	7.462
1900	98.719	381.384	312.798	130.313	-461.776	-245.770	6.757
2000	99.507	386.468	316.355	140.225	-461.655	-234.404	6.122
2100	100.203	391.340	319.811	150.212	-461.520	-223.045	5.548
2200	100.822	396.016	323.169	160.263	-461.373	-211.693	5.026
2300	101.373	400.510	326.435	170.374	-461.215	-200.347	4.550
2400	101.866	404.835	329.612	180.536	-461.047	-189.009	4.114
2500	102.308	409.003	332.704	190.745	-460.868	-177.677	3.712
2600	102.706	413.023	335.717	200.996	-460.677	-166.353	3.342
2700	103.065	416.906	338.652	211.285	-460.473	-155.037	2.999
2800	103.391	420.660	341.514	221.608	-460.255	-143.729	2.681
2900	103.686	424.294	344.307	231.962	-460.022	-132.428	2.385
3000	103.955	427.813	347.032	242.344	-459.773	-121.136	2.109
3100	104.201	431.226	349.693	252.752	-459.507	-109.853	1.851
3200	104.426	434.538	352.293	263.184	-459.223	-98.578	1.609
3300	104.632	437.754	354.834	273.637	-458.922	-87.312	1.382
3400	104.822	440.881	357.319	284.110	-458.602	-76.056	1.168
3500	104.997	443.922	359.750	294.601	-458.264	-64.810	0.967
3600	105.158	446.882	362.130	305.109	-457.908	-53.573	0.777
3700	105.307	449.765	364.459	315.632	-457.534	-42.347	0.598
3800	105.445	452.576	366.741	326.170	-457.143	-31.131	0.428
3900	105.573	455.316	368.978	336.721	-456.735	-19.925	0.267
4000	105.693	457.991	371.170	347.284	-456.310	-8.730	0.114
4100	105.804	460.602	373.319	357.859	-455.870	2.454	-0.031
4200	105.907	463.153	375.428	368.445	-455.415	13.627	-0.169
4300	106.004	465.646	377.497	379.040	-454.947	24.789	-0.301
4400	106.095	468.084	379.528	389 645	-454.465	35.940	-0.427
4500	106.180	470.469	381.523	400.259	-453.970	47.080	-0.546
4600	106.259	472.804	383.482	410.881	-453.465	58.209	-0.661
4700	106.334	475.090	385.407	421.511	-452.948	69.327	-0.770
4800	106.404	477.329	387.299	432.148	-452.421	80.434	-0.875
4900	106.471	479.524	389.158	442.791	-451.885	91.529	-0.976
5000	106.533	481.676	390.987	453.442	-451.340	102.614	-1.072
5100	106.592	483.786	392.786	464.098	-450.787	113.687	-1.164
5200	106.647	485.856	394.556	474.760	-450.226	124.750	-1.253
5300	106.700	487.888	396.298	485.427	-449.658	135.802	-1.338
5400	106.750	489.883	398.013	496.100	-449.083	146.843	-1.420
5500	106.797	491.842	399.701	506.777	-448.501	157.873	-1.499
5600	106.842	493.767	401.364	517.459	-447.912	168.893	-1.575
5700	106.884	495.658	403.001	528.145	-447.317	179.902	-1.649
5800	106.925	497.518	404.615	538.836	-446.716	190.901	-1.719
5900	106.963	499.346	406.205	549.530	-446.108	201.889	-1.787
6000	106.999	501.144	407.772	560.228	-445.494	212.866	-1.853

PREVIOUS: December 1969 (1 atm) CURRENT: December 1969 (1 bar)

Formaldehyde (H_2CO) IDEAL GAS $M_r = 30.02628$ Formaldehyde (H_2CO) $C_1H_2O_1(g)$

$\Delta H_f°(0\ K) = -112.057 \pm 6.3\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -115.897 \pm 6.3\ kJ{\cdot}mol^{-1}$

$S°(298.15\ K) = 218.950 \pm 0.4\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

Vibrational Levels and Degeneracies

ν, cm^{-1}	ν, cm^{-1}
2766.4 (1)	2843.4(1)
1746.07(1)	1247.4(1)
1500.6 (1)	1163.5(1)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: C_{2v}
Bond Distances: C–H = 1.12 ± 0.01 Å; C–O = 1.21 ± 0.01 Å
Bond Angle· H–C–H = 118 ± 2°
Product of the Moments of Inertia: $I_A I_B I_C = 1.6597 \times 10^{-117}\ g^3{\cdot}cm^6$

Enthalpy of Formation

Delepine and Badoche[1] measured the enthalpy of combustion of a formaldehyde polymer. Their value is revised to $\Delta_f H°(298.15\ K) = -25.0$ kcal·mol^{-1} based on the following thermochemical cycle:

I $C(cr) + 1/2O_2(g) + H_2(g) = \frac{1}{n}(CH_2O)_n(cr)$ −42.3 kcal·mol^{-1}
II $[1/n]\ (CH_2O)_n(cr) + H_2O = CH_2O(aq)$ 2.4
III $CH_2O(g) = CH_2O(aq)$ 14.9

Equation I and II are based upon data listed by Delepine and Badoche.[1] For reaction III, Delepine and Badoche obtained 15 kcal·mol^{-1}. Whereas, Walker[2] obtained 14.8 kcal·mol^{-1}. A value of −27.7 kcal·mol^{-1} is obtained from the combustion experiments of Wartenberg and Lerner–Steinberg.[3] Corrections of −0.6 and 0.1 kcal·mol^{-1} were applied to obtain a enthalpy of reaction at constant pressure and at 298.15 K.

Equilibrium constant determinations of reaction (IV) by Newton and Dodge[4] lead to a $\Delta_f H°(298.15\ K) = -29.0$ kcal·mol^{-1}.

IV $H_2(g) + CO(g) = H_2CO(g)$

The value obtained from the measurements of Wartenberg and Lerner–Steinberg[3] is believed to be the most reliable.

Heat Capacity and Entropy

Frequencies were measured by Blau and Nielson[5] in the I. R. Microwave determinations of Lawrence and Strandberg,[6] and those of Erlandson[7] are in essential agreement. The principal moments of inertia are: $I_A = 0.3085 \times 10^{-39}$, $I_B = 2.1701 \times 10^{-39}$, and $I_C = 2.4786 \times 10^{-39}\ g{\cdot}cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.021	−112.057	−112.057	INFINITE
100	33.258	182.208	249.156	−6.695	−113.243	−112.630	58.832
200	33.502	205.292	222.109	−3.363	−114.387	−111.598	29.146
250	34.194	212.831	219.525	−1.673	−115.118	−110.819	23.154
298.15	35.402	218.950	218.950	0.	−115.897	−109.921	19.258
300	35.458	219.169	218.951	0.066	−115.928	−109.884	19.132
350	37.203	224.761	219.388	1.880	−116.771	−108.810	16.239
400	39.264	229.861	220.383	3.791	−117.616	−107.615	14.053
450	41.489	234.613	221.703	5.810	−118.445	−106.314	12.341
500	43.766	239.102	223.220	7.941	−119.245	−104.923	10.961
600	48.216	247.478	226.575	12.542	−120.731	−101.917	8.873
700	52.319	255.224	230.121	17.572	−122.039	−98.675	7.363
800	55.983	262.455	233.716	22.991	−123.162	−95.259	6.220
900	59.199	269.239	237.290	28.754	−124.111	−91.712	5.323
1000	61.995	275 624	240.807	34.817	−124.906	−88.068	4.600
1100	64.411	281.649	244.249	41.140	−125.570	−84.351	4.005
1200	66.494	287.345	247.605	47.688	−126.127	−80.578	3.507
1300	68.290	292.740	250.871	54.429	−126.596	−76.763	3.084
1400	69.840	297.859	254.046	61.338	−126.998	−72.914	2.720
1500	71.182	302.724	257.131	68.390	−127.349	−69.039	2.404
1600	72.346	307.356	260.126	75.568	−127.661	−65.141	2.127
1700	73.360	311.773	263.035	82.855	−127.946	−61.225	1.881
1800	74.246	315.992	265.861	90.236	−128.213	−57.292	1.663
1900	75.023	320.028	268.606	97.700	−128.470	−53.345	1.467
2000	75.709	323.894	271.275	105.237	−128.724	−49.385	1.290
2100	76.314	327.602	273.869	112.839	−128.979	−45.411	1.130
2200	76.852	331.165	276.393	120.498	−129.240	−41.426	0.984
2300	77.331	334.592	278.850	128.208	−129.510	−37.428	0.850
2400	77.759	337.893	281.241	135.963	−129.792	−33.419	0.727
2500	78.143	341.075	283.572	143.758	−130.090	−29.397	0.614
2600	78.489	344.146	285.843	151.590	−130.404	−25.363	0.510
2700	78.801	347.115	288.057	159.455	−130.736	−21.317	0.412
2800	79.083	349 986	290.218	167.349	−131.088	−17.258	0.322
2900	79.339	352 765	292.327	175.270	−131.461	−13.186	0.238
3000	79.573	355.459	294.387	183.216	−131.855	−9.101	0.158
3100	79 786	358.072	296.399	191.184	−132.272	−5.002	0.084
3200	79.981	360.608	298.366	199.173	−132.713	−0.890	0.015
3300	80.159	363.072	300.290	207.180	−133.177	3.236	−0.051
3400	80.323	365.467	302.172	215.204	−133.666	7.377	−0.113
3500	80.475	367.798	304 014	223.244	−134.179	11.533	−0.172
3600	80.614	370.067	305.817	231.299	−134.717	15.704	−0.228
3700	80.743	372.277	307.584	239.367	−135.281	19.890	−0.281
3800	80.863	374.432	309.315	247.447	−135.871	24.092	−0.331
3900	80.974	376.534	311.011	255.539	−136.486	28.310	−0.379
4000	81.077	378.586	312.675	263.641	−137.128	32.543	−0.425
4100	81.173	380.589	314.307	271.754	−137.796	36.793	−0.469
4200	81.263	382.546	315.909	279.876	−138.491	41.060	−0.511
4300	81.346	384.459	317.481	288.006	−139.213	45.343	−0.551
4400	81.425	386.330	319.024	296.145	−139.962	49.643	−0.589
4500	81.498	388.161	320.541	304.291	−140.738	53.961	−0.626
4600	81.567	389.953	322.030	312.444	−141.540	58.296	−0.662
4700	81.631	391.708	323.494	320.604	−142.371	62.650	−0.696
4800	81.692	393.427	324.933	328.771	−143.228	67.021	−0.729
4900	81.749	395.112	326.348	336.943	−144.113	71.410	−0.761
5000	81.803	396.764	327.740	345.120	−145.025	75.818	−0.792
5100	81.854	398.384	329.109	353.303	−145.964	80.244	−0.822
5200	81.902	399.974	330.457	361.491	−146.930	84.689	−0.851
5300	81 948	401.535	331.783	369.683	−147.924	89.153	−0.879
5400	81 991	403.067	333.089	377.880	−148.944	93.636	−0.906
5500	82.031	404.572	334.375	386.082	−149.991	98.137	−0.932
5600	82.070	406.050	335.642	394.287	−151.064	102.659	−0.958
5700	82.107	407.503	336.890	402.495	−152.164	107.199	−0.982
5800	82.141	408.932	338.120	410.708	−153.290	111.759	−1.007
5900	82.175	410.336	339.332	418.924	−154.442	116.338	−1.030
6000	82.206	411.717	340.527	427.143	−155.619	120.938	−1.053

PREVIOUS· March 1961 (1 atm) CURRENT: March 1961 (1 bar)

Methyl (CH$_3$) IDEAL GAS $M_r = 15.03482$ Methyl (CH$_3$) C$_1$H$_3$(g)

$S°(298.15\ K) = 194.171 \pm 1.3\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 149.031 \pm 0.8\ kJ{\cdot}mol^{-1}$

$\Delta_f H°(298.15\ K) = 145.687 \pm 0.8\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights	
ϵ_i, cm^{-1}	g_i
0	2
46205	2

Vibrational Frequencies and Degeneracies
ν, cm^{-1}
[3002] (1)
580 (1)
[3184] (2)
1383 (2)

Point Group: D_{3h} $\sigma = 6$
Bond Distance: C–H = 1.079 Å
Bond Angle: H–C–H = 120°
Product of the Moments of Inertia: $I_A I_B I_C = 4.99 \times 10^{-119}\ g^3{\cdot}cm^6$

Enthalpy of Formation

Chupka[1] measured the photoionization spectrum of methane and from the onset of CH_3^+ production has reported $\Delta_a H°(CH_3–H) = 103.244 \pm 0.12\ kcal{\cdot}mol^{-1}$. The value was corrected for the thermal rotation energy of the fragment ions and is the value adopted here.

Dibeler *et al.*[2] had earlier reported $\Delta_a H°(CH_3–H) = 101.7 \pm 0.5\ kcal{\cdot}mol^{-1}$ but they did not apply the rotational energy correction, which bring them closer to Chupka.

The photoionization values are in good agreement with earlier electron impact determiantions as summarized by Stevenson[3] who gives $\Delta_a H°(CH_3–H) = 101.9 \pm 1\ kcal{\cdot}mol^{-1}$. Kinetic determinations have been recently reviewed by Kerr[4] and yield $\Delta_a H°(CH_3–H) = 102.5 \pm 1\ kcal{\cdot}mol^{-1}$ again in excellent agreement.

Heat Capacity and Entropy

The structure, bond length, angles and electronic levels are those reported by Herzberg.[5] A set of vibrational frequencies have been reported by Andrews and Pimentel[6] in an argon matrix, of which only two were observed. Milligan and Jacox[7] observed $\nu_2 = 611\ cm^{-1}$ in an argon matrix and disagreed with Andrews and Pimentel who reported 730 cm^{-1}. Later, Tan and Pimentel[8] agreed that the earlier values were for a methyl radical interacting with an alkali halide molecule. This would affect the ν_2 mode strongest, thus, we adopt the remaining in plane frequencies which appear to be of the correct magnitudes. The ν_2 mode is taken fro mthe analysis of Herzberg[5] since this represents the gas phase molcule and is in resonable agreement with the matrix value of Milligan and Jacox.[7] The uncertainity in the entropy reflects the uncertainties in the vibrational frequencies.

The principal moments of inertia are: $I_A = I_B = 0.2923 \times 10^{-39}$, and $I_C = 0.5846 \times 10^{-39}\ g{\cdot}cm^2$.

References

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−10.407	149.031	149.031	INFINITE
100	33.395	155.665	226.465	−7.080	147.800	147.438	−77 014
200	35.638	179.380	197.609	−3.646	146.868	147.432	−38.505
250	37.162	187.495	194.799	−1.826	146.297	147.637	−30.847
298.15	38.693	194.170	194.170	0.	145.687	147.950	−25.920
300	38.753	194.410	194.171	0.072	145.663	147.964	−25.763
350	40.392	200.506	194.649	2.050	144.997	148.400	−22.147
400	42.041	206.008	195.730	4.111	144.320	148.932	−19.449
450	43.668	211.054	197.156	6.254	143.644	149.549	−17.359
500	45.252	215.737	198.783	8.477	142.976	150.241	−15.696
600	48.288	224.258	202.333	13.155	141.682	151.817	−13.217
700	51.174	231.921	206.021	18.130	140 477	153.602	−11 462
800	53.926	238.935	209.703	23.386	139.383	155.554	−10.157
900	56.527	245.438	213.316	28.910	138.411	157.635	−9 149
1000	58.954	251.521	216.836	34.686	137.557	159.817	−8.348
1100	61.187	257.247	220.252	40.694	136.814	162.080	−7.697
1200	63.217	262.659	223.562	46.916	136.167	164.406	−7.156
1300	65.048	267.793	226.769	53.331	135.602	166.783	−6.701
1400	66.690	272.675	229.875	59.919	135.105	169.201	−6.313
1500	68.156	277.327	232.885	66.663	134.662	171.652	−5.977
1600	69.463	281.768	235.802	73.545	134.262	174.131	−5.685
1700	70.628	286.015	238.632	80.551	133.896	176.634	−5.427
1800	71.667	290.082	241.378	87.667	133.554	179.158	−5.199
1900	72.594	293.982	244.045	94.881	133.230	181.701	−4.995
2000	73.422	297.727	246.636	102.182	132.917	184.260	−4.812
2100	74.165	301.327	249.155	109.562	132.610	186.835	−4 647
2200	74.831	304.793	251.606	117.013	132.305	189.424	−4 497
2300	75.430	308.133	253.991	124.526	131.999	192.027	−4.361
2400	75.971	311.355	256.315	132.097	131.688	194 644	−4.236
2500	76.459	314.466	258.579	139.719	131.369	197.273	−4.122
2600	76.902	317.474	260.787	147.387	131.041	199.916	−4.016
2700	77.304	320.384	262.940	155.098	130.701	202.571	−3.919
2800	77.670	323.202	265.042	162.847	130.348	205.239	−3.829
2900	78.003	325.933	267.095	170.630	129.980	207.921	−3.745
3000	78.309	328.583	269.101	178.446	129.595	210.615	−3.667
3100	78.588	331.155	271.061	186.291	129.193	213.322	−3.594
3200	78.845	333.655	272.979	194.163	128.772	216.042	−3.527
3300	79.082	336.084	274.854	202.060	128.331	218.777	−3.463
3400	79.300	338.449	276.690	209.979	127.869	221.524	−3 403
3500	79.501	340.750	278.488	217.919	127.385	224.286	−3.347
3600	79.687	342.992	280.248	225.879	126.879	227.061	−3.295
3700	79.860	345.178	281.974	233.856	126.349	229.852	−3.245
3800	80.020	347.310	283.665	241.850	125.796	232.656	−3.198
3900	80.169	349.391	285.324	249.860	125.217	235.476	−3.154
4000	80.308	351.422	286.951	257.884	124.613	238.311	−3.112
4100	80.438	353.407	288.548	265.921	123.984	241.161	−3.072
4200	80.559	355.346	290.115	273.971	123.328	244.027	−3.035
4300	80.672	357.243	291.654	282.033	122.645	246.909	−2.999
4400	80.778	359.099	293.166	290.105	121.936	249.807	−2.966
4500	80.878	360.916	294.652	298.188	121.199	252.721	−2.934
4600	80.972	362.694	296.112	306.281	120.436	255.652	−2.903
4700	81.060	364.437	297.547	314.382	119.645	258.600	−2.874
4800	81.143	366.144	298.958	322.492	118.827	261.565	−2.846
4900	81.221	367.818	300.347	330.611	117.982	264.547	−2.820
5000	81.295	369.460	301.712	338.737	117.111	267.548	−2.795
5100	81.365	371.070	303.057	346.870	116.214	270.565	−2.771
5200	81.432	372.651	304.380	355.009	115.292	273.601	−2.748
5300	81.495	374.203	305.683	363.156	114.345	276.654	−2.727
5400	81.554	375.726	306.966	371.308	113.373	279.726	−2.706
5500	81.611	377.223	308.230	379.467	112.379	282.815	−2.686
5600	81.666	378.694	309.475	387.630	111.362	285.923	−2.667
5700	81.718	380.140	310.702	395.800	110.324	289.050	−2.649
5800	81.767	381.562	311.911	403.974	109.266	292.195	−2.631
5900	81.815	382.960	313.104	412.153	108.188	295.357	−2.615
6000	81.860	384.336	314.280	420.337	107.094	298.539	−2.599

PREVIOUS: June 1969 (1 atm)   CURRENT. June 1969 (1 bar)

Chloromethane (CH_3Cl) IDEAL GAS $M_r = 50.48782$ Chloromethane (CH_3Cl) $C_1H_3Cl_1(g)$

$S°(298.15\ K) = 234.367 \pm 0.42\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -75.753 \pm 2.1\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -83.680 \pm 2.1\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	 ν, cm^{-1}
2968 (1)	3054 (2)
1355 (1)	1455 (2)
732 (1)	1017 (2)

Ground State Quantum Weight: 1 $\sigma = 3$
Point Group: C_{3v}
Bond Distances: C–H = 1.0959 Å; C–Cl = 1.7812 Å
Bond Angles: H–C–H = 108°; H–C–Cl = 110°55′
Product of the Moments of Inertia: $I_A I_B I_C = 2.14799 \times 10^{-116}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The enthalpy of formation has been determined by hydrogenation of methyl chloride to give methane and hydrogen chloride by Lacher *et al.*,[1] and by Lacher *et al.*[2] They reported an average enthalpy of hydrogenation at 248°C to be $-19{,}655 \pm 45\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$. Using this value, together with JANAF data[5] for $H_2(g)$, $CH_4(g)$, HCl(g), the enthalpy of formation of methyl chloride is calculated to be $\Delta_f H°(298.15\ K) = -20.69\ kcal{\cdot}mol^{-1}$. Fowell *et al.*,[3] using a similar hydrogenation technique almost ten years later, report a value $\Delta_f H°(CH_3Cl, g, 298.15\ K) = -20.741\ kcal{\cdot}mol^{-1}$.

Fletcher and Pilcher[4] derived the enthalpy of formation by measuring the enthalpy of combustion of methyl chloride by flame calorimetry. They reported a value $\Delta_f H°(CH_3Cl, g, 298.15\ K) = -19.59 \pm 0.16\ kcal{\cdot}mol^{-1}$ where the error, according to the authors, is twice the standard deviation of the mean including the uncertainty in calibration, measurement, determination of ignition energy, and values of auxiliary data used.

In support of their results, Fletcher and Pilcher[4] have compared the enthalpies of formation of $C_2H_5Cl(g)$ and i-$C_3H_7Cl(g)$ as determined by equilibrium studies (2nd and 3rd law) with their work via flame calorimetry. The agreement is excellent ($<0.2\ kcal{\cdot}mol^{-1}$ difference) but in both cases results for hydrogenation studies are at least $1\ kcal{\cdot}mol^{-1}$ less negative. In the case of $CH_3Cl(g)$ no equilibrium results are currently available and the results of $\Delta_f H°(298.15\ K)$ from hydrogenation studies are approximately $1\ kcal{\cdot}mol^{-1}$ more negative than the results from flame calorimetry.

The value chosen as the enthalpy of formation is $\Delta_f H°(CH_3Cl, g, 298.15\ K) = -20.0 \pm 0.5\ kcal{\cdot}mol^{-1}$. This value is close to the median value and is arbitrarily chosen as it is uncertain whether the flame calorimetry or hydrogenation studies are the more accurate. Slightly more weight was given to the flame calorimetry work due to favorable comparisons with equilibrium studfies in related compounds. An error of $\pm 0.5\ kcal{\cdot}mol^{-1}$ is chosen so as to encompass the current $\Delta_f H°(298.15\ K)$ experimental values even though the actual experimental error is considerably less.

Heat Capacity and Entropy

The vibrational frequencies are essentially typical values which were taken from the experimental work of Plyler and Benedict,[6] Reichman and Overend,[7] Morino and Nakamura,[8] Jones *et al.*,[9] Fletcher,[10] and King *et al.*[11] The value of ω_1 as given by Plyler and Benedict[6] appears too low and was not included. Costain[12] has calculated the bond distances and angles based on a isotopic substitution method. From this latter data, the moments of inertia are calculated to be: $I_A = 0.5263 \times 10^{-39}$ and $I_B = I_C = 6.3887 \times 10^{-39}\ g{\cdot}cm^2$.

References

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[5] JANAF Thermochemical Tables: $H_2(g)$, 3–31–61, $CH_4(g)$, 3–31–61; HCl(g), 9–30–64.
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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.415	−75.753	−75.753	INFINITE
100	33.284	195.966	266.858	−7.089	−78.441	−73.383	38.331
200	35.151	219.389	237.889	−3.700	−80.938	−67.379	17.598
250	37.631	227.482	235.019	−1.884	−82.322	−63.831	13.337
298.15	40.731	234.367	234.367	0.	−83.680	−60.146	10.537
300	40.859	234.619	234.368	0.075	−83.732	−60.000	10.447
350	44.466	241.186	234.878	2.208	−85.103	−55.936	8.348
400	48.155	247.365	236.056	4.523	−86.401	−51.679	6.749
450	51.745	253.245	237.642	7.022	−87.609	−47.266	5.486
500	55.145	258.875	239.486	9.695	−88.725	−42.722	4.463
600	61.284	269.485	243.613	15.523	−90.685	−33.332	2.902
700	66.605	279.341	248.021	21.924	−92.300	−23.640	1.764
800	71.239	288.545	252.518	28.822	−93.602	−13.740	0.897
900	75.294	297.175	257.005	36.153	−94.627	−3.692	0.214
1000	78.845	305.296	261.432	43.864	−95 414	6 456	−0.337
1100	81.952	312.960	265.771	51.907	−95.998	16.672	−0.792
1200	84.669	320.209	270.009	60.241	−96.413	26.935	−1.172
1300	87.043	327.082	274.137	68.829	−96.691	37.226	−1.496
1400	89.119	333.611	278.154	77.640	−96.857	47.534	−1.774
1500	90.936	339.823	282.060	86.644	−96.935	57.851	−2.015
1600	92.529	345.743	285.856	95.819	−96.941	68.170	−2.226
1700	93.929	351.396	289.547	105.144	−96.894	78.488	−2.412
1800	95 162	356.800	293.134	114.599	−96.804	88.803	−2.577
1900	96.253	361.975	296.622	124.171	−96.684	99.111	−2.725
2000	97.219	366.937	300.015	133.846	−96.543	109.412	−2.858
2100	98.079	371.702	303.316	143.612	−96.388	119.706	−2.978
2200	98.845	376.283	306.529	153.459	−96.227	129.993	−3.086
2300	99.531	380.692	309.658	163.378	−96.064	140.272	−3.186
2400	100.147	384.941	312.707	173.362	−95.906	150.544	−3.277
2500	100.701	389.041	315.679	183.405	−95.755	160.810	−3.360
2600	101.201	393.000	318.577	193.501	−95.617	171.069	−3.437
2700	101.654	396.828	321.405	203.644	−95.495	181.324	−3.508
2800	102.065	400.533	324.165	213.830	−95.390	191.575	−3.574
2900	102.439	404.121	326.860	224.056	−95.306	201.822	−3.635
3000	102.780	407.600	329.494	234.317	−95.244	212.067	−3.692
3100	103.092	410.975	332.068	244.611	−95.206	222.309	−3.746
3200	103.378	414.253	334.586	254.934	−95.194	232.551	−3.796
3300	103.640	417.438	337.048	265.286	−95.207	242.794	−3.843
3400	103.882	420.535	339.458	275.662	−95.247	253.037	−3.887
3500	104.105	423.550	341.818	286.061	−95.314	263.281	−3.929
3600	104.311	426.486	344.129	296.482	−95.408	273.528	−3.969
3700	104.502	429.346	346.394	306.923	−95.530	283.778	−4.006
3800	104.678	432.135	348.614	317.382	−95.678	294.032	−4.042
3900	104.843	434.857	350.790	327.858	−95.852	304.289	−4.075
4000	104.996	437.513	352.925	338.350	−96.053	314.552	−4.108
4100	105.138	440.107	355.020	348.857	−96.278	324.820	−4.138
4200	105.271	442.643	357.076	359.378	−96.529	335.094	−4.167
4300	105.395	445.121	359.095	369.911	−96.802	345.373	−4.195
4400	105.512	447.545	361.078	380.456	−97.098	355.660	−4.222
4500	105.621	449.918	363.026	391.013	−97.416	365.953	−4.248
4600	105.723	452.240	364.940	401.580	−97.755	376.254	−4.272
4700	105.819	454.515	366.822	412.158	−98.113	386.562	−4.296
4800	105.910	456.744	368.672	422.744	−98.489	396.879	−4.319
4900	105.995	458.929	370.492	433.339	−98.883	407.203	−4.341
5000	106.076	461.071	372.282	443.943	−99.293	417.536	−4.362
5100	106.151	463.172	374.044	454.554	−99.717	427.876	−4.382
5200	106.223	465.234	375.778	465.173	−100.156	438.225	−4.402
5300	106.291	467.258	377.485	475.799	−100.606	448.583	−4.421
5400	106.355	469.246	379.166	486.431	−101.068	458.950	−4.439
5500	106.416	471.198	380.821	497.070	−101.539	469.324	−4.457
5600	106.474	473.116	382.452	507.714	−102.018	479.708	−4.475
5700	106.529	475.001	384.060	518.364	−102.505	490.101	−4.491
5800	106.581	476.854	385.643	529.020	−102.997	500.502	−4.508
5900	106.630	478.676	387.205	539.680	−103.493	510.910	−4.523
6000	106.677	480.469	388.744	550.346	−103.992	521.328	−4.539

PREVIOUS: June 1972 (1 atm) CURRENT: June 1972 (1 bar)

Trichloromethylsilane ($Si(CH_3)Cl_3$) IDEAL GAS M_r = 149.47932 Trichloromethylsilane ($SiCH_3Cl_3$) $C_1H_3Cl_3Si_1(g)$

$S°(298.15\ K) = 351.147\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K)$ = Unknown

$\Delta_f H°(298.15\ K) = [-528.858]\ kJ \cdot mol^{-1}$

Enthalpy of Formation

Source unknown.

Heat Capacity and Entropy

$C_p°$ values are taken from Janz *et al.*[1]

Reference

[1] G. J. Janz, Y. Mikawa, and F. Behnke, Silanes Vibrational Spectra, Molecular Parameters, and Thermodynamic Properties, Rensselaer Polytechnic Institute, Troy, N. Y., (1960).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	102.382	351.147	351.147	.000	−528.858	−468.020	81.995
300	102.634	351.781	351.149	.190	−528.895	−467.642	81.424
400	114.725	383.033	355.328	11.082	−530.711	−446.939	58.364
500	123.888	409.653	363.596	23.029	−532.110	−425.826	44.486
600	131.127	432.901	373.250	35 791	−533.144	−404.466	35.212
700	137.026	453.570	383.275	49.206	−533.864	−382.959	28.577
800	141.963	472.197	393.245	63.161	−534.317	−361.368	23.595
900	146.231	489.170	402.974	77.576	−534.541	−339.733	19.718
1000	149.871	504.769	412.384	92.385	−534.577	−318.084	16.615
1100	153.051	519.206	421.447	107.535	−534.460	−296.440	14.077
1200	155.770	532.643	430.160	122.979	−534.227	−274.811	11.962
1300	158.155	545.207	438.532	138.678	−533.906	−253.206	10.174
1400	160.205	557 004	446.577	154.598	−533.527	−231.627	8.642
1500	162.004	568.120	454.313	170.711	−533.112	−210.077	7.316

PREVIOUS: December 1960 (1 atm) CURRENT: December 1960 (1 bar)

Fluoromethane (CH_3F) IDEAL GAS $M_r = 34.033223$ Fluoromethane (CH_3F) $C_1H_3F_1(g)$

$S°(298.15\ K) = 222.843\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = -226.3 \pm 33\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -234.3 \pm 29\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}
2965 (1)	3006 (2)
1464 (1)	1467 (2)
1049 (1)	1182 (2)

Ground State Quantum Weight: 1 $\sigma = 3$
Point Group: C_{3v}
Bond Distances: C–F = 1.391 ± 0.005 Å; C–H = 1.095 ± 0.010 Å
Bond Angle: H–C–H = 109.5° ± 2°
Product of the Moments of Inertia: $I_A I_B I_C = 5.8630 \times 10^{-117}\ g^3 \cdot cm^6$

Enthalpy of Formation

Appearance potentials for CH_3^+ from CH_4 and CH_3F reported by Lossing *et al.*[1] the enthalpies of dissociation of hydrogen (104.20 $kcal \cdot mol^{-1}$) and fluorine (37.72 $kcal \cdot mol^{-1}$), and the enthalpy of formation of methane (−17.90 $kcal \cdot mol^{-1}$) were used to calculate the enthalpy of formation of gaseous CH_3F. These authors measured an appearance potential for CH_3^+ from CH_3F of 14.6 ± 0.6 eV, which would give an uncertainty of about ±15 $kcal\ mol^{-1}$ in the enthalpy of formation of methyl fluoride. However, a correlation of the enthalpy of formation from the atoms of the methyl fluorides and methyl chlorides indicates that the uncertainty can be reduced to ±7 $kcal \cdot mol^{-1}$.

Heat Capacity and Entropy

Fundamental vibrational frequencies were taken from the summary reported by Smith and Mills.[2] Moments of inertia from the microwave results of Gilliam *et al.*[3] are: $I_A = 0.5354 \times 10^{-39}$, $I_B = I_C = 3.3093 \times 10^{-39}\ g \cdot cm^2$. Bond parameters are the values of Brockway *et al.*[4] from electron diffraction results. These values are in close agreement with the microwave parameters reported by Gilliam *et al.*[3]

References

[1] F. P. Lossing, K. V. Ingold, and I. H. S. Henderson, J Chem. Phys. 22, 1489 (1954).
[2] W. L. Smith and I. M. Mills, J. Mol. Spectrosc. 11, 11 (1963).
[3] O. R. Gilliam, H. D Edwards, and W Gordy, Phys. Rev. 75, 1014 (1949).
[4] L. O. Brockway, C G. Thornton, and L. S. Bartell, Ann. Rev. Phys. Chem. 5, 397 (1954).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.135	−226.275	−226.275	INFINITE
100	33.258	185.647	253.738	−6.809	−228.961	−223.802	116.902
200	33.825	208.776	226.124	−3.470	−231.453	−217.703	56.858
250	35.227	216.456	223.446	−1.748	−232.872	−214.103	44.734
298.15	37.500	222.843	222.843	0.	−234.304	−210.359	36.854
300	37.603	223.075	222.843	0.069	−234.359	−210.210	36.601
350	40.695	229.097	223.312	2.025	−235.843	−206.068	30.754
400	44.167	234.755	224.392	4.145	−237.275	−201.716	26.341
450	47.751	240.164	225.846	6.443	−238.629	−197.188	22.889
500	51.280	245.378	227.540	8.919	−239.894	−192.515	20.112
600	57.871	255.322	231.350	14.383	−242.139	−182.822	15.916
700	63.705	264.690	235.450	20.468	−244.010	−172.783	12.893
800	68.812	273.538	239.663	27.100	−245.533	−162.500	10.610
900	73.269	281.906	243.896	34.209	−246.747	−152.045	8.824
1000	77.150	289.831	248.097	41.734	−247.695	−141.470	7.390
1100	80.526	297.347	252.236	49.622	−248.420	−130.810	6.212
1200	83.459	304.482	256.295	57.825	−248.959	−120.093	5.228
1300	86.009	311.265	260.265	66.301	−249.347	−109.338	4.393
1400	88.227	317.723	264.140	75.016	−249.614	−98.557	3.677
1500	90.161	323.877	267.919	83.937	−249.784	−87.761	3.056
1600	91.851	329.751	271.601	93.040	−249.878	−76.956	2.512
1700	93.332	335.365	275.188	102.300	−249.912	−66.147	2.032
1800	94.633	340.737	278.682	111.700	−249.900	−55.338	1.606
1900	95.780	345.885	282.084	121.222	−249.852	−44.530	1.224
2000	96.795	350.824	285.399	130.852	−249.777	−33.725	0.881
2100	97.696	355.569	288.628	140.577	−249.682	−22.925	0.570
2200	98.499	360.133	291.775	150.388	−249.571	−12.130	0.288
2300	99.216	364.527	294.843	160.274	−249.449	−1.339	0.030
2400	99.858	368.764	297.835	170.228	−249.318	9.445	−0.206
2500	100.436	372.852	300.755	180.243	−249.180	20.224	−0.423
2600	100.957	376.802	303.604	190.314	−249.038	30.998	−0.623
2700	101.429	380.621	306.386	200.433	−248.892	41.765	−0.808
2800	101.856	384.317	309.104	210.598	−248.743	52.528	−0.980
2900	102.245	387.899	311.760	220.803	−248.593	63.285	−1.140
3000	102.599	391.371	314.356	231.046	−248.441	74.037	−1.289
3100	102.923	394.741	316.895	241.322	−248.290	84.783	−1.429
3200	103.220	398.013	319.379	251.630	−248.138	95.525	−1.559
3300	103.492	401.193	321.810	261.965	−247.988	106.262	−1.682
3400	103.743	404.287	324.191	272.327	−247.839	116.995	−1.797
3500	103.974	407.297	326.522	282.713	−247.693	127.723	−1.906
3600	104.187	410.229	328.807	293.122	−247.550	138.447	−2.009
3700	104.385	413.087	331.046	303.550	−247.410	149.168	−2.106
3800	104.568	415.873	333.242	313.998	−247.276	159.884	−2.198
3900	104.738	418.591	335.396	324.463	−247.147	170.597	−2.285
4000	104.896	421.245	337.509	334.945	−247.024	181.307	−2.368
4100	105.044	423.837	339.583	345.442	−246.908	192.014	−2.446
4200	105.181	426.370	341.619	355.954	−246.800	202.718	−2.521
4300	105.310	428.847	343.619	366.478	−246.700	213.420	−2.593
4400	105.430	431.269	345.584	377.015	−246.609	224.119	−2.661
4500	105.543	433.640	347.514	387.564	−246.528	234.816	−2.726
4600	105.649	435.961	349.412	398.124	−246.457	245.512	−2.788
4700	105.748	438.234	351.278	408.694	−246.397	256.206	−2.847
4800	105.842	440.461	353.113	419.273	−246.348	266.900	−2.904
4900	105.930	442.644	354.918	429.862	−246.309	277.592	−2.959
5000	106.013	444.785	356.694	440.459	−246.282	288.284	−3.012
5100	106.091	446.885	358.442	451.064	−246.266	298.974	−3.062
5200	106.165	448.946	360.162	461.677	−246.261	309.666	−3.111
5300	106.235	450.969	361.857	472.297	−246.267	320.357	−3.157
5400	106.302	452.956	363.525	482.924	−246.283	331.048	−3.202
5500	106.364	454.907	365.169	493.557	−246.310	341.739	−3.246
5600	106.424	456.824	366.789	504.197	−246.347	352.431	−3.287
5700	106.481	458.708	368.385	514.842	−246.392	363.124	−3.328
5800	106.534	460.560	369.958	525.493	−246.446	373.818	−3.367
5900	106.585	462.382	371.509	536.149	−246.508	384.512	−3.404
6000	106.634	464.174	373.039	546.810	−246.576	395.208	−3.441

PREVIOUS: December 1963 (1 atm) CURRENT December 1963 (1 bar)

Trifluoromethylsilane ($Si(CH_3)F_3$) IDEAL GAS M_r = 100.115529 Trifluoromethylsilane ($SiCH_3F_3$) $C_1H_3F_3Si_1(g)$

$S°(298.15 K) = 314.2 J·K^{-1}·mol^{-1}$

$\Delta_f H°(0 K)$ = Unknown

$\Delta_f H°(298.15 K) = [-1232.71] kJ·mol^{-1}$

Enthalpy of Formation

Source unknown.

Heat Capacity and Entropy

Data from Janz *et al.*[1]

Reference

[1] G. J. Janz, Y. Mikawa, and F. Behnke, "Silanes. Vibrational Spectra, Molecular Parameters, and Thermodynamic Properties," Rensselaer Polytechnic Institute, Troy, N. Y., (1960).

Enthalpy Reference Temperature = T_r = 298.15 K

Standard State Pressure = $p°$ = 0.1 MPa

	$J·K^{-1}mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
0							
100							
200							
250							
298.15	90.876	314.202	314.202	.000	−1232.711	−1169.932	204.967
300	91.169	314.765	314.204	.168	−1232.762	−1169.542	203.635
400	105.269	342.993	317.957	10.014	−1235.248	−1148 078	149.924
500	116.483	367.732	325.489	21.122	−1237.178	−1126.052	117.638
600	125.311	389.777	334.400	33.226	−1238.632	−1103.683	96.084
700	132.382	409.640	343.753	46.121	−1239.692	−1081.103	80.673
800	138.239	427.710	353.135	59.660	−1240.426	−1058.393	69.106
900	143.135	444.282	362.355	73.735	−1240.891	−1035.609	60.105
1000	147.277	459.582	371.322	88.260	−1241.140	−1012.785	52.902
1100	150.875	473.793	379.999	103.173	−1241.216	−989.944	47.009
1200	153.888	487.052	388.374	118.414	−1241.161	−967.103	42.097
1300	156.523	499.476	396.448	133.937	−1241.012	−944.270	37.941
1400	158.825	511.161	404.228	149.706	−1240.797	−921.451	34.380
1500	160.917	522.192	411.728	165.695	−1240.535	−898.650	31.294

PREVIOUS: December 1960 (1 atm) CURRENT: December 1960 (1 bar)

Trifluoromethylsilane ($SiCH_3F_3$) $C_1H_3F_3Si_1(g)$

Methane (CH_4) IDEAL GAS M_r = 16.04276 Methane (CH_4) $C_1H_4(g)$

$S°(298.15\ K) = 186.251 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -66.911 \pm 0.34\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -74.873 \pm 0.34\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
2916.5 (1)
1534.0 (2)
3018.7 (3)
1306 (3)

Ground State Quantum Weight: [1] $\sigma = 12$
Point Group: T_d
Bond Distance: C–H = 1.091 ± 0.002 Å
Bond Angle: H–C–H = 109.4712°
Product of the Moments of Inertia: $I_AI_BI_C = 1.499 \times 10^{-118}\ g^3{\cdot}cm^6$.

Enthalpy of Formation

Rossini[1] measured the enthalpy of combustion of methane gas. His value at 298.15 K was corrected to the presently accepted molecular weight of water. The enthalpy of formation was calculated using −68.3174 and −94.0540 kcal·mol^{-1} for the enthalpy of formation of $H_2O(l)$ and $CO_2(g)$, respectively.

Heat Capacity and Entropy

Stevenson and Ibers,[2] calculated the bond distance from an analysis of available spectroscopic data. Vibrational frequencies listed by Jones and McDowell,[3] are consistent with their results of a force constant calculation. The principal moments of inertia are: $I_A = I_B = I_C = 0.5313 \times 10^{-39}\ g{\cdot}cm^2$.

References

[1] F. D. Rossini, J. Res. Nat. Bur. Stand. 6, 37 (1931).
[2] D. P. Stevenson and J. A. Ibers, J. Chem. Phys. 33, 100 (1960).
[3] L. H. Jones and R. S. McDowell, J. Mol. Spectrosc. 3, 632 (1959).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
0	0.	0.	INFINITE	−10.024	−66.911	−66.911	INFINITE
100	33.258	149.500	216.485	−6.698	−69.644	−64.353	33.615
200	33.473	172.577	189.418	−3.368	−72.027	−58.161	15.190
250	34.216	180.113	186.829	−1.679	−73.426	−54.536	11.395
298.15	35.639	186.251	186.251	0.	−74.873	−50.768	8.894
300	35.708	186.472	186.252	0.066	−74.929	−50.618	8.813
350	37.874	192.131	186.694	1.903	−76.461	−46.445	6.932
400	40.500	197.356	187.704	3.861	−77.969	−42.054	5.492
450	43.374	202.291	189.053	5.957	−79.422	−37.476	4.350
500	46.342	207.014	190.614	8.200	−80.802	−32.741	3.420
600	52.227	215.987	194.103	13.130	−83.308	−22.887	1.993
700	57.794	224.461	197.840	18.635	−85.452	−12.643	0.943
800	62.932	232.518	201.675	24.675	−87.238	−2.115	0.138
900	67.601	240.205	205.532	31.205	−88.692	8.616	−0.500
1000	71.795	247.549	209.370	38.179	−89.849	19.492	−1.018
1100	75.529	254.570	213.162	45.549	−90.750	30.472	−1.447
1200	78.833	261.287	216.895	53.270	−91.437	41.524	−1.807
1300	81.744	267.714	220.558	61.302	−91.945	52.626	−2.115
1400	84.305	273.868	224.148	69.608	−92.308	63.761	−2.379
1500	86.556	279.763	227.660	78.153	−92.553	74.918	−2.609
1600	88.537	285.413	231.095	86.910	−92.703	86.088	−2.810
1700	90.283	290.834	234.450	95.853	−92.780	97.265	−2.989
1800	91.824	296.039	237.728	104.960	−92.797	108.445	−3.147
1900	93.188	301.041	240.930	114.212	−92.770	119.624	−3.289
2000	94.399	305.853	244.057	123.592	−92.709	130.802	−3.416
2100	95.477	310.485	247.110	133.087	−92.624	141.975	−3.531
2200	96.439	314.949	250.093	142.684	−92.521	153.144	−3.636
2300	97.301	319.255	253.007	152.371	−92.409	164.308	−3.732
2400	98.075	323.413	255.854	162.141	−92.291	175.467	−3.819
2500	98.772	327.431	258.638	171.984	−92.174	186.622	−3.899
2600	99.401	331.317	261.359	181.893	−92.060	197.771	−3.973
2700	99.971	335.080	264.020	191.862	−91.954	208.916	−4.042
2800	100.489	338.725	266.623	201.885	−91.857	220.058	−4.105
2900	100.960	342.260	269.171	211.958	−91.773	231.196	−4.164
3000	101.389	345.690	271.664	222.076	−91.705	242.332	−4.219
3100	101.782	349.021	274.106	232.235	−91.653	253.465	−4.271
3200	102.143	352.258	276.498	242.431	−91.621	264.598	−4.319
3300	102.474	355.406	278.842	252.662	−91.609	275.730	−4.364
3400	102.778	358.470	281.139	262.925	−91.619	286.861	−4.407
3500	103.060	361.453	283.391	273.217	−91.654	297.993	−4.447
3600	103.319	364.360	285.600	283.536	−91.713	309.127	−4.485
3700	103.560	367.194	287.767	293.881	−91.798	320.262	−4.521
3800	103.783	369.959	289.894	304.248	−91.911	331.401	−4.555
3900	103.990	372.658	291.982	314.637	−92.051	342.542	−4.588
4000	104.183	375.293	294.032	325.045	−92.222	353.687	−4.619
4100	104.363	377.868	296.045	335.473	−92.422	364.838	−4.648
4200	104.531	380.385	298.023	345.918	−92.652	375.993	−4.676
4300	104.688	382.846	299.967	356.379	−92.914	387.155	−4.703
4400	104.834	385.255	301.879	366.855	−93.208	398.322	−4.729
4500	104.972	387.612	303.758	377.345	−93.533	409.497	−4.753
4600	105.101	389.921	305.606	387.849	−93.891	420.679	−4.777
4700	105.223	392.182	307.424	398.365	−94.281	431.869	−4.800
4800	105.337	394.399	309.213	408.893	−94.702	443.069	−4.822
4900	105.445	396.572	310.973	419.432	−95.156	454.277	−4.843
5000	105.546	398.703	312.707	429.982	−95.641	465.495	−4.863
5100	105.642	400.794	314.414	440.541	−96.157	476.722	−4.883
5200	105.733	402.847	316.095	451.110	−96.703	487.961	−4.902
5300	105.818	404.861	317.750	461.688	−97.278	499.210	−4.920
5400	105.899	406.840	319.382	472.274	−97.882	510.470	−4.938
5500	105.976	408.784	320.990	482.867	−98.513	521.741	−4.955
5600	106.049	410.694	322.575	493.469	−99.170	533.025	−4.972
5700	106.118	412.572	324.137	504.077	−99.852	544.320	−4.988
5800	106.184	414.418	325.678	514.692	−100.557	555.628	−5.004
5900	106.247	416.234	327.197	525.314	−101.284	566.946	−5.019
6000	106.306	418.020	328.696	535.942	−102.032	578.279	−5.034

PREVIOUS. March 1961 (1 atm) CURRENT: March 1961 (1 bar)

Cyanogen Iodide (ICN) IDEAL GAS $M_r = 152.9222$ Cyanogen Iodide (CNI) $C_1I_1N_1(g)$

$S°(298.15\ K) = 257.34 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 226.5 \pm 6.3\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = 225.9 \pm 6.3\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
485.8 (1)
304.5 (2)
2188 (1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: $C_{\infty v}$
Bond Distances: C–I = 1.994 Å; C–N = 1.159 Å
Bond Angle: I–C–N = 180°
Rotational Constant: $B_0 = 0.107604\ cm^{-1}$

Enthalpy of Formation

The enthalpy of formation is calculated from $\Delta_fH°$(ICN, cr, 298.15 K) = 39.71 kcal·mol^{-1} [1] and $\Delta_{sub}H°$(298.15 K) = 14.29 ± 0.15 kcal·mol^{-1}. This latter value is obtained from a 2nd and 3rd law analysis of the vapor pressure data of Yost and Stone[2] and Ketelaar and Kruyer,[3] which are in good agreement after dropping the lowest point in the first set and the lowest 3 points in the second set.

The enthalpy of formation of the crystal is calculated from $\Delta_rH°$(298.15 K) = −46.3 ± 0.08 kcal·mol^{-1} obtained by Lord and Woolf[4] for the reaction ICN(cr) + 2 NaOH(56 H_2O) = NaCNO(2800 H_2O) + NaI(2800 H_2O) + H_2O(l). The auxiliary data used were $\Delta_fH°$(NaOH·56 H_2O, 298.15 K) = −112.26 kcal·mol^{-1};[1,5] $\Delta_fH°$(NaCNO·2800 H_2O, 298.15 K) = −92.25 kcal·mol^{-1} [1,5] and $\Delta_fH°$(NaI 2800·H_2O, 298.15 K) = −70.54 kcal·mol^{-1}.[1,5] The uncertainty in the final value reflects the uncertainty in $\Delta_fH°$(NaCNO·2800 H_2O, 298.15 K) which was determined by Lord and Woolf to be −93.6 kcal·mol^{-1} in excess NaOH·56 H_2O.

Heat Capacity and Entropy

The molecular structure, bond distances and angle were determined using microwave spectroscopy by Tyler and Sheridan.[6] The infrared spectrum of the gas has been reported by Hemple and Nixon[7] using a 10m folded path cell. The fundamentals have been confirmed by the Raman data of West and Farnsworth[8] on a solution in methanol; and by the infrared data of Freitag and Nixon[9] on solid ICN.

References:

[1] U. S. Nat. Bur. Stand. Tech. Note 270–3, (1968).
[2] D. M. Yost and W. E. Stone, J. Amer. Chem. Soc. 55, 1889 (1933).
[3] J. A. A. Ketelaar and S. Kruyer, Rec. Trav. Chem. 62, 550 (1943).
[4] G. Lord and A. A. Woolf, J. Chem. Soc. (London), 2546 (1954).
[5] V. B. Parker, U. S. Nat. Bur. Stand. NSRDS–NBS 2, (1965).
[6] J. K. Tyler and J. Sheridan, Trans. Faraday Soc. 59, 2661 (1963).
[7] S. Hemple and E. R. Nixon, J. Chem. Phys. 47, 4273 and 48, 5288 (1968).
[8] W. West and M. Farnsworth, J. Chem. Phys. 1, 402 (1933).
[9] W. O. Freitag and E. R Nixon, J. Chem. Phys. 24, 109 (1956).

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−11.470	226.451	226.451	INFINITE
100	33.571	212.187	296.813	−8.463	226.423	216.340	−113.004
200	43.694	238.890	261.644	−4.551	226.087	206.419	−53.911
250	46.561	248.970	258.128	−2.289	226.011	201.512	−42.104
298.15	48.420	257.340	257.340	0.	225.936	196.800	−34.478
300	48.479	257.640	257.341	0.090	225.932	196.619	−34.234
350	49.827	265.220	257.937	2.549	225.787	191.743	−28.616
400	50.845	271.942	259.275	5.067	217.609	187.166	−24.441
450	51.676	277.980	261.024	7.631	216.795	183.409	−21.290
500	52.398	283.463	262.998	10.233	195.880	181.645	−18.976
600	53.662	293.131	267.235	15.537	196.238	178.762	−15.563
700	54.769	301.488	271.545	20.960	196.483	175.828	−13.120
800	55.742	308.866	275.758	26.487	196.644	172.866	−11.287
900	56.587	315.482	279.811	32.104	196.744	169.887	−9.860
1000	57.312	321.482	283.682	37.800	196.796	166.899	−8.718
1100	57.930	326.975	287.372	43.563	196.808	163.909	−7.783
1200	58.456	332.038	290.886	49.383	196.786	160.919	−7.005
1300	58.903	336.735	294.234	55.252	196.731	157.932	−6.346
1400	59.284	341.115	297.428	61.161	196.641	154.950	−5.781
1500	59.610	345.217	300.479	67.107	196.514	151.977	−5.292
1600	59.890	349.073	303.397	73.082	196.346	149.013	−4.865
1700	60.132	352.711	306.192	79.083	196.135	146.061	−4.488
1800	60.342	356.154	308.872	85.107	195.877	143.122	−4.153
1900	60.525	359.422	311.448	91.151	195.572	140.200	−3.854
2000	60.684	362.530	313.925	97.211	195.218	137.294	−3.586
2100	60.825	365.495	316.310	103.287	194.819	134.408	−3.343
2200	60.949	368.327	318.611	109.376	194.376	131.541	−3.123
2300	61.059	371.039	320.832	115.476	193.894	128.696	−2.923
2400	61.157	373.640	322.978	121.587	193.377	125.872	−2.740
2500	61.245	376.138	325.055	127.708	192.832	123.070	−2.571
2600	61.323	378.542	327.066	133.836	192.264	120.291	−2.417
2700	61.394	380.858	329.016	139.972	191.680	117.534	−2.274
2800	61.458	383.091	330.908	146.115	191.084	114.799	−2.142
2900	61.516	385.249	332.744	152.263	190.483	112.085	−2.019
3000	61.568	387.335	334.530	158.418	189.881	109.392	−1.905
3100	61.616	389.355	336.266	164.577	189.283	106.719	−1.798
3200	61.660	391.312	337.956	170.741	188.692	104.065	−1.699
3300	61.700	393.210	339.601	176.909	188.112	101.429	−1.605
3400	61.736	395.053	341.205	183.081	187.545	98.811	−1.518
3500	61.770	396.843	342.769	189.256	186.992	96.209	−1.436
3600	61.801	398.583	344.296	195.435	186.456	93.623	−1.358
3700	61.830	400.277	345.786	201.616	185.938	91.051	−1.285
3800	61.857	401.926	347.242	207.801	185.438	88.494	−1.216
3900	61.881	403.533	348.665	213.987	184.956	85.949	−1.151
4000	61.904	405.100	350.056	220.177	184.493	83.416	−1.089
4100	61.925	406.629	351.417	226.368	184.049	80.895	−1.031
4200	61.945	408.122	352.750	232.562	183.622	78.384	−0.975
4300	61.964	409.579	354.054	238.757	183.213	75.883	−0.922
4400	61.981	411.004	355.333	244.954	182.822	73.391	−0.871
4500	61.997	412.397	356.585	251.153	182.446	70.909	−0.823
4600	62.012	413.760	357.813	257.354	182.087	68.434	−0.777
4700	62.027	415.094	359.018	263.556	181.741	65.967	−0.733
4800	62.040	416.400	360.200	269.759	181.410	63.508	−0.691
4900	62.053	417.679	361.360	275.964	181.092	61.055	−0.651
5000	62.065	418.933	362.499	282.170	180.785	58.608	−0.612
5100	62.076	420.162	363.618	288.377	180.490	56.167	−0.575
5200	62.086	421.368	364.717	294.585	180.205	53.732	−0.540
5300	62.096	422.550	365.797	300.794	179.930	51.303	−0.506
5400	62.106	423.711	366.858	307.004	179.663	48.878	−0.473
5500	62.115	424.851	367.902	313.215	179.404	46.459	−0.441
5600	62.123	425.970	368.929	319.427	179.152	44.044	−0.411
5700	62.131	427.070	369.940	325.640	178.906	41.633	−0.382
5800	62.139	428.150	370.934	331.853	178.666	39.227	−0.353
5900	62.146	429.213	371.913	338.068	178.430	36.825	−0.326
6000	62.153	430.257	372.877	344.283	178.197	34.427	−0.300

PREVIOUS June 1969 (1 atm)   CURRENT June 1969 (1 bar)

Potassium Cyanide (KCN) CRYSTAL $M_r = 65.1160$ Potassium Cyanide (KCN) $C_1K_1N_1(cr)$

$\Delta_f H°(0\ K) = -118.34 \pm 0.8\ kJ \cdot mol^{-1}$
$S°(298.15\ K) = 127.780 \pm 1.05\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = -113.47 \pm 0.8\ kJ \cdot mol^{-1}$
$T_{trs} = 168.3 \pm 0.1\ K$ $\Delta_{trs} H° = 1.167\ kJ \cdot mol^{-1}$
$T_{fus} = 895 \pm 2\ K$ $\Delta_{fus} H° = 14.644\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The enthalpy change, $\Delta_r H°(298.15\ K) = 2.80 \pm 0.10\ kcal \cdot mol^{-1}$, for the reaction $KCN(cr) \rightarrow KCN(aq, \infty)$ was reported by Parker.[1] Incorporating these data with the enthalpy of formation for $K^+(aq, \infty)$ and $CN^-(aq, \infty)$, reported by Wagman *et al.*,[2] the value of $\Delta_f H°(KCN, cr, 298.15\ K)$ was evaluated to be $-27.12 \pm 0.2\ kcal \cdot mol^{-1}$.

Heat Capacity and Entropy

The heat capacity for KCN(cr) has been measured with a heat conduction method by Messer and Ziegler,[3] 101.6–345 8 K, and adiabatically by Suga *et al.*,[4] 14.23–308.5 K. The data of Suga[4] were adopted after correction for curvature. The anomaleous region between 50–105 K has been treated as second order by inclusion of the enthalpy in the heat capacity. The $C_p°$ values above 310 K were estimated by graphical extrapolation. The value of $S°(298\ 15\ K)$ was evaluated based on $S°(15\ K) = 0.193\ cal \cdot K^{-1} \cdot mol^{-1}$ This extrapolated value appears more reasonable than the value, $S°(15\ K) = 0.307\ cal \cdot K^{-1} \cdot mol^{-1}$ reported by Suga *et al.*[4]

Transition Data

T_{trs} was taken from Suga *et al.*[4] $\Delta_{trs} H°$ was calculated as the difference between the total enthalpy change, $H°(173.80\ K) - H°(159.02\ K) = 0.533\ kcal\ mol^{-1}$ obtained from $C_p°$ values measured by Messer and Ziegler,[3] and the enthalpy change, $0.254\ kcal \cdot mol^{-1}$, calculated from the arbitrarily smoothed $C_p°$ curve. Suga *et al*[4] reported $\Delta_{trs} H° = 0\ 339\ kcal\ mol^{-1}$, however, their $C_p°$ data do not adequately define the total enthalpy change through the transition region. The values of T_{trs} and $\Delta_{trs} H°$ reported by Messer and Ziegler[3] were $168.3 \pm 0.4\ K$ and $0.30\ kcal \cdot mol^{-1}$, respectively. The lower transition, $T_{trs} = 82.9 \pm 0.2\ K$ and $\Delta_t H° = 0.095 \pm 0.001\ kcal \cdot mol^{-1}$ reported by Suga *et al*[4] was treatment as second order by inclusion of the enthalpy in the heat capacity.

Fusion Data

Refer to the liquid table for details.

Sublimation Data

The difference between $\Delta_f H°(298.15\ K)$ for $(KCN)_2(g)$ and 2 KCN(cr) is $\Delta_{sub} H°(cr \rightarrow dimer, 298.15\ K)$ and for KCN(g) and KCN(cr) is $\Delta_{sub} H°(cr \rightarrow monomer, 298.15\ K)$.

References

[1] V B. Parker, NSRDS–NBS 2, (1965).
[2] U. S. Nat. Bur. Stand. Tech. Note 270–1, (1965).
[3] C. E. Messer and W T. Ziegler, J. Amer. Chem. Soc. 63, 2703 (1941).
[4] H. Suga, T. Matsuo and S Seki, Bull Chem. Soc. Japan 38, 1115 (1965).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−17.343	−118.345	−118.345	INFINITE
100	55.483	49.213	191.980	−14.277	−118.522	−111.797	58.397
168.300	76.283	82.687	141.073	−9.826		I <--> II	
168.300	67.280	89.623	141.073	−8.659		TRANSITION	
200	66.828	101 196	133.862	−6.533	−115.154	−106.080	27 705
298.15	66.391	127.780	127.780	0.	−113.470	−102.011	17.872
300	66.383	128 191	127.781	0.123	−113.445	−101.940	17.749
400	66.316	147.269	130.383	6.755	−114 772	−97.829	12.775
500	66.354	162.072	135.295	13.388	−114.043	−93 681	9.787
600	66.392	174.173	140.797	20.025	−113.515	−89.662	7.806
700	66.431	184.410	146.315	26.667	−113.164	−85.716	6.396
800	66.471	193.283	151.644	33.312	−112.972	−81.810	5.342
895.000	66.509	200.744	156.467	39.628		----- I <--> LIQUID -----	
900	66.511	201.115	156.714	39.961	−112.928	−77.919	4.522
1000	66.551	208.124	161.510	46.614	−113.031	−74.025	3.867
1100	66.590	214 469	166.041	53.271	−192.235	−65.504	3 111
1200	66.629	220.265	170.322	59.932	−191.578	−54.012	2.351
1300	66.669	225.600	174.371	66.597	−190 988	−42.573	1.711
1400	66.708	230.542	178.209	73.266	−190 455	−31 177	1.163
1500	66.747	235 146	181.853	79.938	−189.970	−19.817	0.690
1600	66.787	239.455	185.320	86.615	−189.529	−8 488	0.277
1700	66.826	243.505	188.625	93.296	−189.125	2.815	−0.086
1800	66.865	247.325	191.781	99.980	−188.757	14.094	−0 409
1900	66.905	250.942	194.800	106.669	−188.422	25.355	−0.697
2000	66.944	254.375	197.694	113.361	−188.117	36.598	−0.956

PREVIOUS: June 1962 CURRENT. March 1966

Potassium Cyanide (KCN) LIQUID $M_r = 65.1160$

$S°(298.15\ K) = [134.321]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$T_{fus} = 895 \pm 2\ K$

$\Delta_f H°(298.15\ K) = [-104.148]\ kJ{\cdot}mol^{-1}$

$\Delta_{fus}H° = 14.644\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(l,\ 298.15\ K)$ is calculated from $\Delta_f H°(cr,\ 298.15\ K)$ by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(895\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

Heat capacity is estimated and assumed constant in the temperature range 298.15–3000 K. The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

The melting temperature was reported by Truthe.[1] The value of $\Delta_{fus}H°$ was taken from Kelly[2] on phase diagrams of the systems KCN–AgCN, KCN–$Cu_2(CN)_2$, KCN–KCl, KCN–NaCN, and KCN–$Zn(CN)_2$ reported by Truthe.[1]

Vaporization Data

T_{vap} is the temperature at which the Gibbs energy change for the reaction KCN(l) = KCN(g) becomes zero. The difference between $\Delta_f H°$ for KCN(g) and KCN(l) at T_{vap} is $\Delta_{vap}H°$.

References

[1] W. Truthe, Z. Anorg. Chem. 76, 129 (1912).

[2] K. K. Kelley, U. S. Bur. Mines Bull. 393, (1936).

Potassium Cyanide (KCN) $C_1K_1N_1(l)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	75.312	134.321	134.321	0.	−104.148	−94.638	16.580
300	75.312	134.787	134.323	0.139	−104.106	−94.580	16.468
400	75.312	156.453	137.277	7.671	−104.534	−91.264	11.918
500	75.312	173.258	142.855	15.202	−102.907	−88.139	9.208
600	75.312	186.989	149.101	22.733	−101.485	−85.322	7.428
700	75.312	198.599	155.364	30.264	−100.244	−82.729	6.173
800	75.312	208.655	161.411	37.795	−99.166	−80.302	5.243
895.000	75.312	217.106	166.883	44.950	----- I <--> LIQUID -----		
900	75.312	217.526	167.163	45.327	−98.240	−78.001	4.527
1000	75.312	225.461	172.603	52.858	−97.465	−75.795	3.959
1100	75.312	232.639	177.740	60.389	−175.795	−69.050	3.279
1200	75.312	239.192	182.592	67.920	−174.268	−59.414	2.586
1300	75.312	245.220	187.180	75.451	−172.811	−49.902	2.005
1400	75.312	250.801	191.528	82.983	−171.416	−40.500	1.511
1500	75.312	255.997	195.655	90.514	−170.073	−31.197	1.086
1600	75.312	260.858	199.580	98.045	−168.777	−21.981	0.718
1700	75.312	265.423	203.320	105.576	−167.523	−12.844	0.395
1800	75.312	269.728	206.891	113.107	−166.308	−3.781	0.110
1900	75.312	273.800	210.306	120.639	−165.130	5.216	−0.143
2000	75.312	277.663	213.578	128.170	−163.986	14.152	−0.370
2100	75.312	281.337	216.718	135.701	−162.878	23.031	−0.573
2200	75.312	284.841	219.735	143.232	−161.804	31.859	−0.756
2300	75.312	288.189	222.639	150.763	−160.764	40.638	−0.923
2400	75.312	291.394	225.438	158.295	−159.761	49.373	−1.075
2500	75.312	294.468	228.138	165.826	−158.794	58.067	−1.213
2600	75.312	297.422	230.746	173.357	−157.867	66.723	−1.340
2700	75.312	300.264	233.269	180.888	−156.980	75.344	−1.458
2800	75.312	303.003	235.711	188.419	−156.136	83.933	−1.566
2900	75.312	305.646	238.077	195.951	−155.338	92.493	−1.666
3000	75.312	308.199	240.372	203.482	−154.588	101.026	−1.759

PREVIOUS: June 1962 CURRENT: March 1966

Potassium Cyanide (KCN) CRYSTAL(I, II)-LIQUID

0	to	168.3	K	crystal, I
168.3	to	895	K	crystal, II
above		895	K	liquid

Refer to the individual tables for details.

$M_r = 65.1160$ Potassium Cyanide (KCN) $C_1K_1N_1(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	Δ_fH°	Δ_fG°	log K_f
0	0.	0.	INFINITE	−17.343	−118.345	−118.345	INFINITE
100	55.483	49.213	191.980	−14.277	−118.522	−111.797	58.397
168.300	76.283	82.687	141.073	−9.826		I <−−> II	
168.300	67.280	89.623	141.073	−8.659		TRANSITION	
200	66.828	101.196	133.862	−6.533	−115.154	−106.080	27.705
298.15	66.391	127.780	127.780	0.	−113.470	−102.011	17.872
300	66.383	128.191	127.781	0.123	−113.445	−101.940	17.749
400	66.316	147.269	130.383	6.755	−114.772	−97.829	12.775
500	66.354	162.072	135.295	13.388	−114.043	−93.681	9.787
600	66.392	174.173	140.797	20.025	−113.515	−89.662	7.806
700	66.431	184.410	146.315	26.667	−113.164	−85.716	6.396
800	66.471	193.283	151.644	33.312	−112.972	−81.810	5.342
895.000	66.509	200.744	156.467	39.628		I <−−> LIQUID	
895.000	75.312	217.106	156.467	54.272		TRANSITION	
900	75.312	217.526	156.805	54.649	−98.240	−78.001	4.527
1000	75.312	225.461	163.281	62.180	−97.465	−75.795	3.959
1100	75.312	232.639	169.265	69.711	−175.795	−69.050	3.279
1200	75.312	239.192	174.823	77.242	−174.268	−59.414	2.586
1300	75.312	245.220	180.009	84.774	−172.811	−49.902	2.005
1400	75.312	250.801	184.869	92.305	−171.416	−40.500	1.511
1500	75.312	255.997	189.440	99.836	−170.073	−31.197	1.086
1600	75.312	260.858	193.753	107.367	−168.777	−21.981	0.718
1700	75.312	265.423	197.836	114.898	−167.523	−12.844	0.395
1800	75.312	269.728	201.712	122.430	−166.308	−3.781	0.110
1900	75.312	273.800	205.400	129.961	−165.130	5.216	−0.143
2000	75.312	277.663	208.917	137.492	−163.986	14.152	−0.370
2100	75.312	281.337	212.279	145.023	−162.878	23.031	−0.573
2200	75.312	284.841	215.498	152.554	−161.804	31.859	−0.756
2300	75.312	288.189	218.586	160.086	−160.764	40.638	−0.923
2400	75.312	291.394	221.554	167.617	−159.761	49.373	−1.075
2500	75.312	294.468	224.409	175.148	−158.794	58.067	−1.213
2600	75.312	297.422	227.161	182.679	−157.867	66.723	−1.340
2700	75.312	300.264	229.816	190.210	−156.980	75.344	−1.458
2800	75.312	303.003	232.381	197.742	−156.136	83.933	−1.566
2900	75.312	305.646	234.862	205.273	−155.338	92.493	−1.666
3000	75.312	308.199	237.265	212.804	−154.588	101.026	−1.759

PREVIOUS: CURRENT: March 1966

Potassium Cyanide (KCN) IDEAL GAS $M_r = 65.1160$ Potassium Cyanide (KCN) $C_1K_1N_1(g)$

$S°(298.15\ K) = [253.15]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = [80 \pm 21]\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = [79 \pm 21]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[370] (1)
207 (2)
2158 (1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: $C_{\infty v}$
Bond Distances: C–N = 1.16 ± 0.01 Å; K–C = [2.294] Å
Bond Angle: K–C–C = 180°
Rotational Constant: $B_0 = [0.118914]\ cm^{-1}$

Enthalpy of Formation

The vapor pressure of KCN(g) at 870°C was estimated to be 1–10 mm Hg by Villars.[1] Assuming the vapor pressure at this temperature to be 1 mm Hg, the enthalpy of vaporization, $\Delta_{vap}H°(298.15\ K)$, for KCN(l) was evaluated as 44 kcal·mol⁻¹. Based on $\Delta_fH°(298.15\ K) = -24.89\ kcal{\cdot}mol^{-1}$ for KCN(l), the value of $\Delta_fH°$(KCN, g, 298.15 K) is calculated to be 19 ± 5 kcal·mol⁻¹.

Heat Capacity and Entropy

The molecular structure of KCN(g) has not been determined. It was assumed to be linear by comparison with that for HCN(g). The C–N bond distance was determined by Elliott and Hastings[2] by use of neutron diffraction measurements. The K–C bond distance was taken from Leroi,[3] which was estimated. The vibrational frequencies, ν_2 and ν_3, were obtained from Leroi and Klemperer.[4] The value of ν_1 was calculated by valence force method described by Herzberg[5] using appropriate force constants.

References

[1] D. S. Villars, J. Am. Chem. Soc. 53, 405 (1931).
[2] N. Elliott and J. Hastings, Acta Cryst. 14, 1018 (1961).
[3] G. E. Leroi, Ph. D. Dissertation, Harvard University, (1961).
[4] G. E. Leroi and W. Klemperer, J. Chem. Phys. 35, 774 (1961).
[5] G. Herzberg, "Infrared and Raman Spectra," D. Van Nostrand, Inc., New York, (1945).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−12.456	79.509	79.509	INFINITE
100	38.592	203.295	295.884	−9.259	79.462	70.779	−36.971
200	47.724	233.411	257.718	−4.861	79.484	62.115	−16.223
250	49.674	244.289	253.978	−2.422	79.525	57.767	−12.070
298.15	50.857	253.146	253.146	0.	79.496	53.578	−9.387
300	50.894	253.461	253.147	0.094	79.493	53.417	−9.301
350	51.734	261.373	253.770	2.661	76.969	49.177	−7.339
400	52.384	268.325	255.164	5.264	76.703	45.225	−5.906
450	52.944	274.528	256.977	7.898	76.412	41.307	−4.795
500	53.465	280.133	259.017	10.558	76.093	37.424	−3.910
600	54 456	289.969	263.378	15.955	75.380	29.755	−2.590
700	55.391	298.435	267.795	21.447	74.583	22.213	−1.658
800	56.246	305.888	272.100	27.030	73.713	14.790	−0.966
900	57.006	312.558	276.231	32.694	72.771	7.481	−0.434
1000	57.666	318.599	280.171	38.428	71.749	0.280	−0.015
1100	58.234	324.122	283.919	44.224	−8.316	−2.203	0.105
1200	58.719	329.211	287.484	50.072	−8.472	−1.641	0.071
1300	59.133	333.927	290.877	55.965	−8.654	−1.065	0.043
1400	59.487	338.323	294.111	61.896	−8.858	−0.473	0.018
1500	59.790	342.438	297.197	67.861	−9.082	0.133	−0.005
1600	60.051	346.305	300.147	73.853	−9.325	0.756	−0.025
1700	60.277	349.952	302.970	79.870	−9.585	1.393	−0.043
1800	60.472	353.403	305.677	85.907	−9.864	2.047	−0.059
1900	60.643	356.678	308.276	91.963	−10.161	2.717	−0.075
2000	60.792	359.792	310.774	98.035	−10.477	3.403	−0.089
2100	60.923	362.761	313.180	104.121	−10.814	4.105	−0.102
2200	61.039	365.598	315.499	110.219	−11.173	4.824	−0.115
2300	61.142	368.314	317.736	116.329	−11.555	5.559	−0.126
2400	61.234	370.918	319.898	122.448	−11.964	6.312	−0.137
2500	61.316	373.420	321.989	128.575	−12.401	7.083	−0.148
2600	61.389	375.826	324.014	134.710	−12.870	7.871	−0.158
2700	61.456	378.144	325.976	140.853	−13.372	8.678	−0.168
2800	61.515	380.380	327.880	147.001	−13.911	9.505	−0.177
2900	61.569	382.540	329.727	153.156	−14.489	10.351	−0.186
3000	61.619	384.628	331.523	159.315	−15.111	11.218	−0.195
3100	61.663	386.649	333.269	165.479	−15.779	12.106	−0.204
3200	61.704	388.607	334.967	171.648	−16.498	13.017	−0.212
3300	61.742	390.507	336.622	177.820	−17.261	13.951	−0.221
3400	61.776	392.350	338.234	183.996	−18.088	14.909	−0.229
3500	61.808	394.142	339.806	190.175	−18.972	15.892	−0.237
3600	61.837	395.883	341.339	196.357	−19.924	16.901	−0.245
3700	61.864	397.578	342.837	202.542	−20.946	17.938	−0.253
3800	61.888	399.228	344.299	208.730	−22.041	19.003	−0.261
3900	61.912	400.836	345.728	214.920	−23.215	20.099	−0.269
4000	61.933	402.404	347.126	221.112	−24.465	21.224	−0.277
4100	61.953	403.933	348.492	227.307	−25.804	22.383	−0.285
4200	61.971	405.426	349.830	233.503	−27.239	23.575	−0.293
4300	61.989	406.885	351.140	239.701	−28.772	24.803	−0.301
4400	62.005	408.310	352.423	245.900	−30.129	26.040	−0.309
4500	62.020	409.704	353.681	252.102	−31.800	27.336	−0.317
4600	62.034	411.067	354.914	258.304	−33.571	28.669	−0.326
4700	62.048	412.401	356.123	264.509	−35.422	30.040	−0.334
4800	62.060	413.708	357.309	270.714	−37.267	31.440	−0.342
4900	62.072	414.987	358.473	276.921	−39.319	32.892	−0.351
5000	62.083	416.241	359.616	283.128	−41.475	34.387	−0.359
5100	62.094	417.471	360.738	289.337	−43.736	35.927	−0.368
5200	62.104	418.677	361.841	295.547	−46.103	37.512	−0.377
5300	62.113	419.860	362.924	301.758	−48.577	39.143	−0.386
5400	62.122	421.021	363.990	307.970	−51 157	40.822	−0.395
5500	62.130	422.161	365.037	314.182	−53.843	42.550	−0.404
5600	62.138	423.280	366.067	320.396	−56.633	44.328	−0.413
5700	62.146	424.380	367.080	326.610	−59.183	46.109	−0.423
5800	62.153	425.461	368.078	332.825	−62.136	47.981	−0.432
5900	62.160	426.524	369.059	339.040	−65.186	49.906	−0.442
6000	62.166	427.569	370.026	345.257	−68.329	51.883	−0.452

PREVIOUS: March 1966 (1 atm) CURRENT March 1966 (1 bar)

Potassium Cyanide (KCN) $C_1K_1N_1(g)$

Potassium Carbonate (K_2CO_3) CRYSTAL M_r = 138.2058 Potassium Carbonate (K_2CO_3) $C_1K_2O_3$(cr)

$\Delta_f H°$(0 K) = −1144.61 ± 2.1 kJ·mol^{-1}

$S°$(298.15 K) = 155.519 ± 0.4 J·K^{-1}·mol^{-1} $\Delta_f H°$(298.15 K) = −1150.18 ± 2.1 kJ·mol^{-1}

T_{fus} = 1174 ± 1 K $\Delta_{fus} H°$ = 27.614 ± 0.4 kJ·mol^{-1}

Enthalpy of Formation

The enthalpy of formation was obtained from the enthalpy of solution $\Delta_{\infty}H°$ = −7.6 ± 0.5 kcal·mol^{-1} and the enthalpies of formation for K^+(aq) and $CO_3^{=}$(aq), −60.32 and −161.84 kcal·mol^{-1}, respectively. The standard enthalpy solution, $\Delta_{\infty}H°$ = −7.6 ± 0.5 kcal·mol^{-1}, was calculated by extrapolation to infinite dilution of the calorimetric data of Benjamin,[1] using the methods suggested by Rupert *et al.*[2] The equilibrium constant for the hydrolysis $CO_3^{=}(aq, \infty) + H_2O(l) \rightarrow HCO_3^-(aq, \infty) + OH^-(\infty H_2O)$ was taken as K = 2.1 × 10^{-4} based on the selected values of Wagman *et al.*[3] The resulting extrapolations were not so consistent as those of Rupert *et al.*[2] for Na_2CO_3. The ionic enthalpies of formation were taken from Wagman *et al.*[3] This procedure was adopted even though it may involve an inconsistency between the extrapolations for $\Delta_{\infty}H°$ and $CO_3^{=}(\infty H_2O)$. The alternative evaluation of $\Delta_f H°$(298.15 K) for K_2CO_3(~1900 H_2O) from the enthalpies of mixing given by Muller[4] and Berthelot[5] may be subject to significant error if dissolved CO_2 was not excluded from the solutions. Presumably, this path was used by Wagman[6] in the selection of $\Delta_f H°$(298.15 K) = −274.3 kcal·mol^{-1}. This value is 0.6 kcal·mol^{-1} less negative than the value adopted here.

Heat Capacity and Entropy

The low temperature heat capacity, 14.0–315 K was measured by Oetting.[7] Janz *et al*[8] measured the heat content by drop calorimetry in the temperature range 630–1250 K, and gave enthalpy and heat capacity equations based on their measurements. The above information was used in a Shomate analysis in order to smooth the enthalpy and calculate heat capacity above 298 15 K. The values from the low and high temperature sources join smoothly at 298.15 K. The heat capacity was graphically extrapolated above the melting point. The entropy at 14.0 K was calculated from the extrapolated low temperature $C_p°$ data, using the cubic law. The value of $S°$(14 K) = 0.109 cal·K^{-1}·mol^{-1}.

Fusion Data

T_{fus} was obtained from Reisman[9] and $\Delta_{fus}H°$ was taken from Janz.[8]

References

[1] L. Benjamin, J. Chem. Eng. Data 7, 239–40 (1962).
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[6] D. D. Wagman, U. S. Nat. Bur. Stand. Report 8628, (1965).
[7] F. L. Oetting, unpublished data, Thermal Research Laboratory, Dow Chemical Company, Midland, Michigan, (1963).
[8] G. I. Janz, E. Neuenschwander and F. J. Kelly, Trans. Faraday Soc. 59, 841 (1963).
[9] A. Reisman, J. Amer. Chem. Soc. 80, 3558 (1958).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−22.673	−1144.614	−1144.614	INFINITE
100	72.383	53.095	246.061	−19.297	−1149.119	−1121.217	585.664
200	99.140	113.018	165.506	−10.498	−1150.202	−1092.747	285.396
298.15	114.437	155.519	155.519	0.	−1150.182	−1064.528	186.501
300	114.699	156.228	155.521	0.212	−1150.176	−1063.997	185.258
400	128.135	191.103	160.186	12.367	−1154.457	−1034.430	135.083
500	140.049	221.005	169.426	25.790	−1153.165	−1004.553	104.945
600	150.666	247.493	180.270	40.334	−1151.017	−975.020	84.883
700	160.483	271.462	191.611	55.896	−1148.102	−945.907	70.584
800	170.043	293.516	202.989	72.422	−1144.456	−917.262	59.891
900	179.515	314.092	214.202	89.901	−1140.085	−889.118	51.603
1000	188.949	333.495	225.170	108.325	−1135.003	−861.499	45.000
1100	198.321	351.944	235.863	127.688	−1287.134	−825.202	39.186
1174.000	205.259	365.079	243.596	142.621	--- CRYSTAL <--> LIQUID ---		
1200	207.695	369.602	246.277	147.989	−1278.565	−783.580	34.108
1300	217.066	386.596	256.421	169.227	−1269.158	−742.707	29.842
1400	226.438	403.026	266.309	191.403	−1258.901	−702.590	26.214
1500	235.810	418.968	275.958	214.515	−1247.784	−663.237	23.096
1600	245.182	434 486	285.383	238.565	−1235.802	−624.653	20.393
1700	254.555	449.631	294.601	263.552	−1222.949	−586.845	18.032
1800	263.927	464.446	303.626	289.476	−1209.226	−549.819	15.955
1900	273.299	478.967	312.474	316.337	−1194.631	−513.579	14.119
2000	282.671	493.224	321.156	344.135	−1179.164	−478.131	12.487

PREVIOUS: December 1961 CURRENT: March 1966

Potassium Carbonate (K_2CO_3) LIQUID $M_r = 138.2058$ Potassium Carbonate (K_2CO_3) $C_1K_2O_3(l)$

$S°(298.15\ K) = [170.373]\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = [-1130.609]\ kJ \cdot mol^{-1}$

$T_{fus} = 1174 \pm 1\ K$ $\Delta_{fus}H° = 27.614 \pm 0.4\ kJ \cdot mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(l, 298\ 15\ K)$ is calculated from $\Delta_f H°(cr, 298.15\ K)$ by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(1174\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

A glass transition is assumed at 800 K. The heat capacity below 800 K is obtained from the heat capacity of the crystal. Above 800 K the heat capacity is adopted as $50.0\ cal \cdot K^{-1} \cdot mol^{-1}$, based on the enthalpy measurements in the range 1169–1250 K reported by Janz *et al.*[1] The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Refer to the crystal table for details.

Reference

[1] G. J Janz, E. Neuenschwander and F. J. Kelly, Trans. Faraday Soc. 59, 841 (1963).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	114.437	170.373	170.373	0.	−1130.609	−1049.385	183.848
300	114.699	171.082	170.375	0.212	−1130.604	−1048.881	182.626
400	128.135	205.957	175.039	12.367	−1134.885	−1020.799	133.303
500	140.049	235.859	184.280	25.790	−1133.593	−992.408	103.676
600	150.666	262.347	195.124	40.334	−1131.445	−964.360	83.955
700	160.483	286.316	206.465	55.896	−1128.530	−936.732	69.900
800	183.110	308.360	217.832	72.422	−1124.884	−909.565	59.388
800.000	183.110	308.360	217.832	72.422	GLASS <--> LIQUID		
800.000	209.200	308.360	217.832	72.422	TRANSITION		
900	209.200	333.000	229.286	93.342	−1117.071	−883.121	51.255
1000	209.200	355.041	240.779	114.262	−1109.493	−857.535	44.793
1100	209.200	374.980	252.087	135.182	−1260.068	−823.476	39.104
1174.000	209.200	388.601	260.267	150.663	--- CRYSTAL <--> LIQUID ---		
1200	209.200	393.183	263.098	156.102	−1250.880	−784.193	34.135
1300	209.200	409.928	273.757	177.022	−1241.791	−745.671	29.961
1400	209.200	425.431	284.044	197.942	−1232.789	−707.846	26.410
1500	209.200	439.865	293.957	218.862	−1223.865	−670.663	23.355
1600	209.200	453.366	303.502	239.782	−1215.012	−634.072	20.700
1700	209.200	466.049	312.695	260.702	−1206.226	−598.032	18.375
1800	209.200	478.006	321.550	281.622	−1197.507	−562.508	16.324
1900	209.200	489.317	330.084	302.542	−1188.853	−527.467	14.501
2000	209.200	500 048	338.317	323.462	−1180.265	−492.879	12.873
2100	209.200	510.255	346.263	344.382	−1171.745	−458.720	11.410
2200	209.200	519.987	353.940	365.302	−1163.295	−424.964	10.090
2300	209.200	529.286	361.363	386.222	−1154.918	−391.592	8.893
2400	209.200	538.189	368.547	407.142	−1146 618	−358.582	7.804
2500	209.200	546.729	375.504	428.062	−1138.398	−325.917	6.810

PREVIOUS: December 1961 CURRENT: March 1966

Potassium Carbonate (K_2CO_3) $C_1K_2O_3(l)$

Potassium Carbonate (K_2CO_3) CRYSTAL-LIQUID

0 to 1174 K crystal
above 1174 K liquid

Refer to the individual tables for details.

M_r = 138.2058 Potassium Carbonate (K_2CO_3) $C_1K_2O_3(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−22.673	−1144.614	−1144.614	INFINITE
100	72.383	53.095	246.061	−19.297	−1149.119	−1121.217	585.664
200	99.140	113.018	165.506	−10.498	−1150.202	−1092.747	285.396
298.15	114.437	155.519	155.519	0.	−1150.182	−1064.528	186.501
300	114.699	156.228	155.521	0.212	−1150.176	−1063.997	185.258
400	128.135	191.103	160.186	12.367	−1154.457	−1034.430	135.083
500	140.049	221.005	169.426	25.790	−1153.165	−1004.553	104.945
600	150.666	247.493	180.270	40.334	−1151.017	−975.020	84.883
700	160.483	271.462	191.611	55.896	−1148.102	−945.907	70.584
800	170.043	293.516	202.989	72.422	−1144.456	−917.262	59.891
900	179.515	314.092	214.202	89.901	−1140.085	−889.118	51.603
1000	188.949	333.495	225.170	108.325	−1135.003	−861.499	45.000
1100	198.321	351.944	235.863	127.688	−1287.134	−825.202	39.186
1174.000	205.259	365.079	243.596	142.621	CRYSTAL <−−> LIQUID		
1174.000	209.200	388.601	243.596	170.235	TRANSITION		
1200	209.200	393.183	246.788	175.675	−1250.880	−784.193	34.135
1300	209.200	409.928	258.701	196.595	−1241.791	−745.671	29.961
1400	209.200	425.431	270.064	217.515	−1232.789	−707.846	26.410
1500	209.200	439.865	280.908	238.435	−1223.865	−670.663	23.355
1600	209.200	453.366	291.270	259.355	−1215.012	−634.072	20.700
1700	209.200	466.049	301.181	280.275	−1206.226	−598.032	18.375
1800	209.200	478.006	310.676	301.195	−1197.507	−562.508	16.324
1900	209.200	489.317	319.783	322.115	−1188.853	−527.467	14.501
2000	209.200	500.048	328.530	343.035	−1180.265	−492.879	12.873
2100	209.200	510.255	336.943	363.955	−1171.745	−458.720	11.410
2200	209.200	519.987	345.044	384.875	−1163.295	−424.964	10.090
2300	209.200	529.286	352.854	405.795	−1154.918	−391.592	8.893
2400	209.200	538.189	360.392	426.715	−1146.618	−358.582	7.804
2500	209.200	546.729	367.676	447.635	−1138.398	−325.917	6.810

PREVIOUS.   CURRENT: March 1966

$S°(298.15\ K) = 90.171 \pm 0.21\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{trs1} = 623\ K$
$T_{trs2} = 683 \pm 3\ K$
$T_{fus} = 993 \pm 1\ K$

$\Delta_fH°(0\ K) = -1207.891 \pm 0.17\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -1216.038 \pm 0.17\ kJ{\cdot}mol^{-1}$
$\Delta_{trs1}H° = [0.561]\ kJ{\cdot}mol^{-1}$
$\Delta_{trs2}H° = [2.238]\ kJ{\cdot}mol^{-1}$
$\Delta_{fus}H° = 44.769 \pm 0.4\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

The enthalpy of formation was derived from the enthalpy change of the following reactions:

	$\Delta_rH°(298.15K)$ kcal·mol^{-1}	References
$2\ Li^+(aq, \infty) + CO_3^=(aq, \infty) = Li_2CO_3(cr)$	4.20	1
$2\ Li(cr) + 2\ H_2O(l) = 2\ Li^+(aq, \infty) + 2\ OH^-(aq, \infty) + H_2(g)$	−106.310	2, 3, 4, 5

Summation of these two reactions gives

$$2\ Li(cr) + 2\ H_2O(l) + CO_3^=(aq, \infty) = Li_2CO_3(cr) + 2\ OH^-(aq, \infty) + H_2(g) = -102.110$$

Using $\Delta_fH°$[6] of $H_2O(l)$, $CO_3^=(aq, \infty)$ and $OH^-(aq, \infty)$ yields $\Delta_fH°$ (Li_2CO_3, cr, 298.15 K) = −290.64 kcal·mol^{-1}.

Heat Capacity and Entropy

The low temperature heat capacity, 16 68–300.20 K, was measured by Brown and Latimer.[1] Janz *et al.*[7] measured the heat content by drop calorimetry in the temperature range 560–1150 K and gave enthalpy and heat capacity equations based on their measurement. The above information was used in a Shomate analysis in order to smooth the enthalpy and calculate heat capacity The values from the low and high temperature sources join smoothly at 298 K. The heat capacity was graphically extrapolated above the melting point The entropy at 16.68 K was calculated from the extrapolated low temperature $C_p°$ data, using the cubic law. The value of $S°(16.68\ K) = 0.053\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$.

Transition Data

T_{trs} were taken from Reisman.[8] The enthalpies of transition were estimated from the relative areas of the transitions and the heat of fusion of the differential analysis curve reported by Reisman.[8]

Fusion Data

T_{fus} was obtained from Reisman[8] and $\Delta_{fus}H°$ was taken from Janz *et al.*[7]

References

[1] O L. I Brown and W. M. Latimer, J Amer. Chem. Soc 58, 2228 (1936).
[2] JANAF Thermochemical tables LiOH(cr), 3–31–66.
[3] S R Gunn and L. G. Green, J Amer. Chem. Soc. 80, 4782 (1958), S R Gunn, "Note Concerning an Electrical Heater Error in the Rocking-Bomb Solution Calorimeters," UCRL-7992, (October 1964).
[4] C B. Messer, L. G. Fasolino and C. E Thalmayer, J. Amer. Chem. Soc. 77, 4524 (1955).
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[6] U. S Nat. Bur. Stand. Tech. Note 270–1, (1965).
[7] G. I. Janz, E. Neuenschwander and F. J Kelly, Trans. Faraday Soc. 59, 841 (1963).
[8] A. Reisman, J Amer. Chem. Soc. 80, 3558 (1958).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	S°	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−15.174	−1207.891	−1207.891	INFINITE
100	34.811	20.048	158.357	−13.831	−1211.955	−1186.400	619.712
200	72.425	56.513	98.271	−8.352	−1214.852	−1159.562	302.847
298.15	96.232	90.171	90.171	0.	−1216.038	−1132.120	198.343
300	96.567	90.767	90.172	0.178	−1216.048	−1131.600	197.029
400	112.173	120.752	94.156	10.638	−1216.269	−1103.403	144.090
500	128.951	147.525	102.190	22.668	−1222.020	−1074.589	112.262
600	149.369	172.780	111.863	36.550	−1220.421	−1045.224	90.995
623.150	154.643	178.533	114.233	40.069	I <--> II		
623.150	154.638	179.433	114.233	40.630	TRANSITION		
683.150	170.212	194.286	120.612	50.331	II <--> III		
683 150	138.782	197.563	120.612	52.569	TRANSITION		
700	140.875	200.969	122.505	54.925	−1214.552	−1016.396	75.844
800	158.992	220.962	133.565	69.917	−1212.279	−988.225	64.524
900	177.025	240.727	144.376	86.716	−1208.404	−960.434	55.742
993.150	194.096	258.989	154.270	104.001	----- III <--> LIQUID -----		
1000	194.723	260.350	154.993	105.357	−1202.852	−933.163	48.743
1100	205.936	279.471	165.446	125.428	−1196.001	−906.517	43.047
1200	212.673	297.699	175.714	146.382	−1188.373	−880.533	38.329
1300	216.564	314.883	185.765	167.853	−1180.320	−855.204	34.363
1400	219.325	331.040	195.571	189.656	−1172.009	−830.506	30.987
1500	221.083	346.233	205.114	211.678	−1163.538	−806.408	28.082
1600	222.589	360.553	214.386	233.868	−1154.954	−782.878	25.558
1700	223.426	374.072	223.385	256.168	−1436.778	−745.536	22.908
1800	224.262	386.867	232.115	278.553	−1426.584	−705.169	20 463
1900	225.099	399.014	240.582	301.021	−1416.368	−665.369	18.292
2000	225.936	410.582	248.795	323.572	−1406.127	−626.107	16.352

PREVIOUS. CURRENT: March 1966

Lithium Carbonate (Li_2CO_3) LIQUID $M_r = 73.8912$

S°(298.15 K) = [130.567] J·K^{-1}·mol^{-1}
T_{fus} = 993.15 ± 1 K

$\Delta_f H^\circ$(298.15 K) = [−1175.083] kJ·mol^{-1}
$\Delta_{fus} H^\circ$ = 44.769 ± 0.4 kJ·mol^{-1}

Enthalpy of Formation

$\Delta_f H^\circ$(l, 298.15 K) is calculated from $\Delta_f H^\circ$(cr, 298.15 K) by adding $\Delta_{fus} H^\circ$ and the difference in enthalpy, H°(993.15 K)–H°(298.15 K), between the crystal and liquid.

Heat Capacity and Entropy

A glass transition is assumed at 683.15 K. The heat capacity below 683.15 K is obtained from the heat capacity of the crystal. Above 683.15 K the heat capacity is adopted as 44.32 cal·deg^{-1}·mol^{-1}, based on the enthalpy measurements in the range 996–1150 K reported by Janz *et al.*[1] The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Refer to the crystal table for details.

Reference

[1] G. J. Janz, E. Neuenschwander and F. J. Kelly, Trans. Faraday Soc. 59, 841 (1963).

Lithium Carbonate (Li_2CO_3) $C_1Li_2O_3(l)$

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = p° = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0							
100							
200							
298.15	96.232	130.567	130.567	0.	−1175.083	−1103.210	193.278
300	96.567	131.163	130.569	0.178	−1175.094	−1102.764	192.008
400	112.173	161.148	134.553	10.638	−1175.314	−1078.607	140.852
500	128.951	187.921	142.586	22.668	−1181.066	−1053.833	110.093
600	149.369	213.176	152.259	36.550	−1179.467	−1028.507	89.540
623.150	154.643	218.930	154.629	40.069	I <--> II		
623.150	154.638	219.829	154.629	40.630	TRANSITION		
683.150	170.212	234.683	161.008	50.331	II <--> III		
683.150	185.435	234 683	161 008	50.331	TRANSITION		
700	185.435	239.201	162.836	53.455	−1175.067	−1003.674	74.895
800	185.435	263.962	173.964	71.999	−1169.242	−979.589	63.961
900	185.435	285.803	185.201	90.542	−1163.624	−956.222	55.498
993.150	185 .435	304.066	195.507	107.816	----- III <--> LIQUID -----		
1000	185.435	305.341	196.255	109.086	−1158.169	−933.471	48.760
1100	185.435	323.015	206.988	127.629	−1152.845	−911.260	43.272
1200	185.435	339.150	217.339	146.173	−1147.628	−889.528	38.720
1300	185.435	353.992	227.288	164.716	−1142.503	−868.229	34.886
1400	185.435	367.735	236.835	183.260	−1137.451	−847.320	31.614
1500	185.435	380.528	245.993	201.803	−1132.459	−826.772	28.791
1600	185.435	392.496	254.779	220.347	−1127.520	−806.554	26.331
1700	185.435	403.738	263.214	238.890	−1413.101	−772.291	23.730
1800	185.435	414.337	271.318	257.434	−1406.749	−734.781	21.323
1900	185.435	424.363	279.112	275.977	−1400.457	−697.621	19.179
2000	185.435	433.875	286.614	294.521	−1394.224	−660.791	17.258

PREVIOUS.   CURRENT March 1966

Lithium Carbonate (Li_2CO_3) CRYSTAL(I, II, III)-LIQUID

0	to	623 K	crystal, I
623	to	683 K	crystal, II
683	to	993 K	crystal, III
above		993 K	liquid

Refer to the individual tables for details.

$M_r = 73.8912$ Lithium Carbonate (Li_2CO_3) $C_1Li_2O_3(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−15.174	−1207.891	−1207.891	INFINITE
100	34.811	20.048	158.357	−13.831	−1211.955	−1186 400	619.712
200	72.425	56.513	98.271	−8.352	−1214.852	−1159.562	302.847
298.15	96.232	90.171	90.171	0.	−1216.038	−1132.120	198.343
300	96.567	90.767	90.172	0.178	−1216.048	−1131.600	197.029
400	112.173	120.752	94.156	10.638	−1216.269	−1103.403	144.090
500	128.951	147.525	102.190	22.668	−1222.020	−1074.589	112.262
600	149.369	172.780	111.863	36.550	−1220.421	−1045.224	90.995
623.150	154.643	178.533	114.233	40.069		I <--> II	
623.150	154.638	179.433	114.233	40.630		TRANSITION	
683.150	170.212	194.286	120.612	50.331		II <--> III	
683.150	138.782	197.563	120.612	52.569		TRANSITION	
700	140.875	200.969	122.505	54.925	−1214.552	−1016.396	75.844
800	158.992	220.962	133.565	69.917	−1212.279	−988.225	64.524
900	177.025	240.727	144.376	86.716	−1208.404	−960.434	55.742
993 150	194.096	258.989	154.270	104.001		III <--> LIQUID	
993.150	185.435	304.066	154.270	148.770		TRANSITION	
1000	185.435	305.341	155.301	150.040	−1158.169	−933.471	48.760
1100	185.435	323.015	169.757	168.584	−1152.845	−911.260	43.272
1200	185.435	339.150	183.210	187.127	−1147.628	−889.528	38.720
1300	185.435	353.992	195.784	205.671	−1142.503	−868.229	34.886
1400	185.435	367.735	207.582	224.214	−1137.451	−847.321	31.614
1500	185.435	380.528	218.690	242.758	−1132.459	−826.772	28.791
1600	185.435	392.496	229.183	261.301	−1127.520	−806.554	26.331
1700	185.435	403.738	239.124	279.845	−1413.101	−772.291	23.730
1800	185.435	414.337	248.566	298.388	−1406.749	−734.781	21.323
1900	185.435	424.363	257.557	316.932	−1400.457	−697.621	19.179
2000	185.435	433.875	266.137	335.475	−1394.224	−660.791	17.258

PREVIOUS: CURRENT· March 1966

Magnesium Carbonate ($MgCO_3$) CRYSTAL $M_r = 84.3142$ Magnesium Carbonate ($MgCO_3$) $C_1Mg_1O_3(cr)$

$S°(298.15\ K) = 65.854\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -1104.3 \pm 8\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -1111.7 \pm 8\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

The adopted $\Delta_fH°(298.15\ K) = -265.7 \pm 2\ kcal{\cdot}mol^{-1}$ ($-1111.689 \pm 8\ kJ{\cdot}mol^{-1}$) is the average value derived from the dissociation pressures of $MgCO_3(cr)$ in the temperature range 671–782 K measured by Marc and Simek[1] and from the $\Delta_rH°(923\ K) = 25.9 \pm 0.6\ kcal{\cdot}mol^{-1}$ determined by Thomasson and Cunningham[2] using a high temperature differential calorimeter. The decomposition of $MgCO_3$ has been studied in a bomb calorimeter by Roth;[3] this yields $\Delta_rH°(293\ K) = 23.8\ kcal{\cdot}mol^{-1}$ when corrected to constant pressure. The value is derived from the small difference between two large heats of combustion, so the uncertainty is probably large. Roth also reported $\Delta_rH°(363\ K) = 26.15\ kcal{\cdot}mol^{-1}$ from calorimetric data on the heat of solution in HCl. Berthelot[4] measured the heat of solution of $MgSO_4(aq)$ with $K_2CO_3(aq)$. Analyzing his data we find $\Delta_fH°(298.15\ K) = -268.6\ kcal{\cdot}mol^{-1}$.

Discrepancies are apparent in the wide range of the calorimetric results and in the 3rd law drift of the equilibrium data. Possible sources for the drift include lack of true equilibrium (e.g., excess surface energy for MgO) and uncertainty in the high temperature entropy of $MgCO_3$ (refer to entropy write-up). Non-standard state behavior of the crystal phases may also be a problem in the calorimetric studies. The data of Thomasson and Cunningham,[2] based on a high temperature differential thermal analysis technique, are probably the most reliable of the calorimetric values; however, there are uncertainties in the absolute energy calibration. The first result of Roth[3] may be dismissed as too discrepant and the remaining two calorimetric values are within $\pm 3\ kcal{\cdot}mol^{-1}$ of the selected enthalpy of formation.

Source	Method	Reaction	T/K	$\Delta_rH°(298.15\ K)$ kcal·mol		Drift cal·K⁻¹·mol⁻¹	$\Delta_fH°(298.15\ K)$ kcal·mol⁻¹
1	*Kp*	$MgCO_3(cr) = MgO(cr) + CO_2(g)$	671–782	–	28.3	4.8 ± 0.9	−266.04
2	Calorimetric	$MgCO_3(cr) = MgO(cr) + CO_2(g)$	923	25.9	27.7		−265.45
3	Calorimetric	$MgCO_3(cr) = MgO(cr) + CO_2(g)$	293	23.8	23.8		−260.35
3	Calorimetric	$MgCO_3(cr) = MgO(cr) + CO_2(g)$	363	26.15	26.10		−263.95
4	Calorimetric	$K_2CO_3(\sim.5m) + MgSO_4(\sim.5m) = MgCO_3(cr) + K_2SO_4(\sim.5m)$	288	1.05	1.35		−268.6

Heat Capacity and Entropy

Low temperature heat capacities (56.3–291.6 K) were measured by Anderson.[5] The high temperature heat capacities are derived by a Shomate analysis of smoothed enthalpies reported by Kelley.[6] Kelley obtained the smoothed values from unpublished high temperature (400–743 K) enthalpy measurements by Shomate.[7] The data were joined smoothly at 298.15 K and extrapolated graphically above 743 K. The entropy was obtained from the heat capacities using $S°(56.2) = 0.57\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$.

Because of the drift in the decomposition pressure data, it is pertinent to assess the uncertainty in the functions. The greatest potential source for error is in the values above room temperature where the increment of entropy is about $20\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ between 298.15 and 700 K. Unfortunately, no evaluation of the unpublished enthalpies is possible, but an increase of 10% in the entropy increment would reduce the drift to a tolerable level.

Decomposition Data

T_{dcm} is calculated as the temperature at which $\Delta_rG°$ equals zero for $MgCO_3(cr) = MgO(cr) + CO_2(g)$.

References

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Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	$S°$ (J·K⁻¹mol⁻¹)	$-[G°-H°(T_r)]/T$ (J·K⁻¹mol⁻¹)	$H°-H°(T_r)$ (kJ·mol⁻¹)	$\Delta_fH°$ (kJ·mol⁻¹)	$\Delta_fG°$ (kJ·mol⁻¹)	log K_f
0	0.	0.	INFINITE	−11.689	−1104.304	−1104.304	INFINITE
100	24.683	10.780	119.865	−10.909	−1108.582	−1082.618	565.502
200	57.572	39.145	72.274	−6.626	−1110.999	−1055.538	275.678
298.15	76.210	65.854	65.854	0.	−1111.689	−1028.124	180.123
300	76.501	66.327	65.856	0.141	−1111.691	−1027.606	178.922
400	89.855	90.253	69.028	8.490	−1111.377	−999.603	130.535
500	100.061	111.423	75.430	17.996	−1110.452	−971.756	101.519
600	109.035	130.486	83.043	28.466	−1109.068	−944.140	82.195
700	116.232	147.849	91.080	39.739	−1107.322	−916.786	68.411
800	122.256	163.771	99.185	51.669	−1105.306	−889.702	58.092
900	127.612	178.491	107.189	64.172	−1103.064	−862.883	50.080
1000	131.796	192.163	115.011	77.152	−1109.256	−835.612	43.648

PREVIOUS: December 1960 CURRENT: December 1966

Cyanogen (CN) **IDEAL GAS** $M_r = 26.0177$ **Cyanogen (CN)** $C_1N_1(g)$

$S°(298.15\ K) = 202.64 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 436.8 \pm 10\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = 435.1 \pm 10\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

ϵ_i, cm^{-1}	g_i	ϵ_i, cm^{-1}	g_i
0	2	58960	2
9118	4	59683	4
25798	2	60939	4
53955	4	64782	4

$\omega_e = 2068.61\ cm^{-1}$ $\omega_ex_e = 13.114\ cm^{-1}$ $\sigma = 1$
$B_e = 1.8989\ cm^{-1}$ $\alpha_e = 0.0172\ cm^{-1}$ $r_e = 1.175$ Å

Enthalpy of Formation

The enthalpy of formation of CN has been the subject of considerable uncertainty for many years. Berkowitz[1] has reviewed the earlier work and he concludes that $\Delta_fH°$(CN, g, 0 K) = 109 kcal·mol^{-1}. Since this review a considerable body of work has emerged which supports a value near 100 kcal·mol^{-1}.

Tsang *et al.*[2] obtained $\Delta_fH°$(CN, g, 298.15 K) = 100 ± 4 kcal·mol^{-1} from shock tube studies of the decomposition of cyanogen.

Dibeler and Liston[3,4] have studied a series of cyanogen compounds and obtained their enthaplies of dissociation from photoionization threshold measurements. The values below are obtained from the halogen ion threshold measurements, except for HCN which is from the CN$^+$ threshold measurements. The value below is calculated using the IP from CNCl measurements.[3]

Davis and Okabe[5] employed a direct photodissociation technique to obtain dissociation energies for many of the same molecules. The method determines the disappearance threshold for fluorescence due to decay of excited CN $B^2\Sigma^+ - X^2\Sigma^+$. This corresponds to the energy needed to just break the bond and form excited cyanogen in the $B^2\Sigma^+$ state, whose energy above ground is well known.

Setser and Steadman[6] used metastable excited argon atoms with a maximum electronic energy of 270 kcal·mol^{-1} to break the bonds in HCN and $(CN)_2$. From the emission spectra of the excited $B^2\Sigma^+$ CN they were able to calculate the highest populated vibrational level and thus a maximum limit to the dissociation energy.

Berkowitz *et al.*[7] have recently examined the photoionization spectrum of HCN using the H$^+$ ion threshold. They also determined the threshold for the CN$^+$ ion which agrees exactly with that of Diebeler and Liston[4] when the latter is corrected for rotational energy contributions (0.7 kcal·mol^{-1}). Berkowitz *et al.*[7] suggest that the HCN limit of Setser and Steadman[6] should be <105 due to neglect of the significant vibrational population of the first harmonic of the bending mode. However, if the same allowance is made for the C_2N_2 data the limit is only ≤104 and this presumes significant occupation of the third harmonic of the bending mode of C_2N_2.

It is apparent from the data that considerable scatter still exists and several sources of error are probable. HCN and the cyanogen halides all have significant uncertainties in their enthalpy of formation, and the effects of rotational and vibrational contributions at 300 K are uncertain, but could be eliminated by using refrigerated gases. We choose to adopt a median value within the range of almost all determinations of $\Delta_fH°$(CN, g, 0 K) = 103.2 ± 2.5 kcal·mol^{-1}.

	$\Delta_rH°$(CNX → CN + X, 0 K), kcal·mol^{-1}					$\Delta_fH°$(CN, g, 0 K), kcal·mol^{-1}				
Reference	2	3,4	5	6	7	2	3 4	5	6	7
Cl		99.23 ± 0.5	99.86 ± 1.2				103.5 ± 2.0	104.1 ± 2.5		
Br		84.72 ± 0.5	86.94 ± 1.2				102.6 ± 2.0	104.8 ± 2.5		
I		72.95 ± 0.5	71.72 ± 1.0				101.4 ± 2.0	100.2 ± 2.5		
H		119.99 ± 0.5	119.92 ± 1.2	≤124	124.57 ± 0.3		100.7 ± 2.5	100.7 ± 3.0	≤103	105.3 ± 2.5
CN	125 ± 8		129.61 ± 1.2	≤133		100 ± 4		101.5 ± 0.8	≤103	

Heat Capacity and Entropy

The therodynamic functions are taken from Johnston *et al.*[8] calculated based on the direct summation of the energy levels. All the electronic levels and molecular constants listed above are from Carroll.[9] Johnston *et al.* used only the first two excited electronic states but the contribution of the higher levels is negligible.

References

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.000	0.000	INFINITE	−8.672	431.850	431.850	INFINITE
100	29.104	170.835	228.528	−5.769	433.242	424.244	−221.603
200	29.108	191.009	205.304	−2.859	434.371	414.784	−108.330
298.15	29.154	202.638	202.638	0 000	435.136	404.995	−70.953
300	29.157	202.819	202.639	054	435 147	404.808	−70.483
400	29.408	211.235	203.785	2.980	435.592	394.619	−51.532
500	29.936	217.849	205.959	5.945	435.760	384.352	−40.153
600	30.650	223.368	208.413	8.973	435.719	374 071	−32.566
700	31.423	228.151	210.898	12.077	435.528	363.810	−27.148
800	32.171	232.396	213.325	15.257	435.233	353.583	−23.087
900	32.852	236.226	215.660	18.509	434.862	343.399	−19.930
1000	33.456	239.719	217.894	21.825	434.435	333.258	−17.408
1100	33.987	242.933	220.026	25.198	433.965	323.163	−15.346
1200	34.457	245.911	222.060	28.620	433.462	313.112	−13.629
1300	34.882	248.686	224.003	32.088	432.933	303.105	−12.179
1400	35.277	251.285	225.860	35.596	432.385	293.138	−10.937
1500	35.656	253.732	227.637	39.143	431.823	283.211	−9.862
1600	36.031	256.046	229.341	42.727	431.253	273.323	−8.923
1700	36.408	258.241	230.977	46.349	430.680	263 469	−8.095
1800	36.795	260.333	232.550	50.009	430.109	253.650	−7 361
1900	37.194	262.333	234.066	53.708	429.544	243.862	−6.704
2000	37.608	264.251	235.527	57.448	428.990	234 104	−6.114
2100	38.033	266 097	236.939	61.230	428.451	224.373	−5.581
2200	38.474	267.876	238.305	65.055	427.930	214.667	−5 097
2300	38.921	269.596	239.629	68.925	427.429	204.985	−4 655
2400	39.374	271.262	240.912	72.840	426.952	195.324	−4.251
2500	39.829	272.879	242.159	76.800	426.499	185.682	−3.880
2600	40.282	274.450	243.371	80.806	426.071	176.058	−3.537
2700	40.730	275 978	244.550	84.856	425.670	166.449	−3.220
2800	41.169	277.467	245.699	88.951	425.295	156.856	−2.926
2900	41.596	278.920	246.820	93.090	424.945	147.275	−2.653
3000	42.008	280.337	247.913	97.270	424.621	137.705	−2.398
3100	42.403	281.721	248.982	101.491	424.321	128.147	−2.159
3200	42.779	283.073	250.026	105.750	424 044	118.597	−1.936
3300	43.135	284.395	251.048	110 046	423 788	109.056	−1.726
3400	43.470	285.688	252.048	114.376	423.552	99.522	−1.529
3500	43.783	286.952	253.027	118 739	423.333	89.995	−1.343
3600	44 073	288.190	253.986	123.132	423 130	80.474	−1.168
3700	44 341	289.401	254.927	127.553	422 941	70.958	−1.002
3800	44.586	290.587	255 850	131.999	422.764	61 448	−.845
3900	44.810	291.748	256 756	136 469	422.597	51.942	−.696
4000	45 013	292.885	257 645	140.961	422.437	42.440	−.554
4100	45.196	293.999	258.518	145.471	422.284	32.942	− 420
4200	45.359	295.090	259.376	149.999	422.134	23 447	−.292
4300	45.504	296 159	260.219	154.542	421.987	13.956	− 170
4400	45.631	297.207	261.048	159.099	421.841	4.469	− 053
4500	45.742	298.233	261.863	163.668	421.694	−5.015	.058
4600	45.838	299.240	262.664	168.247	421.544	−14.496	.165
4700	45.920	300.226	263.453	172.835	421.391	−23.973	.266
4800	45.988	301.194	264.229	177.431	421.233	−33.447	.364
4900	46.044	302.143	264.993	182.032	421.068	−42.918	.458
5000	46.090	303.073	265.746	186 639	420.896	−52.386	.547
5100	46.126	303.986	266.486	191.250	420.716	−61.849	.633
5200	46.153	304.882	267.216	195.864	420.527	−71.310	.716
5300	46.171	305.762	267.935	200.480	420.327	−80.766	.796
5400	46.183	306.625	268.644	205.098	420.117	−90.219	.873
5500	46.187	307.472	269.342	209.717	419.896	−99.667	.947
5600	46.186	308.305	270.030	214.335	419.662	−109.112	1.018
5700	46.175	309.122	270.709	218.953	419.415	−118.552	1.086
5800	46.166	309.925	271.378	223.571	419.155	−127.988	1.153
5900	46.145	310.714	272.038	228.186	418.881	−137.419	1.217
6000	46.129	311.489	272.689	232.800	418.593	−146.846	1.278

PREVIOUS June 1969 (1 atm)   CURRENT: June 1969 (1 bar)

Cyanogen (CN) $C_1N_1(g)$

Cyanogen, Ion (CN^+) IDEAL GAS M_r = 26.01715 Cyanogen, Ion (CN^+) $C_1N_1^+(g)$

$\Delta_fH°(0\ K) = 1793.26 \pm 12.6\ kJ\cdot mol^{-1}$
$S°(298.15\ K) = 213.44 \pm 6.3\ J\cdot K^{-1}\cdot mol^{-1}$ $\Delta_fH°(298.15\ K) = 1802.76 \pm 12.6\ kJ\cdot mol^{-1}$

Electronic Levels and Quantum Weights

ϵ_i, cm^{-1}	g_i
0	[6]
[1500]	[1]
[6000]	[2]
[8000]	[3]
[15000]	[2]

$\omega_e = [1580]\ cm^{-1}$ $\omega_ex_e = [12.5]\ cm^{-1}$ $\sigma = 1$
$B_e = [1.566]\ cm^{-1}$ $\alpha_e = [0.017]\ cm^{-1}$ $r_e = [1.29]$ Å

Enthalpy of Formation

Dibeler and Liston[1] have measured the photoionization thresholds for the processes:

$ClCN + h\nu \rightarrow Cl^+ + CN + e^-$ $\Delta_rH°(0\ K) = 399.44 \pm 0.5\ kcal\cdot mol^{-1}$
$ClCN + h\nu \rightarrow Cl + CN^+ + e^-$ $\Delta_rH°(0\ K) = 426.65 \pm 0.5\ kcal\cdot mol^{-1}$

By subtraction we obtain

$Cl + CN^+ \rightarrow Cl^+ + CN$ $\Delta_rH°(0\ K) = -27.21 \pm 0.7\ kcal\cdot mol^{-1}$

Using JANAF vlaues for Cl, Cl⁺ and CN we obtain $\Delta_fH°(CN^+\ 0\ K) = 430.6 \pm 3.0\ kcal\cdot mol^{-1}$ and $IP(CN) = 327.42 \pm 0.7\ kcal\cdot mol^{-1}$ Berkowitz *et al.*[2] have measured the photoionization thresholds for the processes:

$HCN + h\nu \rightarrow H^+ + CN + e^-$ $\Delta_rH°(0\ K) = 438.18 \pm 0.3\ kcal\cdot mol^{-1}$
$HCN + h\nu \rightarrow H + CN^+$ $\Delta_rH°(0\ K) = 448.09 \pm 0.3\ kcal\cdot mol^{-1}$

By subtraction we obtain

$H + CN^+ \rightarrow H^+ + CN$ $\Delta_rH°(0\ K) = -9.91 \pm 0.4\ kcal\cdot mol^{-1}$

Using JANAF values for H, H⁺ and CN we obtain $\Delta_fH°(CN^+\ 0\ K) = 426.7 \pm 3.0\ kcal\cdot mol^{-1}$ and $IP(CN) = 323.51 \pm 0.4\ kcal\cdot mol^{-1}$. We adopt a median value for $\Delta_fH°(CN^+, 0\ K) = 428.6 \pm 3.0\ kcal\cdot mol^{-1}$ and $325.4 \pm 2\ kcal\cdot mol^{-1}$ for IP(CN).

Heat Capacity and Entropy

The molecule has eight valence electrons and thus we expect that its molecular constants should fall between those for C_2 and BN. The ground electronic state is either $^1\Sigma$ or $^3\Pi$ and the two levels are likely to be very close. As a consequence the thermodynamic functions are dominated by the $^3\Pi$ contribution and so we choose this to be the ground state. The other levels are estimated based on the values of Fougere and Nesbet[3] for C_2 and of Verhaegen *et al.*[4] for BN. The vibrational constants and bond length are estimated between those for the $^3\Pi$ states of BN and C_2. The rotational constants B_e is obtained from the estimated bond length and α_e is calculated from the other constants assuming a Morse potential function.

References

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[2] J. Berkowitz, W. A. Chupka and T. A. Walter, J. Chem. Phys. 50, 1497 (1969).
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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J\cdot K^{-1}mol^{-1}$			$kJ\cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	-8.685	1793.264		
100	29.106	181.588	239.398	-5.781			
200	29.130	201.766	216.115	-2.870			
250	29.221	208.274	213.920	-1.411			
298.15	29.431	213.437	213.437	0.	1802.760	1763.145	-308.896
300	29.442	213.619	213.437	0.054	1802.810	1762.899	-306.948
350	29.809	218.183	213.797	1.535	1804.131	1756.142	-262.090
400	30.294	222.194	214.601	3.037	1805.390	1749.199	-228.422
450	30.852	225.794	215.648	4.566	1806.597	1742.102	-202.218
500	31.440	229.075	216.829	6.123	1807.758	1734.874	-181.241
600	32.585	234.910	219.368	9.325	1809.969	1720.087	-149.747
700	33.585	240.010	221.960	12.635	1812.063	1704.940	-127.224
800	34.412	244.551	224.505	16.036	1814 068	1689.498	-110.313
900	35.083	248.644	226.964	19.512	1815.999	1673.811	-97.145
1000	35.630	252.370	229.321	23.049	1817.871	1657.911	-86.600
1100	36.083	255.788	231.574	26.635	1819.694	1641.826	-77.964
1200	36.469	258.944	233.725	30.263	1821.475	1625.578	-70.760
1300	36.807	261.877	235.779	33.927	1823.221	1609.182	-64.658
1400	37.112	264.616	237.742	37.624	1824.940	1592.653	-59.423
1500	37.394	267.186	239.620	41.349	1826.635	1576.001	-54.881
1600	37.659	269.608	241.419	45.102	1828.312	1559.238	-50.904
1700	37.912	271.899	243.146	48.881	1829.975	1542.370	-47.391
1800	38.155	274 073	244.804	52.684	1831.626	1525.404	-44.266
1900	38.389	276.142	246.399	56.511	1833.267	1508.347	-41.467
2000	38.615	278.117	247.936	60.362	1834.903	1491.203	-38.946
2100	38.832	280.006	249.419	64.234	1836.532	1473.978	-36.663
2200	39.042	281.818	250.850	68.128	1838.158	1456.676	-34.586
2300	39.242	283.557	252.235	72.042	1839.781	1439.299	-32.688
2400	39.435	285.232	253.575	75.976	1841.401	1421.852	-30.946
2500	39.618	286.845	254.874	79.929	1843.019	1404.338	-29.342
2600	39.792	288.402	256.134	83.899	1844.635	1386.759	-27.860
2700	39.957	289.907	257.357	87.887	1846.249	1369.118	-26.487
2800	40.113	291.363	258.545	91.890	1847.861	1351.416	-25.211
2900	40.261	292.774	259.702	95.909	1849.471	1333.658	-24.022
3000	40.400	294.141	260.827	99.942	1851.078	1315.844	-22.911
3100	40.530	295.468	261.923	103.989	1852.683	1297.976	-21.871
3200	40.652	296.756	262.991	108.048	1854.284	1280.057	-20.895
3300	40.766	298.009	264.034	112.119	1855.882	1262.088	-19.977
3400	40.873	299.228	265.051	116.201	1857.476	1244.070	-19.113
3500	40.972	300.414	266.045	120.293	1859.065	1226.005	-18.297
3600	41.065	301.570	267.015	124.395	1860.650	1207.896	-17.526
3700	41.151	302.696	267.965	128.506	1862.230	1189.742	-16.796
3800	41.231	303.794	268.893	132.625	1863.804	1171.545	-16.104
3900	41.305	304.866	269.802	136.752	1865.372	1153.307	-15.447
4000	41.373	305.913	270.691	140.886	1866.933	1135.030	-14.822
4100	41.436	306.935	271.563	145.026	1868.488	1116.713	-14.227
4200	41.495	307.935	272.417	149.173	1870.036	1098.358	-13.660
4300	41.548	308.912	273.255	153.325	1871.576	1079.966	-13.119
4400	41.598	309.867	274.076	157.483	1873.109	1061.539	-12.602
4500	41.643	310.803	274.882	161.645	1874.634	1043.077	-12.108
4600	41.685	311.718	275.673	165.811	1876.150	1024.581	-11.634
4700	41.724	312.615	276.449	169.982	1877.658	1006.053	-11.181
4800	41.759	313.494	277.212	174.156	1879.157	987.492	-10.746
4900	41.791	314.355	277.961	178.333	1880.647	968.900	-10.329
5000	41.820	315.200	278.697	182.514	1882.128	950.278	-9.927
5100	41.846	316.028	279.421	186.697	1883.599	931.627	-9.542
5200	41.871	316.841	280.133	190.883	1885.060	912.946	-9.171
5300	41.893	317.639	280.833	195.071	1886.511	894.238	-8.813
5400	41.913	318.422	281.522	199.261	1887.952	875.502	-8.469
5500	41.931	319.192	282.200	203.454	1889.382	856.740	-8.137
5600	41.947	319.947	282.867	207.647	1890.803	837.952	-7.816
5700	41.962	320.690	283.524	211.843	1892.212	819.138	-7.507
5800	41.975	321.420	284.171	216.040	1893.610	800.300	-7.207
5900	41.987	322.137	284.809	220.238	1894.997	781.438	-6.918
6000	41.997	322.843	285.437	224 437	1896.373	762.553	-6.639

PREVIOUS: December 1970 (1 atm) CURRENT December 1970 (1 bar)

Cyanide (CN⁻) IDEAL GAS $M_r = 26.01825$

$S°(298.15\ K) = 195.98 \pm 2.1\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 63.6 \pm 13\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 60.7 \pm 13\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights State	ϵ_i, cm^{-1}	g_i
[$^1\Sigma^+$]	0	[1]
	[67000]	[2]

$\omega_e = [2250]\ cm^{-1}$ $\quad \omega_e x_e = [13.8]\ cm^{-1}$ $\quad \sigma = 1$
$B_e = [2.116]\ cm^{-1}$ $\quad \alpha_e = [0.0177]\ cm^{-1}$ $\quad r_e = [1.11]\ Å$

Enthalpy of Formation

Berkowitz *et al.*[1] reported 88 ± 0.5 kcal·mol^{-1} for the electron affinity of CN from the photoionization thresholds of the reactions $HCN \rightarrow N^+ + CN^-$ and $HCN \rightarrow H^+ = CN + e^-$.

Other values have been reported by Page,[2] who reinterpreted his earlier data,[3] *to yield* 73 ± 1 kcal·mol^{-1}; Bakulina and Ionov[4] in conjunction with the data of Branscomb and Smith[5] reported 78 ± 5 kcal·mol^{-1} and Inoue[6] who obtained 83 ± 7 kcal·mol^{-1}.

We adopt the value given by Berkowitz *et al.*[1] as being the most well defined in terms of both the precision of measurements and the reactions being studied. This leads to $\Delta_f H°(CN^-, g, 0\ K) = 15.2 \pm 3\ kcal{\cdot}mol^{-1}$ or $\Delta_f H°(CN^-, g, 298.15\ K) = 14.5 \pm 3\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

The electronic structure and molecular constants are estimated by analogy with the isoelectronic species CO and N_2. The uncertainties in the constants are generally small since N_2 and CO are quite similar, thus the entropy has an uncertainty of only 0.5 cal·K^{-1}·mol^{-1}.

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[2] F. M. Page, J. Chem. Phys. 49, 2466 (1968).
[3] R. Napper and F. M. Page, Trans. Faraday Soc. 59, 1086 (1963).
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[5] L. M. Branscomb and S. J. Smith, J. Chem. Phys. 25, 598 (1956).
[6] M. Inoue, J. Chim. Phys. 63, 1061 (1966).

Cyanide (CN⁻) $C_1N_1^-(g)$

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−8.670	63.581		
100	29.105	164.176	221.860	−5.768			
200	29.109	184.351	198.640	−2.858			
250	29.114	190.847	196.456	−1.402			
298.15	29.133	195.976	195.976	0.	60.668	38.768	−6.792
300	29.135	196.156	195.977	0.054	60.641	38.632	−6.726
350	29.190	200.651	196.332	1.512	59.860	35.025	−5.227
400	29.297	204.555	197.121	2.974	59.001	31.535	−4.118
450	29.466	208.015	198.143	4.443	58.069	28.157	−3.268
500	29.695	211.131	199.288	5.921	57.073	24.886	−2.600
600	30.291	216.595	201.730	8.919	54.923	18.647	−1.623
700	30.986	221.316	204 198	11.983	52.613	12.782	−0.954
800	31.693	225.500	206 604	15 117	50.193	7.256	−0.474
900	32.362	229.272	208.917	18.320	47.695	2.038	−0.118
1000	32.969	232.714	211.127	21.587	45.140	−2.898	0.151
1100	33.506	235.882	213.235	24.912	42.544	−7.576	0.360
1200	33.976	238.818	215.246	28.286	39.914	−12.017	0.523
1300	34.385	241.554	217.166	31.705	37.258	−16.237	0.652
1400	34.741	244.116	219.000	35.161	34.580	−20.252	0.756
1500	35.050	246.523	220 756	38.651	31.882	−24.074	0.838
1600	35.321	248.794	222.438	42.170	29.168	−27.716	0.905
1700	35.557	250.943	224.052	45.714	26.439	−31.188	0.958
1800	35.766	252.981	225.603	49.281	23.695	−34.499	1.001
1900	35.950	254.920	227.095	52.867	20.939	−37.657	1.035
2000	36.114	256.768	228.533	56.470	18.170	−40.669	1.062
2100	36.260	258.534	229.920	60.089	15.389	−43.542	1.083
2200	36.391	260.224	231.259	63.722	12.596	−46.283	1.099
2300	36.510	261.844	232.554	67.367	9.793	−48.897	1.110
2400	36.617	263.400	233.807	71.023	6.978	−51.388	1.118
2500	36.714	264.897	235.021	74.690	4.153	−53.762	1.123
2600	36.804	266.339	236.198	78.366	1.317	−56.023	1.126
2700	36.885	267.729	237.340	82.050	−1.529	−58.174	1.125
2800	36.961	269.072	238.450	85.743	−4.386	−60.220	1.123
2900	37.030	270.370	239.528	89.442	−7.252	−62.164	1.120
3000	37.095	271.627	240.577	93.149	−10.129	−64.008	1.114
3100	37.155	272.844	241.599	96.861	−13.016	−65.757	1.108
3200	37.212	274.025	242.593	100.579	−15.912	−67.412	1.100
3300	37.265	275.170	243.563	104.303	−18.819	−68.976	1.092
3400	37.314	276.284	244.509	108.032	−21.735	−70.452	1.082
3500	37.361	277.366	245.433	111.766	−24.661	−71.843	1.072
3600	37.406	278.419	246.335	115.504	−27.597	−73.149	1.061
3700	37.448	279.445	247.216	119.247	−30.543	−74.374	1.050
3800	37.488	280.444	248.077	122.994	−33.499	−75.519	1.038
3900	37.526	281.418	248.919	126.745	−36.464	−76.586	1.026
4000	37.563	282.369	249.744	130.499	−39.439	−77.577	1.013
4100	37.598	283.297	250.551	134.257	−42.424	−78.493	1.000
4200	37.632	284.203	251.341	138.019	−45.418	−79.337	0.987
4300	37.664	285.089	252.116	141.784	−48.422	−80.109	0.973
4400	37.696	285.955	252.875	145.552	−51.436	−80.811	0.959
4500	37 726	286.803	253.620	149.323	−54.460	−81.445	0.945
4600	37.755	287.632	254.350	153.097	−57.493	−82.011	0.931
4700	37.783	288.444	255.067	156.874	−60.536	−82.511	0.917
4800	37.811	289.240	255.771	160.653	−63.588	−82.947	0.903
4900	37.838	290.020	256.462	164.436	−66.650	−83.318	0.888
5000	37.864	290.785	257.141	168.221	−69.723	−83.627	0.874
5100	37.889	291.535	257.808	172.009	−72.805	−83.875	0.859
5200	37.914	292.271	258.463	175.799	−75.897	−84.062	0.844
5300	37.939	292.993	259.108	179.591	−78.998	−84.189	0.830
5400	37.962	293.703	259.742	183.386	−82.110	−84.258	0.815
5500	37.986	294.399	260.366	187.184	−85.231	−84.269	0.800
5600	38.009	295.084	260.980	190.984	−88.362	−84.223	0.786
5700	38.031	295.757	261.584	194.786	−91.504	−84.121	0.771
5800	38.053	296.419	262.179	198.590	−94.655	−83.964	0.756
5900	38.075	297.069	262.765	202.396	−97.817	−83.753	0.741
6000	38.096	297.709	263.342	206.205	−100.989	−83.488	0.727

PREVIOUS December 1970 (1 atm) — CURRENT: December 1970 (1 bar)

Cyanide (CN⁻) $C_1N_1^-(g)$

Sodium Cyanide (NaCN) CRYSTAL $M_r = 49.00747$ Sodium Cyanide (NaCN) $C_1N_1Na_1(cr)$

$S°(298.15\ K) = [118.47 \pm 2.1]\ J \cdot K^{-1} \cdot mol^{-1}$
$T_{fus} = 835\ K$

$\Delta_f H°(0\ K) = -98.3 \pm 1.3\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -90.7 \pm 1.3\ kJ \cdot mol^{-1}$
$\Delta_{fus} H° = [8.786]\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The enthalpy change for the reaction NaCN(cr) → NaCN(aq, ∞) was reported to be 0.29 ± 0.20 kcal·mol^{-1} by Parker.[1] Incorporating this data with the heats of formation for Na$^+$(aq, ∞), −57.39, and CN$^-$(aq, ∞), 36.0 kcal·mol^{-1}, reported by Wagman *et al.*,[2] the value of $\Delta_f H°(298.15\ K)$ for NaCN(cr) was derived and adopted.

Lord and Woolf[3] determined the value, $\Delta_f H°$(NaCN, cr, 298.15 K) = −21.4 kcal·mol^{-1}, by solution calorimetry. This value is in agreement with the adopted one.

Heat Capacity and Entropy

The low temperature heat capacities, 101.6–345.8 K, were reported by Messer and Ziegler.[4] The $C_p°$ values above 345.8 K were estimated by graphical extrapolation. $S°(298.15\ K)$ was derived from low temperature heat capacities, based on $S°(100\ K) = 8.4\ cal \cdot deg^{-1} \cdot mol^{-1}$ which was estimated by comparison with the $S°(298.15\ K)$ values for NaCl, KCl, and KCN crystals.

Transition Data

The transition temperatures, T_{trs} and T_{trs}, were determined by Messer and Ziegler.[4] The corresponding enthalpies of transition were reported to be 0.15 and 0.70 kcal·mol^{-1}, respectively However, these quantities were incorporated with $C_p°$ values used to evaluate $H°(0\ K)$–$H°(298.15\ K)$. Therefore $\Delta_{trs} H°$ values are not listed.

Fusion Data

Refer to the liquid table for details.

Sublimation Data

The difference between $\Delta_f H°(298.15\ K)$ for $(NaCN)_2(g)$ and 2 NaCN(cr) is $\Delta_{sub} H°$(cr → dimer, 298.15 K); for NaCN(g) and NaCN(cr) is $\Delta_{sub} H°$(cr→ monomer, 298.15 K).

References

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[2] U. S. Nat. Bur. Stand. Tech. Note 270–1, (1965).
[3] G. Lord and A. A. Woolf, J. Chem. Soc. 2546 (1954).
[4] C. E. Messer and W. T. Ziegler, J. Amer Chem. Soc. 63, 2703 (1941).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−19.422	−98.299	−98.299	INFINITE
100	47.363	35.146	200.082	−16.494	−98.220	−91.268	47.673
172.100	93.722	69.586	138.127	−11.796	I <−−> II TRANSITION		
172.100	93.724	69.588	138.127	−11.796			
200	67.877	80.075	129.338	−9.853	−95.817	−85.077	22.220
288.500	1548.088	111.062	118.520	−2.152	II <−−> III TRANSITION		
288.500	1548.129	111.063	118.520	−2.151			
298.15	68.681	118.467	118.467	0.	−90.709	−80.413	14.088
300	68.575	118.892	118.469	0.127	−90.677	−80.349	13.990
400	68.659	138.659	121.165	6.998	−91.909	−76.931	10.046
500	68.752	153.990	126.254	13.868	−90.937	−73.303	7.658
600	68.848	166.534	131.953	20.748	−90.143	−69.854	6.081
700	68.945	177.154	137.671	27.638	−89.499	−66.526	4.964
800	69.046	186.367	143.195	34.537	−88.985	−63.280	4.132
835.000	69.082	189.324	145.067	36.955	−−−−− III <−−> LIQUID −−−−−		
900	69.145	194.505	148.453	41.447	−88.585	−60.092	3.488
1000	69.245	201.795	153.429	48.367	−88.296	−56.943	2.974
1100	69.354	208.400	158.131	55.297	−88.117	−53.817	2.556
1200	69.462	214.439	162.575	62.237	−184.812	−48.263	2.101
1300	69.570	220.004	166.781	69.189	−183.935	−36.920	1.483
1400	69.676	225.163	170.769	76.151	−183.108	−25.642	0.957
1500	69.781	229.974	174.558	83.124	−182.322	−14.422	0.502
1600	69.885	234.481	178.164	90.107	−181.572	−3.254	0.106
1700	69.988	238.721	181.602	97.101	−180.852	7.869	−0.242
1800	70.090	242.724	184.888	104.105	−180.158	18.950	−0.550
1900	70.191	246.516	188.032	111.119	−179.488	29.993	−0.825
2000	70.291	250.119	191.047	118.143	−178.837	41.002	−1.071

PREVIOUS: December 1960 CURRENT: March 1966

Sodium Cyanide (NaCN) **LIQUID** **$M_r = 49.00747$**

$S°(298.15\ K) = [125.507]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_f H°(298.15\ K) = [-84.398]\ kJ{\cdot}mol^{-1}$

$T_{fus} = 835\ K$ $\Delta_{fus}H° = [8.7]\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

$\Delta_f H°$(l, 298.15 K) was obtained from $\Delta_f H°$(cr, 298.15 K) by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(835\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

The heat capacity is estimated by comparison with those for NaCN(cr), KCN(cr) and KCN(l). A glass transition temperature is assumed at 600 K. The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

The melting temperature was reported by Truthe.[1] $\Delta_{fus}H°$ is estimated such that the derived third law value for $\Delta_{vap}H°$(NaCN, l) agrees with the 2nd law value. Refer to the ideal gas table for details.

Vaporization Data

T_{vap} is the temperature at which the Gibbs energy change for the reaction NaCN(l) = NaCN(g) becomes zero. The difference between $\Delta_f H°$ for NaCN(g) and NACN(l) at T_{vap} is $\Delta_{vap}H°$.

Reference

[1] W. Truthe, Z. Anorg. Chem. 76, 129 (1912).

Sodium Cyanide (NaCN) **$C_1N_1Na_1(l)$**

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	68.680	125.507	125.507	0.	−84.398	−76.201	13.350
300	68.575	125.931	125.508	0.127	−84.366	−76.150	13.259
400	68.659	145.699	128.205	6.998	−85.598	−73.436	9.590
500	68.749	161.029	133.293	13.868	−84.626	−70.512	7.366
600	68.848	173.572	138.993	20.748	−83.832	−67.767	5.900
600.000	68.848	173.573	138.993	20.748	GLASS <--> LIQUID TRANSITION		
600.000	79.496	173.573	138.993	20.748			
700	79.496	185.827	144.830	28.698	−82.128	−65.226	4.867
800	79.496	196.443	150.633	36.647	−80.563	−62.920	4.108
835.000	79.496	199.847	152.625	39.430	----- III <--> LIQUID -----		
900	79 496	205.806	156.254	44.597	−79.124	−60.802	3.529
1000	79.496	214.182	161.635	52.547	−77.805	−58.838	3.073
1100	79.496	221.758	166.762	60.496	−76.606	−57.000	2.707
1200	79.496	228.675	171.637	68.446	−172.292	−52.827	2.299
1300	79.496	235.039	176.273	76.395	−170.417	−42.948	1.726
1400	79.496	240.930	180.683	84.345	−168.603	−33.211	1.239
1500	79.496	246.414	184.885	92.295	−166.841	−23.601	0.822
1600	79.496	251.545	188.892	100.244	−165.124	−14.108	0.461
1700	79.496	256.364	192.721	108.194	−163.448	−4.722	0.145
1800	79.496	260.908	196.384	116.143	−161.809	4.568	−0.133
1900	79.496	265.206	199.894	124.093	−160.203	13.767	−0.378
2000	79.496	269.284	203.263	132.043	−158.627	22.883	−0.598
2100	79.496	273.163	206.500	139.992	−157.079	31.920	−0.794
2200	79.496	276.861	209.615	147.942	−155.559	40.884	−0.971
2300	79.496	280.395	212.616	155.891	−154.064	49.780	−1.131
2400	79.496	283.778	215.511	163.841	−152.593	58.611	−1.276
2500	79.496	287.023	218.307	171.791	−151.148	67.381	−1.408
2600	79.496	290.141	221.010	179.740	−149.726	76.094	−1.529
2700	79.496	293.141	223.626	187.690	−148.329	84.753	−1.640
2800	79.496	296.032	226.161	195.639	−146.956	93.360	−1.742
2900	79.496	298.822	228.619	203.589	−145.608	101.919	−1.836
3000	79.496	301.517	231.004	211.539	−144.287	110.432	−1.923

PREVIOUS: December 1960 CURRENT: March 1966

Sodium Cyanide (NaCN) **$C_1N_1Na_1(l)$**

Sodium Cyanide (NaCN) **CRYSTAL–LIQUID** M_r = 49.00747 **Sodium Cyanide (NaCN)** $C_1N_1Na_1(cr,l)$

0	to	835 K	crystal
above		835 K	liquid

Refer to the individual tables for details.

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	Δ_fH°	Δ_fG°	log K_f
0	0.	0.	INFINITE	−19.422	−98.299	−98.299	INFINITE
100	47.363	35.146	200.082	−16.494	−98.220	−91.268	47.673
172.100	93.722	69.586	138.127	−11.796		I <--> II	
172.100	93.724	69.588	138.127	−11.796		TRANSITION	
200	67.877	80.075	129.338	−9.853	−95.817	−85.077	22.220
288.500	1548.088	111.062	118.520	−2.152		II <--> III	
288.500	1548.129	111.063	118.520	−2.151		TRANSITION	
298.15	68.681	118.467	118.467	0.	−90.709	−80.413	14.088
300	68.575	118.892	118.469	0.127	−90.677	−80.349	13.990
400	68.659	138.659	121.165	6.998	−91.909	−76.931	10.046
500	68.752	153.990	126.254	13.868	−90.937	−73.303	7.658
600	68.848	166.534	131.953	20.748	−90.143	−69.854	6.081
700	68.945	177.154	137.671	27.638	−89.499	−66.526	4.964
800	69.046	186.367	143.195	34.537	−88.985	−63.280	4.132
835.000	69.082	189.324	145.067	36.955		III <--> LIQUID	
835.000	79.496	199.847	145.067	45.741		TRANSITION	
900	79.496	205.806	149.241	50.908	−79.124	−60.802	3.529
1000	79.496	214.182	155.324	58.858	−77.805	−58.838	3.073
1100	79.496	221.758	161.024	66.807	−76.606	−57.000	2.707
1200	79.496	228.675	166.378	74.757	−172.292	−52.826	2.299
1300	79.496	235.039	171.418	82.707	−170.417	−42.947	1.726
1400	79.496	240.930	176.175	90.656	−168.603	−33.210	1.239
1500	79.496	246.414	180.677	98.606	−166.840	−23.601	0.822
1600	79.496	251.545	184.948	106.555	−165.124	−14.108	0.461
1700	79.496	256.364	189.009	114.505	−163.448	−4.721	0.145
1800	79.496	260.908	192.878	122.455	−161.809	4.568	−0.133
1900	79.496	265.206	196.573	130.404	−160.202	13.767	−0.378
2000	79.496	269.284	200.107	138.354	−158.627	22.883	−0.598
2100	79.496	273.163	203.494	146.303	−157.079	31.920	−0 794
2200	79.496	276.861	206.746	154.253	−155.559	40.884	−0.971
2300	79.496	280.395	209.872	162.203	−154.064	49.780	−1.131
2400	79.496	283.778	212.881	170.152	−152.593	58.611	−1.276
2500	79.496	287.023	215.782	178.102	−151.147	67.381	−1.408
2600	79.496	290.141	218.583	186.051	−149.726	76.094	−1.529
2700	79.496	293.141	221.289	194.001	−148.328	84.753	−1.640
2800	79.496	296.032	223.907	201.951	−146.956	93.361	−1.742
2900	79.496	298.822	226.442	209.900	−145.608	101.919	−1.836
3000	79.496	301.517	228.900	217.850	−144.287	110.432	−1.923

PREVIOUS·   CURRENT: March 1966

Sodium Cyanide (NaCN) $C_1N_1Na_1(cr,l)$

Sodium Cyanide (NaCN) **IDEAL GAS** **$M_r = 49.00747$** **Sodium Cyanide (NaCN)** **$C_1N_1Na_1(g)$**

$\Delta_f H°(0\ K) = 93.97 \pm 2.1\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = [243.37]\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = 94.27 \pm 2.1\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[400] (1)
239 (2)
2176 (1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: $C_{\infty v}$
Bond Distances: Na–C = [1.992] Å; C–N = [1.16] Å
Bond Angle. Na–C–N = [180]°
Rotational Constant: $B_0 = [0.182724]\ cm^{-1}$

Enthalpy of Formation

The vapor pressures of NaCN(l) at temperatures 805–1353 K were measured by Ingold.[1] According to the investigation reported by Porter,[2] the vapor consists of NaCN and $(NaCN)_2$. Based on his data the dimer/monomer ratios at temperatures 805–1353°C(1078.2–1626.2 K) were calculated to be 0.29–0.09. Hence the respective partial pressures for NaCN(g) and $(NaCN)_2$)(g) were derived. By the 2nd and 3rd law methods, the values of $\Delta_{vap}H°(l \rightarrow \text{monomer}, 298.15\ K)$ were evaluated to be 43.43 and 42.69 $kcal \cdot mol^{-1}$, respectively. The enthalpy of formation for NaCN(g) is calculated from $\Delta_f H°(NaCN, cr, 298.15\ K)$ and the 3rd law value for $\Delta_{vap}H°$.

Heat Capacity and Entropy

The molecular structure of NaCN(g) has not been determined. It was assumed to be linear by comparison with that for HCN(g). The C–N bond distance was assumed to be the same as that in KCN(g) and the Na–C bond distance was taken from Leroi,[3] which was calculated. The vibrational frequencies, ν_2 and ν_3, were measured by Leroi and Klemperer[4] from infrared absorption spectra. The value of ν_1 was calculated by valence force method described by Herzberg,[5] using appropriate force constants.

References

[1] C. K. Ingold, J. Chem. Soc. **123**, 885 (1923).
[2] R. F. Porter, J. Chem. Phys. 35, 318 (1961).
[3] G. E. Leroi, Ph. D. Dissertation, Harvard University, 1960.
[4] G. E. Leroi and W. Klemperer, J. Chem. Phys. 35, 774 (1961).
[5] G. Herzberg, "Infrared and Raman Spectra," D. Van Nostrand, Inc., New York, (1945).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−12.125	93.973	93.973	INFINITE
100	36.717	195.016	285.125	−9.011	94.237	85.203	−44.505
200	46.524	224.002	247.863	−4.772	94.238	76.192	−19.899
250	48.786	234.647	244.186	−2.385	94.278	71.676	−14.976
298.15	50.178	243.367	243.367	0.	94.266	67.323	−11.795
300	50.222	243.678	243.368	0.093	94.263	67.155	−11.693
350	51.210	251.498	243.983	2.630	94.148	62.645	−9.349
400	51.962	258.387	245.362	5.210	91.278	58.365	−7.622
450	52.595	264.544	247.157	7.824	90.968	54.269	−6.299
500	53.168	270.116	249.179	10.469	90.638	50.209	−5.245
600	54.227	279.904	253.506	15.839	89.923	42.189	−3.673
700	55.203	288.338	257.893	21.311	89.149	34.294	−2.559
800	56 088	295.768	262.172	26.877	88.329	26.513	−1.731
900	56.870	302.420	266.281	32.525	87.468	18.837	−1.093
1000	57.548	308.448	270.201	38.247	86.559	11.259	−0.588
1100	58.130	313.961	273.932	44.032	85.593	3.776	−0.179
1200	58.627	319.041	277.483	49.870	−12.205	−1.177	0.051
1300	59.051	323.751	280.863	55.755	−12.395	−0.251	0.010
1400	59.414	328.141	284.085	61.678	−12.606	0.691	−0.026
1500	59.725	332.251	287.160	67.636	−12.836	1.649	−0.057
1600	59.992	336.114	290.100	73.622	−13.083	2.622	−0.086
1700	60.223	339.758	292.915	79.633	−13.346	3.612	−0.111
1800	60.424	343.206	295.614	85.666	−13.623	4.617	−0.134
1900	60.598	346.478	298.206	91.717	−13.915	5.639	−0.155
2000	60.752	349.590	300.698	97.784	−14.221	6.676	−0.174
2100	60.886	352.558	303.097	103.867	−14.542	7.728	−0.192
2200	61.005	355.393	305.410	109.961	−14.876	8.797	−0.209
2300	61.111	358.107	307.643	116.067	−15.224	9.880	−0.224
2400	61.205	360.710	309.800	122.183	−15.588	10.980	−0.239
2500	61.289	363.210	311.887	128.308	−15.967	12.094	−0.253
2600	61.364	365.615	313.907	134.440	−16.362	13.225	−0.266
2700	61.432	367.933	315.866	140.580	−16.774	14.370	−0.278
2800	61.493	370.168	317.765	146.727	−17.205	15.532	−0.290
2900	61.549	372.327	319.610	152.879	−17.655	16.709	−0.301
3000	61.599	374.414	321.402	159.036	−18.126	17.902	−0.312
3100	61.645	376.435	323.145	165.199	−18.619	19.110	−0.322
3200	61.687	378.393	324.841	171.365	−19.135	20.336	−0.332
3300	61.725	380.291	326.493	177.536	−19.676	21.577	−0.342
3400	61.761	382.135	328.102	183.710	−20.245	22.836	−0.351
3500	61.793	383.925	329.672	189.888	−20.842	24.112	−0.360
3600	61.823	385.667	331.203	196.069	−21.470	25.405	−0.369
3700	61.851	387.361	332.698	202.252	−22.131	26.716	−0.377
3800	61.876	389.011	334.158	208.439	−22.827	28.045	−0.386
3900	61.900	390.618	335.585	214.628	−23.559	29.394	−0.394
4000	61.922	392.186	336.981	220.819	−24.332	30.761	−0.402
4100	61.942	393.715	338.346	227.012	−25.147	32.149	−0 410
4200	61.961	395.208	339.682	233.207	−26.004	33.556	−0.417
4300	61.979	396.666	340.991	239.404	−26.910	34.985	−0.425
4400	61.996	398.091	342.272	245.603	−27.824	36.432	−0.432
4500	62.011	399.484	343.528	251.803	−28.811	37.902	−0.440
4600	62.026	400.848	344.759	258.005	−29.858	39.396	−0.447
4700	62.040	402.182	345.967	264.208	−30.961	40.914	−0.455
4800	62.052	403.488	347.152	270.413	−32.121	42.455	−0.462
4900	62.065	404.767	348.315	276.619	−33.343	44.021	−0.469
5000	62.076	406.021	349.456	282.826	−34.620	45.612	−0.477
5100	62.087	407.251	350.578	289.034	−35.970	47.230	−0.484
5200	62.097	408.457	351.679	295.243	−37.388	48.875	−0.491
5300	62.106	409.639	352.762	301.453	−38.878	50.548	−0.498
5400	62.116	410.800	353.826	307.664	−40.441	52.250	−0.505
5500	62.124	411.940	354.872	313.876	−42.081	53.982	−0.513
5600	62.132	413.060	355.901	320.089	−43.800	55.744	−0.520
5700	62.140	414.160	356.913	326.303	−45.601	57.537	−0.527
5800	62.147	415.240	357.910	332.517	−47.485	59.363	−0.535
5900	62.154	416.303	358.891	338.732	−49.455	61.222	−0.542
6000	62.161	417.347	359.856	344.948	−51.355	63.097	−0.549

PREVIOUS· March 1966 (1 atm) CURRENT· March 1966 (1 bar)

NCO Radical (NCO) IDEAL GAS $M_r = 42.0171$ NCO Radical (NCO) $C_1N_1O_1(g)$

$\Delta_f H°(0\ K) = 159.0 \pm 10.5\ kJ \cdot mol^{-1}$
$S°(298.15\ K) = 232.2 \pm 0.8\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = 159.4 \pm 10.5\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$X^2\Pi_{3/2}$	0	2
$X^2\Pi_{1/2}$	95.6	2
$A^2\Sigma^+$	22802	2
$B^2\Pi$	31811	4

Vibrational Frequencies and Degeneracies ν, cm^{-1}
1922 (1)
536 (2)
1275 (1)

Point Group: $C_{\infty v}$ $\sigma = 1$
Bond Distances: N–C = [1.23] Å; C–O = [1.18] Å
Bond Angle: N–C–O = 108°
Rotational Constant: $B_0 = 0.388394\ cm^{-1}$

Enthalpy of Formation

Okabe[1] has measured the onset of photodissociation for the process $HNCO(g) \rightarrow H(g) + NCO(A^2\Sigma)$ as 7.73 ± 0.01 eV (178.25 ± 0.25 kcal·mol^{-1}). This result in combination with JANAF auxiliary data[2] results in $\Delta_f H°$(NCO, g, 0 K) = 38 ± 2.5 kcal·mol^{-1}.

Dixon[3] has discussed the diffusencess in the $^2\Pi$–$^2\Pi$ bands of NCO above 33700 cm^{-1} and concludes this is due to either predissociation or unresolved groups of lines due to a perturbing state. Assuming the dissociation is to $N(^2D) + CO(^1\Sigma)$ yields $D_0°$(N–CO) ≤ 41 kcal·mol^{-1}, or $\Delta_f H°$(NCO, 0 K) ≥ 44 kcal·mol^{-1}; assuming the products $CN(^2\Sigma) + O(^3P)$ then $D_0°$(NC–O) ≤ 97 kcal·mol^{-1}, or $\Delta_f H°$(NCO, 0 K) ≥ 65 kcal·mol^{-1}. Milligan and Jacox[4] confirm the diffuseness and observe increased amounts of CO. Thus, they prefer the first dissociation mechanism which favors $\Delta_f H°$(NCO, 0 K) ≥ 44 kcal·mol^{-1}. An upper limit to the enthalpy formation can be obtained from HNCO(g)[2] by assuming a maximum $D_0°$(H–NCO) ≤ 122 kcal·mol^{-1}, equal to $D_0°$(H–CN), which yields $\Delta_f H°$(NCO, 0 K) ≤ 45 kcal·mol^{-1}. Another estimate may be obtained by making the reasonable assumption that the sum of the atomization energies of NCN + NNO equal those of NNN + NCO, where the central atoms are simply interchanged. Using respective atomization values[2] of 282, 264 and 242 kcal·mol^{-1} yields 304 kcal·mol^{-1} for NCO, or $\Delta_f H°$(NCO, 0 K) = 38 kcal·mol^{-1}. It appears that the diffuseness in the spectrum is not due to predissociation, since all the estimates and measurements fall below the vlaues calculated on that basis. We adopt $\Delta_f H°$(NCO, g, 0 K) = 38 ± 2.5 kcal·mol^{-1}.

Heat Capacity and Entropy

The electronic levels, structure, and ν_2 are from Dixon.[3] The ν_1 and ν_3 vibrational frequencies are from the matrix isolation data of Milligan and Jacox.[4] The individual bond lengths are those selected by Milligan and Jacox[4] to fit the overall length determined by Dixon.[3]

References

[1] H. Okabe, J. Chem. Phys. 53, 3507 (1970).
[2] JANAF Thermochemical Tables: HNCO(g), 12–31–70; HCN(g), 12–31–69; NCN(g), 12–31–70; NNO(g), 12–31–64; NNN(g), 12–31–70; CN(g), 6–30–69; H(g), 9–30–65.
[3] R. N. Dixon, Phil. Trans. Roy. Soc. (London) 252A, 165 (1960) and Can. J. Phys. 38, 10 (1960).
[4] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 47, 5157 (1967).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.196	158.943	158.943	INFINITE
100	32.077	194.218	264.724	−7.051	159.125	156.454	−81.723
200	35.509	217.193	235.771	−3.716	159.222	153.747	−40.155
250	37.940	225.381	232.896	−1.879	159.307	152.369	−31.836
298.15	40.053	232.248	232.248	0.	159.410	151.024	−26.459
300	40.130	232.496	232.249	0.074	159.415	150.972	−26.286
350	42.089	238.832	232.744	2.131	159.533	149.555	−22.320
400	43.865	244.570	233.869	4.280	159.654	148.121	−19.343
450	45.485	249.831	235.355	6.514	159.768	146.673	−17.025
500	46.967	254.701	237.049	8.826	159.874	145.212	−15.170
600	49.543	263.500	240.740	13.656	160.054	142.262	−12.385
700	51.652	271.301	244.559	18.719	160.196	139.285	−10.394
800	53.361	278.314	248.347	23.973	160.305	136.290	−8.899
900	54.740	284.681	252.036	29.381	160.387	133.283	−7.736
1000	55.855	290.508	255.596	34.912	160.445	130.268	−6.805
1100	56.761	295.876	259.017	40.545	160.480	127.249	−6.043
1200	57.503	300.848	262.298	46.259	160.495	124.227	−5.407
1300	58.114	305.475	265.444	52.041	160.489	121.205	−4.870
1400	58.622	309.801	268.459	57.878	160.463	118.184	−4.409
1500	59.048	313.861	271.352	63.763	160.418	115.165	−4.010
1600	59.408	317.683	274.130	69.686	160.353	112.150	−3.661
1700	59.713	321.294	276.799	75.642	160.269	109.140	−3.353
1800	59.975	324.715	279.367	81.627	160.165	106.135	−3.080
1900	60.201	327.964	281.840	87.636	160.040	103.137	−2.835
2000	60.397	331.057	284.224	93.666	159.895	100.146	−2.616
2100	60.568	334.008	286.525	99.715	159.730	97.162	−2.417
2200	60.718	336.829	288.748	105.779	159.544	94.187	−2.236
2300	60.851	339.531	290.897	111.858	159.337	91.221	−2.072
2400	60.968	342.123	292.978	117.949	159.109	88.264	−1.921
2500	61.073	344.614	294.994	124.051	158.860	85.317	−1.783
2600	61.167	347.012	296.949	130.163	158.591	82.381	−1.655
2700	61.251	349.322	298.846	136.284	158.301	79.455	−1.537
2800	61.328	351.551	300.689	142.413	157.992	76.541	−1.428
2900	61.398	353.704	302.480	148.550	157.661	73.637	−1.326
3000	61.462	355.787	304.222	154.693	157.312	70.746	−1.232
3100	61.521	357.803	305.918	160.842	156.942	67.866	−1.144
3200	61.576	359.757	307.570	166.997	156.554	64.999	−1.061
3300	61.627	361.652	309.181	173.157	156.147	62.144	−0.984
3400	61.676	363.493	310.751	179.322	155.721	59.302	−0.911
3500	61.722	365.281	312.284	185.492	155.278	56.472	−0.843
3600	61.766	367.021	313.780	191.666	154.817	53.656	−0.779
3700	61.808	368.714	315.242	197.845	154.338	50.852	−0.718
3800	61.850	370.363	316.671	204.028	153.843	48.062	−0.661
3900	61.891	371.970	318.068	210.215	153.332	45.285	−0.607
4000	61.931	373.537	319.436	216.406	152.804	42.521	−0.555
4100	61.971	375.067	320.774	222.601	152.261	39.771	−0.507
4200	62.011	376.561	322.084	228.800	151.702	37.034	−0.461
4300	62.052	378.020	323.368	235.003	151.128	34.311	−0.417
4400	62.092	379.447	324.627	241.211	150.539	31.601	−0.375
4500	62.134	380.843	325.861	247.422	149.936	28.904	−0.336
4600	62.176	382.209	327.071	253.637	149.317	26.221	−0.298
4700	62.219	383.547	328.258	259.857	148.685	23.552	−0.262
4800	62.263	384.857	329.424	266.081	148.038	20.896	−0.227
4900	62.308	386.142	330.568	272.310	147.376	18.255	−0.195
5000	62.355	387.401	331.692	278.543	146.700	15.626	−0.163
5100	62.402	388.636	332.797	284.781	146.010	13.012	−0.133
5200	62.451	389.848	333.882	291.023	145.305	10.411	−0.105
5300	62.501	391.038	334.950	297.271	144.585	7.824	−0.077
5400	62.552	392.207	335.999	303.524	143.851	5.250	−0.051
5500	62.605	393.355	337.031	309.782	143.101	2.690	−0.026
5600	62.659	394.484	338.047	316.045	142.337	0.144	−0.001
5700	62.714	395.593	339.047	322.313	141.556	−2.388	0.022
5800	62.771	396.685	340.032	328.588	140.759	−4.906	0.044
5900	62.829	397.758	341.001	334.868	139.946	−7.412	0.066
6000	62.888	398.815	341.956	341.154	139.116	−9.902	0.086

PREVIOUS: December 1970 (1 atm) CURRENT: December 1970 (1 bar)

CNN Radical (CNN) IDEAL GAS $M_r = 40.0244$ CNN Radical (CNN) $C_1N_2(g)$

$\Delta_f H°(0\ K) = 584 \pm 126\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = 231.716\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = 585 \pm 126\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
1241 (1)
393 (2)
2847 (1)

Ground State Quantum Weight: [3]
Point Group: $C_{\infty v}$ $\sigma = 1$
Bond Distances: C–N = [1.15] Å; N-N = [1.25] Å
Bond Angle: C–N–N = 180°
Rotational Constant: $B_0 = [0.450392]\ cm^{-1}$

Enthalpy of Formation

The enthalpy of formation is calculated from the estimated enthalpy of reaction $\Delta_r H°(0\ K) = 255 \pm 30\ kcal \cdot mol^{-1}$ for $CNN(g) \rightarrow C(g) + 2\ N(g)$. Since CNN radical can dissociate to give $C + N_2$ or $CN + N$, the molecule must have more energy than either CN or N_2. It is assumed that the extra bond will be quite weak, for this we estimate $30 \pm 30\ kcal \cdot mol^{-1}$ which gives $\Delta_r H°(0\ K) = 255 \pm 30\ kcal \cdot mol^{-1}$ ($583.856 \pm 126\ kJ \cdot mol^{-1}$) for the first path and $\Delta_r H° = 204 \pm 30\ kcal \cdot mol^{-1}$ for the second. We adopt the former value.

Heat Capacity and Entropy

Milligan and Jacox[1] have measured three fundamental vibrational frequencies for CNN radical (g) in the infrared and ultraviolet spectra by matrix-isolation, and proposed a linear molecular configuration with a $^3\Sigma$ ground state which has been confirmed by Wasserman *et al.*[2] in the electron paramagnetic resonance observations. Also Milligan and Jacox[1] suggested a C ≡ N = N bond structure, based on the agreement between the C–N and N–N stretching force constants (calculated from observed vibrational frequencies in the CNN radical) and the typical C ≡ N and N = N stretching force constants. In addition, they estimated the bond distances r(C–N) = 1.15 Å and r(N–N) = 1.25 Å from the proposed structure.

References

[1] D. E. Milligan, M. E. Jacox, J. Chem. Phys. 44, 3149 (1966).
[2] E. Wasserman, L. Barash and W. A. Yager, J. Amer. Chem. Soc. 87, 2075 (1965).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.372	583.854	583.854	INFINITE
100	30.975	191.895	266.206	−7.431	583.833	580.720	−303.337
200	38.075	215.660	235.463	−3.961	584.066	577.548	−150.840
250	40.478	224 427	232.403	−1.994	584.282	575.894	−120.326
298.15	42.281	231.716	231.716	0.	584.505	574.258	−100.608
300	42.343	231.978	231.717	0.078	584.513	574.195	−99.976
350	43.883	238.624	232.238	2.235	584.742	572.457	−85.435
400	45.200	244.572	233.415	4.463	584.958	570.687	−74.524
450	46.353	249.964	234.959	6.752	585.154	568.891	−66.035
500	47.377	254.902	236.709	9.096	585.325	567.075	−59.242
600	49.142	263.700	240.493	13.925	585.592	563.398	−49.048
700	50.642	271.391	244.369	18.916	585.768	559.684	−41.764
800	51.950	278.241	248.182	24.047	585.868	555.950	−36.300
900	53.100	284.427	251.871	29.300	585.911	552.207	−32.049
1000	54.111	290.075	255.413	34.662	585.909	548.462	−28.649
1100	54.997	295.275	258.804	40.118	585.874	544.718	−25.867
1200	55.772	300.095	262.046	45.658	585.814	540.979	−23.548
1300	56.449	304.586	265.148	51.270	585.733	537.246	−21.587
1400	57.040	308.791	268.117	56.945	585.634	533.520	−19.906
1500	57.556	312.745	270.961	62.675	585.522	529.802	−18.449
1600	58.007	316.474	273.691	68.454	585.397	526.091	−17.175
1700	58.404	320.003	276.312	74.275	585.260	522.388	−16.051
1800	58.752	323.351	278.833	80.133	585.113	518.694	−15.052
1900	59.060	326.536	281.261	86.024	584.954	515.009	−14.159
2000	59.332	329.573	283.601	91.944	584.786	511.332	−13.355
2100	59.573	332.473	285.860	97.889	584.608	507.663	−12.627
2200	59.788	335.250	288.042	103.857	584.420	504.004	−11.967
2300	59.981	337.912	290.153	109.846	584.222	500.353	−11.363
2400	60.153	340.468	292.196	115.853	584.014	496.711	−10.811
2500	60.308	342.927	294.177	121.876	583.795	493.078	−10.302
2600	60.448	345.295	296.097	127.914	583.567	489.453	−9.833
2700	60.574	347.579	297.962	133.965	583.328	485.838	−9.399
2800	60.689	349.784	299.774	140.028	583.079	482.232	−8.996
2900	60.793	351.915	301.535	146.102	582.819	478.635	−8.621
3000	60.888	353.978	303.249	152.187	582.550	475.047	−8.271
3100	60.975	355.976	304.918	158.280	582.269	471.468	−7.944
3200	61.054	357.913	306.544	164.381	581.978	467.898	−7.638
3300	61.127	359.793	308.129	170.490	581.676	464.338	−7.350
3400	61.195	361.619	309.676	176.607	581.363	460.787	−7.079
3500	61.257	363.394	311.185	182.729	581.039	457.245	−6.824
3600	61.314	365.120	312.660	188.858	580.704	453.713	−6.583
3700	61.367	366.801	314.100	194.992	580.359	450.190	−6.356
3800	61.416	368.438	315.509	201.131	580.002	446.677	−6.140
3900	61.461	370.034	316.886	207.275	579.634	443.173	−5.936
4000	61.504	371.590	318.235	213.423	579.255	439.679	−5.742
4100	61.543	373.110	319.555	219.576	578.865	436.194	−5.557
4200	61.580	374.593	320.847	225.732	578.463	432.719	−5.382
4300	61.614	376.043	322.114	231.891	578.050	429.254	−5.214
4400	61.647	377.459	323.356	238.055	577.626	425.799	−5.055
4500	61.677	378.845	324.574	244.221	577.190	422.353	−4.903
4600	61.705	380.201	325.768	250.390	576.743	418.917	−4.757
4700	61.732	381.528	326.941	256.562	576.284	415.491	−4.618
4800	61.757	382.828	328.092	262.736	575.813	412.075	−4.484
4900	61.780	384.102	329.222	268.913	575.331	408.668	−4.356
5000	61.803	385.350	330.332	275.092	574.837	405.272	−4.234
5100	61.824	386.574	331.423	281.274	574.331	401.886	−4.116
5200	61.844	387.775	332.495	287.457	573.812	398.510	−4.003
5300	61.862	388.953	333.549	293.642	573.282	395.143	−3.894
5400	61.880	390.110	334.586	299.829	572.740	391.787	−3.790
5500	61.897	391.245	335.606	306.018	572.186	388.442	−3.689
5600	61.913	392.361	336.609	312.209	571.619	385.106	−3.592
5700	61.928	393.457	337.597	318.401	571.039	381.780	−3.499
5800	61.942	394.534	338.569	324.594	570.447	378.465	−3.408
5900	61.956	395.593	339.527	330.789	569.842	375.160	−3.321
6000	61.969	396 634	340.470	336.985	569.223	371.866	−3.237

PREVIOUS: June 1966 (1 atm) CURRENT: June 1966 (1 bar)

CNN Radical (CNN) $C_1N_2(g)$

NCN Radical (NCN) IDEAL GAS $M_r = 40.0244$ NCN Radical (NCN) $C_1N_2(g)$

$S°(298.15\text{ K}) = 226.21 \pm 0.42\text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_fH°(0\text{ K}) = 472 \pm 21\text{ kJ·mol}^{-1}$

$\Delta_fH°(298.15\text{ K}) = 473 \pm 21\text{ kJ·mol}^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$X^3\Sigma_g^-$	0	3
$A^3\Pi_u$	30384	6
$a^1\Delta$	[38000]	2

Vibrational Frequencies and Degeneracies ν, cm^{-1}
1197 (1)
423 (2)
1475 (1)

Point Group: $D_{\infty h}$ $\sigma = 2$

Bond Distance: C–N = 1.232 Å

Bond Angle: N–C–N = 180°

Rotational Constant: $B_0 = 0.396469\text{ cm}^{-1}$

Enthalpy of Formation

Okabe and Mele[1] have measured the photodissociation onset of the process

$$CNN_3(g) \rightarrow NCN(g) + N_2(A^3\Sigma) \qquad \Delta_rH°(0\text{ K}) = 149.3 \pm 2.5\text{ kcal·mol}^{-1}$$

Using $\Delta_fH°(N_2, A^3\Sigma, 298.15\text{ K}) = 143.5\text{ kcal·mol}^{-1}$ [2] and $\Delta_fH°(CNN_3, g, 298.15\text{ K}) = 107 \pm 3\text{ kcal·mol}^{-1}$,[3] we obtain $\Delta_fH°(NCN, g, 298.15\text{ K}) = 113 \pm 5\text{ kcal·mol}^{-1}$.

Heat Capacity and Entropy

The X and A electronic levels, ground state structure, and rotational constants are from Herzberg and Travis,[4] the $a^1\Delta$ level is estimated from the work of Schoen.[5] The vibrational frequencies have been observed in the matrix-isolated species by Milligan and Jacox.[6,7] Wasserman *et al.*[8] have confirmed the ground state is linear and triplet by electron paramagnetic resonance.

References

[1] H. Okabe and A. Mele, J. Chem. Phys. 51, 2100 (1969).
[2] G. Herzberg, "Spectra of Diatomic Molecules," D. Van Nostrand Co., Inc., New York, (1950).
[3] JANAF Thermochemical Tables: $N_3(g)$, 12-31-70.
[4] G. Herzberg and D. N. Travis, Can. J. Phys. 42, 1658 (1964).
[5] L. J. Schoen, J. Chem. Phys. 45, 2773 (1966).
[6] D. E. Milligan, M. E. Jacox and A. M. Bass, J. Chem. Phys. 43, 3149 (1965).
[7] D. E. Milligan and M. E. Jacox, J. Chem. Phys. 45, 1387 (1966).
[8] E. Wasserman, L. Barash and W. A. Yager, J. Amer. Chem. Soc. 87, 2075 (1965).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K$_f$
0	0.	0.	INFINITE	−10.244	472.269	472.269	INFINITE
100	30.508	187.072	260.196	−7.312	472.239	469.608	−245.298
200	37.333	210.338	229.916	−3.916	472.399	466.945	−121.953
250	40.004	218.965	226.885	−1.980	472.583	465.561	−97.274
298.15	42.192	226.203	226.203	0.	472.792	464.189	−81.324
300	42.271	226.464	226.203	0.078	472.800	464.136	−80.813
350	44.309	233.135	226.726	2.243	473.038	462.673	−69.050
400	46.171	239.175	227.910	4.506	473.288	461.176	−60.223
450	47.866	244.713	229.474	6.858	473.546	459.646	−53.354
500	49.391	249.837	231.257	9.290	473.806	458.088	−47.856
600	51.948	259.078	235.141	14.362	474.317	454.896	−39.602
700	53.928	267.241	239.155	19.660	474.799	451.621	−33.700
800	55.451	274.546	243.130	25.133	475.241	448.279	−29.270
900	56.627	281.148	246.993	30.739	475.636	444.884	−25.820
1000	57.545	287.163	250.714	36.449	475.984	441.448	−23.059
1100	58.270	292.683	254.282	42.242	476.285	437.980	−20.798
1200	58.849	297.779	257.697	48.099	476.542	434.486	−18.913
1300	59.317	302.509	260.964	54.008	476.758	430.972	−17.317
1400	59.700	306.919	264.091	59.959	476.936	427.443	−15.948
1500	60.017	311.049	267.086	65.945	477.080	423.903	−14.762
1600	60.282	314.931	269.956	71.961	477.191	420.354	−13.723
1700	60.505	318.593	272.710	78.000	477.273	416.799	−12.807
1800	60.695	322.057	275.356	84.061	477.328	413.240	−11.992
1900	60.857	325.343	277.901	90.138	477.356	409.678	−11.263
2000	60.997	328.468	280.352	96.231	477.361	406.116	−10.607
2100	61.119	331.447	282.715	102.337	477.344	402.554	−10.013
2200	61.225	334.293	284.995	108.455	477.304	398.994	−9.473
2300	61.318	337.016	287.198	114.582	477.245	395.435	−8.981
2400	61.400	339.628	289.329	120.718	477.166	391.880	−8.529
2500	61.473	342.136	291.391	126.862	477.068	388.329	−8.114
2600	61.538	344.548	293.390	133.012	476.952	384 781	−7.730
2700	61.597	346.872	295.328	139.169	476.819	381.239	−7.376
2800	61.649	349.113	297.209	145.331	476.669	377.701	−7.046
2900	61.697	351.277	299.036	151.499	476.503	374.170	−6.740
3000	61.740	353.369	300.812	157.671	476.321	370.644	−6.453
3100	61.779	355.394	302.541	163.847	476.123	367.125	−6.186
3200	61.816	357.356	304.223	170.026	475.910	363.612	−5.935
3300	61.849	359.259	305.862	176.210	475.682	360.106	−5.700
3400	61.881	361.106	307.460	182.396	475.439	356.607	−5.479
3500	61.910	362.900	309.019	188.586	475.183	353.116	−5.270
3600	61.938	364 645	310.540	194.778	474.912	349.632	−5.073
3700	61.966	366.342	312.025	200.973	474.628	346.156	−4.887
3800	61.992	367.995	313.476	207.171	474.329	342.688	−4.711
3900	62.018	369.606	314.895	213.372	474.018	339.228	−4.543
4000	62.043	371.176	316.282	219.575	473.694	335 776	−4.385
4100	62.069	372.708	317.640	225.780	473.357	332.332	−4.234
4200	62.095	374.204	318.969	231.989	473.007	328.896	−4.090
4300	62.122	375.666	320.271	238.199	472.645	325.469	−3.954
4400	62.150	377.094	321.546	244.413	472.272	322.051	−3.823
4500	62.179	378.491	322.796	250.629	471.886	318.641	−3.699
4600	62.209	379.858	324.022	256.849	471.489	315.240	−3.580
4700	62.241	381.196	325.224	263.071	471.081	311.848	−3.466
4800	62.274	382.507	326.404	269.297	470.662	308.464	−3.357
4900	62.309	383.792	327.562	275.526	470.231	305.090	−3.252
5000	62.347	385.051	328.699	281.759	469.791	301.724	−3.152
5100	62.386	386.286	329.816	287.996	469.340	298.367	−3.056
5200	62.428	387.498	330.914	294.236	468.879	295.019	−2.964
5300	62.472	388.687	331.993	300.481	468.408	291.680	−2.875
5400	62.519	389.855	333.053	306.731	467.929	288.350	−2.789
5500	62.568	391.003	334.097	312.985	467.440	285.029	−2.707
5600	62.620	392.131	335.123	319.244	466.942	281.717	−2.628
5700	62.674	393.240	336.133	325.509	466.435	278.414	−2.551
5800	62.732	394.330	337.127	331.779	465.919	275.119	−2.478
5900	62.792	395.403	338.105	338.056	465.395	271.834	−2.407
6000	62.854	396.459	339.069	344.338	464.863	268.558	−2.338

PREVIOUS: December 1970 (1 atm) CURRENT December 1970 (1 bar)

Sodium Carbonate (Na_2CO_3) CRYSTAL $M_r = 105.98874$

$S°(298.15\ K) = 138.797 \pm 0.8\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{trs} = 723.15\ K$
$T_{fus} = 1123.15\ K$

$\Delta_f H°(0\ K) = -1124.610 \pm 0.21\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -1130.768 \pm\ kJ{\cdot}mol^{-1}$
$\Delta_{trs} H° = 0.690\ kJ{\cdot}mol^{-1}$
$\Delta_{fus} H° = 29.665\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

The enthalpy of formation was obtained from the enthalpy of solution $\Delta_{sol}H = -6.36\ kcal{\cdot}mol^{-1}$ and the enthalpies of formation for $Na^+(aq, \infty)$ and $CO_3^{=}(aq, \infty)$, −57.39 and −161.84 $kcal{\cdot}mol^{-1}$, respectively. The enthalpy of solution was taken from Rupert *et al.*[1] The ionic enthalpies of formation were taken from Wagman *et al.*[2]

A value of $\Delta_f H°(298.15\ K) = -270.9\ kcal{\cdot}mol^{-1}$ has been selected by Wagman.[3]

Heat Capacity and Entropy

The low temperature heat capacities, 54.6–292.1 K, were measured by Anderson.[4] In the temperature range 473.15–873.15 K, Popov and Galchenko[5] measured the heat capacities (by heat conduction calorimetry) and observed two transformations, one at about 623 K and the other at about 750 K. Popov and Ginzburg[6] measured enthalpies in the temperature range 480–1350 K and tabulated their data only in the range 476–872 K. Ginzburg[7] has given heat capacity equations based on the data from[5] [6] and has tabulated thermodynamic functions in the range 500–1500 K. There appear to be inconsistencies among the data, equations and functions. Rolin and Recapet[8] also measured the enthalpy in the temperature range 645–1322 K. Janz *et al.*[9] have given an enthalpy equation based on their heat content measured data in the range 707–1127 K. May[10] has tabulated smoothed measured enthalpy values in the range 400–1500 K. All the above information was used in a Shomate analysis in order to smooth the enthalpies and calculate heat capacities. The values from the low and high temperature sources join smoothly at 298 K. The heat capacity was graphically extrapolated above the melting point.

The entropy was calculated at 54.60 using the Debye and Einstein function $D(138/T) + 2E(266/T) + 2D(737/T)$ given by Anderson.[4] The value of $S°(54.6\ K) = 3.943\ cal{\cdot}deg^{-1}{\cdot}mole^{-1}$.

Transition Data

T_{trs} was taken from Ginzburg[7] and $\Delta_{trs}H°$ was obtained from the above reported enthalpy measurements by means of Shomate function analysis. The heat of transition at 593.15 K has been incorporated in the heat capacity.

Fusion Data

T_{fus} was taken from Ginzburg[7] and $\Delta_{fus}H°$ was obtained from the above reported enthalpy measurements by means of Shomate function analysis.

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[1] J. P. Rupert, H. P. Hopkins, Jr., and C. A. Wulff, J. Phys. Chem. 69, 3059–62 (1965).
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[10] M. N. May, Tappi, 35, 511 (1952).

Sodium Carbonate (Na_2CO_3) $C_1Na_2O_3(cr)$

Enthalpy Reference Temperature = T_r = 298.15 K | Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−20.812	−1124 610	−1124.610	INFINITE
100	61.241	43.237	225.158	−18.192	−1129.086	−1102.556	575.916
200	94.140	97.766	148.470	−10.141	−1130.640	−1075.252	280.827
298.15	111.003	138.797	138.797	0.	−1130.768	−1048.009	183.607
300	111.253	139.484	138.799	0.206	−1130.764	−1047.496	182.385
400	125.102	173.307	143.317	11.996	−1135.696	−1019.370	133.116
500	142.214	203.007	152.332	25.337	−1134.473	−990.400	103.466
600	163.302	230.759	163.106	40.592	−1131.568	−961.826	83.734
700	187.569	257.722	174.702	58.115	−1126.604	−933.897	69.688
723.150	193.385	263.919	177.459	62.524	I <−−> II		
723.150	143.762	264.873	177.459	63.214	TRANSITION		
800	153.344	279.866	186.580	74.628	−1122.835	−906.701	59.202
900	166.230	298.668	197.996	90.605	−1119.776	−879.857	51.066
1000	179.201	316.851	208.977	107.874	−1115.597	−853.412	44.578
1100	192.046	334.537	219.591	126.441	−1110.305	−827.441	39.292
1123.150	195.101	338.569	222.002	130.922	−−−−− II <−−> LIQUID −−−−−−		
1200	200.748	351.719	229.891	146.194	−1297.547	−797.118	34.698
1300	206.188	368.015	239.895	166.556	−1289.016	−755.759	30.367
1400	209.744	383.430	249.602	187.359	−1280.130	−715.071	26.680
1500	212.547	398.000	259.014	208.478	−1271.004	−675.027	23.507
1600	214.765	411.789	268.136	229.845	−1261.701	−635.598	20.750
1700	216.899	424.875	276.974	251.431	−1252.242	−596.755	18.336
1800	218.656	437.323	285.539	273.210	−1242.651	−558.473	16.206
1900	220.204	449.186	293.843	295.153	−1232.955	−520.727	14.316
2000	221.752	460.521	301.895	317.251	−1223.161	−483.495	12.628

PREVIOUS: December 1960 CURRENT: March 1966

Sodium Carbonate (Na_2CO_3) LIQUID $M_r = 105.98874$ Sodium Carbonate (Na_2CO_3) $C_1Na_2O_3(l)$

$S°(298.15\ K) = [156.423]\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = [-1108.515]\ kJ \cdot mol^{-1}$

$T_{fus} = 1123.15\ K$ $\Delta_{fus} H° = 29.665\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The $\Delta_f H°(l, 298.15\ K)$ is calculated from $\Delta_f H°(cr, 298.15\ K)$ by adding $\Delta_{fus} H°$ and the difference enthalpy, $H°(1123.15\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

A glass transition is assumed at 723.15 K. The heat capacity below 723.15 K is obtained from the heat capacity of the crystal. Above 723.15 K the heat capacity is adopted as $45.30\ cal \cdot K^{-1} \cdot mol^{-1}$, based on the enthalpy measurements in the range 1127–1210 K reported by Janz *et al.*[1] The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Refer to the crystal table for details.

Reference

[1] G. J. Janz, E. Neuenschwander and F. J. Kelly, Trans. Faraday Soc. 59, 841 (1963).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p° = 0.1$ MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	111.002	156.423	156.423	0.	−1108.515	−1031.011	180.629
300	111.253	157.110	156.425	0.206	−1108.511	−1030.531	179.431
400	125.102	190.934	160.944	11.996	−1113.443	−1004.168	131.131
500	142.214	220.614	169.957	25.329	−1112.228	−976.960	102.062
600	163.302	248.359	180.729	40.578	−1109.329	−950.147	82.718
700	187.569	275.336	192.322	58.110	−1104.356	−923.979	68.948
723.150	193.387	281.533	195.079	62.519	I <−−> II TRANSITION		
723 150	189.535	281.533	195.079	62.519			
800	189.535	300.675	204.319	77.085	−1098.125	−898.639	58.675
900	189.535	322.999	216.289	96.039	−1092.089	−874.068	50.730
1000	189.535	342.969	227.976	114.992	−1086.226	−850.159	44.408
1100	189.535	361.033	239.264	133.946	−1080.547	−826.828	39.263
1123.150	189.535	364.981	241.815	138.333	−−−−− II <−−> LIQUID −−−−−−		
1200	189.535	377.525	250.109	152.899	−1268.589	−799.127	34.785
1300	189.535	392.696	260.501	171.853	−1261.466	−760.294	30.549
1400	189.535	406.742	270.452	190.806	−1254.430	−722.007	26.938
1500	189.535	419.818	279.979	209.760	−1247.470	−684.221	23.827
1600	189.535	432.051	289.105	228.713	−1240.579	−646.896	21.119
1700	189.535	443.541	297.855	247.667	−1233.753	−610.000	18.743
1800	189.535	454.375	306.252	266.620	−1226.988	−573.504	16.643
1900	189.535	464.622	314.320	285.574	−1220.282	−537.383	14.774
2000	189.535	474.344	322.081	304.527	−1213.632	−501.613	13.101
2100	189.535	483.592	329.553	323.481	−1207.037	−466.174	11.595
2200	189.535	492.409	336.757	342.434	−1200.497	−431.048	10.234
2300	189.535	500.834	343.709	361.388	−1194.012	−396.219	8.998
2400	189.535	508.901	350.425	380.341	−1187.582	−361.671	7.872
2500	189.535	516.638	356.920	399.295	−1181.206	−327.389	6.840

PREVIOUS: December 1960 CURRENT: March 1966

Sodium Carbonate ($NaCO_3$) CRYSTAL(I, II)–LIQUID

0	to	723.15	K	crystal, I
723.15	to	1123.15	K	crystal, II
above		1123.15	K	liquid

Refer to the individual tables for details

M_r 105.98874 Sodium Carbonate (Na_2CO_3) $C_1Na_2O_3$(cr,l)

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−20.812	−1124.610	−1124.610	INFINITE
100	61.241	43.237	225.158	−18.192	−1129.086	−1102.556	575.916
200	94.140	97.766	148.470	−10.141	−1130.640	−1075.252	280.827
298.15	111.003	138.797	138.797	0.	−1130.768	−1048.009	183.607
300	111.253	139.484	138.799	0.206	−1130.764	−1047.496	182.385
400	125.102	173.307	143.317	11.996	−1135.696	−1019.370	133.116
500	142.214	203.007	152.332	25.337	−1134.473	−990.400	103.466
600	163.302	230.759	163.106	40.592	−1131.568	−961.826	83.734
700	187.569	257.722	174.702	58.115	−1126.604	−933.897	69.688
723.150	193.387	263.919	177.459	62.524	I <--> II		
723.150	143.761	264.873	177.459	63.214	TRANSITION		
800	153.344	279.866	186.580	74.628	−1122.835	−906.701	59.202
900	166.230	298.668	197.996	90.605	−1119.776	−879.857	51.066
1000	179.201	316.851	208.977	107.874	−1115.597	−853.412	44.578
1100	192.046	334.537	219.591	126.441	−1110.305	−827.441	39.292
1123.150	195.101	338.569	222.002	130.922	II <--> LIQUID		
1123.150	189.535	364.981	222.002	160.586	TRANSITION		
1200	189.535	377.525	231.565	175.152	−1268.589	−799.127	34.785
1300	189.535	392.696	243.384	194.106	−1261.466	−760.294	30.549
1400	189.535	406.742	254.557	213.059	−1254.430	−722.007	26.938
1500	189.535	419.818	265.143	232.013	−1247.470	−684.221	23.827
1600	189.535	432.051	275.197	250.966	−1240.579	−646.896	21.119
1700	189.535	443.541	284.765	269.920	−1233.753	−610.000	18.743
1800	189.535	454.375	293.890	288.873	−1226.988	−573.504	16.643
1900	189.535	464.622	302.608	307.827	−1220.282	−537.383	14.774
2000	189.535	474.344	310.954	326.780	−1213.632	−501.613	13.101
2100	189.535	483.592	318.957	345.734	−1207.037	−466.174	11.595
2200	189.535	492.409	326.642	364.687	−1200.497	−431.048	10.234
2300	189.535	500.834	334.034	383.641	−1194.012	−396.219	8.998
2400	189.535	508.901	341.153	402.594	−1187.582	−361.671	7.872
2500	189.535	516.638	348.019	421.548	−1181.206	−327.389	6.840

PREVIOUS: CURRENT: March 1966

Carbon Monoxide (CO) **IDEAL GAS** **$M_r = 28.0104$ Carbon Monoxide (CO)** **$C_1O_1(g)$**

$S°(298.15\ K) = 197.65 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -113.81 \pm 0.17\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -110.53 \pm 0.17\ kJ{\cdot}mol^{-1}$

Electronic Level and Quantum Weight		
State	ϵ_i, cm^{-1}	g_i
$^1\Sigma$	0	1

$\omega_e = 2169.52\ cm^{-1}$ $\omega_e x_e = 13.453\ cm^{-1}$ $\sigma = 1$
$B_e = 1.9302\ cm^{-1}$ $\alpha_e = 0.01746\ cm^{-1}$ $r_e = 1.1281\ Å$

Enthalpy of Formation

The enthalpy change $\Delta_f H°(298.15\ K)$ for the reaction: $CO(g) + 1/2\ O_2(g) = CO_2(g)$ was reported to be $-67.636 \pm 0.029\ kcal{\cdot}mol^{-1}$, based on molecular weight of $CO_2 = 44.010$, by Rossini.[1] It was recalculated to be $-67.638 \pm 0.03\ kcal{\cdot}mol^{-1}$, using molecular weight of $CO_2 = 44.011$, for internal consistency. From the value of $\Delta_r H°(298.15\ K)$, the enthalpy of formation $\Delta_f H°(298.15\ K)$ for CO(g) was derived to be $-26.417 \pm 0.04\ kcal{\cdot}mol^{-1}$, which yields $D_0^\circ(CO) = 11.09$ eV.

The $D_0^\circ(CO)$ value has been proposed to be 6.92 to 11.11 eV in the past few decades in order to explain data collected from spectroscopic, flame, shock–wave, detonation, and electron–impact studies. Recent evaluations by Brewer and Searcy,[2] Fineman and Petrocelli,[3] and Giese and Maier[4] favored the value 11.11 eV, reported by Gaydon.[5]

The enthaply of combustion of CO(g) was also determined by Awbery and Griffiths,[6] Fenning and Cotton,[7] and Roth and Banse.[8]

Heat Capacity and Entropy

The functions adopted here were obtained from Belzer *et al.*,[9] assuming the thermodynamic functions for the naturally occurring isotopic mixture to be the same as those for $C^{12}O^{16}(g)$. The spectroscopic constants employed for calculation were reported by Herzberg.[10] The tabulated functions include the second order corrections to the rigid–rotator and harmonic–oscillator molecular model for vibrational anharmonicity, rotational stretching and rotational–vibrational interaction.

The spectroscopic constants listed above are for the naturally occurring isotopic composition given by Strominger *et al.*[11]

Thermodynamic properties for CO from 70 to 300 K, with pressures to 300 atmospheres were reported by Hust *et al.*[12] Calculations of the vapor pressure and enthalpies of vaporization and sublimation of CO and CO_2 below one atmosphere were reported by Mullins *et al.*[13]

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[13] J. C. Mullins, B. S. Kirk, and W. T. Ziegler, U.S. Atomic Energy Commission, NP–13862 (1963).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.000	0.000	INFINITE	−8.671	−113.805	−113.805	INFINITE
100	29.104	165.850	223.539	−5.769	−112.415	−120.239	62.807
200	29.108	186.025	200.317	−2.858	−111.286	−128.526	33.568
298.15	29.142	197.653	197.653	0.000	−110.527	−137.163	24.030
300	29.142	197.833	197.653	0.054	−110.516	−137.328	23.911
400	29.342	206.238	198.798	2.976	−110.102	−146.338	19.110
500	29.794	212.831	200.968	5.931	−110.003	−155.414	16.236
600	30.443	218.319	203.415	8.942	−110.150	−164.486	14.320
700	31.171	223.066	205.890	12.023	−110.469	−173.518	12.948
800	31.899	227.277	208.305	15.177	−110.905	−182.497	11.916
900	32.577	231.074	210.628	18.401	−111.418	−191.416	11.109
1000	33.183	234.538	212.848	21.690	−111.983	−200.275	10.461
1100	33.710	237.726	214.967	25.035	−112.586	−209.075	9.928
1200	34.175	240.679	216.988	28.430	−113.217	−217.819	9.481
1300	34.572	243.431	218.917	31.868	−113.870	−226.509	9.101
1400	34.920	246.006	220.761	35.343	−114.541	−235.149	8.774
1500	35.217	248.426	222.526	38.850	−115.229	−243.740	8.488
1600	35.480	250.707	224.216	42.385	−115.933	−252.284	8.236
1700	35.710	252.865	225.839	45.945	−116.651	−260.784	8.013
1800	35.911	254.912	227.398	49.526	−117.384	−269.242	7.813
1900	36.091	256.859	228.897	53.126	−118.133	−277.658	7.633
2000	36.250	258.714	230.342	56.744	−118.896	−286.034	7.470
2100	36.392	260.486	231.736	60.376	−119.675	−294.372	7.322
2200	36.518	262.182	233.081	64.021	−120.470	−302.672	7.186
2300	36.635	263.808	234.382	67.679	−121.282	−310.936	7.062
2400	36.740	265.369	235.641	71.348	−122.109	−319.165	6.946
2500	36.836	266.871	236.860	75.027	−122.953	−327.358	6.840
2600	36.924	268.318	238.043	78.715	−123.813	−335.517	6.741
2700	37.003	269.713	239.190	82.411	−124.689	−343.643	6 648
2800	37.083	271.060	240.304	86.116	−125.582	−351.736	6.562
2900	37.150	272.362	241.387	89.827	−126.490	−359.797	6.481
3000	37.217	273.623	242.441	93.546	−127.415	−367.826	6.404
3100	37.279	274.844	243.467	97.271	−128.356	−375.824	6.333
3200	37.338	276.029	244.466	101.001	−129.312	−383.792	6.265
3300	37.392	277.178	245.440	104.738	−130.283	−391.730	6.201
3400	37.443	278.295	246.390	108.480	−131.270	−399.638	6.140
3500	37.493	279.382	247.317	112.227	−132.271	−407.517	6.082
3600	37.543	280.438	248.222	115.978	−133.288	−415.366	6.027
3700	37.589	281.468	249.107	119.735	−134.318	−423.188	5.974
3800	37.631	282.471	249.972	123.496	−135.363	−430.981	5.924
3900	37.673	283.449	250.818	127.261	−136.422	−438.746	5.876
4000	37.715	284.403	251.645	131.031	−137.495	−446.485	5.830
4100	37.756	285.335	252.456	134.804	−138.581	−454.196	5.787
4200	37.794	286.245	253.250	138.582	−139.681	−461.881	5.744
4300	37.832	287.135	254.027	142.363	−140.794	−469.539	5.704
4400	37.869	288.005	254.790	146.148	−141.921	−477.171	5.665
4500	37.903	288.856	255.537	149.937	−143.062	−484.778	5.627
4600	37.941	289.690	256.271	153.729	−144.215	−492.359	5.591
4700	37.974	290.506	256.990	157.525	−145.383	−499.915	5.556
4800	38.007	291.306	257.697	161.324	−146.563	−507.446	5.522
4900	38.041	292.090	258.391	165.126	−147.758	−514.951	5.489
5000	38.074	292.859	259.073	168.932	−148.967	−522.433	5.458
5100	38.104	293.613	259.743	172.741	−150.190	−529.890	5.427
5200	38.137	294.354	260.401	176.553	−151.427	−537.323	5.397
5300	38.171	295.080	261.049	180.368	−152.679	−544.732	5.369
5400	38.200	295.794	261.685	184.187	−153.946	−552.118	5.341
5500	38.233	296.495	262.312	188.008	−155.228	−559.480	5.313
5600	38.263	297.184	262.929	191.833	−156.527	−566.818	5.287
5700	38.296	297.862	263.535	195.661	−157.841	−574.133	5.261
5800	38.325	298.528	264.133	199.492	−159.172	−581.424	5.236
5900	38.355	299.184	264.722	203.326	−160.521	−588.694	5.212
6000	38.388	299.829	265.301	207.163	−161.887	−595.939	5.188

PREVIOUS· September 1965 (1 atm) CURRENT: September 1965 (1 bar)

$S^\circ(298.15\ K) = 231.581\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH^\circ(0\ K) = -138.531 \pm 1.05\ kJ{\cdot}mol^{-1}$
$\Delta_fH^\circ(298.15\ K) = -138.407 \pm 1.05\ kJ{\cdot}mol^{-1}$

Vibrational Levels and Degeneracies ν, cm^{-1}
859(1)
524(2)
2064(1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: $C_{\infty v}$
Rotational Constant: $B_{000} = 0.20287\ cm^{-1}$
Spectroscopic constants used in calculating corrections to rigid rotator–harmonic oscillator approximation (cm^{-1}):

$\alpha_1 = 0.0006044$ $x_{11} = -4.0$ $x_{12} = -6.8$ $A_{000} = 0$ $g_{22} = 3.2$
$\alpha_2 = 0.0003539$ $x_{22} = -0.4$ $x_{23} = -11.5$ $C_{000} = 0$
$\alpha_3 = 0.001838$ $x_{33} = -7.0$ $x_{13} = -4.5$ $D_{000} = 4.37 \times 10^{-8}$

Enthalpy of Formation

Terres and Wesemann,[1] report equilibrium constants from 623 to 873 K for the reaction $CO_2(g) + H_2S(g) \rightarrow COS(g) + H_2O(g)$. These yield $\Delta_rH^\circ(700\ K) = 8.19 \pm 0.23\ kcal{\cdot}mol^{-1}$, whence $\Delta_fH^\circ(298.15\ K)$ for COS is $-33.08 \pm 0.25\ kcal{\cdot}mol^{-1}$. The same authors report equilibrium constants for the reaction $COS(g) + H_2S(g) \rightarrow CS_2\ (g) + H_2O(g)$, but regard these as less reliable than the others. The resulting value of $-26.39\ kcal{\cdot}mol^{-1}$ for $\Delta_fH^\circ(298.15\ K)$ of COS has been disregarded.

Heat Capacity

Gordon[2] has used the constants listed above to calculate C_p° from 298 15 to 6000 K by the method of Pennington and Kobe,[3] which takes anharmonicity, vibration–rotation interaction, and centrifugal stretching into account. The constants have been taken from.[4-8] The thermodynamic functions below 298.15 K have been calculated for the rigidly rotating harmonic oscillator.

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	Δ_fH°	Δ_fG°	log K_f
0	0.	0.	INFINITE	−9.929	−138.531	−138.531	INFINITE
100	29.610	194.193	264.316	−7.012	−137.816	−147.223	76.901
200	35.472	216.276	235.229	−3.791	−138.018	−156.581	40.895
298.15	41.497	231.581	231.581	0.	−138.407	−165.601	29.013
300	41.589	231.838	231.582	0.077	−138.415	−165.770	28.863
400	45.852	244.415	233.268	4.459	−141.138	−174.727	22.817
500	48.903	254.988	236.582	9.203	−143.179	−182.902	19.108
600	51.250	264.118	240.428	14.214	−144.910	−190.679	16.600
700	53.137	272.164	244.398	19.436	−146.435	−198.184	14.789
800	54.677	279.363	248.327	24.829	−147.842	−205.480	13.416
900	55.940	285.878	252.143	30.362	−202.304	−211.523	12.276
1000	56.990	291.828	255.818	36.010	−202.366	−212.544	11.102
1100	57.861	297.302	259.344	41.754	−202.442	−213.559	10.141
1200	58.597	302.369	262.721	47.577	−202.531	−214.565	9.340
1300	59.216	307.084	265.954	53.469	−202.633	−215.564	8.661
1400	59.748	311.492	269.051	59.418	−202.748	−216.555	8.080
1500	60.208	315.631	272.020	65.416	−202.878	−217.536	7.575
1600	60.605	319.529	274.869	71.457	−203.024	−218.509	7.134
1700	60.957	323.214	277.605	77.535	−203.187	−219.472	6.744
1800	61.266	326.707	280.237	83.647	−203.366	−220.425	6.397
1900	61.547	330.027	282.771	89.788	−203.563	−221.367	6.086
2000	61.798	333.191	285.213	95.955	−203.778	−222.299	5.806
2100	62.024	336.211	287.570	102.146	−204.011	−223.219	5.552
2200	62.233	339.102	289.847	108.359	−204.261	−224.128	5.321
2300	62.423	341.872	292.050	114.592	−204.529	−225.025	5.110
2400	62.601	344.533	294.181	120.843	−204.815	−225.910	4.917
2500	62.764	347.092	296.247	127.112	−205.118	−226.783	4.738
2600	62.919	349.556	298.250	133.396	−205.437	−227.643	4.573
2700	63.065	351.934	300.195	139.695	−205.773	−228.491	4.420
2800	63.203	354.230	302.084	146.009	−206.124	−229.326	4.278
2900	63.333	356.450	303.920	152.336	−206.491	−230.148	4.145
3000	63.459	358.599	305.707	158.675	−206.873	−230.958	4.021
3100	63.576	360.682	307.447	165.027	−207.270	−231.754	3.905
3200	63.691	362.702	309.143	171.390	−207.681	−232.537	3.796
3300	63.802	364.664	310.795	177.765	−208.107	−233.308	3.693
3400	63.910	366.570	312.408	184.151	−208.546	−234.064	3.596
3500	64.015	368.424	313.982	190.547	−208.998	−234.809	3.504
3600	64.114	370.229	315.520	196.954	−209.464	−235.539	3.418
3700	64.211	371.987	317.022	203.370	−209.944	−236.257	3.335
3800	64.306	373.701	318.491	209.796	−210.436	−236.962	3.257
3900	64.400	375.372	319.928	216.231	−210.942	−237.653	3.183
4000	64.492	377.004	321.335	222.676	−211.462	−238.331	3.112
4100	64.582	378.597	322.712	229.129	−211.994	−238.997	3.045
4200	64.670	380.155	324.061	235.592	−212.540	−239.649	2.980
4300	64.757	381.677	325.384	242.063	−213.100	−240.287	2.919
4400	64.843	383.167	326.680	248.543	−213.673	−240.913	2.860
4500	64.927	384.625	327.952	255.032	−214.261	−241.526	2.804
4600	65.009	386.053	329.199	261.529	−214.863	−242.125	2.749
4700	65.090	387.452	330.424	268.034	−215.479	−242.711	2.697
4800	65.170	388.823	331.626	274.547	−216.111	−243.284	2.647
4900	65.250	390.168	332.807	281.068	−216.759	−243.843	2.599
5000	65.329	391.487	333.968	287.597	−217.422	−244.389	2.553
5100	65.407	392.781	335.108	294.133	−218.101	−244.922	2.509
5200	65.484	394.052	336.230	300.678	−218.797	−245.441	2.465
5300	65.561	395.300	337.332	307.230	−219.511	−245.946	2.424
5400	65.638	396.527	338.417	313.790	−220.242	−246.439	2.384
5500	65.714	397.732	339.485	320.358	−220.991	−246.917	2.345
5600	65.789	398.916	340.536	326.933	−221.759	−247.381	2.307
5700	65.864	400.082	341.570	333.516	−222.546	−247.832	2.271
5800	65.939	401.228	342.589	340.106	−223.353	−248.268	2.236
5900	66.013	402.355	343.592	346.704	−224.180	−248.692	2.202
6000	66.086	403.466	344.581	353.308	−225.028	−249.099	2.169

PREVIOUS: March 1961 (1 atm) CURRENT. March 1961 (1 bar)

Carbon Dioxide (CO_2) IDEAL GAS $M_r = 44.0098$ Carbon Dioxide (CO_2) $C_1O_2(g)$

$\Delta_f H°(0\ K) = -393.151 \pm 0.05\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = 213.795 \pm 0.12\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = -393.522 \pm 0.05\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
1384.86 (1)
667.30 (2)
2349.30 (1)

Ground State Quantum Weight: 1
Point Group: $D_{\infty h}$ $\sigma = 2$
Bond Distances: C–O = 1.16 Å
Bond Angle: O–C–O = 180°
Rotational Constant: $B_0 = 0.391514\ cm^{-1}$

Enthalpy of Formation

The enthalpy change of the reaction $C(c, graphite) + O_2(g) = CO_2(g)$ has been measured by Dewey and Harper.[1] Jessup,[2] and Prosen and Rossini.[3] Based on these data, the enthalpy of formation for $CO_2(g)$ was reported to be $-94.0518 \pm 0.0108\ kcal \cdot mol^{-1}$, using molecular weight of $CO_2 = 44.010$, by Prosen *et al.*[4] This value was recalculated to be $-94.054 \pm 0.011\ kcal \cdot mol^{-1}$, based on molecular weight of $CO_2 = 44.011$, for internal consistency.

Heat Capacity and Entropy

The functions adopted here were obtained from Woolley,[5] who calculated the thermodynamic functions by means of a direct summation for the naturally occurring isotopic composition. The spectroscopic constants used are essentially those selected by Wentnik.[6] Slightly different sets of spectroscopic constants were obtained by Courtoy[7] and Stull *et al.*[8] The high-resolution infrared spectrum of O^{18} – enriched CO_2 was examined in the region 5400–1620 cm^{-1}, using an Ebert grating Spectrometer with spectral slit widths ranging from 0.4 to 0.2 cm^{-1} by Berney.[9]

The molecular structure was reported by Herzberg.[10] The rotational constant, B_o, was obtained from Woolley.[5] The value of bond distance, r_e, was calculated from B_e which was derived from B_o, using $B_e - B_o = 0.0011\ cm^{-1}$ given in Herzberg.[10] Heat capacities of $CO_2(g)$ at high pressures were reported by Vukalovich *et al.*,[11] Krueger,[12] and Vukalovich and Gureev.[13]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−9.364	−393.151	−393.151	INFINITE
100	29.208	179.009	243.568	−6.456	−393.208	−393.683	205.639
200	32.359	199.975	217.046	−3.414	−393.404	−394.085	102.924
298.15	37.129	213.795	213.795	0.	−393.522	−394.389	69.095
300	37.221	214.025	213.795	0.069	−393.523	−394.394	68.670
400	41.325	225.314	215.307	4.003	−393.583	−394.675	51.539
500	44.627	234.901	218.290	8.305	−393.666	−394.939	41.259
600	47.321	243.283	221.772	12.907	−393.803	−395.182	34.404
700	49.564	250.750	225.388	17.754	−393.983	−395.398	29.505
800	51.434	257.494	228.986	22.806	−394.188	−395.586	25.829
900	52.999	263.645	232.500	28.030	−394.405	−395.748	22.969
1000	54.308	269.299	235.901	33.397	−394.623	−395.886	20.679
1100	55.409	274.528	239.178	38.884	−394.838	−396.001	18.805
1200	56.342	279.390	242.329	44.473	−395.050	−396.098	17.242
1300	57.137	283.932	245.356	50.148	−395.257	−396.177	15.919
1400	57.802	288.191	248.265	55.896	−395.462	−396.240	14.784
1500	58.379	292.199	251.062	61.705	−395.668	−396.288	13.800
1600	58.886	295.983	253.753	67.569	−395.876	−396.323	12.939
1700	59.317	299.566	256.343	73.480	−396.090	−396.344	12.178
1800	59.701	302.968	258.840	79.431	−396.311	−396.353	11.502
1900	60.049	306.205	261.248	85.419	−396.542	−396.349	10.896
2000	60.350	309.293	263.574	91.439	−396.784	−396.333	10.351
2100	60.622	312.244	265.822	97.488	−397.039	−396.304	9.858
2200	60.865	315.070	267.996	103.562	−397.309	−396.262	9.408
2300	61.086	317.781	270.102	109.660	−397.596	−396.209	8.998
2400	61.287	320.385	272.144	115.779	−397.900	−396.142	8.622
2500	61.471	322.890	274.124	121.917	−398.222	−396.062	8.275
2600	61.647	325.305	276.046	128.073	−398.562	−395.969	7.955
2700	61.802	327.634	277.914	134.246	−398.921	−395.862	7.658
2800	61.952	329.885	279.730	140.433	−399.299	−395.742	7.383
2900	62.095	332.061	281.497	146.636	−399.695	−395.609	7.126
3000	62.229	334.169	283.218	152.852	−400.111	−395.461	6.886
3100	62.347	336.211	284.895	159.081	−400.545	−395.298	6.661
3200	62.462	338.192	286.529	165.321	−400.998	−395.122	6.450
3300	62.573	340.116	288.124	171.573	−401.470	−394.932	6.251
3400	62.681	341.986	289.681	177.836	−401.960	−394.726	6.064
3500	62.785	343.804	291.202	184.109	−402.467	−394.506	5.888
3600	62.884	345.574	292.687	190.393	−402.991	−394.271	5.721
3700	62.980	347.299	294.140	196.686	−403.532	−394.022	5.563
3800	63.074	348.979	295.561	202.989	−404.089	−393.756	5.413
3900	63.166	350.619	296.952	209.301	−404.662	−393.477	5.270
4000	63.254	352.219	298.314	215.622	−405.251	−393.183	5.134
4100	63.341	353.782	299.648	221.951	−405.856	−392.874	5.005
4200	63.426	355.310	300.955	228.290	−406.475	−392.550	4.882
4300	63.509	356.803	302.236	234.637	−407.110	−392.210	4.764
4400	63.588	358.264	303.493	240.991	−407.760	−391.857	4.652
4500	63.667	359.694	304.726	247.354	−408.426	−391.488	4.544
4600	63.745	361.094	305.937	253.725	−409.106	−391.105	4.441
4700	63.823	362.466	307.125	260.103	−409.802	−390.706	4.342
4800	63.893	363.810	308.292	266.489	−410.514	−390.292	4.247
4900	63.968	365.128	309.438	272.882	−411.242	−389.862	4.156
5000	64.046	366.422	310.565	279.283	−411.986	−389.419	4 068
5100	64.128	367.691	311.673	285.691	−412.746	−388.959	3.984
5200	64.220	368.937	312.762	292.109	−413.522	−388.486	3.902
5300	64.312	370.161	313.833	298.535	−414.314	−387.996	3.824
5400	64.404	371.364	314.888	304.971	−415.123	−387.493	3.748
5500	64.496	372.547	315.925	311.416	−415.949	−386.974	3.675
5600	64.588	373.709	316.947	317.870	−416.794	−386.439	3.605
5700	64.680	374.853	317.953	324.334	−417.658	−385.890	3.536
5800	64.772	375.979	318.944	330.806	−418.541	−385.324	3.470
5900	64.865	377.087	319.920	337.288	−419.445	−384 745	3.406
6000	64.957	378.178	320.882	343.779	−420.372	−384.148	3.344

PREVIOUS: September 1965 (1 atm) CURRENT September 1965 (1 bar)

Carbon Dioxide, Ion (CO_2^-) IDEAL GAS $M_r = 44.010348$ Carbon Dioxide, Ion (CO_2^-) $C_1O_2^-(g)$

$S°(298.15\ K) = [240.65]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = [-435.6 \pm 113]\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = [-441.4 \pm 113]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[1400] (1)
[800] (1)
1671 (1)

Ground State Quantum Weight: [2] $\sigma = 2$
Point Group: $[C_{2v}]$
Bond Distances: C–O = [1.25] Å
Bond Angle: O–C–O = 127° ± 8°
Product of the Moments of Inertia: $I_AI_BI_C = [2.13011 \times 10^{-116}]$

Enthalpy of Formation

$\Delta_fH°(CO_2^-, g, 298.15\ K) = -105.5 \pm 27\ kcal{\cdot}mol^{-1}$ is estimated from $\Delta_rH°(298.15\ K) = 88.6 \pm 10\ kcal{\cdot}mol^{-1}$ for $HCO_2^-(g) \rightarrow H(g) + CO_2^-(g)$, using the $\Delta_fH°(HCO_2^-, g, 298.15\ K) = 142 \pm 17\ kcal{\cdot}mol^{-1}$ and $\Delta_fH°(H, g, 298.15\ K) = 52.1\ kcal{\cdot}mol^{-1}$. The value of $\Delta_rH°(298.15\ K)$ is assumed to be the same as that for $HCOOH(g) \rightarrow H(G) + COOH(g)$. The values of $\Delta_fH°(HCOOH, g, 298.15\ K)$ and $\Delta_fH°(H, g, 298.15\ K)$, −90.5 and 52.1 $kcal{\cdot}mol^{-1}$, respectively, are from NBS,[1] and the value of $\Delta_fH°(COOH, g, 298.15\ K) = -54 \pm 3\ kcal{\cdot}mol^{-1}$ is from Benson.[2] The value of $\Delta_fH°(HCO_2^-, g, 298.15\ K)$ is estimated from an approximate lattice energy calculation for sodium formate. The derived electron affinity of $CO_2(g)$ is 11.5 $kcal{\cdot}mol^{-1}$ (0.5 eV) with an estimated uncertainty range of 0–40 $kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

The correlations of Walsh[3] predict a bent molecular structure of CO_2^- based on its 17 valence electrons. Hartman and Hisatsune[4] measured the asymmetric C–O stretching frequency and derived the bond angle of 127 ± 8° from the infrared spectrum of matrix isolated CO_2^-. They also estimated the bond distance C–O and the symmetric stretching and the bending vibrational frequencies by the valence force method. These molecular constants are adopted in the tabulation. The principal moments of inertia are: $I_A = 0.4511 \times 10^{-39}$, $I_B = 6.6497 \times 10^{-39}$, and $I_C = 7.1008 \times 10^{-39}\ g{\cdot}cm^2$.

Ovenall and Whiffen[5] have derived a bond angle of 134° which is in good agreement with the value selected. This result was obtained from electron spin resonance for the CO_2^- radical trapped in sodium formate.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	$\log K_f$
0	0.	0.	INFINITE	−10.147	−435.628		
100	33.269	203.352	271.567	−6.822			
200	34.178	226.586	243.909	−3.465			
250	35.280	234.325	241.243	−1.730			
298.15	36.593	240.648	240.648	0.	−441.412	−444.030	77.792
300	36.647	240.875	240.649	0.068	−441.453	−444.047	77.315
350	38.163	246.636	241.100	1.938	−442.570	−444.391	66.322
400	39.737	251.835	242.122	3.885	−443.708	−444.573	58.055
450	41.295	256.606	243.470	5.911	−444.867	−444.612	51.609
500	42.785	261.034	245.008	8.013	−446.044	−444.521	46.439
600	45.454	269.078	248.363	12.429	−448.445	−443.992	38.653
700	47.653	276.256	251.844	17.088	−450.891	−443.057	33.061
800	49.420	282.739	255.307	21.945	−453.371	−441.769	28.845
900	50.828	288.644	258.688	26.960	−455.874	−440.168	25.547
1000	51.952	294.060	261.958	32.101	−458.397	−438.288	22.894
1100	52.854	299.055	265.106	37.343	−460.937	−436.154	20.711
1200	53.586	303.686	268.131	42.667	−463.492	−433.789	18.882
1300	54.183	308.000	271.034	48.056	−466.063	−431.209	17.326
1400	54.677	312.034	273.820	53.500	−468.651	−428.431	15.985
1500	55.088	315.821	276.495	58.989	−471.257	−425.468	14.816
1600	55.433	319.387	279.065	64.515	−473.881	−422.330	13.788
1700	55.725	322.757	281.537	70.073	−476.525	−419.027	12.875
1800	55.974	325.949	283.917	75.659	−479.191	−415.568	12.059
1900	56.188	328.981	286.209	81.267	−481.880	−411.960	11.326
2000	56.374	331.868	288.421	86.895	−484.592	−408.210	10.661
2100	56.535	334.623	290.556	92.541	−487.329	−404.324	10.057
2200	56.676	337.256	292.619	98.202	−490.092	−400.306	9.504
2300	56.800	339.778	294.615	103.876	−492.881	−396.163	8.997
2400	56.910	342.198	296.548	109.561	−495.697	−391.898	8.529
2500	57.008	344.523	298.420	115.257	−498.539	−387.514	8.097
2600	57.095	346.761	300.237	120.962	−501.409	−383.017	7.695
2700	57.173	348.917	302.000	126.676	−504.305	−378.408	7.321
2800	57.243	350.998	303.713	132.397	−507.229	−373.691	6.971
2900	57.306	353.008	305.378	138.124	−510.179	−368.871	6.644
3000	57.363	354.951	306.999	143.858	−513.156	−363.947	6.337
3100	57.415	356.833	308.576	149.597	−516.159	−358.924	6.048
3200	57.462	358.657	310.113	155.341	−519.187	−353.804	5.775
3300	57.505	360.426	311.611	161.089	−522.241	−348.589	5.518
3400	57.545	362.143	313.072	166.842	−525.319	−343.280	5.274
3500	57.581	363.811	314.498	172.598	−528.422	−337.881	5.043
3600	57.615	365.434	315.890	178.358	−531.548	−332.393	4.823
3700	57.645	367.013	317.251	184.121	−534.698	−326.818	4.614
3800	57.674	368.551	318.581	189.887	−537.871	−321.156	4.415
3900	57.700	370.049	319.881	195.655	−541.066	−315.411	4.224
4000	57.724	371.510	321.154	201.427	−544.283	−309.585	4.043
4100	57.747	372.936	322.399	207.200	−547.523	−303.677	3.869
4200	57.768	374.328	323.619	212.976	−550.783	−297.691	3.702
4300	57.788	375.687	324.814	218.754	−554.066	−291.625	3.543
4400	57.806	377.016	325.986	224.533	−557.370	−285.485	3.389
4500	57.823	378.315	327.134	230.315	−560.695	−279.268	3.242
4600	57.839	379.586	328.261	236.098	−564.041	−272.978	3.100
4700	57.854	380.830	329.366	241.883	−567.409	−266.614	2.963
4800	57.869	382.049	330.451	247.669	−570.799	−260.178	2.831
4900	57.882	383.242	331.516	253.456	−574.211	−253.671	2.704
5000	57.894	384.411	332.562	259.245	−577.646	−247.094	2.581
5100	57.906	385.558	333.590	265.035	−581.103	−240.449	2.463
5200	57.917	386.683	334.601	270.826	−584.584	−233.736	2.348
5300	57.928	387.786	335.594	276.619	−588.089	−226.955	2.237
5400	57.938	388.869	336.570	282.412	−591.620	−220.109	2.129
5500	57.947	389.932	337.531	288.206	−595.175	−213.197	2.025
5600	57.956	390.976	338.476	294.001	−598.757	−206.218	1.924
5700	57.965	392.002	339.406	299.797	−602.367	−199.177	1.825
5800	57.973	393.010	340.322	305.594	−606.005	−192.071	1.730
5900	57.980	394.001	341.223	311.392	−609.672	−184.905	1.637
6000	57.987	394.976	342.111	317.190	−613.369	−177.673	1.547

PREVIOUS: December 1966 (1 atm) CURRENT· December 1966 (1 bar)

Carbon Phosphide (CP) IDEAL GAS $M_r = 2.98476$ Carbon Phosphide (CP) $C_1P_1(g)$

$S°(298.15\ K) = 216.26 \pm 0.2\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 447.6 \pm 9\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = 449.9 \pm 9\ kJ{\cdot}mol^{-1}$

Electronic States and Molecular Constants

State	T_e, cm^{-1}	ω_e, cm^{-1}	ω_ex_e, cm^{-1}	B_e, cm^{-1}	α_e, cm^{-1}	D_e, cm^{-1}	r_e, Å
X $^2\Sigma^+$	0	1239.67	6.86	0.7986	0.00597	[1.33]	1.5622
A $^2\Pi_i$	7053.2	1061.99	6.035	0.7135	0.0058	[1.3]	1.653
B $^2\Sigma^+$	29100.4	836.32	5.917	0.6829	0.00628	[1.82]	1.6894

Enthalpy of Formation

We adopt the value which Huber and Herzberg[1] recommended, D_0°(CP, g) = 5.28 eV (509.4 kJ·mol^{-1}), based on the mass–spectrometric studies of Gingerich,[2] Smoes *et al*.,[3] and Kordis and Gingerich.[4] Smoes *et al*.[3] studied the equilibrium between graphite and mono– and di–atomic phosphorus vapor when gadolinium phosphide was heated in a graphite Knudsen cell in the absence of excess graphite powder (2120–2500 K). Kordis and Gingerich[4] studied the effusate from a graphite–lined tantalum Knudsen cell containing a mixture of graphite(-excess)–TiP–Rh.

Heat Capacity and Entropy

The molecular constants for the three electronic states are taken from Huber and Herzberg[1] based on their review in 1976 of the data of Barwald *et al*.,[5] Thakur and Singh,[6] Chaudhry and Upadhya,[7] and Wentink and Spindler.[8]

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−8.715	447.589	447.589	INFINITE
100	29.105	184.299	242.380	−5.808	449.549	432.983	−226.167
200	29.207	204.487	218.963	−2.895	449.872	416.016	−108.652
250	29.473	211.029	216.745	−1.429	449.951	407.540	−85.151
298.15	29.910	216.255	216.255	0.	449.893	399.375	−69.969
300	29.930	216.440	216.256	0.055	449.888	399.062	−69.483
350	30.515	221.097	216.622	1.566	448.992	390.674	−58.305
400	31.154	225.213	217.444	3.108	448.666	382.365	−49.932
450	31.789	228.919	218.516	4.681	448.295	374.099	−43.424
500	32.388	232.300	219.728	6.286	447.885	365.877	−38.223
600	33.423	238.300	222.336	9.578	446.967	349.559	−30.432
700	34.239	243.516	224.997	12.963	445.946	333.404	−24.879
800	34.872	248.131	227.606	16.420	444.849	317.401	−20.724
900	35.364	252.268	230.120	19.933	443.695	301.538	−17.501
1000	35.752	256.015	232.526	23.489	442.496	285.807	−14.929
1100	36.061	259.438	234.819	27.081	441.261	270.198	−12.831
1200	36.312	262.586	237.003	30.700	376.424	255.781	−11.134
1300	36.519	265.501	239.085	34.342	375.909	245.748	−9.874
1400	36.692	268.214	241.070	38.002	375.367	235.756	−8.796
1500	36.838	270.751	242.965	41.679	374.803	225.803	−7.863
1600	36.964	273.132	244.777	45.369	374.218	215.888	−7.048
1700	37.074	275.377	246.511	49.071	373.614	206.011	−6.330
1800	37.170	277.499	248.174	52.784	372.994	196.170	−5.693
1900	37.256	279.511	249.771	56.505	372.357	186.364	−5.123
2000	37.333	281.424	251.306	60.235	371.706	176.592	−4.612
2100	37.403	283.247	252.784	63.972	371.041	166.852	−4.150
2200	37.466	284.988	254.209	67.715	370.362	157.145	−3.731
2300	37.525	286.655	255.583	71.465	369.671	147.468	−3.349
2400	37.579	288.253	256.912	75.220	368.967	137.822	−3.000
2500	37.630	289.788	258.196	78.980	368.252	128.206	−2.679
2600	37.678	291.265	259.440	82.746	367.525	118.619	−2.383
2700	37.723	292.688	260.645	86.516	366.786	109.059	−2.110
2800	37.765	294.061	261.814	90.290	366.037	99.528	−1.857
2900	37.806	295.387	262.949	94.069	365.277	90.023	−1.621
3000	37.845	296.669	264.052	97.851	364.506	80.544	−1.402
3100	37.882	297.911	265.124	101.638	363.725	71.092	−1.198
3200	37.918	299.114	266.168	105.428	362.933	61.665	−1.007
3300	37.953	300.281	267.184	109.221	362.131	52.262	−0.827
3400	37.987	301.415	268.174	113.018	361.319	42.885	−0.659
3500	38.019	302.516	269.140	116.819	360.497	33.531	−0.500
3600	38.051	303.588	270.082	120.622	359.666	24.201	−0.351
3700	38.082	304.631	271.001	124.429	358.824	14.894	−0.210
3800	38.113	305.647	271.900	128.239	357.973	5.610	−0.077
3900	38.143	306.637	272.778	132.052	357.112	−3.652	0.049
4000	38.172	307.603	273.636	135.867	356.241	−12.891	0.168
4100	38.201	308.546	274.476	139.686	355.360	−22.109	0.282
4200	38.229	309.467	275.299	143.507	354.471	−31.304	0.389
4300	38.257	310.367	276.104	147.332	353.571	−40.479	0.492
4400	38.285	311.247	276.892	151.159	352.662	−49.632	0.589
4500	38.312	312.107	277.665	154.989	351.744	−58.765	0.682
4600	38.339	312.950	278.423	158.821	350.816	−67.877	0.771
4700	38.366	313.775	279.167	162.657	349.879	−76.969	0.855
4800	38.392	314.583	279.896	166.495	348.933	−86.041	0.936
4900	38.418	315.375	280.612	170.335	347.977	−95.093	1.014
5000	38.444	316.151	281.315	174.178	347.012	−104.126	1.088
5100	38.470	316.912	282.006	178.024	346.038	−113.139	1.159
5200	38.496	317.660	282.684	181.872	345.054	−122.133	1.227
5300	38.521	318.393	283.351	185.723	344.061	−131.108	1.292
5400	38.546	319.114	284.007	189.576	343.059	−140.064	1.355
5500	38.571	319.821	284.652	193.432	342.048	−149.001	1.415
5600	38.596	320.516	285.286	197.291	341.028	−157.920	1.473
5700	38.621	321.200	285.910	201.151	339.998	−166.821	1.529
5800	38.645	321.872	286.524	205.015	338.959	−175.703	1.582
5900	38.670	322.532	287.129	208.881	337.911	−184.568	1.634
6000	38.694	323.182	287.724	212.749	336.854	−193.414	1.684

PREVIOUS June 1962 (1 atm)   CURRENT: June 1962 (1 bar)

Carbon Phosphide (CP) $C_1P_1(g)$

Carbon Sulfide (CS) IDEAL GAS $M_r = 44.071$ Carbon Sulfide (CS) $C_1S_1(g)$

$S°(298.15\ K) = 210.55 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 277.1 \pm 25\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = 280.3 \pm 25\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$X^1\Sigma^+$	0	1
a^3	27509	2
	27590	2
	27607	2
$a(^3\pi)$	38613.9	6
$A^1\pi$	38797.6	2
$a'^3\Sigma^+$	38851.8	3
$c^3\Sigma^-$	39160.8	3
$(^1\Delta)$	39170	2
$(^1\Delta)$	39950	2

$\omega_e = 1285.08\ cm^{-1}$ $\omega_ex_e = 6.46\ cm^{-1}$ $\sigma = 1$
$B_e = 0.820046\ cm^{-1}$ $\alpha_e = 0.005922\ cm^{-1}$ $r_e = 1.5349$ Å

Enthalpy of Formation

Several values have been proposed for the enthalpy of formation or the dissociation energy of CS(g).[1-17] Many of these have been summarized by Hubin–Franksin *et al.*[16] although distinction was not made between $\Delta_fH°$(0 K) and $\Delta_fH°$(298.15 K). The values proposed or derivable for $\Delta_fH°$(298.15 K) vary from <32 kcal·mol^{-1} (electron impact of COS) to 77 ± 4 kcal·mol^{-1}(photodissociation of COS).[15] We give more weight to the equilibrium measurements — Δ_fH(298.15 K) = 69 kcal·mol^{-1} derived from,[3] 58 ± 5 and 60 ± 6 kcal·mol^{-1},[5] 55 ± 1 kcal·mol^{-1},[7] and 70 ± 2 kcal·mol^{-1} [11] (lack of data prohibits a complete re–analysis of these values) — and adopt $\Delta_fH°$(CS, g, 298.15 K) = 67 ± 6 kcal·mol^{-1} (280.328 ± 25 kJ·mol^{-1}). This leads to $\Delta_fH°$(0 K) = 66.2 ± 6 kcal·mol^{-1} and to D_0° = 169.1 ± 6 kcal·mol^{-1} for the process CS(g) = C(g) + S(g), using JANAF values for the heats of formation of C(g) and S(g).[18]

Heat Capacity and Entropy

The molecular constants and electronic levels are those compiled by Rosen[19] except that the value of ω_ex_e = 8.46 cm^{-1} given by Rosen[19] and by Suchard[20] appears to be a transcription error for the original ω_ex_e = 6.46 cm^{-1} by Lagerqvist *et al.*[4]

The microwave spectra of carbon monosulfide have been critically reviewed by Lovas and Krupenie.[21] Their derived rotational constants are in agreement with those adopted.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−8.708	277.083	277 083	INFINITE
100	29.105	178.626	236.638	−5.801	279.240	262.725	−137.234
200	29.184	198.810	213.254	−2.889	280.184	245.766	−64.188
250	29.409	205.343	211.042	−1.425	280.333	237.141	−49.548
298 15	29.798	210.554	210.554	0.	280.328	228.820	−40.088
300	29.816	210.738	210.555	0.055	280.325	228.501	−39 786
350	30.358	215.374	210.920	1.559	280.192	219.872	−32.814
400	30.965	219.467	211.737	3.092	277.742	211.358	−27.601
450	31.583	223.150	212.804	4.656	276.753	203.110	−23.576
500	32.174	226.509	214.009	6.250	275.646	194.988	−20.370
600	33.214	232.470	216.601	9.521	273.754	179.039	−15.587
700	34.046	237.655	219.247	12.886	271.999	163.393	−12.193
800	34.698	242.245	221.840	16.324	270.305	147.994	−9.663
900	35.208	246.363	224.340	19.820	215.510	133.886	−7.771
1000	35.612	250.094	226.732	23.362	215.073	124.839	−6.521
1100	35.934	253.504	229.013	26.940	214.585	115.839	−5.501
1200	36.197	256.642	231.186	30.547	214.054	106.886	−4 653
1300	36.412	259.548	233.257	34.178	213.483	97.978	−3.937
1400	36.593	262.253	235.233	37.828	212.876	89.115	−3.325
1500	36.745	264.783	237.120	41.496	212.235	80.297	−2.796
1600	36 876	267.159	238.924	45.177	211.563	71.523	−2.335
1700	36.989	269.398	240.651	48.870	210.862	62.792	−1.929
1800	37.088	271.515	242.307	52.574	210.133	54.103	−1.570
1900	37.176	273.523	243.898	56.287	209.378	45.455	−1.250
2000	37.255	275.432	245.427	60.009	208.598	36.848	−0.962
2100	37.326	277.251	246.900	63.738	207.796	28.280	−0.703
2200	37.391	278.989	248.319	67.474	206.973	19.751	−0.469
2300	37.450	280.653	249.689	71.216	206.129	11.259	−0.256
2400	37.505	282.248	251.013	74.964	205.267	2.805	−0 061
2500	37.557	283.780	252.293	78.717	204.386	−5.613	0.117
2600	37.605	285.254	253.532	82.475	203.489	−13.995	0.281
2700	37.651	286.674	254.734	86.238	202.575	−22.342	0 432
2800	37.696	288.044	255.899	90.005	201.647	−30.656	0.572
2900	37.740	289.367	257.031	93.777	200.704	−38.936	0 701
3000	37.783	290.648	258.130	97.553	199.746	−47.183	0.822
3100	37.827	291.887	259.199	101.334	198.776	−55.398	0.933
3200	37.871	293.089	260.239	105.119	197.793	−63.581	1.038
3300	37.917	294.255	261.253	108.908	196.798	−71.734	1 135
3400	37.966	295.388	262.240	112.702	195.791	−79.856	1.227
3500	38.017	296.489	263.203	116.501	194.774	−87.949	1.313
3600	38.072	297.561	264.142	120.306	193.745	−96.012	1 393
3700	38.132	298.605	265.060	124.116	192.707	−104.046	1.469
3800	38.198	299.622	265.956	127.932	191.659	−112.053	1.540
3900	38.269	300.615	266.832	131.756	190.602	−120.031	1.608
4000	38.348	301.585	267.689	135.586	189.537	−127.983	1.671
4100	38.435	302.533	268.527	139.426	188.464	−135.908	1.731
4200	38.530	303.461	269.348	143.274	187.384	−143.806	1.788
4300	38.636	304.368	270.152	147.132	186.298	−151.679	1.843
4400	38.752	305.258	270.940	151.001	185.206	−159.526	1.894
4500	38.879	306.130	271.712	154.883	184.111	−167.348	1.943
4600	39.018	306.986	272.469	158.777	183.012	−175.147	1.989
4700	39.171	307.827	273.213	162.687	181.911	−182.921	2.033
4800	39.337	308.653	273.943	166.612	180.809	−190.671	2.075
4900	39.517	309.466	274.659	170.555	179.707	−198.399	2.115
5000	39.712	310.267	275.363	174.516	178.607	−206.105	2.153
5100	39.922	311.055	276.056	178.497	177.509	−213.788	2.190
5200	40.148	311.832	276.736	182.501	176.416	−221.450	2.224
5300	40.391	312.599	277.406	186.528	175.329	−229.091	2.258
5400	40.651	313.357	278.064	190.580	174.249	−236.711	2.290
5500	40.927	314.105	278.713	194.658	173.178	−244.312	2.320
5600	41.221	314.845	279.351	198.766	172.118	−251.893	2.350
5700	41.532	315.578	279.981	202.903	171.070	−259.455	2.378
5800	41.861	316.303	280.601	207.073	170.036	−266.999	2.405
5900	42.207	317.021	281.212	211.276	169.018	−274.525	2.430
6000	42.571	317.734	281.815	215.515	168.018	−282.035	2.455

PREVIOUS: December 1976 (1 atm) CURRENT December 1976 (1 bar)

Carbon Disulfide (CS_2) IDEAL GAS $M_r = 76.131$ Carbon Disulfide (CS_2) $C_1S_2(g)$

$S°(298.15\ K) = 237.977 \pm 0.08\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 116.131 \pm 0.84\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 116.943 \pm 0.84\ kJ \cdot mol^{-1}$

Vibrational Frequencies, Degeneracies, and Anharmonicity and Rotational Constants

ν, cm^{-1}	x_{ij} cm^{-1}	x_{ij} cm^{-1}	α_i,cm^{-1}
657.98 (1)	$x_{11} = -0.83$	$x_{12} = -1.75$	$\alpha_1 = 0.0002144$
395.93 (2)	$x_{22} = 0.82$	$x_{23} = -6.49$	$\alpha_2 = 0.0007130$
1535.35 (1)	$x_{33} = -6.54$	$x_{13} = -7.59$	$\alpha_3 = 0.0002148$

Point Group: $D_{\infty h}$ $\sigma = 2$
Bond Distance: C–S = 1.553 Å
Bond Angle: S–C–S = 180°
$B_e = 0.109277\ cm^{-1}$; $g_{22} = -0.74\ cm^{-1}$
$D_o = 1.05 \times 10^{-8}\ cm^{-1}$

Enthalpy of Formation

Good *et al.*[1] have determined $\Delta_f H°(CS_2, l, 298.15\ K) = 21.37 \pm 0.17\ kcal \cdot mol^{-1}$ by rotating bomb combustion calorimetry. They combined this with an unpublished measurement of $\Delta_{vap} H°(298.15\ K) = 6.61 \pm 0.02\ kcal \cdot mol^{-1}$ to obtain $\Delta_f H°(CS_2, g, 298.15\ K) = 27.98 \pm 0.19\ kcal \cdot mol^{-1}$. We adopt $\Delta_{vap} H°(298.15\ K) = 6.578 \pm 0.003\ kcal \cdot mol^{-1}$ determined by Weddington *et al.*[2] by vapor flow calorimetry and obtain the adopted $\Delta_f H°(CS_2, g, 298.15\ K) = 27.95 \pm 0.20\ kcal \cdot mol^{-1}$.

The resulting $\Delta_f H°(CS_2, g, 0\ K) = 27.75 \pm 0.20\ kcal \cdot mol^{-1}$ leads to $\Delta_a H°(0\ K) = 273.33 \pm 0.66\ kcal \cdot mol^{-1}$ for the process $CS_2(g) = C(g) + 2\ S(g)$. Auxiliary data are from the JANAF Tables.[12]

Heat Capacity and Entropy

The fundamental ground state vibrational frequencies are those from a re–analysis of infra–red and Raman spectra by Guenther and Stoicheff, referenced by Kleman[3] as a private communication. Several sets of anharmonicity constants and/or rotational constants have been published.[2,4-9] Some are corrected for Fermi resonance to some degree in some manner,[6,7,9] others are not.[2,4] We adopt the x_{ii}, x_{ij}, α_i, and g_{22} terms determined from the least–square estimates of the force constants in the general quartic force field by Giguere *et al.*[9] The rotational constants B_e and D_o are from McBride and Gordon.[7] The bond distance, r_e, is a rounded average of 1.5529 ± 0.0005 Å[4] and 1.5523 ± 0.0005 Å[5] and is consistent with the adopted B_e. The bond angle of 180° is from Cross and Brockway.[10]

Waddington *et al.*[2] have measured $C_p°$ of carbon disulfide gas in the 325.65–502.25 K range. At 325.65 K, the value calculated by Waddington *et al.*,[2] where Fermi resonance was not considered explicitly, is approximately 0.03% lower than the observed value; at 300 K, the present table is higher than the table calculated by Waddington *et al.*[2] by about 0.3%. At 502.25 K, the present table is approximately 0.6% higher ($0.074\ cal \cdot K^{-1} \cdot mol^{-1}$) than the measured value of $12.484\ cal \cdot K^{-1}\ mol^{-1}$. The value calculated by Waddington *et al.*[2] is 0.2% higher ($0.025\ cal \cdot K^{-1} \cdot mol^{-1}$) than the observed value. At 6000 K, the value of $C_p°$ in the present table is approximately 1.1% higher ($0.17\ cal \cdot K^{-1} \cdot mol^{-1}$) than the value calculated with the anharmonicity constants used by Waddington *et al.*[2]

The tabulated functions have been generated by the NASA–Lewis computer program.[11] We adopted these functions directly for 0 to 298.15 K and reproduce the functions at higher temperatures by integration of $C_p°$.

The allowed error of $\pm 0.02\ cal\ K^{-1} \cdot mol^{-1}$ for $S°(298.15\ K)$ includes the values calculated using other anharmonicity correction constants.[2,6,7]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.687	116.131	116.131	INFINITE
100	30.995	196.787	274.228	−7.744	117.634	100.555	−52.525
200	39.648	220.929	241.981	−4.210	117.558	83.443	−21.793
298.15	45.664	237.977	237.977	0.	116.943	66.816	−11.706
300	45.751	238.260	237.978	0.085	116.927	66.505	−11.580
400	49.677	251.995	239.824	4.868	111.494	50.016	−6.531
500	52.494	263.398	243.431	9.984	107.427	35.091	−3.666
600	54.616	273.165	247.592	15.344	104.039	20.954	−1.824
700	56.242	281.711	251.868	20.890	101.119	7.342	−0.548
800	57.503	289.307	256.082	26.580	98.466	−5.871	0.383
900	58.493	296.140	260.160	32.382	−10.281	−16.601	0.963
1000	59.283	302.345	264.073	38.272	−10.226	−17.306	0.904
1100	59.923	308.026	267.814	44.233	−10.201	−18.016	0.855
1200	60.450	313.263	271.386	50.253	−10.207	−18.726	0.815
1300	60.891	318.120	274.796	56.320	−10.243	−19.435	0.781
1400	61.266	322.646	278.054	62.429	−10.311	−20.139	0 751
1500	61.588	326.884	281.170	68.572	−10.409	−20.838	0.726
1600	61.869	330.868	284.153	74.745	−10.537	−21.530	0.703
1700	62.118	334.627	287.012	80.944	−10.695	−22.212	0.682
1800	62.340	338.184	289.757	87.167	−10.882	−22.884	0.664
1900	62.539	341.560	292.396	93.412	−11.095	−23.545	0.647
2000	62.722	344.772	294.935	99.675	−11.335	−24.194	0.632
2100	62.889	347.837	297.382	105.955	−11.598	−24.831	0.618
2200	63.045	350.766	299.742	112.252	−11.882	−25.455	0.604
2300	63.189	353.571	302.022	118.564	−12.188	−26.065	0.592
2400	63.325	356.264	304.226	124.890	−12.514	−26.661	0.580
2500	63.453	358.851	306.360	131.229	−12.857	−27.244	0.569
2600	63.575	361.342	308.427	137.580	−13.217	−27.812	0.559
2700	63.691	363.744	310.432	143.943	−13.592	−28.366	0.549
2800	63.802	366.062	312.377	150.318	−13.981	−28.906	0.539
2900	63.909	368.303	314.267	156.704	−14.384	−29.432	0.530
3000	64.012	370.471	316.105	163.100	−14.800	−29.944	0.521
3100	64.111	372.572	317.893	169.506	−15.228	−30.442	0.513
3200	64.208	374.609	319.633	175.922	−15.668	−30.926	0.505
3300	64.303	376.586	321.329	182.348	−16.118	−31.396	0.497
3400	64.394	378.507	322.983	188.782	−16.580	−31.852	0.489
3500	64.484	380.375	324.596	195.226	−17.054	−32.294	0.482
3600	64.572	382.193	326.171	201.679	−17.538	−32.723	0.475
3700	64.658	383.963	327.709	208.141	−18.034	−33.138	0.468
3800	64.742	385.689	329.212	214.611	−18.541	−33.539	0.461
3900	64.825	387.371	330.682	221.089	−19.060	−33.927	0.454
4000	64.907	389.014	332.120	227.576	−19.591	−34.302	0.448
4100	64.988	390.617	333.527	234.070	−20.135	−34.663	0.442
4200	65.067	392.184	334.905	240.573	−20.692	−35.010	0.435
4300	65.145	393.716	336.255	247.084	−21.261	−35.344	0.429
4400	65.223	395.215	337.578	253.602	−21.845	−35.665	0.423
4500	65.299	396.682	338.875	260.128	−22.443	−35.973	0.418
4600	65.375	398.118	340.148	266.662	−23.056	−36.267	0.412
4700	65.450	399.524	341.396	273.203	−23.684	−36.547	0.406
4800	65.524	400.903	342.621	279.752	−24.327	−36.814	0.401
4900	65.598	402.255	343.825	286.308	−24.987	−37.067	0.395
5000	65.671	403.581	345.007	292.871	−25.663	−37.307	0.390
5100	65 743	404.882	346.168	299.442	−26.355	−37.533	0.384
5200	65.815	406.159	347.309	306.020	−27.065	−37.745	0.379
5300	65.886	407.414	348.432	312.605	−27.793	−37.944	0.374
5400	65.957	408.646	349.535	319.197	−28.538	−38.128	0.369
5500	66.027	409.857	350.621	325 796	−29.301	−38.299	0.364
5600	66.097	411.047	351 690	332.403	−30.082	−38.455	0.359
5700	66 166	412.218	352.741	339.016	−30.882	−38.598	0.354
5800	66.235	413.369	353.777	345.636	−31.700	−38.726	0.349
5900	66.303	414.502	354.796	352.263	−32.536	−38.840	0.344
6000	66.372	415.617	355.801	358.896	−33.392	−38 940	0.339

PREVIOUS December 1976 (1 atm) CURRENT December 1976 (1 bar)

$\Delta_f H°(0\ K) = -70.530 \pm 6.3\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = 16.485 \pm 0.13\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = -71.546 \pm 6.3\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The enthalpy of formation is calculated from $\Delta_r H°(298.15\ K) = -591.9\ kcal \cdot mol^{-1}$ for $SiC(\alpha) + 4F_2(g) \rightarrow SiF_4(g) + CF_4(g)$ based on the tentative value of $\Delta_f H°(298.15\ K) = -223 \pm 1\ kcal \cdot mol^{-1}$ for $CF_4(g)$. Greenberg *et al.*[1] determined the enthalpy of reaction by fluorine bomb calorimetry. Data of Humphrey *et al.*[2] obtained by oxygen bomb calorimetry yield a $\Delta_f H°$ which is over 2 $kcal \cdot mol^{-1}$ more negative; however, this difference is probably within the uncertainties due to use of large amounts of Ti as a kindling agent and to corrections for incomplete combustion. Decomposition pressure data obtained mass spectrometrically by Drowart *et al.*[3] are in close agreement with the selected $\Delta_f H°$, but Knudsen weight loss data of Grieveson and Alcock[4] and solubility–activity data of Kirkwood and Chipman[5] yield values less negative by 2 and 3 $kcal \cdot mol^{-1}$, respectively. The results are summarized below.

The data of Drowart *et al.*[3] show a significant drift while those of Grieveson and Alcock[4] do not, but the latter should be corrected for $C_2Si(g)$ and $CSi_2(g)$ which are present in amounts of about 4 and 3%, respectively, at 2000 K. Silicon carbide may have a small vaporization coefficient, since rates of free evaporation reported by Voronin *et al.*[6] and Ghoshtagore[7] yield apparent pressures which are smaller by factors of 1/30 to 1/10000.

Source	Method	Reaction	T/K	Data Points	$\Delta_r H°(298.15\ K)$, $kcal \cdot mol^{-1}$ 2nd law	3rd law	Drift $cal \cdot K^{-1} \cdot mol^{-1}$	$\Delta_f H°(298.15\ K)$ $kcal \cdot mol^{-1}$
1	F_2 Calorimetry	A	298	–	−591.9		–	−17.1
2	O_2Calorimetry	B	303	–	−292.0		–	−19.6
3	Mass Spec.	C	2149–2316	7	136.9 ± 0.7	124.61	−5.6 ± 0.3	−16.9(−17.6)*
4	Knudsen Wt. Loss	C	1785–2004	10	122.9 ± 0.7	122.66	−0.2 ± 0.4	−15.0
5	Soly. in Pb	D	1693	1	–	25.66	–	−14.1

A) $SiC(\alpha) + 4F_2(g) \rightarrow SiF_4(g) + CF_4(g)$

B) $SiC(\alpha) + 2O_2(g) \rightarrow SiO_2(low\text{–}quartz) + CO_2(g)$

C) $SiC(\alpha) \rightarrow C(graph) + Si(g)$

D) $SiC(\alpha) \rightarrow C(graph) + Si(l)$

*Value in parentheses is based on authors' data for $Si(l) \rightarrow Si(g)$ rather than JANAF value.

Heat Capacity and Entropy

Low temperature heat capacities are from data (54–296 K) of Humphrey *et al.*[2] and are in good agreement with earlier data (54–295 K) of Kelley.[8] The entropy is obtained from $C_p°$ using $S°(50\ K) = 0.038\ cal \cdot K^{-1} \cdot mol^{-1}$. $C_p°$ above room temperature is based on enthalpy data of Humphrey *et al.*[2] [389–1789 K], Walker *et al.*[9] [373–1073 K] and Magnus[10] [372–1172 K]. Maximum deviations of the data from the selected values are 1.4, 2 and −1.7%, respectively; these occur in the range 370–621 K. Kirillin *et al.*[11] obtained enthalpy data (1114–2843 K) for SiC mixed with 12% free carbon. When corrected for free carbon but not for 0.73% iron impurity, these data deviate by −1 ± 1.5% from the selected values. Enthalpies (793–1790 K) of Fieldhouse and Hedge[12] are high by 1–8% while those of Maksimenko and Polubelova[13] were not available for analysis.

Transition Data

SiC(α), also called hexagonal II or 6H, is one of the more common of many hexagonal forms which arise from various possible stacking sequences of the hexagonal SiC layers.[14] The properties of these phases are so similar that they have not been adequately differentiated thermodynamically. It has frequently been assumed that cubic SiC(β) transforms to alpha at about 2300 K, but this seems unlikely since both phases have been prepared over temperature ranges of 1700–3000 K.[14] Heat of formation and equilibrium data indicate that alpha is less stable up to 2000 K. The adopted functions suggest that this is the case at all temperatures; however, the stability difference is small.

Decomposition Data

The decomposition temperature, $T_{dcm} = \sim 3245$ K, is calculated as the value at which the total pressure reaches one atm for vapor consisting of C_2Si(44.3 mol %), Si(32.0%), CSi_2(21.2%), Si_2(1.9%), CS_i(0.27%), and Si_3(0.25%). The tables predict decomposition to graphite and pure liquid silicon at about 3280 K; however, Scace and Slack[15] observed peritectic decomposition to graphite and solution containing 19 atom % of carbon at 3103 ± 40 K. In contrast, Dolloff[16] reported the peritectic at 2813 ± 40 K and 27% carbon. Badami[17] has shown that decomposition in vacuum at lower temperatures (2400 K) leads to graphite.

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−3.252	−70.530	−70.530	INFINITE
100	4.197	1.414	32.865	−3.145	−70.748	−70.411	36.779
200	16.246	7.954	18.613	−2.132	−71.240	−69.881	18.251
298.15	26.761	16.485	16.485	0.	−71.546	−69.139	12.113
300	26.932	16.651	16.485	0.050	−71.550	−69.124	12.036
400	34.100	25.466	17.639	3.131	−71.613	−68.301	8.919
500	38.610	33.593	20.030	6.781	−71.567	−67.477	7.049
600	41.723	40.922	22.912	10.806	−71.496	−66.666	5.804
700	44.007	47.534	25.965	15.098	−71.425	−65.866	4.915
800	45.769	53.530	29.042	19.590	−71.363	−65.076	4.249
900	47.170	59.004	32.071	24.239	−71.310	−64.294	3.732
1000	48.321	64.035	35.019	29.016	−71.268	−63.517	3.318
1100	49.283	68.687	37.871	33.897	−71.236	−62.743	2.979
1200	50.108	73.011	40.622	38.868	−71.216	−61.972	2.698
1300	50.823	77.051	43.270	43.915	−71.208	−61.202	2.459
1400	51.451	80.841	45.820	49.029	−71.216	−60.432	2.255
1500	52.011	84.410	48.275	54.203	−71.241	−59.661	2.078
1600	52.518	87.783	50.640	59.430	−71.285	−58.888	1.922
1700	52.974	90.981	52.919	64.704	−121.527	−57.665	1.772
1800	53.396	94.021	55.119	70.023	−121.385	−53.912	1.564
1900	53.781	96.918	57.243	75.382	−121.224	−50.168	1.379
2000	54.141	99.686	59.297	80.779	−121.047	−46.432	1.213
2100	54.476	102.336	61.284	86.210	−120.854	−42.706	1.062
2200	54.785	104.877	63.208	91.673	−120.647	−38.990	0.926
2300	55.082	107.319	65.073	97.166	−120.427	−35.283	0.801
2400	55.363	109.669	66.882	102.689	−120.194	−31.586	0.687
2500	55.630	111.935	68.640	108.238	−119.949	−27.899	0.583
2600	55.881	114.122	70.347	113.814	−119.693	−24.222	0.487
2700	56.124	116.235	72.008	119.414	−119.426	−20.555	0.398
2800	56.358	118.281	73.624	125.039	−119.149	−16.898	0.315
2900	56.580	120.262	75.198	130.686	−118.864	−13.251	0.239
3000	56.798	122.184	76.732	136.355	−118.569	−9.615	0.167
3100	57.007	124.050	78.229	142.045	−118.266	−5.988	0.101
3200	57.208	125.863	79.689	147.756	−117.955	−2.371	0.039
3300	57.404	127.626	81.115	153.486	−117.636	1.236	−0.020
3400	57.593	129.343	82.509	159.236	−117.310	4.833	−0.074
3500	57.781	131.015	83.871	165.005	−116.978	8.421	−0.126
3600	57.961	132.645	85.203	170.792	−500.790	22.460	−0.326
3700	58.137	134.236	86.507	176.597	−500.031	36.984	−0.522
3800	58.312	135.789	87.783	182.420	−499.268	51.488	−0.708
3900	58.480	137.305	89.034	188.259	−498.500	65.971	−0.884
4000	58.647	138.788	90.259	194.116	−497.728	80.435	−1.050

PREVIOUS: December 1962   CURRENT: March 1967

Silicon Carbide, Beta (SiC) CRYSTAL $M_r = 40.0965$ Silicon Carbide, Beta (SiC) $C_1Si_1(cr)$

$S°(298.15\text{ K}) = 16.610 \pm 0.13\ \text{J·K}^{-1}\text{·mol}^{-1}$

$\Delta_fH°(0\text{ K}) = -72.221 \pm 6.3\ \text{kJ·mol}^{-1}$

$\Delta_fH°(298.15\text{ K}) = -73.220 \pm 6.3\ \text{kJ·mol}^{-1}$

Enthalpy of Formation

The enthalpy of formation is calculated from $\Delta_rH°(298.15\text{ K}) = -591.5\ \text{kcal·mol}^{-1}$ for $SiC(\beta) + 4F_2(g) \rightarrow SiF_4(g) + CF_4(g)$, based on the tentative value of $\Delta_fH°(CF_4, g, 298.15\text{ K}) = -223 \pm 1\ \text{kcal·mol}^{-1}$. Greenberg *et al.*[1] determined the enthalpy of reaction by fluorine bomb calorimetry. Data of Humphrey *et al.*[2] obtained by oxygen bomb calorimetry yield a $\Delta_fH°$ which is over 3 kcal·mol^{-1} more negative; however, this difference is probably within the uncertainties due to use of large amounts of Ti as a kindling agent and to corrections for incomplete combustion. Decomposition pressure data obtained with the Knudsen weight loss method by Davis *et al.*[3] are in good agreement with the selected $\Delta_fH°$, but similar data of Grieveson and Alcock[4] and solubility–activity data of Rein and Chipman[5] and d'Entremont and Chipman[6] yield values less negative by 1.6 to 2.5 kcal·mol^{-1}. The results ar summarized below. Other equilibrium data[5] relating SiC and SiO_2 are not included, pending the revision of tables for SiO_2.

The data of Davis *et al.* show a serious drift, while those of Grieveson *et al.* do not; but the latter should be corrrected for $C_2Si(g)$ and $CSi_2(g)$ which are present in amounts of about 4 and 3%, respectively, at 2000 K. Silicon carbide may have a small vaporization coefficient, since rates of free evaporation reported by Voronin *et al.*[7] and Ghoshtagore[8] yield apparent pressures which are smaller by factors of 1/30 to 1/10000.

Source	Method	Reaction	T/K	Data Points	$\Delta_rH°$(298.15 K), kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_fH°$(298.15 K) kcal·mol^{-1}
1	F_2 Calorimetry	A	298	–	−591.5		–	−17.5
2	O_2 Calorimetry	B	303	–	−290.9		–	−20.6
3	Knudsen Wt. Loss	C	2117–2171	8	167 ± 28	126.10	−19 ± 13	−18.4(−17.6)*
4	Knudson Wt. Loss	C	1808–1973	6	123.3 ± 0.3	122.65	−04 ± 0.2	−15.0
5	Soly. in C–Fe	D	1823–1873	2	32.0	27.43	−2.5	−15.9
6	Soly. in Ag	D	1693	1	–	27.31	–	−15.7

A) $SiC(\beta) + 4F_2(g) \rightarrow SiF_4(g) + CF_4(g)$

B) $SiC(\beta) + 2O_2(g) \rightarrow SiO_2(\text{low quartz}) + CO_2(g)$

C) $SiC(\beta) \rightarrow C(\text{graph}) + Si(g)$

D) $SiC(\beta) \rightarrow C(\text{graph}) + Si(l)$

*Value in parentheses is based on author's data for $Si(l) \rightarrow Si(g)$ rather than JANAF value.

Heat Capacity and Entropy

Low temperature heat capacities are from data (54–296 K) of Humphrey *et al.*[2] The entropy is obtained from $C_p°$ using $S°(50\text{ K}) = 0.041$ cal·K^{-1}·mol^{-1}. $C_p°$ above room temperature is based on Humphrey's enthalpy data (389–1693 K), which show a maximum deviation of ±1.2% from the selected functions. Humphrey's sample contained about 1% of α–SiC and about 0.6% of other impurities. Kirillin *et al.*[9] obtained enthalpy data (1114–2843 K) for SiC mixed with 12% free carbon. When corrected for free carbon but not for 0.73% iron impurity, these data deviate by −1 ± 2% from the selected values.

Transition Data

SiC(β), also called cubic or 3C, has a structure of the diamond or zinc blend type.[10] The cubic phase differs from the many hexagonal forms only in the order of the stacking sequence of the hexagonal SiC layers. It has frequently been assumed that β transforms into α at about 2300 K, but this seems unlikely, since both phases have been prepared over temperature ranges of 1700–3000 K.[10] Heat of formation and equilibrium data indicate that β is more stable up to 2000 K. The adopted functions suggest that this is the case at all temperatures; however, the stability difference is small.

Decomposition Data

The decomposition temperature, $T_{dcm} = \sim 3259$ K, is calculated as the value at which the total pressure reaches one atm for vapor consisting of C_2Si(45.4 mol %), Si(32.1%), CSi_2(20.1%), Si_2(1.8%), CSi(0.28%) and Si_3(0.23%). The tables predict decomposition to graphite and pure liquid silicon at about 3337 K, however, Scace and Slack[11] observed peritectic decomposition to graphite and solution containing 19 atom % of carbon at 3103 ± 40 K. In contrast, Dolloff[12] reported the peritectic at 2813 ± 40 K and 27% carbon.

References

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Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_fH°$ (kJ·mol^{-1})	$\Delta_fG°$ (kJ·mol^{-1})	log K_f
0	0.	0.	INFINITE	−3.270	−72.221	−72.221	INFINITE
100	4.263	1.460	33.062	−3.160	−72.437	−72.104	37.664
200	16.301	8.033	18.740	−2.141	−72.923	−71.580	18.695
298.15	26.840	16.610	16.610	0.	−73.220	−70.850	12.413
300	27.008	16.777	16.611	0.050	−73.223	−70.835	12.333
400	34.100	25.598	17.765	3.133	−73.284	−70.025	9.144
500	38.639	33.727	20.158	6.784	−73.237	−69.215	7.231
600	41.790	41.066	23.042	10.814	−73.161	−68.417	5.956
700	44.108	47.690	26.098	15.115	−73.082	−67.633	5.047
800	45.878	53.700	29.178	19.618	−73.009	−66.859	4.365
900	47.283	59.188	32.212	24.278	−72.945	−66.094	3.836
1000	48.421	64.231	35.165	29.065	−72.892	−65.336	3.413
1100	49.363	68.891	38.022	33.956	−72.851	−64.583	3.067
1200	50.158	73.221	40.777	38.932	−72.824	−63.832	2.779
1300	50.840	77.263	43.430	43.983	−72.813	−63.084	2.535
1400	51.430	81.053	45.984	49.097	−72.821	−62.335	2.326
1500	51.944	84.619	48.442	54.266	−72.851	−61.585	2.145
1600	52.400	87.986	50.809	59.484	−72.904	−60.832	1.986
1700	52.806	91.176	53.090	64.745	−123.160	−59.629	1.832
1800	53.170	94.204	55.291	70.044	−123.038	−55.895	1.622
1900	53.497	97.088	57.416	75.377	−122.903	−52.169	1.434
2000	53.798	99.840	59.469	80.742	−122.757	−48.450	1.265
2100	54.070	102.471	61.454	86.136	−122.601	−44.738	1.113
2200	54.321	104.992	63.376	91.556	−122.438	−41.034	0.974
2300	54.555	107.412	65.239	97.000	−122.267	−37.338	0.848
2400	54.769	109.739	67.045	102.466	−122.090	−33.649	0.732
2500	54.965	111.979	68.797	107.953	−121.908	−29.967	0.626
2600	55.153	114.138	70.500	113.459	−121.722	−26.294	0.528
2700	55.329	116.223	72.155	118.983	−121.531	−22.627	0.438
2800	55.492	118.238	73.765	124.524	−121.338	−18.967	0.354
2900	55.643	120.188	75.332	130.081	−121.142	−15.315	0.276
3000	55.789	122.077	76.859	135.653	−120.944	−11.669	0.203
3100	55.928	123.908	78.348	141.239	−120.746	−8.030	0.135
3200	56.057	125.686	79.799	146.838	−120.546	−4.397	0.072
3300	56.183	127.413	81.216	152.450	−120.346	−0.770	0.012
3400	56.300	129.092	82.600	158.074	−120.146	2.850	−0.044
3500	56.413	130.726	83.951	163.710	−119.946	6.465	−0.096
3600	56.522	132.316	85.273	169.357	−503.899	20.535	−0.298
3700	56.626	133.866	86.565	175.014	−503.288	35.094	−0.495
3800	56.722	135.378	87.830	180.681	−502.679	49.637	−0.682
3900	56.819	136.853	89.068	186.359	−502.074	64.163	−0.859
4000	56.911	138.292	90.281	192.045	−501.472	78.675	−1.027

PREVIOUS: CURRENT. March 1967

Silicon Carbide (SiC) **IDEAL GAS** $M_r = 40.0965$ **Silicon Carbide (SiC)** **$C_1Si_1(g)$**

$S°(298.15\ K) = [213\ 04]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 714\ 7 \pm 3.3\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = 719.6 \pm 33\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
[$^1\Sigma$]	0	[1]
	[1000]	[6]
	[5000]	[3]
	[8000]	[2]
	[14000]	[2]
	[18000]	[1]

$\omega_e = [1226]\ cm^{-1}$ $\omega_ex_e = [5]\ cm^{-1}$ $\alpha = 1$
$B_e = [0.6933]\ cm^{-1}$ $\alpha_e = [0.006]\ cm^{-1}$ $r_e = [1.7]$ Å

Enthalpy of Formation

Drowart *et al.* have used the Knudsen effusion–mass spectrometric technique to determine the vapor equilibrium over the systems SiC–graphite[1] and boron–silicon–graphite.[2] 3rd law analysis of the partial pressures of Si and SiC yields the results summarized below. The adopted value, $\Delta_fH°(298.15\ K) = 172 \pm 8$ is the mean of the two results and the uncertainty reflects the possible effect of an error of up to 4 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$ in the functions. The corresponding dissociation energy is $D_0^\circ = 106.5 \pm 8\ kcal{\cdot}mol^{-1}$.

Source	Method	Reaction*	T/K	Data Points	$\Delta_fH°(298.15\ K)$, kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_fH°(298.15\ )$ kcal·mol^{-1}
1	Mass Spec.	A	2181–2316	3	27.1 ± 4	65.94	17 ± 2	173.6
2	Mass Spec.	A	2249–2344	3	48.7 ± 4	62.67	6 ± 2	170.4

*Reaction: (A) C(graphite) + Si(g) = SiC(g)

Heat Capacity and Entropy

The ground state is assumed to be $^1\Sigma$, as suggested by Weltner and McLeod.[3] By analogy with C_2, there should be a low–lying $^3\Pi$ excited state; this would dominate the thermodynamic functions at temperatures above 2000 K if the level lies below 5000 cm^{-1}. The $^3\Pi$ level is assumed to lie at 1000 cm^{-1}, intermediate between the value[4] observed for C_2 and that estimated for Si_2 (see JANAF table). Additional excited states, $^3\Sigma$, $^1\Pi$, $^1\Delta$ and $^1\Sigma$, are estimated by comparison with those observed or predicted[5] for C_2. The estimates for the electronic levels are relatively uncertain and probably yield an upper limit for the entropy at temperatures where SiC(g) is significant. A probable lower limit for the electronic contribution may be obtained by increasing the $^3\Pi$ level to 7000 cm^{-1} and omitting the other excited states. This would reduce the entropy by 3.5 and 2.0 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$ at 2000 and 4000 K.

The vibrational frequency is that estimated by Weltner and McLeod[3] from a valence bond calculation using $k = 7.44 \times 10^5$ dyn/cm obtained from C_2Si. The constants ω_ex_e, α_e, and r_e are estimated by interpolation between those[4,6] for the $^3\Pi_u$ states of Si_2 and C_2. Use of constants based on the $^3\Pi$ state is consistent with the assumption that this state dominates the electronic partition function at high temperatures. B_e is calculated from r_e.

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−9.266	714.651	714.651	INFINITE
100	29 111	178.849	242.437	−6.359	717.232	699.826	−365.552
200	31.133	199.342	216.303	−3.392	718.694	681.775	−178 061
250	34.526	206.629	213.654	−1.756	719.184	672.487	−140.508
298.15	38.417	213.044	213.044	0.	719.648	663.452	−116.234
300	38.562	213.282	213.044	0.071	719.666	663.103	−115.456
350	42.006	219.498	213.527	2.090	720.179	653.636	−97.550
400	44.241	225.267	214.639	4.251	720.702	644.093	−84.110
450	45.276	230.548	216.118	6.494	721.192	634.487	−73.649
500	45.426	235.333	217.804	8.764	721 610	624.830	−65.276
600	44.395	243.540	221.433	13.264	722.156	605.416	−52.706
700	42.946	250.274	225.087	17.631	722.302	585.943	−43.724
800	41.723	255.925	228.598	21.861	722.103	566.473	−36.987
900	40.839	260.785	231.911	25.987	721.631	547.045	−31.750
1000	40.250	265.055	235.016	30.039	720.950	527.681	−27.563
1100	39.884	268.872	237.923	34.044	720.105	508 394	−24.142
1200	39.677	272.333	240.649	38.021	719.132	489.190	−21.294
1300	39.581	275.504	243.210	41.983	718.055	470.071	−18.888
1400	39.561	278.437	245.622	45.940	716.889	451.038	−16.828
1500	39.591	281 167	247.902	49.897	715.648	432.092	−15.047
1600	39.654	283.724	250.062	53.859	714.339	413.231	−13.491
1700	39.737	286.130	252.113	57.828	662.791	394.900	−12.134
1800	39.831	288.404	254.067	61.807	661.593	379.176	−11.003
1900	39.931	290.560	255.931	65.795	660.383	363.519	−9.994
2000	40.031	292.611	257.715	69.793	659.162	347.926	−9.087
2100	40.129	294.567	259.423	73.801	657.931	332.395	−8.268
2200	40.224	296.436	261.063	77.819	656.693	316.922	−7.525
2300	40.314	298.226	262.641	81.846	655.447	301.506	−6.847
2400	40.398	299.943	264.159	85.881	654.193	286.144	−6.228
2500	40.477	301.594	265.624	89.925	652.932	270.834	−5.659
2600	40.550	303.183	267.038	93.976	651.664	255.575	−5.135
2700	40.618	304.714	268.405	98.035	650.389	240.366	−4.650
2800	40.680	306.193	269.729	102.100	649.106	225.203	−4.201
2900	40.738	307.621	271.011	106.171	647.816	210.086	−3.784
3000	40.791	309.003	272.254	110.247	646.518	195.014	−3.396
3100	40.839	310.342	273.461	114.329	645.212	179.986	−3.033
3200	40.884	311.639	274.634	118.415	643.899	164.999	−2.693
3300	40.925	312.898	275.775	122.505	642.577	150.054	−2.375
3400	40.963	314.120	276.885	126.600	641.248	135.149	−2.076
3500	40.998	315.308	277.966	130.698	639.910	120.283	−1.795
3600	41.030	316.463	279.019	134.799	254.411	115.917	−1.682
3700	41.060	317.588	280.046	138.904	253.470	112.082	−1.582
3800	41.087	318.683	281.049	143.011	252.518	108.274	−1.488
3900	41.112	319.751	282.027	147.121	251.557	104.490	−1.399
4000	41.135	320.792	282.984	151.234	250.585	100.732	−1.315
4100	41.157	321.808	283.918	155.348	249.603	96.998	−1.236
4200	41.176	322.800	284.832	159.465	248.612	93.288	−1.160
4300	41.194	323.769	285.727	163.583	247.611	89.601	−1.088
4400	41.211	324.716	286.602	167.704	246.601	85.938	−1.020
4500	41.227	325.643	287.459	171.826	245.582	82.298	−0.955
4600	41.241	326.549	288.299	175.949	244.554	78.681	−0.893
4700	41.254	327.436	289.123	180.074	243.516	75.086	−0.834
4800	41.266	328.305	289.930	184.200	242.470	71.514	−0.778
4900	41.277	329.156	290.722	188.327	241.414	67.963	−0.724
5000	41.287	329.990	291.499	192.455	240.349	64 434	−0.673
5100	41.296	330.807	292.261	196.584	239.274	60.926	−0.624
5200	41.305	331.609	293.010	200.714	238.190	57.440	−0.577
5300	41.312	332.396	293.746	204.845	237.097	53.974	−0.532
5400	41.319	333.168	294.469	208.977	235.993	50.529	−0.489
5500	41.326	333.927	295.180	213.109	234.881	47.105	−0.447
5600	41.331	334.671	295.878	217.242	233.757	43.701	−0.408
5700	41.337	335.403	296.565	221.375	232.623	40.317	−0.369
5800	41.341	336.122	297.241	225.509	231.478	36.954	−0.333
5900	41.346	336.829	297.906	229.643	230.323	33.610	−0.298
6000	41.350	337.524	298.561	233.778	229.156	30.285	−0.264

PREVIOUS. March 1967 (1 atm) CURRENT: March 1967 (1 bar)

Silicon Carbide (Si_2C) **IDEAL GAS** **M_r = 68.1820 Silicon Carbide (Si_2C)** **$C_1Si_2(g)$**

$S°(298.15 K) = [242.286]\ J\cdot K^{-1}\cdot mol^{-1}$

$\Delta_f H°(0 K) = 531.7 \pm 25\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15 K) = 535.6 \pm 25\ kJ\cdot mol^{-1}$

Electronic Levels and Quantum Weights ϵ_i, cm^{-1}	g_i
0	[1]
[12000]	[6]
[19000]	[2]

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[670](1)
[275](2)
[1600](1)

Ground State Quantum Weight: 1
Point Group: [$D_{\infty h}$]
Bond Distance: C–Si = [1.75] Å
Bond Angle: C–Si–Si = [180]°
Rotational Constant: B_0 = [0 097996] cm^{-1}

$\sigma = [2]$

Enthalpy of Formation

The selected value is an average based on the equilibrium data summarized below. Drowart *et al.*[1] have used the Knudsen effusion–mass spectrometric technique to determine the vapor species over the SiC–graphite,[1] SiC–silicon[2] and boron–carbon–silicon[3] systems. 3rd law analysis of the aprtial pressures of CSi_2 and Si yields the concordant values 127.4, 127.9 and 128.6 kcal·mol^{-1} Two of the drifts are rather large, but they are opposite in sign so that no consistent entropy difference is apparent between the data and the tabulated functions The drifts may be related to the low condensation coefficient for CSi_2 suggested by Drowart and DeMaria.[2] Rates of free evaporation reported by Voronin *et al.*[4] yield apparent pressures which are lower by a factor of 1/30, thus confirming the existence of a low evaporation coefficient. The adopted value of $\Delta_f H°(298.15 K) = 128 \pm 6$ kcal·mol^{-1} (535.552 ± 25 kJ·mol^{-1}) includes allowance for an error in the entropy of up to 3 cal·K^{-1}·mol^{-1}.

Source	Method	Reaction*	T/K	Data Points	$\Delta_f H°$(298.15 K), kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°$(298.15 K) kcal·mol^{-1}
1	Mass Spec.	A	2149–2316	7	−104 ± 7	−88.0	7.4 ± 3.0	127.4
2	Mass Spec.	B	1825–2160	7	141 ± 3	134.4	−3.4 ± 1.7	127.9
3	Mass Spec.	A	2083–2344	6	−68 ± 25	−86.8	−9 ± 12	128.6

*Reactions: A) C(graph) + 2 Si(g) = CSi_2(g) B) SiC(α) + Si(l) = CSi_2(g)

Heat Capacity and Entropy

Weltner and McLeod[5] observed a band system in absorption at 5300 Å in matrix isolation and assigned this tentatively to the transition $^1\Pi_u$ X Σ^{1+}_g of CSi_2. This assignment is adopted, although the evidence is not at all conclusive. A $^3\Pi_u$ excited state is assumed to lie at 12000 cm^{-1}, presumably arising from the same molecular orbital configuration as the $^1\Pi_u$ state. A linear, symmetric structure is assumed, as suggested by Weltner. The bond distance is estimated by comparison with Si_2, C_2 and C_3. Vibrational frequencies are estimated from a valence bond calculation using $k_1 = 7.46 \times 10^5$ and $k\delta/1^2 = 0\ 11 \times 10^5$dyn/cm. The stretching force constant is taken from C_2Si,[5] while the bending force constant is from C_2Si and the $^1\Pi_u$excited state of C_3.[5]

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Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	S°	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−11.389	531.650	531.650	INFINITE
100	34.326	197.543	281.045	−8.350	534.097	515.204	−269.115
200	42.817	224.254	246.492	−4.448	535.316	495.747	−129.476
250	45.453	234.105	243.056	−2.238	535.530	485.825	−101.508
298.15	47.424	242.286	242.286	0.	535.552	476.248	−83.437
300	47.491	242.580	242.287	0.088	535.550	475.880	−82.858
350	49.147	250.029	242.871	2.505	535.427	465.943	−69.538
400	50.550	256.685	244.189	4.998	535.195	456.032	−59.552
450	51.770	262.711	245.918	7.557	534.877	446.155	−51.788
500	52.843	268.222	247.877	10.173	534.487	436.317	−45.582
600	54.631	278.022	252.104	15.550	533.534	416.769	−36.283
700	56.029	286.553	256.429	21.086	532.401	397.395	−29.654
800	57.122	294.108	260.676	26.746	531.122	378.195	−24.694
900	57.979	300.888	264.774	32.503	529.720	359.162	−20.845
1000	58.657	307.033	268.697	38.336	528.208	340.291	−17.775
1100	59.199	312.650	272.441	44.230	526.597	321.576	−15.270
1200	59.640	317.821	276.010	50.172	524.891	303.013	−13.190
1300	60.004	322.609	279.413	56.155	523.093	284.595	−11.435
1400	60.315	327.068	282.659	62.171	521.205	266.319	−9.936
1500	60.592	331.239	285.761	68.217	519.228	248.182	−8.642
1600	60.849	335.157	288.727	74.289	517.163	230.179	−7.515
1700	61.102	338.854	291.568	80.387	414.659	213.201	−6.551
1800	61.363	342.354	294.293	86.510	412.886	201.402	−5.845
1900	61.643	345.679	296.910	92.660	411.118	189.701	−5.215
2000	61.949	348.848	299.429	98.839	409.358	178.093	−4.651
2100	62.289	351.879	301.855	105.051	407.612	166.573	−4.143
2200	62.667	354.785	304.195	111.298	405.884	155.136	−3.683
2300	63.086	357.580	306.456	117.586	404.178	143.776	−3.265
2400	63.546	360.274	308.642	123.917	402.501	132.490	−2.884
2500	64.047	362.879	310.760	130.296	400.856	121.274	−2.534
2600	64.587	365.401	312.813	136.728	399.248	110.123	−2.212
2700	65.162	367.849	314.807	143.215	397.682	99.032	−1.916
2800	65.767	370.230	316.744	149.761	396.161	87.999	−1.642
2900	66.399	372.549	318.628	156.369	394.688	77.020	−1.387
3000	67.050	374.811	320.463	163.042	393.267	66.090	−1.151
3100	67.716	377.020	322.252	169.780	391.898	55.207	−0.930
3200	68.389	379.180	323.998	176.585	390.584	44.367	−0.724
3300	69.065	381.295	325.702	183.458	389.325	33.567	−0.531
3400	69.737	383.367	327.368	190.398	388.122	22.805	−0.350
3500	70.398	385.398	328.997	197.405	386.973	12.077	−0.180
3600	71.045	387.390	330.591	204.477	−382.426	22.303	−0.324
3700	71.672	389.346	332.153	211.613	−382.641	33.548	−0.474
3800	72.275	391.265	333.683	218.811	−382.810	44.799	−0.616
3900	72.849	393.150	335.184	226.067	−382.934	56.054	−0.751
4000	73.393	395.001	336.656	233.379	−383.016	67.311	−0.879
4100	73.902	396.820	338.102	240.744	−383.058	78.570	−1.001
4200	74.376	398.606	339.521	248.159	−383.062	89.829	−1.117
4300	74.812	400.362	340.915	255.618	−383.033	101.088	−1.228
4400	75.209	402.086	342.286	263.120	−382.973	112.346	−1.334
4500	75.568	403.780	343.634	270.659	−382.886	123.602	−1.435
4600	75.888	405.445	344.960	278.232	−382.776	134.856	−1.531
4700	76.169	407.080	346.264	285.835	−382.645	146.108	−1.624
4800	76.411	408.686	347.548	293.464	−382.499	157.356	−1.712
4900	76.617	410.264	348.812	301.116	−382.340	168.602	−1.797
5000	76.787	411.814	350.056	308.787	−382.172	179.844	−1.879
5100	76.923	413.336	351.282	316.472	−381.999	191.082	−1.957
5200	77.025	414.830	352.490	324.170	−381.824	202.318	−2.032
5300	77.097	416.298	353.680	331.876	−381.651	213.550	−2.105
5400	77.139	417.740	354.853	339.588	−381.483	224.778	−2.174
5500	77.153	419.155	356.009	347.303	−381.321	236.004	−2.241
5600	77.142	420.545	357.149	355.018	−381.171	247.226	−2.306
5700	77.108	421.911	358.274	362.731	−381.035	258.446	−2.368
5800	77.051	423.251	359.382	370.439	−380.916	269.664	−2.429
5900	76.974	424.568	360.476	378.140	−380.816	280.880	−2.487
6000	76.880	425.861	361.555	385.833	−380.736	292.095	−2.543

PREVIOUS March 1967 (1 atm) CURRENT: March 1967 (1 bar)

Tantalum Carbide (TaC) **CRYSTAL** $M_r = 192.9589$

$S°(298.15\ \mathrm{K}) = 42.373 \pm 0.84\ \mathrm{J{\cdot}K^{-1}{\cdot}mol^{-1}}$
$T_{fus} = 4273 \pm 200\ \mathrm{K}$

$\Delta_f H°(0\ \mathrm{K}) = -143.9 \pm 3.8\ \mathrm{kJ{\cdot}mol^{-1}}$
$\Delta_f H°(298.15\ \mathrm{K}) = -144.1 \pm 3.8\ \mathrm{kJ{\cdot}mol^{-1}}$
$\Delta_{fus} H° = [104.6 \pm 20.9]\ \mathrm{kJ{\cdot}mol^{-1}}$

Enthalpy of Formation

There are eight oxygen bomb calorimetric studies on TaC reported in the literature[1-8] and one CO(g) equilibrium study.[9] The adopted $\Delta_f H°(298.15\ \mathrm{K})$ value is derived from the calorimetric study of Huber *et al.*[6] These authors studied the combustion of ten TaC_x samples where x covers the range 0.724 to 0.998. For each composition seven or eight combustions were performed. Huber *et al.*[6] reported that the combustions varied from 94.83% to 100% completion but were usually greater than 99%. Corrections of the order 0.4% or less were made to the heat of combustion value to account for impurities. The calculated heats of formation for the ten compositions were fitted to both a quadratic and linear equation by the least squares method by Huber *et al.*[6] Each value was weighted inversely proportional to the square of its uncertainty. Using the linear equation for $\Delta_f H°(298.15\ \mathrm{K})$ and correcting for the JANAF value of $\Delta_f H°(Ta_2O_5,\ cr,\ 298.15\ \mathrm{K})$,[10] we extrapolate to $x = 1.0$, calculate, and adopt $\Delta_f H°(298.15\ \mathrm{K}) = -34.44 \pm 0.9\ \mathrm{kcal{\cdot}mol^{-1}}$ for TaC. The quadratic equation leads to a value of $-33.94 \pm 1.2\ \mathrm{kcal{\cdot}mol^{-1}}$ which is consistent with our adopted value.

Huber *et al.*[6] and Storms[11] have reanalyzed the calorimetric and equilibrium data[1-9] for TaC_x ($x = 0.724$ to 0.998). A graphical comparison of the results (i.e., $\Delta_f H°(298.15\ \mathrm{K})$ values vs. x) indicated that the linear or quadratic equation suggested by Huber *et al.*[6] is a satisfactory representation of all the $\Delta_f H°(298.15\ \mathrm{K})$ results for TaC_x. The shortcomings of the various studies have been discussed by Huber *et al.*[6] and Storms.[11] For comparison, the oxygen combustion study by Mah[8] led to a reported value of $\Delta_f H°(298.15\ \mathrm{K}) = -35.4 \pm 0.5\ \mathrm{kcal{\cdot}mol^{-1}}$ for $TaC_{0.996}$ based on six combustions.

Heat Capacity and Entropy

Kelley[12] measured the heat capacity of TaC in the region 54–294 K (32 points). The reported data refer to stoichiometric TaC with corrections for 0.03% free carbon having been made by Kelley.[12,13] The sample contained less than 0.02% impurities other than free carbon. Using the Debye function suggested by Kelley,[12] we calculate and adopt $S°(50\ \mathrm{K}) = 0.831\ \mathrm{cal{\cdot}K^{-1}{\cdot}mol^{-1}}$ and $H°(50;0) = 30.10\ \mathrm{kcal{\cdot}mol^{-1}}$.

Of the numerous enthalpy and heat capacity studies on TaC,[14-24] the adopted $C_p°$ values for $T > 298$ K are derived primarily from the studies of Pankratz *et al.*,[21] Chang,[23] Levinson,[17] and Bolgar *et al.*[22] The heat capacity data for $200 \leq T \leq 298$ K are used to derive enthalpy values which in turn are used to constrain the high temperature enthalpy data. A polynomial curve fitting technique is used for the Pankratz *et al.*[21] and Levinson[17] data, with the above mentioned constraints, to obtain a smooth joining of the results near 298 K and to provide an equation suitable for extrapolation to T_{fus}. Pankratz *et al.*[21] determined the enthalpy of $TaC_{1.008}$ in the region 405–1700 K (14 data points) while Levinson[17] studied $TaC_{1.007}$ in the range 1289–2778 K (15 data points). Both sets of data are corrected to the stoichiometric composition (TaC) assuming excess free carbon. These corrections are roughly 20 kcal·mol⁻¹ at 1000 K and 90 kcal·mol⁻¹ at 2500 K.[10] Chang[23] determined the enthalpy of a reported stoichiometric TaC sample for 324–985 K (11 data points). Bolgar *et al.*[22] reported an equation for $C_p°$ values as a function of T and x for the 1200–2400 K range. This equation was based on a study of four TaC_x compositions. We use this equation to extrapolate to the TaC composition.

The adopted tabulation yields enthalpy values for $T < 1200$ K which are very similar to those suggested by Pankratz *et al.*,[21] the difference being no more than ±20 kcal·mol⁻¹. Above 1200 K, the data of Pankratz *et al.*[21] lies low approaching roughly 1% in the 1700–1800 K region. The Chang data[23] lies below the tabulated enthalpy values for $T < 600$ K. The average deviation is 0.94% with the maximum of −2.5% occurring at 324.4 K. The Levinson data[17] has an average deviation of 0.5% with considerable scatter. The $C_p°$ values of Bolgar *et al.*[24] has considerable scatter and deviates from our tabulated values by an average deviation of 6%.

Phase Data

Refer to the liquid table for details.

Fusion Data

Refer to the liquid table for details.

References

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[2] M. C. Sanz, North American Aviation, Inc., Report A1-203, (May, 1947).
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[11] E. K. Storms, "The Refractory Carbides," Academic Press, New York, (1967).

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Tantalum Carbide (TaC) $C_1Ta_1(cr)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.514	−143.879	−143.879	INFINITE
100	18.619	12.880	69 673	−5.679	−144.099	−143.677	75.049
200	29.192	29.187	45.519	−3.266	−144.264	−143.168	37.392
298.15	36.790	42.373	42.373	0.	−144.097	−142.654	24.992
300	36.903	42.601	42.374	0.068	−144.091	−142.645	24.837
400	41.664	53.915	43.884	4.012	−143.729	−142.215	18.571
500	44.530	63.537	46.877	8.330	−143.347	−141.882	14.822
600	46.447	71.833	50.361	12.883	−143.033	−141.620	12.329
700	47.890	79.104	53.959	17.602	−142.791	−141.404	10.552
800	49.074	85.578	57.514	22.451	−142.596	−141.220	9.221
900	50.116	91.419	60.962	27.411	−142.426	−141.058	8.187
1000	51.066	96.749	64.278	32.471	−142.270	−140.914	7.361
1100	51.928	101.656	67.456	37.621	−142.124	−140.786	6.685
1200	52.779	106.211	70.498	42.856	−141.987	−140.670	6.123
1300	53.616	110.469	73.411	48.176	−141.850	−140.566	5.648
1400	54.441	114.473	76.202	53.579	−141.697	−140.473	5.241
1500	55.254	118.257	78.881	59.064	−141.513	−140.392	4.889
1600	56.035	121.848	81.455	64.628	−141.291	−140.324	4.581
1700	56.813	125.268	83.932	70.271	−141.035	−140.271	4.310
1800	57.588	128.537	86.320	75.991	−140.761	−140.234	4.069
1900	58.360	131.672	88.625	81.788	−140.482	−140.213	3.855
2000	59.128	134 685	90.853	87.663	−140.200	−140.206	3.662
2100	59.890	137.588	93.010	93.614	−139.913	−140.213	3.488
2200	60.650	140.392	95.100	99.641	−139.621	−140.234	3.330
2300	61.409	143.104	97.129	105.744	−139.325	−140.269	3.186
2400	62.167	145.734	99.100	111.922	−139.030	−140.316	3.054
2500	62.923	148.287	101.016	118.177	−138.741	−140.376	2.933
2600	63.676	150.770	102.882	124.507	−138.467	−140.446	2.822
2700	64.429	153.187	104.701	130.912	−138.218	−140.527	2.719
2800	65.181	155.544	106.475	137.393	−138.006	−140.617	2.623
2900	65.933	157.844	108.207	143.948	−137.845	−140.713	2.535
3000	66.685	160.092	109.899	150.579	−137.753	−140.814	2.452
3100	67.436	162.291	111.554	157.285	−137.746	−140.916	2.374
3200	68.187	164.444	113.173	164.066	−137.846	−141.017	2.302
3300	68.938	166.553	114.759	170.923	−174.531	−140.642	2.226
3400	69.688	168.622	116.312	177.854	−174.488	−139.616	2.145
3500	70.438	170.653	117.836	184.860	−174.382	−138.592	2.068
3600	71.187	172.648	119.331	191.941	−174.213	−137.571	1.996
3700	71.935	174.609	120.799	199.098	−173.981	−136.557	1.928
3800	72.683	176.537	122.240	206.328	−173.686	−135.549	1.863
3900	73.431	178.435	123.657	213.634	−173.328	−134.550	1.802
4000	74.178	180.303	125.050	221.015	−172.905	−133.561	1.744
4100	74.925	182.144	126.420	228.470	−172.420	−132.583	1.689
4200	75.671	183.959	127.768	236.000	−171.871	−131.618	1.637
4273.000	76.216	185.267	128.739	241.544	--- CRYSTAL <--> LIQUID ---		
4300	76.418	185.748	129.096	243.604	−171.259	−130.667	1.587
4400	77.167	187.513	130.403	251.283	−170.582	−129.730	1.540
4500	77.914	189.256	131.692	259.037	−169.842	−128.810	1.495
4600	78.662	190.976	132.962	266.866	−169.038	−127.907	1.452
4700	79.408	192.676	134.215	274.770	−168.170	−127.022	1.412

PREVIOUS: CURRENT December 1973

Tantalum Carbide (TaC) LIQUID $M_r = 192.9589$ Tantalum Carbide (TaC) $C_1Ta_1(l)$

$S°(298.15\ K) = [68.279]\ J·K^{-1}·mol^{-1}$
$T_{fus} = 4273 \pm 200\ K$

$\Delta_fH°(298.15\ K) = [-33.955]\ kJ·mol^{-1}$
$\Delta_{fus}H° = [104.6 \pm 20.9]\ kJ·mol^{-1}$

Enthalpy of Formation

The enthalpy of formation of TaC(l) at 298.15 K is calculated from that of the crystal by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(4273\ K)–H°(298.15\ K)$, between TaC(cr) and TaC(l).

Heat Capacity and Entropy

The heat capacity for TaC(l) is assumed to be 16.0 cal·K⁻¹·mol⁻¹ *for the entire liquid phase. A glass transition is assumed at* 2800 K, below which the heat capacity values of the crystal are used. The entropy at 298.15 K is calculated in a manner analogous to that used for the enthalpy of formation.

Phase Data

TaC has a cubic structure of the NaCl type[1] and has a wide homogeneity range. From the phase diagram for the Ta–C system given by Storms,[1] the temperature dependent homogeneity range extends from $x = 0.58$ at 3603 ± 100 K to $x = 0.998$ or possibly $x = 1.00$. The phase boundary at a eutectic temperature of 3673 ± 50 K is $TaC_{0.98}$. A discussion of the phase diagram for TaC_x ($x = 0.00$ to 1.6) is given by Storms.[1]

Fusion Data

The phase diagram given by Storms[1] indicated a eutectic melting at 3673 ± 50 K. A congruent melting point was estimated by Storms[1] at roughly 4273 K for $TaC_{0.88}$. As an approximation due to the uncertainties in this area of the phase diagram, we adopt $T_{fus} = 4273 \pm 200$ K and assign this melting point to TaC. We assume a heat of melting $\Delta_{fus}H° = 25.0 \pm 5.0\ kcal·mol^{-1}$ ($\Delta_{fus}S° = 5.85\ cal·K^{-1}·mol^{-1}$).

Decomposition Data

Using JANAF auxiliary data,[2] we calculate $T_{dcm} = \sim 5580$ K, as that temperature at which $\Delta_rG°$ is zero for the reaction TaC(l) = Ta(l) + C(g).

References

[1] E. K. Storms, "The Refractory Carbides," Academic Press, New York, (1967).
[2] JANAF Thermochemical Tables: *Ta(l), 12–31–72; C(g), 3–31–61.*

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
0							
100							
200							
298.15	36.790	68.279	68.279	0.	−33.955	−40.236	7.049
300	36.903	68.507	68.279	0.068	−33.950	−40.275	7.013
400	41.664	79.820	69.790	4.012	−33.587	−42.436	5.542
500	44.530	89.443	72.783	8.330	−33.205	−44.693	4.669
600	46.447	97.738	76.267	12.883	−32.891	−47.021	4.094
700	47.890	105.010	79.865	17.602	−32.649	−49.396	3.686
800	49.074	111.484	83.420	22.451	−32.454	−51.802	3.382
900	50.116	117.325	86.868	27.411	−32.285	−54.231	3.148
1000	51.066	122.654	90.184	32.471	−32.128	−56.678	2.961
1100	51.928	127.562	93.362	37.621	−31.982	−59.140	2.808
1200	52.779	132.117	96.404	42.856	−31.846	−61.615	2.682
1300	53.616	136.375	99.316	48.176	−31.708	−64.102	2.576
1400	54.441	140.378	102.108	53.579	−31.555	−66.599	2.485
1500	55.254	144.162	104.786	59.064	−31.371	−69.109	2.407
1600	56.035	147.753	107.361	64.628	−31.149	−71.631	2.339
1700	56.813	151.174	109.838	70.271	−30.894	−74.169	2.279
1800	57.588	154.443	112.226	75.991	−30.620	−76.723	2.226
1900	58.360	157.577	114.531	81.788	−30.340	−79.292	2.180
2000	59.128	160.590	116.759	87.663	−30.058	−81.875	2.138
2100	59.890	163.494	118.916	93.614	−29.771	−84.473	2.101
2200	60.651	166.297	121.006	99.641	−29.479	−87.085	2.068
2300	61.410	169.010	123.035	105.744	−29.183	−89.710	2.037
2400	62.167	171.640	125.005	111.923	−28.888	−92.348	2.010
2500	62.923	174.193	126.922	118.177	−28.599	−94.998	1.985
2600	63.678	176.675	128.788	124.507	−28.325	−97.659	1.962
2700	64 431	179.093	130.607	130.913	−28.075	−100.331	1.941
2800	65.183	181.449	132.380	137.393	−27.863	−103.011	1.922
2800.000	65.183	181.449	132.380	137.393	GLASS <−−> LIQUID TRANSITION		
2800.000	66.944	181.449	132.380	137.393			
2900	66.944	183.799	134.113	144.088	−27.564	−105.701	1.904
3000	66.944	186.068	135.807	150.782	−27.408	−108.398	1.887
3100	66.944	188.263	137.464	157.476	−27.413	−111.098	1.872
3200	66.944	190.389	139.085	164.171	−27.600	−113.795	1.858
3300	66.944	192.449	140.671	170.865	−64.446	−116.013	1.836
3400	66.944	194.447	142.224	177.560	−64.641	−117.572	1.806
3500	66.944	196.388	143.744	184.254	−64.847	−119.126	1.778
3600	66.944	198.273	145.232	190.948	−65.065	−120.674	1.751
3700	66.944	200.108	146.691	197.643	−65.294	−122.215	1.725
3800	66.944	201.893	148.120	204.337	−65.536	−123.751	1.701
3900	66.944	203.632	149.521	211.032	−65.788	−125.279	1.678
4000	66.944	205.327	150.895	217.726	−66.052	−126.801	1.656
4100	66.944	206.980	152.243	224.420	−66.328	−128.317	1.635
4200	66.944	208.593	153.566	231.115	−66.614	−129.825	1.615
4273.000	66.944	209.746	154.516	236.002	−−− CRYSTAL <−−> LIQUID −−−		
4300	66.944	210.168	154.864	237.809	−66.912	−131.327	1.595
4400	66.944	211.707	156.138	244.504	−67.220	−132.821	1.577
4500	66.944	213.212	157.390	251.198	−67.540	−134.309	1.559
4600	66.944	214.683	158.619	257.892	−67.870	−135.789	1.542
4700	66.944	216.123	159.828	264.587	−68.211	−137.262	1.525
4800	66.944	217.532	161.015	271.281	−68.563	−138.727	1.510
4900	66.944	218.912	162.183	277.976	−68.926	−140.185	1.494
5000	66.944	220.265	163.331	284.670	−69.300	−141.636	1.480
5100	66.944	221.591	164.460	291.364	−69.684	−143.078	1.465
5200	66.944	222.890	165.571	298.059	−70.079	−144.514	1.452
5300	66.944	224.166	166.665	304.753	−70.484	−145.941	1.438
5400	66.944	225.417	167.741	311.448	−70.900	−147.361	1.425
5500	66.944	226.645	168.801	318.142	−71.327	−148.773	1.413
5600	66.944	227.852	169.845	324.836	−71.764	−150.177	1.401
5700	66.944	229.036	170.873	331.531	−72.211	−151.574	1.389
5800	66.944	230.201	171.886	338.225	−811.424	−150.161	1.352
5900	66.944	231.345	172.884	344.920	−812.106	−138.754	1.228
6000	66 944	232.470	173.868	351.614	−812.842	−127.335	1.109

PREVIOUS: CURRENT: December 1973

Tantalum Carbide (TaC) CRYSTAL–LIQUID

0 to 4273 K crystal
above 4273 K liquid

Refer to the individual tables for details

M_r = 192.9589 Tantalum Carbide (TaC) $C_1Ta_1(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	$S°$ (J·K⁻¹mol⁻¹)	$-[G°-H°(T_r)]/T$ (J·K⁻¹mol⁻¹)	$H°-H°(T_r)$ (kJ·mol⁻¹)	$\Delta_f H°$ (kJ·mol⁻¹)	$\Delta_f G°$ (kJ·mol⁻¹)	log K_f
0	0.	0.	INFINITE	-6.514	-143.879	-143.879	INFINITE
100	18.619	12.880	69.673	-5.679	-144.099	-143.677	75.049
200	29.192	29.187	45.519	-3.266	-144.264	-143.168	37.392
298.15	36.790	42.373	42.373	0.	-144.097	-142.654	24.992
300	36.903	42.601	42.374	0.068	-144.091	-142.645	24.837
400	41.664	53.915	43.884	4.012	-143.729	-142.215	18.571
500	44.530	63.537	46.877	8.330	-143.347	-141.882	14.822
600	46.447	71.833	50.361	12.883	-143.033	-141.620	12.329
700	47.890	79.104	53.959	17.602	-142.791	-141.404	10.552
800	49.074	85.578	57.514	22.451	-142.596	-141.220	9.221
900	50.116	91.419	60.962	27.411	-142.426	-141.058	8.187
1000	51.066	96.749	64.278	32.471	-142.270	-140.914	7.361
1100	51.928	101.656	67.456	37.621	-142.124	-140.786	6.685
1200	52.779	106.211	70.498	42.856	-141.987	-140.670	6.123
1300	53.616	110.469	73.411	48.176	-141.850	-140.566	5.648
1400	54 441	114.473	76.202	53.579	-141.697	-140.473	5.241
1500	55.254	118.257	78.881	59.064	-141.513	-140.392	4.889
1600	56.035	121.848	81.455	64.628	-141.291	-140.324	4.581
1700	56.813	125.268	83.932	70.271	-141.035	-140.271	4.310
1800	57.588	128.537	86.320	75.991	-140.761	-140.234	4.069
1900	58.360	131.672	88.625	81.788	-140.482	-140.213	3.855
2000	59.128	134.685	90.853	87.663	-140.200	-140.206	3.662
2100	59.890	137.588	93.010	93.614	-139.913	-140.213	3.488
2200	60.650	140.392	95.100	99.641	-139.621	-140.234	3.330
2300	61.409	143.104	97.129	105.744	-139.325	-140.269	3.186
2400	62.167	145.734	99.100	111.922	-139.030	-140.316	3.054
2500	62.923	148.287	101.016	118.177	-138.741	-140.376	2.933
2600	63.676	150.770	102.882	124.507	-138.467	-140.446	2.822
2700	64.429	153.187	104.701	130.912	-138.218	-140.527	2.719
2800	65.181	155.544	106.475	137.393	-138.006	-140.617	2.623
2900	65.933	157.844	108.207	143.948	-137.845	-140.713	2.535
3000	66.685	160.092	109.899	150.579	-137.753	-140.814	2.452
3100	67.436	162.291	111.554	157.285	-137.746	-140.916	2.374
3200	68.187	164.444	113.173	164.066	-137.846	-141.017	2.302
3300	68.938	166.553	114.759	170.923	-174.531	-140.642	2.226
3400	69.688	168.622	116.312	177.854	-174.488	-139.616	2.145
3500	70.438	170.653	117.836	184.860	-174.382	-138.592	2.068
3600	71.187	172.648	119.331	191.941	-174.213	-137.571	1.996
3700	71.935	174.609	120.799	199.098	-173.981	-136.557	1.928
3800	72.683	176.537	122.240	206.328	-173.686	-135.549	1.863
3900	73.431	178.435	123.657	213.634	-173.328	-134.550	1.802
4000	74.178	180.303	125.050	221.015	-172.905	-133.561	1.744
4100	74.925	182.144	126.420	228.470	-172.420	-132.583	1.689
4200	75.671	183.959	127.768	236.000	-171.871	-131.618	1.637
4273.000	76.216	185.267	128.739	241.544	CRYSTAL <--> LIQUID TRANSITION		
4273.000	66.944	209.746	128.739	346.144			
4300	66.944	210.168	129.249	347.951	-66.912	-131.327	1.595
4400	66.944	211.707	131.106	354.645	-67.220	-132.821	1.577
4500	66.944	213.212	132.914	361.340	-67.540	-134.309	1.559
4600	66 944	214.683	134.676	368.034	-67.870	-135.789	1.542
4700	66.944	216.123	136.393	374.729	-68.211	-137.262	1.525
4800	66.944	217.532	138.069	381.423	-68.563	-138.727	1.510
4900	66.944	218.912	139.705	388.117	-68.926	-140.185	1.494
5000	66.944	220.265	141.302	394.812	-69.300	-141.636	1.480
5100	66.944	221.591	142.864	401.506	-69.684	-143.078	1.465
5200	66.944	222.890	144.390	408.201	-70.079	-144.514	1.452
5300	66.944	224.166	145.884	414.895	-70.484	-145.941	1.438
5400	66.944	225.417	147.345	421.589	-70.900	-147.361	1.425
5500	66.944	226.645	148.775	428.284	-71.327	-148.773	1.413
5600	66.944	227.852	150.177	434.978	-71.764	-150.177	1.401
5700	66.944	229.036	151.550	441.673	-72.211	-151.574	1.389
5800	66.944	230.201	152.896	448.367	-811.424	-150.161	1.352
5900	66.944	231.345	154.216	455.061	-812.106	-138.754	1.228
6000	66.944	232.470	155.511	461.756	-812.842	-127.335	1.109

PREVIOUS: CURRENT: December 1973

Titanium Carbide (TiC) CRYSTAL $M_r = 59.891$ Titanium Carbide (TiC) $C_1Ti_1(cr)$

$\Delta_f H°(0\ K) = -182.8 \pm 4\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = 24.229 \pm 0.21\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = -184.1 \pm 4\ kJ \cdot mol^{-1}$

$T_{fus} = 3290 \pm 15\ K$ $\Delta_{fus} H° = [71.128]\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The adopted $\Delta_f H°(298.15\ K) = -44.0\ kcal \cdot mol^{-1}$ ($-184.096\ kJ \cdot mol^{-1}$) is derived from $\Delta_r H°(298.15\ K) = -275.72\ kcal \cdot mol^{-1}$ for reaction (a) determined by Humphrey[1] who burned TiC(cr) in an oxygen bomb calorimeter. The author reported that the combustion product TiO_2 was >95% rutile and <5% anatase, the heat of formation is calculated assuming the above distribution. The uncertainty adopted is due mainly to the uncertainty in TiO_2(rutile).

Using atomic absorbtion spectroscopy Vidale[2] determined that the pressure ($\log P_{Ti} = -7.269$) of Ti(g) at 1666 K was equal to the pressure of TiC(cr) at 2220 K. Using this data for reaction (b) we obtain a $\Delta_f H°(298.15\ K) = -43.02\ kcal \cdot mol^{-1}$. Lowell and Williams[3] measured the $\Delta_f H°(2028\ K) = -43.3 \pm 4\ kcal \cdot mol^{-1}$ of TiC(cr) directly using a high temperature calorimeter, which reduces to $\Delta_f H°(298.15\ K) = -37.7 \pm 4\ kcal \cdot mol^{-1}$.

Fujishiro and Gokcen[4] determined the equilibrium pressure of Ti(g) in reaction (d) in the temperature range 2383–2593 K. 3rd law analysis of the data yields a $\Delta_f H°(298.15\ K) = -31.6\ kcal \cdot mol^{-1}$. Brantley and Beckman[5] measured equilibirum pressures of CO for reaction (e) in the temperature range 1278–1428 K. 3rd law analysis of the data yields a $\Delta_f H°(298.15\ K) = -61.9\ kcal \cdot mol^{-1}$.

Heat Capacity and Entropy

Low temperature heat capacities (55–295 K) have been taken from Kelley.[6] Naylor[7] measured heat contents from 360 to 1738 K and Levinson[8] from 1274 to 2799 K. High temperature heat capacities are derived from the enthalpies by a fitting technique which constrains the curve to join smoothly with the low temperature values. Above 2799 K the heat capacity is graphically extrapolated. The entropy is based on $S°(50;0) = 0.065\ cal \cdot K^{-1} \cdot mol^{-1}$.

Fusion Data

Refer to the liquid table for details.

Source	Method	Reaction	T/K	$\Delta_r H°(298.15\ K)$, $kcal \cdot mol^{-1}$ 2nd law	3rd law	Drift $cal \cdot K^{-1} \cdot mol^{-1}$	$\Delta_f H°(298.15\ K)$ $kcal \cdot mol^{-1}$
1	Calorimetry	(a) $TiC(cr)+2O_2(g) \rightarrow CO_2(g)+TiO_2(rutile)$	298	−275.72			−44.00
2	Equilibrium	(b) $TiC(cr) \rightarrow Ti(g)+C(cr)$			156.02		−43.02
3	Calorimetry	(c) $Ti(cr)+C(cr) \rightarrow TiC(cr)$		−37.7 ± 4			−37.7
4	Equilibrium	(d) $TiC(cr) \rightarrow C(graph)+Ti(g)$	2383–2593	169.5 ± 10.3	144.6	−10.0 ± 4.1	−31.60
5	Equilibrium	(e) $TiO_2(rutile)+3C(graph) \rightarrow TiC(cr)+2CO(g)$	1278–1428	48.07 ± 1.83	111.07	46.7 ± 1.36	−61.90

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−4.607	−182.822	−182.822	INFINITE
100	7.335	2.602	46.702	−4.410	−183.245	−182.584	95.372
200	23.293	12.780	27.026	−2.849	−183.928	−181.622	47.435
298 15	33.807	24.229	24.229	0.	−184.096	−180.438	31.612
300	33.936	24.439	24.230	0.063	−184.096	−180.415	31.413
400	40.685	35.180	25.648	3.813	−183.982	−179.200	23.401
500	45.166	44.777	28.533	8.122	−183.740	−178.031	18.599
600	47.647	53.248	31.962	12.772	−183.494	−176.913	15.402
700	49.032	60.703	35.546	17.610	−183.316	−175.831	13.121
800	49.903	67.310	39.112	22.558	−183.214	−174.770	11.411
900	50.572	73.227	42.579	27.583	−183.215	−173.715	10.082
1000	51.179	78.586	45.916	32.670	−183.372	−172.653	9.018
1100	51.794	83.493	49.112	37.818	−183.732	−171.566	8.147
1200	52.446	88.027	52.169	43.030	−188.267	−170.317	7.414
1300	53.145	92.252	55.091	48.309	−188.267	−168.821	6.783
1400	53.894	96.218	57.889	53.661	−188.314	−167.324	6.243
1500	54 689	99.963	60.570	59.090	−188.410	−165.821	5.774
1600	55.530	103.519	63.144	64.600	−188.559	−164.311	5.364
1700	56.404	106.912	65.620	70.197	−188.767	−162.789	5.002
1800	57.317	110.161	68.005	75.882	−189.042	−161.254	4.679
1900	58.254	113.285	70.306	81.661	−189.390	−159.701	4.390
2000	59.220	116.298	72.531	87.534	−204.508	−157.674	4.118
2100	60.208	119.211	74.685	93.506	−205.780	−155.301	3.863
2200	61.216	122.035	76.773	99.577	−206.969	−152.869	3.630
2300	62.241	124.779	78.801	105.749	−208.073	−150.384	3.415
2400	63.283	127.450	80.773	112.025	−209.091	−147.854	3.218
2500	64.337	130.054	82.692	118.406	−210.019	−145.283	3.036
2600	65.400	132.598	84.563	124.893	−210.856	−142.677	2.866
2700	66.480	135.087	86.388	131.487	−211.600	−140.040	2.709
2800	67.563	137.524	88.171	138.189	−212.249	−137.378	2.563
2900	68.659	139.914	89.914	145.000	−212.803	−134.694	2.426
3000	69.760	142.260	91.620	151.921	−213.261	−131.992	2.298
3100	70.869	144.566	93.291	158.952	−213.621	−129.277	2.178
3200	71.982	146.833	94.929	166.095	−213.882	−126.552	2.066
3290.000	72.987	148.844	96.376	172.618	--- CRYSTAL <--> LIQUID ---		
3300	73.101	149.066	96.536	173.349	−214.044	−123.820	1.960
3400	74.224	151.264	98.113	180.715	−214.106	−121.085	1.860
3500	75.353	153.432	99.663	188.194	−214.068	−118.349	1.766
3600	76.485	155.571	101.186	195.786	−213.928	−115.616	1.678
3700	77.621	157.682	102.684	203.491	−622.785	−105.100	1.484
3800	78.760	159.767	104.159	211.310	−621.207	−91.129	1.253
3900	79.902	161.828	105.612	219.243	−619.582	−77.201	1.034
4000	81.048	163.865	107.042	227.291	−617.908	−63.315	0.827

PREVIOUS December 1964 CURRENT June 1968

Titanium Carbide (TiC) LIQUID $M_r = 59.891$

$S°(298.15\ K) = [47.401]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_f H°(298.15\ K) = [-108.334]\ kJ{\cdot}mol^{-1}$
$T_{fus} = 3290 \pm 15\ K$ $\Delta_{fus}H° = [71.128]\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

The enthalpy of formation is calculated from $\Delta_f H°(cr,\ 298.15\ K)$ by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(3290\ K)–H°(198.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

A glass transition is assumed at 2200 K below which the heat capacity is obtained from that of the crystal; above 2200 K it is assumed constant and estimated as 15 cal·K^{-1}·mol^{-1}. The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

The adopted T_{fus} is taken from the phase diagram of the system Ti–C, at the composition 50% Ti and 50% C, reported by Rudy and Harmon.[1] Earlier reports by Friederich and Sittig[2] and Agte and Moers[3] gave a T_{fus} of 3430 ± 100 K and 3410 ± 90 K, respectively. $\Delta_{fus}H°$ is derived from an estimated $\Delta_{fus}S° = 2.5$ cal·K^{-1} g·atom^{-1}, as suggested by Kubaschewski *et al.*[3]

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Titanium Carbide (TiC) $C_1Ti_1(l)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	33.807	47.401	47.401	0.	−108.334	−111.585	19.549
300	33.936	47.610	47.401	0.063	−108.334	−111.605	19.432
400	40.685	58.352	48.820	3.813	−108.221	−112.707	14.718
500	45.166	67.949	51.705	8.122	−107.978	−113.855	11.894
600	47.647	76.420	55.133	12.772	−107.732	−115.054	10.016
700	49.032	83.875	58.718	17.610	−107.555	−116.290	8.678
800	49.903	90.481	62.283	22.558	−107.452	−117.545	7.675
900	50.572	96.398	65.751	27.583	−107.454	−118.808	6.895
1000	51.179	101.758	69.088	32.670	−107.610	−120.063	6.271
1100	51.794	106.664	72.284	37.818	−107.971	−121.293	5.760
1200	52.446	111.199	75.340	43.030	−112.505	−122.361	5.326
1300	53.145	115.424	78.263	48.309	−112.506	−123.183	4.950
1400	53.894	119.389	81.060	53.661	−112.552	−124 002	4.627
1500	54.689	123.135	83.742	59.090	−112.648	−124.817	4.347
1600	55.530	126.691	86.316	64.600	−112.797	−125.624	4.101
1700	56.404	130.083	88.791	70.197	−113.006	−126.420	3.884
1800	57.317	133.333	91.176	75.882	−113.280	−127.201	3.691
1900	58.254	136.457	93.478	81.661	−113.629	−127.965	3.518
2000	59.220	139.470	95.702	87.534	−128.747	−128.256	3.350
2100	60.208	142.383	97.856	93.506	−130.018	−128.199	3.189
2200	61.216	145.207	99.945	99.577	−131.207	−128.085	3.041
2200.000	61.216	145.207	99.945	99.577	GLASS <--> LIQUID		
2200.000	62.760	145.207	99.945	99.577	TRANSITION		
2300	62.760	147.997	101.974	105.853	−132.209	−127.920	2.905
2400	62.760	150.668	103.947	112.129	−133.226	−127.712	2.780
2500	62.760	153.230	105.868	118.405	−134.259	−127.461	2.663
2600	62.760	155.691	107.737	124.681	−135.307	−127.169	2.555
2700	62.760	158.060	109.557	130.957	−136.369	−126.835	2.454
2800	62.760	160.342	111.330	137.233	−137.444	−126.463	2.359
2900	62.760	162.544	113.059	143.509	−138.534	−126.051	2.270
3000	62.760	164.672	114.744	149.785	−139.636	−125.602	2.187
3100	62.760	166.730	116.388	156.061	−140.751	−125.116	2.108
3200	62.760	168.723	117.992	162.337	−141.879	−124.594	2.034
3290.000	62.760	170.463	119.404	167.985	--- CRYSTAL <--> LIQUID ---		
3300	62.760	170.654	119.559	168.613	−143.019	−124.036	1.963
3400	62.760	172.527	121.089	174.889	−144.171	−123.443	1.896
3500	62.760	174.347	122.585	181.165	−145.336	−122.817	1.833
3600	62.760	176.115	124.048	187.441	−146.512	−122.157	1.772
3700	62.760	177.834	125.478	193.717	−556.798	−113.676	1.605
3800	62.760	179.508	126.878	199.993	−556.763	−101.700	1.398
3900	62.760	181.138	128.249	206.269	−556.795	−89.724	1.202
4000	62.760	182.727	129.591	212.545	−556.892	−77.747	1.015
4100	62.760	184.277	130.906	218.821	−557.053	−65.767	0.838
4200	62.760	185.789	132.195	225.097	−557.277	−53.781	0.669
4300	62.760	187.266	133.458	231.373	−557.560	−41.790	0.508
4400	62.760	188.709	134.698	237.649	−557.902	−29.792	0.354
4500	62.760	190.119	135.914	243.925	−558.301	−17.785	0.206

PREVIOUS: December 1964 CURRENT: June 1968

Titanium Carbide (TiC) CRYSTAL–LIQUID

0 to 3290 K crystal
above 3290 K liquid

Refer to the individual tables for details.

M_r = 59.891 Titanium Carbide (TiC) $C_1Ti_1(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = p° = 0.1 MPa

T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	Δ_fH°	Δ_fG°	log K_f
	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	−4.607	−182.822	−182.822	INFINITE
100	7.335	2.602	46.702	−4.410	−183.245	−182.584	95.372
200	14.924	12.780	27.026	−2.849	−183.928	−181.622	47.435
298.15	33.807	24.229	24.229	0.	−184.096	−180.438	31.612
300	33.936	24.439	24.230	0.063	−184.096	−180.415	31.413
400	40.685	35.180	25.648	3.813	−183.982	−179.200	23.401
500	45.166	44.777	28.533	8.122	−183.740	−178.031	18.599
600	47.647	53.248	31.962	12.772	−183.494	−176.913	15.402
700	49.032	60.703	35.546	17.610	−183.316	−175.831	13.121
800	49.903	67.310	39.112	22.558	−183.214	−174.770	11.411
900	50.572	73.227	42.579	27.583	−183.215	−173.715	10.082
1000	51.179	78.586	45.916	32.670	−183.372	−172.653	9.018
1100	51.794	83.493	49.112	37.818	−183.732	−171.566	8.147
1200	52.446	88.027	52.169	43.030	−188.267	−170.317	7.414
1300	53.145	92.252	55.091	48.309	−188.267	−168.821	6.783
1400	53.894	96.218	57.889	53.661	−188.314	−167.324	6.243
1500	54.689	99.963	60.570	59.090	−188.410	−165.821	5.774
1600	55.530	103.519	63.144	64.600	−188.559	−164.311	5.364
1700	56.404	106.912	65.620	70.197	−188.767	−162.789	5.002
1800	57.317	110.161	68.005	75.882	−189.042	−161.254	4.679
1900	58.254	113.285	70.306	81.661	−189.390	−159.701	4.390
2000	59.220	116.298	72.531	87.534	−204.508	−157.674	4.118
2100	60.208	119.211	74.685	93.506	−205.780	−155.301	3.863
2200	61.216	122.035	76.773	99.577	−206.969	−152.869	3.630
2300	62.241	124.779	78.801	105.749	−208.073	−150.384	3.415
2400	63.283	127.450	80.773	112.025	−209.091	−147.854	3.218
2500	64.337	130.054	82.692	118.406	−210.019	−145.283	3.036
2600	65.400	132.598	84.563	124.893	−210.856	−142.677	2.866
2700	66.480	135.087	86.388	131.487	−211.600	−140.040	2.709
2800	67.563	137.524	88.171	138.189	−212.249	−137.378	2.563
2900	68.659	139.914	89.914	145.000	−212.803	−134.694	2.426
3000	69.760	142.260	91.620	151.921	−213.261	−131.992	2.298
3100	70.869	144.566	93.291	158.952	−213.621	−129.277	2.178
3200	71.982	146.833	94.929	166.095	−213.882	−126.552	2.066
3290.000	72.987	148.844	96.376	172.618	CRYSTAL <−−> LIQUID TRANSITION		
3290.000	62.760	170.463	96.376	243.746			
3300	62.760	170.654	96.601	244.374	−143.019	−124.036	1.963
3400	62.760	172.527	98.807	250.650	−144.171	−123.443	1.896
3500	62.760	174.347	100.939	256.926	−145.336	−122.817	1.833
3600	62.760	176.115	103.003	263.202	−146.512	−122.157	1.772
3700	62.760	177.834	105.002	269.478	−556.798	−113.676	1.605
3800	62.760	179.508	106.941	275.754	−556.763	−101.700	1.398
3900	62.760	181.138	108.823	282.030	−556.795	−89.724	1.202
4000	62.760	182.727	110.650	288.306	−556.892	−77.747	1.015
4100	62.760	184.277	112.427	294.582	−557.053	−65.767	0.838
4200	62.760	185.789	114.156	300.858	−557.277	−53.781	0.669
4300	62.760	187.266	115.839	307.134	−557.560	−41.790	0.508
4400	62.760	188.709	117.479	313.410	−557.902	−29.792	0.354
4500	62.760	190.119	119.078	319.686	−558.301	−17.785	0.206

PREVIOUS: CURRENT: June 1968

Zirconium Carbide (ZrC) CRYSTAL $M_r = 103.231$

$S°(298.15 \text{ K}) = 33.321 \text{ J·K}^{-1}\text{·mol}^{-1}$
$T_{fus} = 3805 \pm 125 \text{ K}$

$\Delta_f H°(0 \text{ K}) = -196.0 \text{ kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = -196.6 \pm 13 \text{ kJ·mol}^{-1}$
$\Delta_{fus} H° = [79.496] \text{ kJ·mol}^{-1}$

Enthalpy of Formation

$\Delta_f H°(298.15 \text{ K}) = -47.16 \pm 1.5 \text{ kcal·mol}^{-1}$ was calculated from the standard Gibbs energy of formation of $-38.9 \pm 1.5 \text{ kcal·mol}^{-1}$ at 2675 K reported by Pollock.[1] Using spectrophotometric data reported by Vidale,[2] we calculated $\Delta_f H°(298.15 \text{ K}) = -46.9 \pm 1 \text{ kcal·mol}^{-1}$. These values were averaged with $\Delta_f H°(298.15 \text{ K}) = 47 0 \pm 0.6 \text{ kcal·mol}^{-1}$ reported by Mah.[3] The equilibria data reported by Prescott[4] and Kutsev *et al.*[5] were considered but not used.

Heat Capacity and Entropy

Enthalpy data over the range 470.8 to 1174.4 K were taken from a preliminary report by Mezaki *et al*[6] These data were smoothed by means of the Shomate plot into low temperature data reported by Westrum and Feick[7] High temperature data reported by Neel *et al.*[8] and McDonald *et al.*[9] were then used to obtain the heat capacity above 1174 K.

Fusion Data

Melting points were measured by Agte and Alterthum[10] and Fredrich and Sittig.[11] The value of 3805 ± 125 K by Agte and Alterthum was chosen. Frederich and Sittig[11] obtained a measurement of 3300 K but estimated 3500 K because of the clouding formation of ZrO_2. Worrell[12] quoted a value of 3480°C taken from Storms.[13] The enthalpy of melting is derived from an estimated $\Delta_{fus}S° = 2.5 \text{ cal·K}^{-1} \text{ g·atom}^{-1}$.

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Zirconium Carbide (ZrC) $C_1Zr_1(cr)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−5.862	−195.961	−195 961	INFINITE
100	12 782	5.832	60.224	−5.439	−196 485	−195.567	102.154
200	28.706	19.970	36.518	−3.310	−196.875	−194.442	50 783
298.15	37 899	33.321	33.321	0.	−196.648	−193.282	33.862
300	37.656	33.555	33.322	0 070	−196.641	−193.262	33.650
400	43.593	45.309	34.885	4.170	−196.123	−192.208	25.100
500	47.133	55.452	38 009	8 721	−195.523	−191.299	19.985
600	49.380	64.257	41 666	13.554	−194.959	−190.508	16.585
700	50.965	72.009	45 459	18.585	−194.468	−189.806	14.164
800	52.070	78.890	49.216	23.740	−194.084	−189 168	12.351
900	52.836	85.070	52.862	28.987	−193.819	−188.570	10 944
1000	53.388	90.662	56.367	34.296	−193.689	−187 995	9.820
1100	54.229	95 794	59.721	39.680	−193.670	−187.428	8.900
1200	54.580	100.528	62.927	45.121	−197.482	−186.635	8.124
1300	54.932	104.910	65.990	50.596	−197.174	−185.744	7.463
1400	55.283	108.994	68.917	56.107	−196.914	−184.875	6.898
1500	55.635	112.820	71.718	61.653	−196.706	−184.023	6.408
1600	55.986	116.422	74 401	67.234	−196.556	−183.182	5.980
1700	56.338	119.827	76 974	72.850	−196.473	−182.349	5.603
1800	56.689	123.057	79.445	78.502	−196.464	−181.519	5.268
1900	57.040	126.131	81.822	84.188	−196.538	−180.687	4.967
2000	57.392	129.066	84.111	89.910	−196.702	−179.849	4.697
2100	57.743	131.875	86.319	95.667	−196.968	−179 001	4.452
2200	58.095	134.569	88.451	101.458	−218.665	−177.391	4.212
2300	58.446	137.159	90.513	107.285	−219.576	−175.494	3.986
2400	58.798	139.654	92.509	113.148	−220 468	−173.559	3.777
2500	59.149	142.061	94.443	119.045	−221.339	−171.586	3.585
2600	59.501	144.388	96.320	124.978	−222.191	−169.579	3.407
2700	59.852	146.640	98.142	130.945	−223.021	−167.540	3.241
2800	60.204	148.823	99.913	136.948	−223.830	−165.470	3.087
2900	60.555	150.942	101.637	142.986	−224 618	−163.372	2.943
3000	60.906	153.001	103.315	149.059	−225.384	−161.247	2.808
3100	61.258	155.004	104.950	155.167	−226.127	−159.097	2.681
3200	61.609	156.954	106.545	161.311	−226.848	−156.923	2.562
3300	61.961	158.855	108.101	167 489	−227.546	−154.727	2.449
3400	62.312	160.710	109.621	173.703	−228.220	−152.510	2.343
3500	62.664	162.522	111.107	179.952	−228.872	−150.274	2.243
3600	63.015	164.292	112.560	186.235	−229.501	−148.019	2.148
3700	63.367	166.023	113.981	192.555	−230.106	−145.747	2.058
3800	63.718	167.718	115.373	198.909	−230.687	−143.459	1.972
3805.000	63.736	167.802	115.442	199.227	--- CRYSTAL <--> LIQUID ---		
3900	64.070	169.377	116.737	205.298	−231.245	−141.157	1.891
4000	64.421	171.004	118.073	211.723	−231.779	−138.840	1.813
4100	64.772	172.599	119.384	218.182	−232.289	−136.510	1.739
4200	65.124	174.164	120.669	224.677	−232.775	−134.168	1.669
4300	65.475	175.701	121.931	231.207	−233.237	−131.815	1.601
4400	65.827	177.210	123.171	237.772	−233.674	−129.451	1.537
4500	66.178	178.693	124.388	244.373	−234.088	−127.078	1.475
4600	66.530	180.151	125.584	251.008	−234.477	−124 695	1.416
4700	66.881	181.586	126.761	257.679	−234.843	−122.305	1.359
4800	67.233	182.998	127.918	264.384	−796.120	−108.289	1.178
4900	67.584	184.388	129.056	271.125	−796.088	−93.960	1.002
5000	67.936	185.757	130.176	277.901	−796.049	−79.631	0.832

PREVIOUS: June 1964 CURRENT: December 1964

Zirconium Carbide (ZrC) LIQUID $M_r = 103.231$ Zirconium Carbide (ZrC) $C_1Zr_1(l)$

$S°(298.15\ K) = [53.577]\ J\cdot K^{-1}\cdot mol^{-1}$

$\Delta_f H°(298.15\ K) = [-118.877]\ kJ\cdot mol^{-1}$

$T_{fus} = 3805 \pm 125\ K$

$\Delta_{fus} H° = [79.496]\ kJ\cdot mol^{-1}$

Enthalpy of Formation

$\Delta_f H°$(ZrC, l, 298.15 K) is calculated from $\Delta_f H°$(ZrC, cr, 298.15 K) by adding $\Delta_{fus} H°$ and the difference in enthalpy, $H°(3805\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

$C_p°$(l) at and below 2500 K is assumed to be equal to that of ZrC(cr). Above 2500 K the heat capacity is estimated to be constant. $S°$(l, 298.15 K) is calculated in a manner similar to that used for the enthalpy of formation.

Fusion Data

Refer to the crystal table for details.

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	$J\cdot K^{-1}mol^{-1}$			$kJ\cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	37.899	53.577	53.577	0.	−118.877	−121.550	21.295
300	38.030	53.811	53.577	0.070	−118.869	−121.567	21.167
400	43.593	65.581	55.144	4.175	−118.347	−122.541	16.002
500	47.133	75.723	58.270	8.727	−117.746	−123.658	12.918
600	49.380	84.529	61.930	13.560	−117.183	−124.895	10.873
700	50.965	92.281	65.723	18.590	−116.692	−126.220	9.419
800	52.070	99.162	69.481	23.745	−116.308	−127.609	8.332
900	52.836	105.341	73.128	28.992	−116.043	−129.039	7.489
1000	53.388	110.934	76.633	34.301	−115.913	−130.491	6.816
1100	54.229	116.066	79.988	39.686	−115.893	−131.950	6.266
1200	54.580	120.799	83.194	45.126	−119.706	−133.185	5.797
1300	54.932	125.182	86.258	50.602	−119.398	−134.321	5.397
1400	55.283	129.266	89.186	56.112	−119.138	−135.479	5.055
1500	55.635	133.092	91.986	61.658	−118.929	−136.654	4.759
1600	55.986	136.694	94.669	67.239	−118.780	−137.841	4.500
1700	56.338	140.098	97.242	72.855	−118.697	−139.035	4.272
1800	56.689	143.329	99.714	78.507	−118.688	−140.232	4.069
1900	57.040	146.403	102.091	84.193	−118.761	−141.427	3.888
2000	57.392	149.338	104.380	89.915	−118.926	−142.617	3.725
2100	57.743	152.146	106.588	95.672	−119.191	−143.795	3.577
2200	58.095	154.841	108.721	101.464	−140.889	−144.213	3.424
2300	58.446	157.431	110.783	107.291	−141.800	−144.343	3.278
2400	58.798	159.926	112.779	113.153	−142.691	−144.435	3.144
2500	59.149	162.333	114.713	119.050	−143.563	−144.489	3.019
2500.000	59.149	162.333	114.713	119.051	GLASS <−−> LIQUID TRANSITION		
2500.000	62.760	162.333	114.713	119.051			
2600	62.760	164.795	116.592	125.327	−144.071	−144.516	2.903
2700	62.760	167.163	118.422	131.603	−144.593	−144.524	2.796
2800	62.760	169.446	120.203	137.879	−145.129	−144.511	2.696
2900	62.760	171.648	121.940	144.155	−145.678	−144.480	2.602
3000	62.760	173.776	123.632	150.431	−146.241	−144.429	2.515
3100	62.760	175.834	125.283	156.707	−146.816	−144.359	2.432
3200	62.760	177.826	126.894	162.983	−147.405	−144.270	2.355
3300	62.760	179.757	128.467	169.259	−148.005	−144.163	2.282
3400	62.760	181.631	130.003	175.535	−148.618	−144.037	2.213
3500	62.760	183.450	131.504	181.811	−149.242	−143.894	2.147
3600	62.760	185.218	132.972	188.087	−149.878	−143.732	2.085
3700	62.760	186.938	134.407	194.363	−150.527	−143.552	2.027
3800	62.760	188.612	135.812	200.639	−151.186	−143.355	1.971
3805.000	62.760	188.694	135.881	200.952	−−− CRYSTAL <−−> LIQUID −−−		
3900	62.760	190.242	137.187	206.915	−151.857	−143.140	1.917
4000	62.760	191.831	138.533	213.191	−152.540	−142.908	1.866
4100	62.760	193.380	139.852	219.467	−153.233	−142.659	1.817
4200	62.760	194.893	141.145	225.743	−153.938	−142.392	1.771
4300	62.760	196.370	142.412	232.019	−154.654	−142.109	1.726
4400	62.760	197.812	143.654	238.295	−155.381	−141.809	1.683
4500	62.760	199.223	144.874	244.571	−156.119	−141.492	1.642
4600	62.760	200.602	146.070	250.847	−156.868	−141.159	1.603
4700	62.760	201.952	147.245	257.123	−157.627	−140.809	1.565
4800	62.760	203.273	148.398	263.399	−719.334	−128.826	1.402
4900	62.760	204.567	149.532	269.675	−719.767	−116.519	1.242
5000	62.760	205.835	150.645	275.951	−720.228	−104.203	1.089
5100	62.760	207.078	151.739	282.227	−720.715	−91.878	0.941
5200	62.760	208.297	152.815	288.503	−721.227	−79.543	0.799
5300	62.760	209.492	153.874	294.779	−721.762	−67.198	0.662
5400	62.760	210.665	154.914	301.055	−722.320	−54.842	0.530
5500	62.760	211.817	155.939	307.331	−722.899	−42.476	0.403
5600	62.760	212.948	156.946	313.607	−723.497	−30.100	0.281
5700	62.760	214.058	157.939	319.883	−724.113	−17.712	0.162
5800	62.760	215.150	158.916	326.159	−724.746	−5.314	0.048
5900	62.760	216.223	159.878	332.435	−725.396	7.096	−0.063
6000	62.760	217.278	160.826	338.711	−726.059	19.517	−0.170

PREVIOUS June 1964 CURRENT December 1964

Zirconium Carbide (ZrC)

CRYSTAL–LIQUID

0	to	3805	K	crystal
above		3805	K	liquid

Refer to the indivicual tables for details.

M_r = 103.231 **Zirconium Carbide (ZrC)** **C_1Zr_1(cr,l)**

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	$J\cdot K^{-1}mol^{-1}$			$kJ\cdot mol^{-1}$			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−5.862	−195.961	−195.961	INFINITE
100	12.782	5.832	60.224	−5.439	−196.485	−195.567	102.154
200	28.706	19.970	36.518	−3.310	−196.875	−194.442	50.783
298.15	37.899	33.321	33.321	0.	−196.648	−193.282	33.862
300	37.656	33.555	33.322	0.070	−196.641	−193.262	33.650
400	43.593	45.309	34.885	4.170	−196.123	−192.208	25.100
500	47.133	55.452	38.009	8.721	−195.523	−191.299	19.985
600	49.380	64.257	41.666	13.554	−194.959	−190.508	16.585
700	50.965	72.009	45.459	18.585	−194.468	−189.806	14.164
800	52.070	78.890	49.216	23.740	−194.084	−189.168	12.351
900	52.836	85.070	52.862	28.987	−193.819	−188.570	10.944
1000	53.388	90.662	56.367	34.296	−193.689	−187.995	9.820
1100	54.229	95.794	59.721	39.680	−193.670	−187.428	8.900
1200	54.580	100.528	62.927	45.121	−197.482	−186.635	8.124
1300	54.932	104.910	65.990	50.596	−197.174	−185.744	7.463
1400	55.283	108.994	68.917	56.107	−196.914	−184.875	6.898
1500	55.635	112.820	71.718	61.653	−196.706	−184.023	6.408
1600	55.986	116.422	74.401	67.234	−196.556	−183.182	5.980
1700	56.338	119.827	76.974	72.850	−196.473	−182.349	5.603
1800	56.689	123.057	79.445	78.502	−196.464	−181.519	5.268
1900	57.040	126.131	81.822	84.188	−196.538	−180.687	4.967
2000	57.392	129.066	84.111	89.910	−196.702	−179.849	4.697
2100	57.743	131.875	86.319	95.667	−196.968	−179.001	4.452
2200	58.095	134.569	88.451	101.458	−218.665	−177.391	4.212
2300	58.446	137.159	90.513	107.285	−219.576	−175.494	3.986
2400	58.798	139.654	92.509	113.148	−220.468	−173.559	3.777
2500	59.149	142.061	94.443	119.045	−221.339	−171.586	3.585
2600	59.501	144.388	96.320	124.978	−222.191	−169.579	3.407
2700	59.852	146.640	98.142	130.945	−223.021	−167.540	3.241
2800	60.204	148.823	99.913	136.948	−223.830	−165.470	3.087
2900	60.555	150.942	101.637	142.986	−224.618	−163.372	2.943
3000	60.906	153.001	103.315	149.059	−225.384	−161.247	2.808
3100	61.258	155.004	104.950	155.167	−226.127	−159.097	2.681
3200	61.609	156.954	106.545	161.311	−226.848	−156.923	2.562
3300	61.961	158.855	108.101	167.489	−227.546	−154.727	2.449
3400	62.312	160.710	109.621	173.703	−228.220	−152.510	2.343
3500	62.664	162.522	111.107	179.952	−228.872	−150.274	2.243
3600	63.015	164.292	112.560	186.235	−229.501	−148.019	2.148
3700	63.367	166.023	113.981	192.555	−230.106	−145.747	2.058
3800	63.718	167.718	115.373	198.909	−230.687	−143.459	1.972
3805.000	63.736	167.802	115.442	199.227	CRYSTAL <--> LIQUID TRANSITION		
3805.000	62.760	188.694	115.442	278.723			
3900	62.760	190.242	117.245	284.686	−151.857	−143.140	1.917
4000	62.760	191.831	119.090	290.962	−152.540	−142.908	1.866
4100	62.760	193.380	120.883	297.238	−153.233	−142.659	1.817
4200	62.760	194.893	122.628	303.514	−153.938	−142.392	1.771
4300	62.760	196.370	124.325	309.790	−154.654	−142.109	1.726
4400	62.760	197.812	125.979	316.066	−155.381	−141.809	1.683
4500	62.760	199.223	127.591	322.342	−156.119	−141.492	1.642
4600	62.760	200.602	129.164	328.618	−156.868	−141.159	1.603
4700	62.760	201.952	130.698	334.894	−157.627	−140.809	1.565
4800	62.760	203.273	132.196	341.170	−719.334	−128.826	1.402
4900	62.760	204.567	133.660	347.446	−719.767	−116.519	1.242
5000	62.760	205.835	135.091	353.722	−720.228	−104.203	1.089
5100	62.760	207.078	136.490	359.998	−720.715	−91.878	0.941
5200	62.760	208.297	137.859	366.274	−721.227	−79.543	0.799
5300	62.760	209.492	139.200	372.550	−721.762	−67.198	0.662
5400	62.760	210.665	140.512	378.826	−722.320	−54.842	0.530
5500	62.760	211.817	141.798	385.102	−722.899	−42.476	0.403
5600	62.760	212.948	143.059	391.378	−723.497	−30.100	0.281
5700	62.760	214.058	144.295	397.654	−724.113	−17.712	0.162
5800	62.760	215.150	145.507	403.930	−724.746	−5.314	0.048
5900	62.760	216.223	146.696	410.206	−725.396	7.096	−0.063
6000	62.760	217.278	147.864	416.482	−726.059	19.517	−0.170

PREVIOUS: CURRENT: December 1964

Zirconium Carbide (ZrC) **C_1Zr_1(cr,l)**

$S°(298.15\ K) = 199.38 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 829.3 \pm 3.8\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 837.7 \pm 3.8\ kJ{\cdot}mol^{-1}$

Electronic Levels and Molecular Constants ($\sigma = 2$)

State	ϵ_i, cm^{-1}	g_i	r_e Å	B_e, cm^{-1}	α_e, cm^{-1}	ω_e, cm^{-1}	$\omega_e x_e$, cm^{-1}
$x^1\Sigma_g^+$	0	1	1.2425	1.81984	0.01765	1854.71	13.34
$X'^3\Pi_u$	610	6	1.3119	1.63246	0.01661	1641.35	11.67
$A'^3\Sigma_g^-$	6243.5	3	1.3693	1.49852	0.01634	1470.45	11.19
$b^1\Pi_u$	8268.33	2	1.3184	1.61634	0.01686	1608.35	12.078
$A''^3\Sigma_u^+$	13365	3	1.23	1.87	[0.018]	1961.6	13.65
$^1\Sigma_g^+$	[18570]	1	[1.38]	[1.475]	[0.013]	[1510]	[10.0]
$A^3\Pi_g$	19916	6	1.266	1.7527	0.01608	1788.2	16.44
$^5\Pi_g$	[22260]	10	[1.46]	[1.324]	[0.012]	[1400]	[9.9]
$^5\Sigma_g^+$	[30320]	5	[1.35]	[1.557]	[0.015]	[1550]	[11.7]
$c^1\Pi_g$	34262	2	1.2552	1.7334	0.018	1809.1	15.81
$^3\Delta_u$	[34530]	6	[1.51]	[1.23]	[0.013]	[1160]	[9.2]
$^1\Sigma_u^-$	[34760]	1	[1.90]	[0.778]	[0.005]	[1025]	[5.8]
$^3\phi_g$	[38020]	6	[1.53]	[1.20]	[0.011]	[1290]	[9.0]
$B^3\Pi_g$	40690	6	1.535	1.1922	0.0242	1106.56	39.26
$^3\Delta_u$	[40780]	6	[1.51]	[1.23]	[0.011]	[1380]	[9.2]
$^3\Pi_g$	[42370]	6	[1.49]	[1.265]	[0.012	[1340]	[9.5]
$^1\phi_g$	[42860]	2	[1.51]	[1.232]	[0.011]	[1360]	[9.2]
$d^1\Sigma_u^+$	43240	1	1.2378	1.8334	0.0204	1829.57	13.97
$^3\Sigma^+_u$	[43360]	3	[1.44]	[1.355]	[0.011]	[1660]	[10.21]

Enthalpy of Formation

Messerle and Krauss[1] have reported the dissociation energy as 49300 ± 300 cm^{-1} from the variation of the rotational structure cut–off with vibrational level in the $c^1\Pi_g$ state. This state dissociates into $C(^3P) + C^3(P)$, due to an avoided crossing,[2] these dissociation products are those of the ground state. The uncertainty in the determination is generous and thus we adopt $D_0^\circ = 140.95 \pm 0.9$ kcal or $\Delta_f H°(C_2,\ g,\ 0\ K) = 198.2 \pm 0.9\ kcal{\cdot}mol^{-1}$, using $\Delta_f H°(C,\ g,\ 0\ K) = 169.576\ kcal{\cdot}mol^{-1}$.[3]

Brewer *et al.*[4] have reviewed several other earlier determinations which confirm $\Delta_f H°(0\ K) = 195 \pm 5\ kcal{\cdot}mol^{-1}$. The extensive mass spectrometric data of Drowart *et al.*[5] yield a 3rd law $\Delta_f H°(0\ K) = 199.2 \pm 1.4\ kcal{\cdot}mol^{-1}$ in excellent agreement with the adopted value.

Heat Capacity and Entropy

The observed molecular constants and electronic levels were taken from Ballik and Ramsay.[2] The estimated parameters are from the correlation calculations of Fougere and Nesbet[6] and Clementi,[7] the electronic levels are T_o values Not all predicted states were included since the contribution of levels above 40000 cm^{-1} is neligible. The functions were calculated from the partition function $Q = Q_t \Sigma Q_v^i Q_r^i g_i \exp(-c_2\epsilon_i/T)$, the values for Q_v^i and Q_r^i were calculated with first order anharmonic corrections. The functions are similar to those reported by Altman[8] and Clementi[7] but include several additional states.

References

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[2] E. A. Ballik and D. A. Ramsay, Astrophys. Journ. **137**, 84 (1963).

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[4] L. Brewer, W. T Hicks, and O. H Krikorian, J Chem. Phys. **36**, 182 (1962).

[5] J. Drowart, R. P. Burns, G. DeMaria and M. G. Inghram, J. Chem. Phys. **31**, 1131 (1959).

[6] P. F Fougere and R. K. Nesbet, J. Chem Phys. **44**, 285 (1966).

[7] E. Clementi, Astrophys. Journ. **133**, 303 (1961).

[8] R. Altman, J. Chem. Phys. **32**, 615 (1960).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	$\Delta_f G°$ (kJ·mol^{-1})	log K_f
0	0.	0.	INFINITE	−10.578	829.262	829.262	INFINITE
100	29.765	158.761	235.431	−7.667	832.053	816.367	−426.427
200	40.456	182.316	203.335	−4.204	834.863	799.633	−208.843
250	43.379	191.730	200.097	−2.092	836.384	790.649	−165.197
298.15	43.145	199.382	199.382	0.	837.737	781.714	−136.953
300	43.100	199.649	199.383	0.080	837.785	781.367	−136.048
350	41.443	206.176	199.902	2.196	838.960	771.867	−115.195
400	39.650	211.590	201.035	4.222	839.882	762.217	−99.535
450	38.191	216.172	202.469	6.166	840.570	752.465	−87.344
500	37.141	220.138	204.042	8.048	841.055	742.648	−77.584
600	36.000	226.793	207.299	11.696	841.547	722.911	−62.935
700	35.622	232.307	210.488	15.273	841.578	703.131	−52.468
800	35.603	237.060	213.520	18.833	841.295	683.369	−44.619
900	35.746	241.261	216.373	22.399	840.793	663.656	−38.518
1000	35.963	245.038	219.054	25.984	840.132	644.008	−33.640
1100	36.212	248.477	221.575	29.593	839.353	624.433	−29.652
1200	36.479	251.639	223.950	33.227	838.484	604.932	−26.332
1300	36.756	254.570	226.194	36.889	837.548	585.507	−23.526
1400	37.038	257.304	228.320	40.579	836.559	566.156	−21.124
1500	37.324	259.869	230.338	44.297	835.528	546.878	−19.044
1600	37.610	262.287	232.260	48.043	834.465	527.669	−17.227
1700	37.896	264.576	234.094	51.819	833.375	508.527	−15.625
1800	38.179	266.750	235.849	55.622	832.266	489.450	−14.203
1900	38.457	268.822	237.530	59.454	831.140	470.436	−12.933
2000	38.729	270.801	239.145	63.314	830.000	451.481	−11.791
2100	38.994	272.697	240.697	67.200	828.849	432.583	−10.760
2200	39.251	274.517	242.194	71.112	827.688	413 741	−9.823
2300	39.500	276.268	243.637	75.050	826.518	394.951	−8.970
2400	39.740	277.954	245.032	79.012	825.341	376.212	−8.188
2500	39.972	279.581	246.382	82.997	824.156	357.523	−7.470
2600	40.197	281.153	247.689	87.006	822.965	338.881	−6.808
2700	40.414	282.674	248.957	91.037	821.767	320.285	−6.196
2800	40.624	284.148	250.188	95.088	820.563	301.734	−5.629
2900	40.827	285.577	251.383	99.161	819.353	283.226	−5.101
3000	41.026	286.964	252.546	103.254	818.136	264.759	−4.610
3100	41.219	288.313	253.678	107.366	816.914	246.333	−4.151
3200	41.409	289.624	254.781	111.498	815.685	227.947	−3.721
3300	41.595	290.901	255.857	115.648	814.450	209.599	−3.318
3400	41.778	292.146	256.906	119.816	813.210	191.289	−2.939
3500	41.960	293.360	257.930	124.003	811.963	173.016	−2.582
3600	42.140	294.544	258.931	128.208	810.712	154.778	−2.246
3700	42.318	295.701	259.909	132.431	809.454	136.574	−1.928
3800	42.496	296.832	260.866	136.672	808.192	118.405	−1.628
3900	42.674	297.938	261.802	140.931	806.924	100.270	−1.343
4000	42.852	299.021	262.719	145.207	805.652	82.166	−1.073
4100	43.030	300.081	263.618	149.501	804.375	64.095	−0.817
4200	43.209	301.120	264.498	153.813	803.093	46.055	−0.573
4300	43.388	302.139	265.362	158.143	801.807	28.046	−0.341
4400	43.568	303.139	266.209	162.490	800.517	10.066	−0.119
4500	43.749	304.120	267.041	166.856	799.223	−7.884	0.092
4600	43.932	305.083	267.857	171.240	797.925	−25.806	0.293
4700	44.115	306.030	268.659	175.643	796.624	−43.699	0.486
4800	44.299	306.961	269.448	180.063	795.320	−61.564	0.670
4900	44.485	307.876	270.222	184.503	794.013	−79.402	0.846
5000	44.671	308.777	270.985	188.960	792.703	−97.214	1.016
5100	44.859	309.663	271.734	193.437	791.390	−114.999	1.178
5200	45.047	310.536	272.472	197.932	790.075	−132.759	1.334
5300	45.237	311.396	273.198	202.446	788.757	−150.493	1.483
5400	45.427	312.243	273.914	206.980	787.438	−168.202	1.627
5500	45.619	313.079	274.618	211.532	786.116	−185.887	1.765
5600	45.811	313.902	275.312	216.103	784.792	−203.548	1.899
5700	46.004	314 715	275.997	220.694	783.467	−221.185	2.027
5800	46.197	315.517	276.671	225.304	782.140	−238.799	2.151
5900	46.391	316.308	277.336	229.933	780.812	−256.390	2.270
6000	46.586	317.089	277.992	234.582	779.482	−273.959	2.385

PREVIOUS December 1969 (1 atm) CURRENT: December 1969 (1 bar)

$S°(298.15\ K) = 196.60 \pm 0.21\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 443 \pm 84\ kJ{\cdot}mol^{-1}$

$\Delta_f H°(298.15\ K) = 444 \pm 84\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights ϵ_i, cm^{-1}	g_i
0	2
[9000]	[4]
18484	[2]

$\omega_e = 1781.04\ cm^{-1}$ $\omega_e x_e = 11.585\ cm^{-1}$ $\sigma = 2$

$B_e = 1.74685\ cm^{-1}$ $\alpha_e = 0.0167\ cm^{-1}$ $r_e = 1.2682$ Å

Enthalpy of Formation

The electron affinity of C_2 has been obtained by Honig[1] as 4 ± 0.8 eV from the difference in enthalpies of sublimation of neutral C_2 and C_2^- and the work function of graphite. Thus, we have the reaction

$$C_2(g) + e^- \rightarrow C_2^-\ (g) \qquad \Delta H(0\ K) = -92.2 \pm 20\ kcal{\cdot}mol^{-1}.$$

Using $\Delta_f H°(C_2, g, 0\ K) = 198.2\ kcal{\cdot}mol^{-1}$,[2] we obtain $\Delta_f H°(C_2^-, g, 0\ K) = 106 \pm 20\ kcal{\cdot}mol^{-1}$, which is adopted.

A value for the enthalpy of formation may be obtained from a linear Birge–Sponer extrapolation of the ground state vibrational levels, which gives 195.8 kcal for the reaction.

$$C_2^-(g) \rightarrow C(g) + C^-(g).$$

With auxiliary data[2] this yields $\Delta_f H°(C_2^-, g, 0\ K) = 114.5\ kcal{\cdot}mol^{-1}$, in good agreement with the adopted value.

Heat Capacity and Entropy

The molecular constants and electronic levels are from Herzberg and Lagerqvist.[3] The values are not definitely ascribed to C_2^- by Herzberg and Lagerqvist, but there is a good deal of evidence to support this assignment. Recently Milligan and Jacox[4] have shown that matrix isolated bands previously attributed to $C_2(g)$ are enhanced in the presence of a photoelectron source. The matrix spectra correspond to the gas system reported by Harzberg and Lagerqvist[3] and leave little doubt that the species is C_2^-.

The estimated electronic level is assumed to be a $^2\Pi$ state and is obtained from the isoelectronic CN(g).[2]

References

[1] R. E. Honig, J. Chem. Phys. **22**, 126 (1954).

[2] JANAF Thermochemical Tables: $C_2(g)$, 12–31–69.

[3] G. Herzberg and A. Lagerqvist, Can. J. Phys. **42**, 2363 (1968).

[4] D. E. Milligan and M. E. Jacox, J. Chem. Phys. **51**, 1952 (1969).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−8.676	443.127		
100	29.106	164.780	222.507	−5.773			
200	29.115	184.957	199.266	−2.862			
250	29.148	191.457	197.078	−1.405			
298.15	29.241	196.597	196.597	0.	443.504	394.566	−69.126
300	29.246	196.778	196.598	0.054	443.488	394.263	−68.647
350	29.438	201.300	196.955	1.521	442.974	386.097	−57.622
400	29.726	205.248	197.750	2.999	442.309	378.015	−49.364
450	30.092	208.770	198.782	4.495	441.509	370.025	−42.951
500	30.511	211.962	199.943	6.010	440.588	362.131	−37.832
600	31.407	217.604	202.428	9.105	438.448	346.635	−30.177
700	32.272	222.511	204.954	12.290	436.008	331.522	−24.738
800	33.042	226.872	207.426	15.556	433.354	316.774	−20.683
900	33.703	230.803	209.809	18.895	430.545	302.369	−17.549
1000	34.263	234.383	212.090	22.294	427.619	288.283	−15.058
1100	34.741	237.672	214.268	25.744	424.604	274.495	−13.035
1200	35.154	240.713	216.347	29.240	421.518	260.985	−11.360
1300	35.522	243.541	218.331	32.774	418.375	247.734	−9.954
1400	35.861	246.186	220.227	36.343	415.187	234.727	−8.758
1500	36.185	248.672	222.041	39.945	411.962	221.950	−7.729
1600	36.503	251.017	223 780	43.580	408.707	209 388	−6.836
1700	36.824	253.240	225.448	47.246	405.431	197.031	−6 054
1800	37.152	255.354	227.051	50.945	402.137	184.867	−5.365
1900	37.490	257.372	228.594	54.677	398.833	172.886	−4.753
2000	37.840	259.303	230.082	58.443	395.522	161.080	−4.207
2100	38.199	261.158	231.518	62.245	392.208	149.440	−3.717
2200	38.568	262.944	232.906	66.083	388.894	137.957	−3.276
2300	38.943	264.666	234.249	69.959	385.584	126.625	−2.876
2400	39.323	266.332	235.552	73.872	382.279	115.437	−2.512
2500	39.704	267.945	236.815	77.823	378.982	104.386	−2.181
2600	40.083	269.509	238.043	81.813	375.692	93.467	−1.878
2700	40.459	271.029	239.237	85.840	372.413	82.675	−1.599
2800	40.828	272.507	240.399	89.904	369.142	72.003	−1.343
2900	41.189	273.946	241.531	94.005	365.882	61.449	−1 107
3000	41.539	275.349	242.635	98.142	362.630	51.007	−0.888
3100	41.876	276.716	243.712	102.313	359.388	40.673	−0.685
3200	42.200	278.051	244.764	106.517	356.153	30 443	−0.497
3300	42.510	279.354	245.793	110.752	352.925	20.315	−0.322
3400	42.803	280.628	246.799	115.018	349.703	10.284	−0.158
3500	43.081	281.872	247.783	119.312	346.486	0.348	−0.005
3600	43.342	283.090	248.747	123.634	343.272	−9.496	0.138
3700	43.587	284.281	249.691	127.980	340.059	−19.251	0.272
3800	43.815	285.446	250.617	132.351	336.848	−28.919	0.398
3900	44.027	286.587	251.525	136.743	333.635	−38.503	0.516
4000	44.223	287.704	252.415	141.155	330.420	−48 004	0.627
4100	44.403	288.798	253.289	145.587	327.202	−57.425	0.732
4200	44.567	289.870	254.148	150.036	323.978	−66.767	0.830
4300	44.717	290.921	254.991	154.500	320.748	−76.032	0.924
4400	44.853	291.951	255.819	158.979	317.510	−85.222	1.012
4500	44.976	292.960	256.633	163.470	314.263	−94.339	1.095
4600	45.085	293.950	257.434	167.973	311.006	−103.383	1.174
4700	45.182	294.920	258.221	172.487	307.738	−112.356	1.249
4800	45.268	295.873	258.996	177.009	304.457	−121.260	1.320
4900	45.343	296.807	259.758	181.540	301.163	−130.095	1.387
5000	45.407	297.723	260.508	186.077	297.854	−138.862	1.451
5100	45.462	298.623	261.246	190.621	294.529	−147.564	1.511
5200	45.507	299.506	261.974	195.169	291.189	−156.200	1.569
5300	45.545	300.374	262.690	199.722	287.831	−164.771	1.624
5400	45.574	301.225	263.396	204.278	284.456	−173.279	1.676
5500	45.596	302.062	264.091	208.837	281.062	−181.725	1.726
5600	45.611	302.883	264.777	213.397	277.649	−190.108	1.773
5700	45.620	303.691	265.452	217.959	274.216	−198.431	1.818
5800	45.624	304.484	266.118	222.521	270.762	−206.693	1.861
5900	45.622	305.264	266.775	227.083	267.288	−214.895	1.903
6000	45.615	306.031	267.423	231.645	263.793	−223.038	1.942

PREVIOUS: December 1969 (1 atm) CURRENT. December 1969 (1 bar)

Beryllium Carbide (BeC_2) IDEAL GAS $M_r = 33.03418$ Beryllium Carbide (BeC_2) $C_2Be_1(g)$

$S°(298.15\ K) = [218.643]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [558.678]\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = [564.840]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[1580](1)
[423](2)
[1947](1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: [$C_{\infty v}$]
Bond Distances: Be–C = [1.407] Å; C≡C = [1.2] Å
Bond Angle: Be–C–C = [180]°
Rotational Constant: $B_0 = [0.481016]\ cm^{-1}$

Enthalpy of Formation

$\Delta_f H°(298.15\ K)$ was estimated as a lower positive limit by U. S. Nat. Bur. Stand.[1]

Heat Capacity and Entropy

The vibrational frequencies, bond angle, and configuration were estimated by Chupka *et al.*[2] Bond distances were calculated assuming the C–C bond distance was the same as in acetylene.

References

[1] G. T. Armstrong and L. A. Krieger, U. S. Nat. Bur. Stand. Report 6645, Chapter A2, (1960).
[2] Chupka, Berkowitz, Giese, and Inghram, J. Phys. Chem. 62, 611 (1958)

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.196	558.678	558.678	INFINITE
100	30.508	179.700	252.347	−7.265	561.451	543.722	−284.011
200	37.212	202.950	222.304	−3.871	563.615	525.092	−137.140
250	39.569	211.521	219.313	−1.948	564.354	515.371	−107.681
298.15	41.282	218.643	218.643	0.	564.840	505.889	−88.630
300	41.341	218.898	218.643	0.076	564.854	505.523	−88.019
350	42.814	225.384	219.152	2.181	565.139	495.610	−73.966
400	44.152	231.189	220.300	4.356	565.246	485.668	−63.422
450	45.426	236.464	221.808	6.595	565.202	475.722	−55.220
500	46.651	241.314	223.519	8.897	565.032	465.787	−48.660
600	48.933	250.025	227.227	13.679	564.390	445.993	−38.827
700	50.936	257.722	231.044	18.675	563.449	426.331	−31.813
800	52.634	264.638	234.818	23.856	562.291	406.819	−26.563
900	54.048	270.921	238.486	29.192	560.965	387.464	−22.488
1000	55.215	276.678	242.021	34.657	559.501	368.263	−19.236
1100	56.179	281.988	245.416	40.228	557.914	349.215	−16.583
1200	56.976	286.911	248.672	45.887	556.212	330.317	−14.378
1300	57.639	291.498	251.792	51.619	554.401	311.565	−12.519
1400	58.194	295.791	254.783	57.411	552.481	292.956	−10.930
1500	58.661	299.822	257.652	63.255	550.455	274.489	−9.559
1600	59.057	303.621	260.408	69.141	533.786	256.686	−8.380
1700	59.395	307.212	263.056	75.064	531.947	239.423	−7.357
1800	59.685	310.615	265.605	81.019	530.068	222.270	−6.450
1900	59.936	313.849	268.060	87.000	528.151	205.222	−5.642
2000	60.155	316.929	270.427	93.005	526.194	188.276	−4.917
2100	60.345	319.869	272.712	99.030	524.197	171.429	−4.264
2200	60.513	322.680	274.919	105.073	522.161	154.678	−3.673
2300	60.660	325.373	277.055	111.132	520.086	138.021	−3.135
2400	60.792	327.958	279.122	117.205	517.971	121.455	−2.643
2500	60.908	330.442	281.126	123.290	515.815	104.977	−2.193
2600	61.013	332.833	283.069	129.386	513.620	88.587	−1.780
2700	61.106	335.137	284.955	135.492	511.385	72.282	−1.398
2800	61.191	337.361	286.787	141.607	218.152	62.283	−1.162
2900	61.267	339.509	288.568	147.730	216.899	56.738	−1.022
3000	61.336	341.588	290.301	153.860	215.622	51.237	−0.892
3100	61.399	343.600	291.988	159.997	214.320	45.779	−0.771
3200	61.456	345.550	293.632	166.139	212.991	40.363	−0.659
3300	61.508	347.442	295.234	172.288	211.634	34.989	−0.554
3400	61.556	349.279	296.796	178.441	210.246	29.657	−0.456
3500	61.600	351.064	298.322	184.599	208.827	24.366	−0.364
3600	61.641	352.800	299.811	190.761	207.373	19.117	−0.277
3700	61.678	354.489	301.266	196.927	205.884	13.908	−0.196
3800	61.712	356.135	302.688	203.096	204.356	8.740	−0.120
3900	61.744	357.738	304.079	209.269	202.788	3.612	−0.048
4000	61.774	359.302	305.440	215.445	201.177	−1.475	0.019
4100	61.802	360.827	306.773	221.624	199.522	−6.520	0.083
4200	61.827	362.317	308.078	227.805	197.819	−11.525	0.143
4300	61.851	363.772	309.356	233.989	196.068	−16.489	0.200
4400	61.874	365.194	310.609	240.176	194.265	−21.412	0.254
4500	61.895	366.585	311.837	246.364	192.409	−26.292	0.305
4600	61.914	367.946	313.042	252.554	190.498	−31.132	0.354
4700	61.933	369.277	314.225	258.747	188.530	−35.928	0.399
4800	61.950	370.581	315.385	264.941	186.503	−40.683	0.443
4900	61.966	371.859	316.525	271.137	184.416	−45.394	0.484
5000	61.982	373.111	317.644	277.334	182.267	−50.063	0.523
5100	61.996	374.339	318.744	283.533	180.054	−54.687	0.560
5200	62.010	375.543	319.825	289.733	177.777	−59.268	0.595
5300	62.023	376.724	320.887	295.935	175.435	−63.804	0.629
5400	62.035	377.883	321.932	302.138	173.026	−68.296	0.661
5500	62.046	379.022	322.959	308.342	170.550	−72.742	0.691
5600	62.057	380.140	323.971	314.547	168.007	−77.143	0.720
5700	62.068	381.238	324.966	320.753	165.395	−81.498	0.747
5800	62.077	382.318	325.945	326.961	162.716	−85.806	0.773
5900	62.087	383.379	326.910	333.169	159.968	−90.067	0.797
6000	62.096	384.423	327.860	339.378	157.151	−94.281	0.821

PREVIOUS: December 1963 (1 atm) CURRENT December 1963 (1 bar)

Dichloroethyne (C_2Cl_2) IDEAL GAS $M_r = 94.928$

$S°(298.15\ K) = [272.027 \pm 13]\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = [206.3 \pm 42]\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [209.6 \pm 42]\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[410](1)
[2200](1)
[925](1)
[380](2)
[165](2)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: $D_{\infty h}$
Bond Distances: C–C = 1.195 Å; C–Cl = 1.64 Å
Bond Angle: Cl–C–C = 180°
Rotational Constant: $B_0 = 0.046368\ cm^{-1}$

Enthalpy of Formation

The enthalpy of formation of dichloroacetylene is calculated from the estimated $\Delta_r H°(298.15\ K) = -53 \pm 10\ kcal \cdot mol^{-1}$ for $ClC \equiv CCl(g) + Cl_2(g) \rightarrow Cl_2C = CCl_2(g)$, using $\Delta_f H°(C_2Cl_4, g, 298.15\ K) = -2.9\ kcal\ mol^{-1}$.[1] The value of $\Delta_r H°(298.15\ K)$ is assumed to be the same as that for the reaction $HC \equiv CH(g) + Cl_2(g) \rightarrow CHCl = CHCl(g)$, using $\Delta_f H°(CHCl = CHCl, g, 298.15\ K) = 1.2\ kcal \cdot mol^{-1}$.[1,2]

Heat Capacity and Entropy

The linear molecular structure and bond distances were determined from electron diffraction studies by Hassel and Viervoll.[3]

All five fundamental vibrational frequencies are calculated by the modified valence force method[4] from estimated force constants which are interpolated from those of C_2I_2,[5] $CH \equiv CF$,[6] $CH \equiv CCl$,[6] $CH \equiv CBr$,[6] and C_2D_2.[4]

References

[1] U. S. Nat. Bur. Stand. Tech. Note 270-3, (1968).
[2] This is an average value of 0.9 and 1.47 kcal·mol^{-1} for cis– and trans– CHCl = CHCl(g), respectively, which are obtained from reference.[1]
[3] O. Hassel and H. Viervoll, Acta Chem. Scand. 1, 149 (1947).
[4] G. Herzberg, "Infrared and Raman Spectra," D. Van Nostrand Co., Inc., New York, pp. 188–189 (1950).
[5] A. G. Meister and F. F. Cleveland, J. Chem. Phys. 17, 212 (1949).
[6] G. R. Hunt and M. K. Wilson, J. Chem. Phys. 34, 1301 (1961).

Dichloroethyne (C_2Cl_2) $C_2Cl_2(g)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−14.565	206.336	206.336	INFINITE
100	42.627	212.575	324.555	−11.198	206.672	204.506	−106.823
200	57.837	247.336	277.809	−6.095	208.085	201.843	−52.716
250	62.360	260.755	273.089	−3.084	208.886	200.190	−41.827
298.15	65.573	272.027	272.027	0.	209.618	198.448	−34.767
300	65.680	272.433	272.028	0.121	209.645	198.378	−34.541
350	68.213	282.756	272.837	3.471	210.335	196.445	−29.318
400	70.218	292.000	274.665	6.934	210.942	194.418	−25.388
450	71.861	300.368	277.063	10.487	211.463	192.320	−22.324
500	73.250	308.013	279.782	14.116	211.900	190.169	−19.867
600	75.515	321.577	285.646	21.559	212.554	185.757	−16.172
700	77.312	333.358	291.639	29.203	212.981	181.255	−13.525
800	78.775	343.780	297.517	37.010	213.246	176.703	−11.538
900	79.977	353.130	303.186	44.950	213.396	172.125	−9.990
1000	80.970	361.610	308.611	52.999	213.462	167.535	−8.751
1100	81.794	369.367	313.787	61.138	213.464	162.942	−7.737
1200	82.480	376.514	318.720	69.353	213.414	158.351	−6.893
1300	83.055	383.139	323.424	77.630	213.322	153.765	−6.178
1400	83.539	389.312	327.912	85.961	213.191	149.189	−5.566
1500	83.950	395.090	332.200	94.336	213.026	144.623	−5.036
1600	84.300	400.520	336.302	102.749	212.829	140.069	−4.573
1700	84.600	405.640	340.232	111.194	212.602	135.528	−4.164
1800	84.859	410.483	344.001	119.667	212.344	131.002	−3.802
1900	85.084	415.077	347.622	128.165	212.056	126.490	−3.477
2000	85.280	419.447	351.105	136.683	211.738	121.995	−3.186
2100	85.452	423.612	354.459	145.220	211.389	117.516	−2.923
2200	85.604	427.590	357.694	153.773	211.008	113.055	−2.684
2300	85.738	431.399	360.816	162.340	210.594	108.611	−2.467
2400	85.857	435.050	363.834	170.920	210.146	104.187	−2.268
2500	85.964	438.557	366.753	179.511	209.662	99.782	−2.085
2600	86.059	441.931	369.580	188.112	209.142	95.397	−1.917
2700	86.144	445.180	372.320	196.723	208.583	91.033	−1.761
2800	86.222	448.315	374.978	205.341	207.987	86.689	−1.617
2900	86.291	451.341	377.560	213.967	207.351	82.368	−1.484
3000	86.355	454.268	380.068	222.599	206.677	78.070	−1.359
3100	86.412	457.100	382.508	231.238	205.963	73.795	−1.243
3200	86.465	459.845	384.882	239.881	205.211	69.543	−1.135
3300	86.513	462.506	387.194	248.530	204.421	65.316	−1.034
3400	86.557	465.090	389.447	257.184	203.595	61.113	−0.939
3500	86.598	467.599	391.644	265.842	202.734	56.935	−0.850
3600	86.635	470.039	393.788	274.503	201.840	52.782	−0.766
3700	86.670	472.413	395.881	283.169	200.915	48.654	−0.687
3800	86.702	474.725	397.926	291.837	199.961	44.551	−0.612
3900	86.731	476.978	399.924	300.509	198.981	40.474	−0.542
4000	86.759	479.174	401.878	309.183	197.978	36.423	−0.476
4100	86.784	481.317	403.790	317.861	196.953	32.396	−0.413
4200	86.808	483.408	405.660	326.540	195.909	28.395	−0.353
4300	86.830	485.451	407.492	335.222	194.850	24.420	−0.297
4400	86.851	487.447	409.287	343.906	193.776	20.468	−0.243
4500	86.870	489.399	411.046	352.592	192.692	16.542	−0.192
4600	86.888	491.309	412.770	361.280	191.599	12.639	−0.144
4700	86.906	493.178	414.461	369.970	190.500	8.761	−0.097
4800	86.922	495.008	416.120	378.661	189.397	4.906	−0.053
4900	86.937	496.800	417.748	387.354	188.291	1.074	−0.011
5000	86.951	498.557	419.347	396.048	187.185	−2.736	0.029
5100	86.964	500.279	420.917	404.744	186.079	−6.523	0.067
5200	86.977	501.967	422.459	413.441	184.977	−10.289	0.103
5300	86.989	503.624	423.975	422.140	183.878	−14.034	0.138
5400	87.000	505.250	425.465	430.839	182.785	−17.758	0.172
5500	87.011	506.847	426.930	439.540	181.698	−21.461	0.204
5600	87.021	508.415	428.372	448.241	180.617	−25.146	0.235
5700	87.031	509.955	429.789	456.944	179.545	−28.811	0.264
5800	87.040	511.469	431.185	465.647	178.481	−32.456	0.292
5900	87.048	512.957	432.558	474.352	177.427	−36.084	0.319
6000	87.057	514.420	433.910	483.057	176.381	−39.695	0.346

PREVIOUS: December 1968 (1 atm) CURRENT: December 1968 (1 bar)

Dichloroethyne (C_2Cl_2) $C_2Cl_2(g)$

Tetrachloroethene (C_2Cl_4) IDEAL GAS $M_r = 165.834$ Tetrachloroethene (C_2Cl_4) $C_2Cl_4(g)$

$S°(298.15\ K) = 343.421\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = -11.873 \pm 2.9\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = -12.426 \pm 2.9\ kJ·mol^{-1}$

Electronic Levels and Quantum Weights

ϵ_i, cm^{-1}	g_i	ϵ_i, cm^{-1}	g_i
0	1	63557	[1]
[37700]	[1]	70097	[1]
[50350]	[1]	72410	[1]
[59000]	[1]		

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
1571 (1)	1000 (1)	918 (1)
447 (1)	347 (1)	176 (1)
235 (1)	324 (1)	777 (1)
110 (1)	512 (1)	288 (1)

Point Group: D_{2h} $\sigma = 4$
Bond Distances: Cl–C = 1.724 Å; C–C = 1.327 Å
Bond Angle: Cl–C–Cl = 113.3°
Product of the Moments of Inertia: $I_A I_B I_C = 3.431926 \times 10^{-112}\ g^3·cm^6$

Enthalpy of Formation

The enthalpy of combustion $\Delta E(Cl_2Cl_4, l, 293\ K)$ has been determined by the ''Quartz Wool'' method by Smith *et al.*[1] The free chlorine produced from combustion was reduced to hydrogen chloride by a quartz spiral moistened with a solution of arsenious acid in the combustion bomb. Based on the reported results, the enthalpy change at 298.15 K for the reaction $C_2Cl_4(l) + O_2(g) + 2H_2O(l) = 2CO_2(g) + 4HCl(aq, 600H_2O)$ is evaluated as $-198.40\ kcal·mol^{-1}$, using recent auxiliary data from[2] and Parker[3] and $C_p°$ for $C_2Cl_4(l)$ from Kurbatov.[4] Employing $\Delta_f H°(298.15\ K) = -94.054, -39.823$ and $-68.315\ kcal·mol^{-1}$ for $CO_2(g)$, $HCl(aq, 600H_2O)$ and $H_2O(l)$, respectively, we calculate the enthalpy of formation for $C_2Cl_4(l)$ as $-12.367\ kcal·mol^{-1}$. Incorporating this value with the value $\Delta_{vap}H°(298.15\ K) = 9.4\ kcal·mol^{-1}$ obtained from Eftring,[5] we derive $\Delta_f H°(298.15\ K) = -2.97 \pm 0.7\ kcal·mol^{-1}$ for $C_2Cl_4(g)$.

Heat Capacity and Entropy

The molecular structure of $C_2Cl_4(g)$ was investigated by the sector–visual method of electron diffraction by Ramachandra and Livingston.[6] The reported bond distances and angle are in agreement with those measured by Karle and Karle,[7] using the sector–microphotometer method, and Lipscomb.[8] The molecular structure has also been determined by Brockway *et al.*,[9] Laszlo,[10] and Dornte[11] by use of electron diffraction. The values reported by Ramachandra and Livingston,[6] are adopted.

The vibrational spectra of tetrachloroethylene have been studied by numerous investigators. The vibrational frequencies assigned by Mann *et al.*[12] are adopted here. These authors also reviewed the results of earlier investigations in detail.

The electronic levels and quantum weights are obtained from Herzberg.[13]

The principal moments of inertia are: $I_A = 48.8379 \times 10^{-39}$, $I_B = 62.8935 \times 10^{-39}$, and $I_C = 111.7314 \times 10^{-39}\ g·cm^2$.

References

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−19.911	−11.873	−11.873	INFINITE
100	56.855	260.362	417.923	−15.756	−13.662	−1.706	0.891
200	81.269	308.108	351.744	−8.727	−13.361	10.236	−2.673
250	89.301	327.140	344.961	−4.455	−12.918	16.086	−3.361
298.15	95.546	343.421	343.421	0.	−12.426	21.628	−3.789
300	95.762	344.013	343.423	0.177	−12.407	21.839	−3.802
350	101.048	359.185	344.609	5.101	−11.861	27.504	−4.105
400	105.411	372.972	347.306	10.266	−11.303	33.089	−4.321
450	109.036	385.603	350.869	15.630	−10.747	38.605	−4.481
500	112.065	397.253	354.933	21.160	−10.205	44.059	−4.603
600	116.755	418.123	363.766	32.614	−9.171	54.814	−4.772
700	120.131	436.388	372.863	44.468	−8.208	65.401	−4.880
800	122.611	452.600	381.836	56.611	−7.306	75.854	−4.953
900	124.471	467.154	390.521	68.969	−6.457	86.198	−5.003
1000	125.893	480.345	398.854	81.490	−5.655	96.449	−5.038
1100	126.999	492.398	406.818	94.137	−4.897	106.623	−5.063
1200	127.874	503.487	414.418	106.883	−4.177	116.729	−5.081
1300	128.576	513.751	421.669	119.706	−3.496	126.776	−5.094
1400	129.147	523.301	428.592	132.593	−2.852	136.773	−5.103
1500	129.616	532.228	435.206	145.532	−2.244	146.725	−5.109
1600	130.007	540.606	441.535	158.514	−1.672	156.637	−5.114
1700	130.336	548.498	447.597	171.532	−1.135	166.515	−5.116
1800	130.614	555.956	453.412	184.579	−0.636	176.362	−5.118
1900	130.852	563.024	458.996	197.653	−0.175	186.182	−5.119
2000	131.057	569.741	464.367	210.749	0.247	195.979	−5.118
2100	131.234	576.140	469.538	223.863	0.627	205.757	−5.118
2200	131.389	582.249	474.524	236.995	0.964	215.517	−5.117
2300	131.525	588.092	479.335	250.141	1.254	225.262	−5.116
2400	131.645	593.692	483.984	263.299	1.496	234.996	−5.115
2500	131.751	599.069	488.481	276.469	1.686	244.721	−5.113
2600	131.845	604.238	492.834	289.649	1.822	254.440	−5.112
2700	131.930	609.215	497.053	302.838	1.903	264.155	−5.110
2800	132.005	614.015	501.145	316.035	1.925	273.867	−5.109
2900	132.074	618.648	505.118	329.239	1.890	283.580	−5 108
3000	132.135	623.127	508.977	342.449	1.796	293.295	−5.107
3100	132.191	627.460	512.730	355.666	1.643	303.013	−5.106
3200	132.242	631.658	516.381	368.887	1.432	312.738	−5.105
3300	132.289	635.728	519.936	382.114	1.166	322.471	−5.104
3400	132.331	639.678	523.400	395.345	0.847	332.212	−5.104
3500	132.370	643.515	526.777	408.580	0.478	341.963	−5.104
3600	132.406	647.244	530.072	421.819	0.063	351.726	−5.103
3700	132.440	650.872	533.288	435.061	−0.395	361.500	−5 103
3800	132.470	654.405	536.429	448.307	−0.891	371.287	−5 104
3900	132.499	657.846	539.498	461.555	−1.419	381.088	−5.104
4000	132.525	661.201	542.499	474.807	−1.976	390.904	−5.105
4100	132.550	664 474	545.434	488.060	−2.555	400 733	−5.105
4200	132.574	667.668	548.307	501.317	−3.151	410.576	−5.106
4300	132.596	670.788	551.119	514.575	−3.760	420.434	−5.107
4400	132.617	673.836	553.874	527.836	−4.376	430.306	−5.108
4500	132.636	676.817	556.573	541.098	−4.994	440.192	−5.110
4600	132.655	679.732	559.219	554.363	−5.609	450.092	−5.111
4700	132.674	682.585	561.813	567.629	−6.217	460.005	−5.112
4800	132.691	685.379	564.358	580.898	−6.814	469.931	−5.114
4900	132.708	688.115	566.856	594.168	−7.395	479.870	−5.115
5000	132.725	690.796	569.308	607.439	−7.957	489.819	−5.117
5100	132.741	693.425	571.716	620.713	−8.496	499.780	−5 119
5200	132.758	696.002	574.082	633.987	−9.010	509.751	−5.121
5300	132.774	698.531	576.406	647.264	−9.496	519.732	−5.122
5400	132.790	701.013	578.691	660.542	−9.951	529.722	−5.124
5500	132.807	703.450	580.937	673.822	−10.372	539.720	−5.126
5600	132.823	705.843	583.146	687.104	−10.759	549.725	−5.128
5700	132.840	708.194	585.319	700.387	−11.110	559.737	−5.129
5800	132.857	710.505	587.458	713.672	−11.422	569.755	−5.131
5900	132.875	712.776	589.563	726.958	−11.696	579.777	−5.133
6000	132.893	715.009	591.635	740.247	−11.930	589.804	−5.135

PREVIOUS: September 1967 (1 atm)   CURRENT: September 1967 (1 bar)

Hexachloroethane (C_2Cl_6) IDEAL GAS $M_r = 236.740$

$S°(298.15\ K) = 397.880\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -135.83 \pm 8.4\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -134.22 \pm 8.4\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies		
ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
976(1)	678(1)	223(1)
431(1)	377(1)	778(2)
164(1)	858(1)	267(2)
Internal Rotation	340(2)	139(2)

Point Group. D_{3d}
Bond Distances: Cl–C = 1.74 Å; C–C = 1.55 Å; $\sigma = 6$
Bond Angles: Cl–C–Cl = 110°; Cl–C–C = 109°
Product of the Moments of Inertia: $I_A I_B I_C = 9.144710 \times 10^{-112}\ g^3{\cdot}cm^6$

Enthalpy of Formation

Smith *et al.*[1] determined the heat of combustion of $C_2Cl_6(cr)$ to be $\Delta E(293\ K) = -718.7 \pm 2\ cal{\cdot}g^{-1}$ (uncorrected) by use of the 'Quartz Wool' method. The free chlorine produced was reduced to HCl by employing the quartz spiral moistened iwth a solution of arsenious acid in the combustion bomb. Adopting the reported results and recent auxiliary data,[2,3,4] we evaluate the values $\Delta_c H°(298\ 15\ K) = -173.525$ and $\Delta_f H°(298.15\ K) = -48.58\ kcal{\cdot}mol^{-1}$ for $C_2Cl_6(cr)$. Kirkbride[5] measured the enthalpy changes as −32.0 and 4.7 kcal·mol^{-1} for the following two reactions by solution calorimetry: $C_2Cl_4(l) + Cl_2(g) = C_2Cl_6(aq)$ and $C_2Cl_6(cr) = C_2Cl_6(aq)$. Hence we obtain $\Delta_f H°(298.15\ K) = -49.07\ kcal{\cdot}mol^{-1}$ for $C_2Cl_6(cr)$, using $\Delta_f H°(C_2Cl_4, l, 298.15\ K) = -12.37\ kcal{\cdot}mol^{-1}$. This value is in reasonable agreement with the adopted value −48.58 kcal·mol^{-1}.

Hexachloroethane (cr) has three modifications, namely triclinic, monoclinic and cubic, with transition temperatures of 318 and 345 K.[4] The sublimiation pressures over the different phases have been measured by Ivin,[8] Lee,[7] and Nitta.[26] Based oin these data, values for $\Delta_{sub}H°$(triclinic, 298.15 K) are derived by a modified second and third law method to be 16.5, 17.1 and 14.8 kcal·mol^{-1}, respectively. The analysis depends on the $C_p°$ and $\Delta_{trs}H°$ data determined by Seki and Momotani.[4] The order of magnitude of the two $\Delta_{trs}H°$ values is confirmed by McDonald, private communication, Thermal Research Laboratory, The Dow Chemical Company, Midland, Michigan. Pressures reported by Nelson[6] are systematically lower than the above data by about 10%, therefore, his data are not used. Third law analysis is not applicable to the pressure data due to lack of $S°$(triclinic, 298.15 K). Adopting $\Delta_{sub}H°(298.15\ K) = 16.5$ and $\Delta_f H°(298.15\ K) = -48.58\ kcal{\cdot}mol^{-1}$ for C_2Cl_6 (triclinic), we obtain $\Delta_f H°(298.15\ K) = -32.08\ kcal{\cdot}mol^{-1}$ for $C_2Cl_6(g)$.

The equilibrium constant at 776 K for the reaction $C_2Cl_6(g) = C_2Cl_4(g) + Cl_2(g)$ was reported as 0.8 ± 0.1 (atm) by Puyo *et al.*[9] The corresponding enthalpy change at 298.15 K is evaluated to be 30.8 kcal·mol^{-1} by the third law method, yielding $\Delta_f H°(C_2Cl_6, g, 298.15\ K) = -33.77\ kcal{\cdot}mol^{-1}$ which is in fair agreement with the adopted one.

Heat Capacity and Entropy

The molecular structure of C_2Cl_6 has been studied previously by means of infrared and Raman spectroscopy,[10] X–ray,[11] and electron diffraction.[12–18] The molecule was found to be in the staggered position in the vapor and solid states. The bond distances and angles adopted here are those reported by Swick *et al.*[16]

Incomplete assignments of vibrational frequencies for $C_2Cl_6(g)$ were reported by many investigators.[21–24] The adopted frequencies, except the torsional mode ν_4, are obtained from Carney *et al.*[19] The torsional mode is treated as a hindered internal rotation, and thermodynamic properties are calculated[25] from the barrier height of $V_0 = 12.8\ kcal{\cdot}mol^{-1}$ which was evaluated by Karle[20] from electron diffraction data. The value of $S°(298.15\ K)$ is calculated based on $S°(400\ K) = 105.355\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ which is derived from the free rotor value $S°(400\ K) = 108.121\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ by subtraction of the entropy difference between a free rotor and hindered rotor at 400 K. Internal rotation contributions to $C_p°$ at temperatures below 350 K could not be calculated since they are beyond the range of the values above 350 K and the corresponding harmonic oscillator values ($\nu_4 = 67\ cm^{-1}$) below 150 K. This calculation presumes that the internal rotation approaches harmonic oscillation as $V/RT >> 1$.

The principal moments of inertia are: $I_A = 79.9217 \times 10^{-39}$, $I_B = 92.8302 \times 10^{-39}$, and $I_C = 123.2582 \times 10^{-39}\ g{\cdot}cm^2$.

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Hexachloroethane (C_2Cl_6) $C_2Cl_6(g)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100	76.371	280.567	504.581	−22.401	−135.834	−106.999	55.890
200	115.964	346.938	409.925	−12.597	−135.796	−77.973	20.364
298.15	138 934	397.880	397.880	0.	−134.223	−49.894	8.741
300	139.267	398.741	397.883	0.257	−134.186	−49.371	8.596
400	153.457	440 913	403.536	14.951	−131.948	−21.427	2.798
500	162.260	476.174	414.636	30.769	−129.496	5.921	−0.619
600	167.954	506.295	427.464	47.298	−127.020	32.772	−2.853
700	171.799	532.488	440.638	64.295	−124.584	59.211	−4.418
800	174.531	555.615	453.593	81.618	−122.203	85.304	−5.570
900	176.536	576.293	466.098	99.175	−119.875	111.102	−6.448
1000	178.033	594.973	478.066	116.907	−117.600	136.644	−7.138
1100	179.128	611.994	489.479	134.766	−115.378	161.960	−7.691
1200	180.012	627.620	500.349	152.725	−113.208	187.076	−8.143
1300	180.651	642.055	510.701	170.760	−111.088	212.014	−8.519
1400	181.150	655.462	520.568	188.851	−109.022	236.790	−8.835
1500	181.478	667.971	529.983	206.983	−107.011	261.420	−9.103
1600	181.732	679.692	538.977	225.144	−105.059	285.919	−9.334
1700	181.832	690.713	547.582	243.322	−103.171	310.296	−9.534
1800	181.910	701.108	555.825	261.510	−101.350	334.565	−9.709
1900	181.968	710.945	563.733	279.704	−99.596	358.734	−9.862
2000	182.004	720.280	571.329	297.902	−97.908	382.813	−9.998
2100	181.922	729.158	578.635	316.099	−96.295	406.809	−10.119
2200	181.841	737.619	585.671	334.287	−94.762	430.730	−10.227
2300	181.761	745.701	592.454	352.467	−93.311	454.584	−10.324
2400	181.681	753.435	599.002	370.639	−91.945	478.375	−10.412
2500	181.602	760.850	605.328	388.803	−90.666	502.112	−10.491
2600	181.523	767.971	611.448	406.960	−89.475	525.800	−10.563
2700	181.445	774.820	617.372	425.108	−88.375	549.443	−10.630
2800	181.367	781.417	623.114	443.249	−87.367	573.047	−10.690
2900	181.290	787.780	628.683	461.381	−86.452	596.617	−10.746
3000	181.213	793.925	634.089	479.506	−85.630	620.157	−10.798
3100	181 128	799.865	639.342	497.624	−84.899	643.670	−10.846
3200	181.045	805.615	644.448	515.732	−84.258	667.162	−10.890
3300	180.965	811.185	649.417	533.833	−83.704	690.636	−10.932
3400	180.888	816.586	654.255	551.925	−83.232	714.093	−10.971
3500	180.813	821.828	658.968	570.010	−82.837	737.538	−11.007
3600	180 740	826.921	663.563	588.088	−82.513	760.972	−11.041
3700	180 671	831.872	668.045	606.158	−82.253	784.399	−11.074
3800	180.603	836.689	672.420	624.222	−82.049	807.818	−11.104
3900	180.539	841.380	676.693	642.279	−81.894	831.234	−11.133
4000	180.477	845.950	680.867	660.330	−81.781	854.646	−11.161
4100	180.423	850.405	684.948	678.375	−81.699	878.056	−11.187
4200	180.370	854.753	688.940	696.414	−81.642	901.464	−11.211
4300	180.319	858.996	692.845	714.449	−81.600	924.871	−11.235
4400	180.269	863.141	696.669	732.478	−81.566	948.277	−11.257
4500	180.221	867.192	700.413	750.503	−81.533	971.682	−11.279
4600	180.174	871.152	704.082	768.522	−81.492	995.087	−11.300
4700	180.128	875.026	707.678	786.538	−81.437	1018.489	−11.319
4800	180.084	878.818	711.204	804.548	−81.362	1041.891	−11.338
4900	180.041	882.531	714.663	822.554	−81.259	1065.292	−11.356
5000	180.000	886.168	718.057	840.556	−81.123	1088.688	−11.373
5100	179.960	889.732	721.388	858.554	−80.950	1112.084	−11.390
5200	179.922	893.226	724.659	876.548	−80.734	1135.474	−11.406
5300	179.885	896.653	727.872	894.539	−80.471	1158.860	−11.421
5400	179.849	900.015	731.029	912.525	−80.157	1182.241	−11.436
5500	179.815	903.315	734.131	930.509	−79.789	1205.616	−11.450
5600	179.782	906.555	737.182	948.488	−79.365	1228.983	−11.463
5700	179.751	909.736	740.181	966.465	−78.881	1252.342	−11.476
5800	179.721	912.862	743.131	984.439	−78.335	1275.693	−11.489
5900	179.692	915.934	746.034	1002.409	−77.726	1299.033	−11.501
6000	179.665	918.954	748.891	1020.377	−77.053	1322.361	−11.512

PREVIOUS: September 1967 (1 atm) CURRENT: September 1967 (1 bar)

Hexachloroethane (C_2Cl_6) $C_2Cl_6(g)$

Chromium Carbide (Cr_3C_2) **CRYSTAL** **M_r = 180.010** **Chromium Carbide (Cr_3C_2)** **$C_2Cr_3(cr)$**

$S°(298.15\ K) = 85.434 \pm 0.42\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = -86.21 \pm 12.6\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -85.35 \pm 12.6\ kJ \cdot mol^{-1}$

Enthalpy of Formation

Mah[1] determined the enthalpy of combustion of $Cr_3C_2(cr)$ using oxygen bomb calorimetry. She reported $\Delta_c H°(298.15\ K) = -574.5 \pm 0.4$ kcal·mol^{-1} based on the reaction $Cr_3C_2(cr) + 17/4O_2(g) = 3/2Cr_2O_3(cr) + 2CO_2(g)$. Using auxiliary JANAF data,[2] we calculate $\Delta_f H°(298.15\ K) = -20.4$ kcal·mol^{-1} for $Cr_3C_2(cr)$ Mah[1] reported that of the six combustion runs four were complete combustions whereas the other two were 99.17% and 98.57% complete. Corrections were made by Mah[1] for incomplete combustion, formation of small amounts of CO(g), and impurities. These corrections amount to less than 1.95% of the $\Delta_c E°v_c$. There are many equilibrium studies involving $Cr_3C_2(cr)$.[3-13] Our analysis of a portion of these studies is tabulated below:

Source	Reaction	T/K	Method	$\Delta_f H°(298.15\ K)$, kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°(298.15\ K)$ kcal·mol^{-1}
4	A(14 pts.)**	1244–1382	CO equilibrium pressure	528.39	533.26	3.7 ± 3.4	−21.29
8	A(18 pts.)	1316–1366	CO equilibrium pressure	495.46	526.56	23.0 ± 6.4	−24.64
10	B(eqn)	880–1100	emf (CaF_2)	−9.34	−12.60	−3.3	−12.60
11	B(eqn)	1073–1303	emf ($ThO_2Y_2O_3$)	−12.70	−15.73	−2.5	−15.73
12	B(eqn)	885–1095	emf (CaF_2)	−15.42	−14.92	0.5	−14.92

Reactions: (A) $3Cr_2O_3(cr) + 13C(cr) = 2Cr_3C_2(cr) + 9CO(g)$. (B) $3Cr(cr) + 2C(cr) = Cr_3C_2(cr)$.
**1374 K point rejected due to statistical test.

The CO(g) equilibrium pressures measured by Heusler[3] in the range 1159–1369 K are higher than those of Kelley *et al.*[4] by a factor varying from 2.0 to 1.4 with increasing temperature. Three studies measured the chromium pressure in equilibrium with C(cr) and $Cr_3C_2(cr)$.[5, 7 9] Reported heats of formation for Cr_3C_2 from these studies are −23.1 kcal·mol^{-1},[5] −14.2 kcal·mol^{-1},[7] and −22 kcal·mol^{-1}.[9] Alekseev and Shvartsman[6] studied the decarburization of the chromium carbides. Mah[1] analyzed their data and reported $\Delta_f H°(298.15\ K) = -16.6$ kcal·mol^{-1} for $Cr_3C_2(cr)$.

The $\Delta_f H°$ results are quite scattered with the emf results being roughly 5 kcal·mol^{-1} more positive than the combustion and pressure equilibrium studies. Possible explanations for these discrepancies are discussed by Kulkarni and Worrell.[16] We adopt $\Delta_f H°(298.15\ K) = -20.4 \pm 3.0$ kcal·mol^{-1} (−85.354 ± 12.6 kJ·mol^{-1}) for $Cr_3C_2(cr)$ based on the combustion study by Mah.[1]

Heat Capacity and Entropy

The heat capacity of $Cr_3C_2(cr)$ has been measured by Kelley *et al.*[4] [53–296 K, 29 pts.) and DeSorbo[14] (12–301 K, 65 pts.). As reported by DeSorbo,[14] the results of these two studies differ by no more than 0.1%. Using the Debye function 3*D* (300/*T*) as suggested by DeSorbo,[14] we calculate and adopt $S°(12\ K) = 0.0297$ cal·K^{-1}·mol^{-1} and $H°(12;0) = 0.268$ kcal·mol^{-1}. The enthalpy has been measured by Kelley *et al.*[4] [481–1576 K, 17 pts.] and Oriani and Murphy[15] [297–1188 K, 11 pts.]. As stated by Oriani and Murphy,[15] their results are somewhat lower than those of Kelley *et al.*;[4] the maximum difference is 1.2% at 970 K. For *T* > 298 15 K, we base our adopted values on the enthalpy data of Kelley *et al.*[4] The enthalpy data is subjected to a curve fit procedure with the constraint that it join smoothly in the 298 K region with the enthalpy derived from the heat capacity data of Kelley *et al.*[4] The deviations between the tabulated and observed enthalpy average 0.26% with a maximum of 0.78% at the lowest observed temperature, 480.7 K.

Phase Data

Storms[17] has summarized the phase information for the Cr–Cr_3C_2 system and reported that Cr_3C_2 has an orthorhombic structure. The range of homogeneity is unknown.[17]

Decomposition Data

The tentative phase diagram for the Cr–Cr_3C_2 system proposed by Storms[17] indicated that Cr_3C_2 has an incongruent melting point at 2168 K.

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Enthalpy Reference Temperature = T_r = 298.15 K						Standard State Pressure = $p°$ = 0.1 MPa	
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−15.132	−86.211	−86.211	INFINITE
100	31.322	14.297	155.599	−14.130	−86.263	−86.216	45.035
200	74.718	50.620	93.807	−8.637	−86.175	−86.144	22.499
298.15	99.299	85.434	85.434	0.	−85.354	−86.277	15.115
300	99.663	86.049	85.436	0.184	−85.331	−86.283	15.023
400	115.478	117.037	89.553	10.994	−84.193	−86.719	11.324
500	125.549	143.964	97.805	23.079	−82.549	−87.540	9.145
600	131.486	167.406	107.496	35.946	−80.997	−88.687	7.721
700	135.658	187.997	117.555	49.309	−79.624	−90.079	6.722
800	139.101	206.340	127.528	63.050	−78.422	−91.657	5.985
900	142.260	222.907	137.220	77.118	−77.406	−93.374	5.419
1000	145.327	238.054	146.556	91.498	−76.621	−95.193	4.972
1100	148.377	252.048	155.518	106.183	−76.120	−97.077	4.610
1200	151.448	265.090	164.112	121.174	−75.926	−98.993	4.309
1300	154.553	277.335	172.355	136.474	−76.068	−100.912	4.055
1400	157.695	288.903	180.270	152.086	−76.569	−102.807	3.836
1500	160.871	299.891	187.882	168.014	−77.437	−104.653	3.644
1600	164.084	310.376	195.213	184.261	−78.678	−106.429	3.475
1700	167.322	320.420	202.284	200.831	−80.296	−108.115	3.322
1800	170.586	330.077	209.117	217.727	−82.294	−109.696	3.183
1900	173.870	339.388	215.730	234.949	−84.677	−111.155	3.056
2000	177.176	348.390	222.139	252.501	−87.445	−112.479	2.938
2100	180.489	357.115	228.360	270.385	−90.603	−113.655	2.827
2200	183.761	365.586	234.406	288.597	−152.162	−112.705	2.676
2300	187.075	373.828	240.289	307.139	−150.527	−110.947	2.520
2400	190.389	381.860	246.021	326.012	−148.592	−109.267	2.378
2500	193.702	389.699	251.612	345.217	−146.356	−107.673	2.250

PREVIOUS· CURRENT: December 1973

Difluoroethyne (C_2F_2) IDEAL GAS $M_r = 62.018806$ Difluoroethyne (C_2F_2) $C_2F_2(g)$

$S°(298.15\ K) = [244.06 \pm 63]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [19.4 \pm 21]\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = [20.9 \pm 21]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}
[1050](1)	[450](2)
[1900](1)	[300](2)
1149 (1)	

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: [$D_{\infty h}$]
Bond Distances: C–F = [1.28] Å; C–C = [1.20] Å
Bond Angle. F–C–C = [180]°
Rotational Constant: $B_0 = [0.117932]\ cm^{-1}$

Enthalpy of Formation

Farber *et al.*,[1] have obtained equilibrium–weight change data over the C–CF_4 system. Our reanalysis of these data assumes that the equilibrium constants for CF_4, CF_3 and CF_2 are those in the JANAF Tables, and that C_2F_2 was the only other C–F species present at equilibrium. This gives maximum possible concentrations of C_2F_2 and places a lower limit on the heat of formation. The $\Delta_f H°(C_2F_2, g, 298.15\ K)$ values so obtained range from +10 kcal·mol^{-1} from data at 2023 K to −10 kcal·mol^{-1} from data at 2373 K; we adopt a weighted mean of +5 ± 5 kcal·mol^{-1} (20.920 ± 21 kJ·mol^{-1}). This value still predicts complete dimerization of CF at 1 atmosphere pressure below about 2200 K, but only CF would exist under experimental conditions such as the study by Farber.

Farber *et al.*[1] also investigated the mass spectrum of the vapor over the C–CF_4 system and did not detect any ion ascribable to C_2F_2. This is additional support for the value adopted.

The C–C bond dissociation energy in C_2F_2 is 113 kcal·mol^{-1}, using JANAF CF(g) table (December 31, 1967). This value is 115 kcal·mol^{-1} weaker than the bond dissociation energy of acetylene. In order to explain such a large decrease, a crossing of the repulsive approach of two $^2\Pi$ CF molecules with an attractive approach of two $^4\Sigma$ CF molecules may be postulated. This follows the reasoning used by Simons[2] to explain the bond dissociation energy of C_2F_4.

Heat Capacity and Entropy

The molecular structure is assumed to be the same as that for $C_2H_2(g)$. The C–F and C–C bond distances are estimated from those in HC = CF reported by Tyler and Sheridan.[3] The assymmetric stretching frequency, $\nu_3 = 1149\ cm^{-1}$, was observed by Heicklen and Knight.[4] The other vibrational frequencies were estimated by comparison with those for $C_2H_2(g)$ and $C_2HF(g)$ reported by Herzberg,[5] Hunt and Wilson,[6] and Brown and Tyler.[7]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−12.403	19.444	19.444	INFINITE
100	34 428	194.599	288.398	−9.380	19.441	17.208	−8.989
200	48.351	223.037	249.016	−5.196	20.043	14.799	−3.865
250	53.162	234.364	244.977	−2.653	20.492	13.436	−2.807
298.15	56.935	244.060	244.060	0.	20.920	12.038	−2.109
300	57.068	244.412	244.061	0.105	20.936	11.983	−2.086
350	60.380	253.465	244.768	3.044	21.344	10.458	−1.561
400	63.249	261.719	246.379	6.136	21.702	8.878	−1.159
450	65.757	269.317	248.511	9.363	22.005	7.256	−0.842
500	67.957	276.361	250.948	12.707	22.253	5.604	−0.585
600	71.592	289.087	256.267	19.692	22.609	2.238	−0.195
700	74.412	300.344	261.775	26.998	22.818	−1.176	0.088
800	76.610	310.429	267.237	34.554	22.922	−4.612	0.301
900	78.336	319.556	272.552	42.304	22.949	−8.056	0.468
1000	79.704	327.883	277.674	50.209	22.917	−11.499	0.601
1100	80.799	335.533	282.591	58.236	22.837	−14.938	0.709
1200	81.685	342.603	287.302	66.362	22.714	−18.366	0.799
1300	82.410	349.171	291.811	74.568	22.553	−21.784	0.875
1400	83.007	355.301	296.130	82.839	22.355	−25.187	0.940
1500	83.506	361.045	300.268	91.166	22.122	−28.575	0.995
1600	83.924	366.448	304.237	99.538	21.855	−31.946	1.043
1700	84.279	371.547	308.048	107.949	21.556	−35.300	1.085
1800	84.582	376.373	311.711	116.392	21.227	−38.635	1.121
1900	84.843	380.953	315.236	124.864	20.868	−41.951	1.153
2000	85.069	385.311	318.631	133.360	20.484	−45.247	1.182
2100	85.265	389.466	321.906	141.876	20.077	−48.524	1.207
2200	85.437	393.437	325 068	150.412	19.649	−51.781	1.229
2300	85.588	397.238	328.124	158.963	19.205	−55.018	1.249
2400	85.722	400.884	331.080	167.529	18.748	−58.235	1.267
2500	85.841	404.386	333.943	176.107	18.282	−61.433	1.284
2600	85.948	407.754	336.717	184.697	17.809	−64.612	1.298
2700	86.043	411.000	339.409	193.296	17.334	−67.773	1.311
2800	86.128	414.131	342.022	201.905	16.859	−70.917	1.323
2900	86.205	417.154	344.561	210.522	16.387	−74.043	1.334
3000	86.275	420.078	347.030	219.146	15.920	−77.154	1.343
3100	86.339	422.908	349.432	227.776	15.462	−80.249	1.352
3200	86.397	425.650	351.771	236.413	15.012	−83.329	1.360
3300	86.449	428.310	354.050	245.056	14.574	−86.395	1.368
3400	86.498	430.891	356.273	253.703	14.148	−89.448	1.374
3500	86.542	433.399	358.440	262.355	13.735	−92.489	1.380
3600	86.583	435.838	360.557	271.011	13.336	−95.518	1.386
3700	86.620	438.210	362.624	279.671	12.951	−98.537	1.391
3800	86.655	440.521	364.643	288.335	12.581	−101.545	1.396
3900	86.687	442.772	366.618	297.002	12.226	−104.544	1.400
4000	86.717	444.967	368.549	305.673	11.885	−107.533	1.404
4100	86.745	447.109	370.439	314.346	11.558	−110.515	1.408
4200	86.771	449.200	372.290	323.022	11.246	−113.488	1.411
4300	86.795	451.242	374.102	331.700	10.947	−116.455	1.415
4400	86.817	453.237	375.878	340.381	10.661	−119.414	1.418
4500	86.838	455.189	377.619	349.063	10.387	−122.367	1.420
4600	86.858	457.097	379.326	357.748	10.125	−125.315	1.423
4700	86.876	458.966	381.001	366.435	9.875	−128.256	1.425
4800	86.894	460.795	382.644	375.123	9.634	−131.192	1.428
4900	86.910	462.587	384.257	383.814	9.403	−134.124	1.430
5000	86.925	464.343	385.842	392.505	9.181	−137.051	1.432
5100	86.940	466.064	387.398	401.199	8.967	−139.973	1.434
5200	86.954	467.752	388.927	409.893	8.760	−142.892	1.435
5300	86.966	469.409	390.430	418.589	8.559	−145.806	1.437
5400	86.979	471.035	391.907	427.287	8.364	−148.717	1.439
5500	86.990	472.631	393.361	435.985	8.174	−151.624	1.440
5600	87.001	474.198	394.790	444.685	7.989	−154.528	1.441
5700	87 011	475.738	396.197	453.385	7.806	−157.429	1.443
5800	87.021	477.252	397.581	462.087	7.626	−160.326	1.444
5900	87.031	478.739	398.944	470.789	7.448	−163.220	1.445
6000	87.039	480.202	400.287	479.493	7.271	−166.111	1.446

PREVIOUS· December 1967 (1 atm) CURRENT: December 1967 (1 bar)

Trifluoroacetonitrile (CF_3CN) IDEAL GAS $M_r = 95.023909$ Trifluoroacetonitrile (CF_3CN) $C_2F_3N_1(g)$

$S°(298.15\ K) = 298.533 \pm 0.4\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = -491.61 \pm 2.9\ kJ \cdot mol^{-1}$

$\Delta_f H°(298.15\ K) = -495.39 \pm 2.9\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}
2271(1)	1215(2)
1228(1)	625(2)
801(1)	464(2)
521(1)	192(2)

Ground State Quantum Weight: [1] $\sigma = 3$

Point Group: C_{3v}

Bond Distances: C–F = 1.335 Å; C–C = 1.461 Å; CN = 1.153 Å

Bond Angles: F–C–F = 107.5°; F–C–C = 111.38°

Product of the Moments of Inertia. $I_A I_B I_C = 1.186732 \times 10^{-113}\ g^3 \cdot cm^6$

Enthalpy of Formation

The selected value is obtained from least squares, simultaneous adjustment of the enthalpies of formation of CF_3, C_2F_4, and CF_3X(X = H, Cl, Br, I, CN). Details of the input data and adjustment are given by Syverud.[1] Input included a calorimetric link to $NF_3(g)$ and $CF_4(g)$ plus an equilibrium link to $C_2F_6(g)$ and $C_2N_2(g)$. The calorimetric study[2] gave $\Delta_r H° = -824.4 \pm 0.6\ kcal \cdot mol^{-1}$ at 298.15 K for the reaction $3CF_3CN(g) + 5NF_3(g) \rightarrow 6CF_4(g) + 4N_2(g)$. Equilibrium data[3] in the range 865–925 K give $\Delta_r H°$(3rd law) = 10.59 and $\Delta_r H°$(2nd law) = $10.59 \pm 0.20\ kcal \cdot mol^{-1}$ at 298.15 K for the reaction $C_2F_6(g) + C_2N_2(g) \rightarrow 2CF_3CN(g)$. The entropy difference, $\Delta_r S°$ (2nd law)–$\Delta_r S°$ (3rd law), is $0.0 \pm 1.5\ cal \cdot K^{-1} \cdot mol^{-1}$. Deviations between the selected $\Delta_f H°$ and the two observations are 1.37 and 0.15 $kcal \cdot mol^{-1}$, respectively, both considerably less than the overall uncertainties including those in auxiliary values of $\Delta_f H°$. Subsequent to the adjustment, Cumutt and Sinke[4] reported $\Delta_r H° = -197.6 \pm 0.9\ kcal \cdot mol^{-1}$ from a calorimetric study of $CF_3CN(g) + 1.25\ O_2(g) + 1.5\ H_2O(l) \rightarrow 2\ CO_2(g) + 0.5\ N_2(g) + 3HF(aq, 120\ H_2O)$. Their result of $\Delta_f H° = -118.4 \pm 1.2\ kcal \cdot mol^{-1}$ is confirmation of the selected value.

Heat Capacity and Entropy

The molecular structure has been derived from electron–diffraction data by Danford and Livingston[5] and from microwave data by Sheridan and Gordy[6] and Thomas *et al.*[7] These studies are in substantial agreement except for a difference of about 0.04 Å in the C–C bond distance. We adopt the results of Thomas *et al.*[7] since they are based on data for several isotopic species. Principal moments of inertia are: $I_A = 14.6267 \times 10^{-39}$ and $I_B = I_C = 28.4842 \times 10^{-39}\ g \cdot cm^2$. Vibrational frequencies are taken from the assignments of Edgell and Potter.[8] All values except ν_8 are from infrared spectra of the vapor phase. Raman spectra of the liquid provide $_8$and confirm the infrared data. Similar assignments have been given by Janz and Wait[9] based on spectra of Wait and Janz.[10]

Pace and Bobka[11] used low temperature calorimetric data to derive the entropy of the ideal gas at the normal boiling point of 205.47 K. The experimental value of $65.01 \pm 0.2\ cal \cdot K^{-1} \cdot mol^{-1}$ is in good agreement with $65.03\ cal \cdot K^{-1} \cdot mol^{-1}$ obtained from this table. The largest uncertainty in $C_p°$ and $S°$ probably arises from neglect of anharmonicity and rotational distortion. Uncertainty in the entropy is estimated to vary from 0.1 to 0.5 $cal \cdot K^{-1} \cdot mol^{-1}$ over the range 300 to 1000 K. Discussions of the neglect of anharmonicity are given on the tables for $CClF_3(g)$ and $CF_4(g)$.

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Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−15.897	−491.608	−491.608	INFINITE
100	43.761	234.503	356.929	−12.243	−493.884	−483.598	252.606
200	62.441	270.513	305.210	−6.939	−495.083	−472.759	123.472
250	71.031	285.389	299.782	−3.598	−495.314	−467.147	97.605
298.15	78.255	298.533	298.533	0.	−495.386	−461.713	80.890
300	78.513	299.017	298.534	0.145	−495.386	−461.505	80.355
350	84.951	311.616	299.514	4.236	−495.349	−455.859	68.033
400	90.470	323.330	301.768	8.625	−495.239	−450.225	58.793
450	95.200	334.266	304.778	13.270	−495.084	−444.607	51.609
500	99.263	344.512	308.244	18.134	−494.902	−439.008	45.863
600	105.795	363.216	315.878	28.402	−494.492	−427.867	37.249
700	110.730	379.912	323.855	39.240	−494.049	−416.797	31.102
800	114.522	394.956	331.818	50.510	−493.589	−405.793	26.496
900	117.482	408.623	339.604	62.116	−493.122	−394.846	22.916
1000	119.823	421.126	347.140	73.986	−492.653	−383.952	20.056
1100	121.700	432.638	354.396	86.066	−492.190	−373.104	17.717
1200	123.221	443.295	361.366	98.314	−491.737	−362.298	15.770
1300	124.468	453.208	368.054	110.701	−491.299	−351.529	14.125
1400	125.500	462.471	374.471	123.201	−490.881	−340.794	12.715
1500	126.362	471.160	380.630	135.795	−490.486	−330.087	11.495
1600	127.089	479.339	386.547	148.469	−490.115	−319.406	10.428
1700	127 706	487.063	392.234	161.209	−489.769	−308.748	9.487
1800	128.234	494.378	397.707	174.007	−489.449	−298.109	8.651
1900	128.690	501.324	402.980	186.854	−489.153	−287.487	7.904
2000	129.084	507.935	408.064	199.743	−488.879	−276.880	7.231
2100	129.428	514.241	412.971	212.669	−488.623	−266.287	6.624
2200	129.730	520.270	417.712	225.627	−488.382	−255.705	6.071
2300	129.996	526.042	422.297	238.614	−488.152	−245.134	5.567
2400	130.232	531.580	426.736	251.625	−487.927	−234.572	5.105
2500	130.441	536.901	431.037	264.659	−487.704	−224.021	4.681
2600	130.629	542.020	435.208	277.713	−487.477	−213.478	4.289
2700	130.797	546.954	439.256	290.784	−487.241	−202.944	3.926
2800	130.948	551.713	443.188	303.872	−486.993	−192.419	3.590
2900	131.084	556.311	447.010	316.973	−486.729	−181.903	3.276
3000	131.208	560.757	450.727	330.088	−486.445	−171.396	2.984
3100	131.320	565.061	454.347	343.214	−486.139	−160.900	2.711
3200	131.422	569.232	457.872	356.352	−485.807	−150.413	2.455
3300	131.516	573.277	461.308	369.499	−485.448	−139.938	2.215
3400	131.601	577.205	464.659	382.654	−485.060	−129.474	1.989
3500	131.680	581.021	467.930	395.819	−484.642	−119.021	1.776
3600	131.752	584.731	471.123	408.990	−484.192	−108.581	1.575
3700	131.819	588.342	474.242	422.169	−483.710	−98.154	1.386
3800	131.881	591.858	477.291	435.354	−483.197	−87.741	1.206
3900	131.938	595.285	480.273	448.545	−482.651	−77.340	1.036
4000	131.991	598.626	483.190	461.741	−482.073	−66.955	0.874
4100	132.040	601.885	486.046	474.943	−481.464	−56.585	0.721
4200	132.086	605.068	488.842	488.149	−480.824	−46.229	0.575
4300	132.128	608.176	491.581	501.360	−480.153	−35.890	0.436
4400	132.168	611.214	494.266	514.575	−479.454	−25.566	0.304
4500	132.206	614.185	496.898	527.793	−478.726	−15.259	0.177
4600	132.241	617.091	499.479	541.016	−477.970	−4.968	0.056
4700	132.274	619.936	502.012	554.241	−477.189	5.307	−0.059
4800	132.304	622.721	504.498	567.470	−476.382	15.564	−0.169
4900	132.333	625.449	506.938	580.702	−475.552	25.804	−0.275
5000	132.361	628.123	509.335	593.937	−474.699	36.027	−0.376
5100	132.386	630.744	511.690	607.174	−473.825	46.233	−0.474
5200	132.411	633.315	514.005	620.414	−472.930	56.422	−0.567
5300	132.434	635.837	516.280	633.656	−472.017	66.593	−0.656
5400	132.455	638.313	518.517	646.901	−471.086	76.747	−0.742
5500	132.476	640.744	520.717	660.147	−470.138	86.883	−0.825
5600	132.495	643.131	522.882	673.396	−469.175	97.002	−0.905
5700	132.514	645.476	525.012	686.646	−468.198	107.103	−0.981
5800	132.531	647.781	527.109	699.899	−467.208	117.187	−1.055
5900	132.548	650.047	529.173	713.153	−466.207	127.256	−1.127
6000	132.564	652.275	531.207	726.408	−465.195	137.305	−1.195

PREVIOUS. December 1969 (1 atm) CURRENT: December 1969 (1 bar)

Tetrafluoroethene (C_2F_4) IDEAL GAS $M_r = 100.015612$ Tetrafluoroethene (C_2F_4) $C_2F_4(g)$

$S°(298.15\ K) = 300.015 \pm 0.4\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -655.14 \pm 2.9\ kJ{\cdot}mol^{-1}$

$\Delta_f H°(298.15\ K) = -658.56 \pm 2.9\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
1872(1)	1340(1)	1337(1)
778(1)	551(1)	218(1)
394(1)	406(1)	1186(1)
190(1)	508(1)	558(1)

Ground State Quantum Weight: 1 $\sigma = 4$
Point Group: D_{2h}
Bond Distances: C–F = 1.313 Å; C–C = 1.313 Å
Bond Angle: F–C–F = 114°
Product of the Moments of Inertia: $I_A I_B I_C = 1.588028 \times 10^{-113}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The selected value is obtained from least squares, simultaneous adjustment of the heats of formation of CF_3, CF_3X (X = H, Cl, Br, I, CF_3) and C_2F_4. Details of the input data and the adjustment are given in[1]. In this case, the selected $\Delta_f H°$ corresponds to the weighted average of three calorimetric studies[2,3] which may be reduced to the following:

Source	Reaction	$\Delta_r H°$(298.15 K) kcal·mol^{-1}	$\Delta_f H°$(298.15 K) kcal·mol^{-1}
2	$C_2F_4(g) \rightarrow CF_4(g) + C(graphite)$	−65.4 ± 0.5	−157.6 ± 0.6
2	$C_2F_4(g) + 2H_2(g) \rightarrow 4HF(50\ H_2O) + 2C(graphite)$	−150.9 ± 1.2	−156.2 ± 1.3
3	$C_2F_4(g) + 4Na(cr) \rightarrow 4NaF(cr) + 2C(graphite)$	−392.9 ± 1.3	−157.2 ± 1.4

Amorphous carbon was formed in all three calorimetric reactions and separate combustions were made to refer the observed product to the standard state of graphite. Other calorimetric studies[4,5,6] are omitted because of apparent uncertainties in the reductions to the standard-state reactions.

Heat Capacity and Entropy

The molecular structure has been derived from electron-diffraction data by Karle and Karle,[7] Broun and Livingston[8] and Young.[9] The resulting structures differ in minor respects, particularly in the exact location of the two carbons. Values from Karle[7] are adopted since they are intermediate between the others. Values from Young[9] and Broun and Livingston[8] correspond to changes of ±2.2% in the product of the moments of inertia. Principal moments of inertia for the adopted structure are: $I_A = 15.3019 \times 10^{-39}$, $I_B = 25.4600 \times 10^{-39}$ and $I_C = 40.7619 \times 10^{-39}\ g{\cdot}cm^2$. Vibrational fundamentals are those selected by Shimanouchi[10] from the data of Mann *et al.*,[11] Monfils and Duchesne[12] and Nielsen *et al.*[13]

Furukawa *et al.*[14] reported low-temperature calorimetric data from which the ideal gas entropy may be derived as 64.54 ± 0.09 cal·K^{-1}·mol^{-1} at 197.53 K. The calculated entropy from this table is also 64.54 cal·K^{-1}·mol^{-1}. The range in values of $I_A I_B I_C$ corresponds to an entropy change of ±0.022 cal·K^{-1}·mol^{-1}.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−16.330	−655.140	−655.140	INFINITE
100	44.191	233.706	360.595	−12.689	−657.432	−646.538	337.717
200	65.202	270.959	306.921	−7.192	−658.446	−635.144	165.883
250	73.646	286.445	301.303	−3.715	−658.565	−629.302	131.485
298.15	80.458	300.015	300.015	0.	−658.562	−623.665	109.263
300	80.698	300.514	300.017	0.149	−658.560	−623.448	108.552
350	86.707	313.416	301.022	4.338	−658.491	−617.601	92.172
400	91.903	325.342	303.326	8.806	−658.387	−611.767	79.889
450	96.426	336.433	306.396	13.517	−658.267	−605.946	70.336
500	100.373	346.802	309.923	18.439	−658.138	−600.140	62.696
600	106.824	365.699	317.676	28.814	−657.867	−588.565	51.239
700	111.747	382.553	325.762	39.753	−657.577	−577.037	43.059
800	115.524	397.732	333.826	51.125	−657.266	−565.553	36.927
900	118.450	411.515	341.704	62.830	−656.939	−554.108	32.160
1000	120.743	424.118	349.324	74.794	−656.601	−542.700	28.348
1100	122.561	435.715	356.658	86.963	−656.259	−531.327	25.231
1200	124.020	446.444	363.699	99.294	−655.922	−519.984	22.634
1300	125.206	456.419	370.452	111.758	−655.595	−508.669	20.439
1400	126.179	465.735	376.929	124.328	−655.285	−497.380	18.557
1500	126.986	474.468	383.143	136.988	−654.995	−486.111	16.928
1600	127.662	482.686	389.110	149.721	−654.729	−474.860	15.503
1700	128.233	490.443	394.845	162.517	−654.489	−463.626	14.245
1800	128.720	497.787	400.362	175.365	−654.274	−452.405	13.128
1900	129.137	504.758	405.675	188.258	−654.082	−441.196	12.129
2000	129.498	511.391	410.796	201.191	−653.911	−429.995	11.230
2100	129.811	517.717	415.738	214.156	−653.757	−418.804	10.417
2200	130.085	523.762	420.512	227.152	−653.614	−407.619	9.678
2300	130.326	529.550	425.128	240.172	−653.477	−396.440	9.003
2400	130.539	535.102	429.595	253.216	−653.339	−385.268	8.385
2500	130.728	540.434	433.923	266.279	−653.195	−374.101	7.816
2600	130.896	545.565	438.119	279.361	−653.038	−362.940	7.292
2700	131.047	550.508	442.190	292.458	−652.862	−351.786	6.806
2800	131.182	555.276	446.144	305.570	−652.662	−340.639	6.355
2900	131.305	559.882	449.987	318.694	−652.432	−329.499	5.935
3000	131.415	564.335	453.725	331.830	−652.167	−318.368	5.543
3100	131.515	568.646	457.363	344.977	−651.865	−307.246	5.177
3200	131.607	572.823	460.906	358.133	−651.521	−296.135	4.834
3300	131.690	576.874	464.359	371.298	−651.132	−285.035	4.512
3400	131.766	580.806	467.727	384.471	−650.697	−273.947	4.209
3500	131.836	584.627	471.012	397.651	−650.214	−262.873	3.923
3600	131.901	588.342	474.220	410.838	−649.681	−251.813	3.654
3700	131.960	591.957	477.354	424.031	−649.097	−240.770	3.399
3800	132.015	595.476	480.416	437.230	−648.463	−229.743	3.158
3900	132.066	598.906	483.410	450.434	−647.778	−218.732	2.930
4000	132.113	602.250	486.340	463.643	−647.042	−207.740	2.713
4100	132.156	605.513	489.207	476.856	−646.257	−196.768	2.507
4200	132.197	608.698	492.014	490.074	−645.422	−185.814	2.311
4300	132.235	611.809	494.764	503.295	−644.539	−174.882	2.124
4400	132.270	614.850	497.459	516.521	−643.609	−163.970	1.947
4500	132.303	617.823	500.101	529.749	−642.633	−153.080	1.777
4600	132.334	620.731	502.692	542.981	−641.613	−142.212	1.615
4700	132.363	623.577	505.233	556.216	−640.550	−131.367	1.460
4800	132.391	626.364	507.728	569.454	−639.446	−120.545	1.312
4900	132.416	629.094	510.177	582.694	−638.301	−109.746	1.170
5000	132.440	631.770	512.582	595.937	−637.118	−98.971	1.034
5100	132.463	634.393	514.945	609.182	−635.899	−88.220	0.904
5200	132.484	636.965	517.267	622.430	−634.644	−77.493	0.778
5300	132.505	639.489	519.549	635.679	−633.356	−66.791	0.658
5400	132.524	641.966	521.793	648.930	−632.036	−56.114	0.543
5500	132.542	644.398	524.001	662 184	−630.686	−45.461	0.432
5600	132.559	646 786	526.172	675.439	−629.307	−34.833	0.325
5700	132.575	649.132	528.309	688.696	−627.900	−24.231	0.222
5800	132.591	651 438	530.412	701.954	−626.468	−13.652	0.123
5900	132.606	653.705	532.482	715.214	−625.011	−3.098	0.027
6000	132.620	655.934	534.521	728.475	−623.532	7.430	−0.065

PREVIOUS. June 1969 (1 atm) CURRENT: June 1969 (1 bar)

Hexafluoroethane (C_2F_6) IDEAL GAS M_r = 138.012418 Hexafluoroethane (C_2F_6) $C_2F_6(g)$

$\Delta_fH°(0\ K) = -1335.6 \pm 5.0\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = 332.185 \pm 0.8\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_fH°(298.15\ K) = -1343.9 \pm 5.0\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
1228(1)	1117(1)	376(2)
807(1)	714(1)	1251(2)
348(1)	1243(2)	523(2)
Torsion	619(2)	220(2)

Ground State Quantum Weight: 1 $\sigma = 6$
Point Group: D_{3d}
Bond Distances: C–F = 1.32 Å; C–C = 1.56 Å
Bond Angle: C–C–F = 109.5 ± 1.5°
Product of the Moments of Inertia: $I_AI_BI_C = 6\ 005449 \times 10^{-113}\ g^3 \cdot cm^6$
Reduced Moment of Inertia: $I_{red} = 7.32 \times 10^{-39}\ g\ cm^2$
Barrier to Internal Rotation: $V = 3.96\ kcal \cdot mol^{-1}$

Enthalpy of Formation

The selected value is obtained from least squares, simultaneous adjustment of the heats of formation of CF_3, CF_3X (X = H, Cl, Br, I, CF_3) and C_2F_4. Details of the input data and the adjustment are given in.[1] Data pertinent to C_2F_6 are summarized below. Calorimetric data[7] for the reaction of C_2F_6 with potassium were omitted from the adjustment due to insufficient characterization of the products.

Source	Method	Reaction	$\Delta_rH°$(298.15 K) kcal^{-1}·mol^{-1}	$\Delta_fH°$(298.15K) kcal^{-1}·mol^{-1}
[2]	Calorimetric	$3\ C_2F_6(g) + 2\ NF_3(g) \rightarrow 6\ CF_4(g) + N_2(g)$	−311.6 ± 3.0	−321.3 ± 1.2
[3]	Calorimetric	$3\ CF_3CN(g) + 5\ NF_3(g) \rightarrow 6\ CF_4(g) + 4\ N_2(g)$	−824.4 ± 0.6	—
[4]	Equilibrium	$2\ CF_3CN(g) \rightarrow C_2F_6(g) + C_2N_2(g)$	−10.59 ± 0.5	−322.2 ± 1.8
[5]	Equilibrium	$C_2F_6(g) + Br_2(g) \rightarrow 2\ CBrF_3(g)$	3.30 ± 0.7	−320.9 ± 1.6
[6,5]	Kinetic	$C_2F_6(g) \rightarrow 2\ CF_3(g)$	97.6 ± 6	−322.4 ± 6

Heat Capacity and Entropy

The adopted molecular structure was derived from electron–diffraction data by Swick and Karle.[8] The vibrational frequencies are from the assignment of Carney *et al.*,[9] who reviewed the extensive spectral data. Shimanouchi[10] has selected the same frequencies. Low–temperature calorimetric data were used by Pace and Aston[11] to derive a value for the entropy of the ideal gas of 69.88 ± 0.20 cal·K^{-1}·mol^{-1} at 194.87 K. This value is used to fix the barrier to internal rotation at 3960 cal/mol. Thermodynamic functions are calculated from these parameters, using hindered internal rotation in place of a torsional vibration. Principal moments of inertia are: $I_A = 29.3165 \times 10^{-39}$, and $I_B = I_C = 45.2602 \times 10^{-39}\ g \cdot cm^2$.

An uncertainty of ±0.2 cal·K^{-1}·mol^{-1} in the 3rd law entropy corresponds to a variation in the barrier to internal rotation of about ±700 cal·mol^{-1}. This range easily includes the barrier of 4300 cal·mol^{-1} derived by Karle[12] from analysis of the electron–diffraction data.[8] Uncertainty in the entropy of this table should not exceed 0.5 cal·K^{-1}·mol^{-1} at 1000 K.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−20.255	−1335.579	−1335.579	INFINITE
100	53.137	248.355	409.522	−16.117	−1340.281	−1313.815	686.267
200	82.437	294.717	341.306	−9.318	−1342.922	−1286.241	335.932
298.15	106.407	332.185	332.185	0.	−1343.901	−1258.134	220.420
300	106.809	332.845	332.187	0.197	−1343.909	−1257.602	218.968
400	125.545	366.266	336.617	11.859	−1343.950	−1228.806	160.466
500	139.139	395.825	345.562	25.132	−1343 428	−1200.072	125.371
600	148.708	422.089	356.170	39.551	−1342.585	−1171.476	101.986
700	155.465	445.549	367.293	54.779	−1341.558	−1143.037	85.294
800	160.310	466.640	378.416	70.579	−1340.428	−1114.753	72.786
900	163.804	485.732	389.296	86.792	−1339.247	−1086 614	63.065
1000	166.486	503.134	399.823	103.311	−1338.044	−1058.608	55.296
1100	168.458	519.097	409.951	120.061	−1336.841	−1030.723	48.945
1200	170.088	533.827	419.668	136.991	−1335.652	−1002.946	43.657
1300	171.296	547.490	428.981	154.062	−1334.487	−975.268	39.187
1400	172.318	560.223	437.906	171.244	−1333.356	−947.679	35.358
1500	173.114	572.140	446.462	188.517	−1332.263	−920.169	32.043
1600	173.808	583.335	454 670	205.864	−1331.213	−892.731	29.145
1700	174.312	593.887	462.552	223.270	−1330.207	−865.356	26.589
1800	174.770	603.864	470.128	240.725	−1329.245	−838.040	24.319
1900	175.182	613.325	477.418	258.222	−1328.321	−810.777	22.290
2000	175.548	622.320	484.440	275.759	−1327.426	−783.560	20.465
2100	175.816	630.891	491.211	293.328	−1326.556	−756.389	18.814
2200	176.065	639.076	497.748	310.922	−1325.704	−729.258	17.315
2300	176.293	646.908	504.064	328.540	−1324.858	−702.166	15.947
2400	176.502	654.415	510.173	346.180	−1324.007	−675.110	14.693
2500	176.690	661.624	516.088	363.840	−1323.141	−648.091	13.541
2600	176.839	668.557	521.820	381.516	−1322.251	−621.106	12.478
2700	176.978	675.234	527.379	399.207	−1321.328	−594.156	11.495
2800	177.107	681.672	532.775	416.912	−1320.362	−567.242	10.582
2900	177.226	687.889	538.017	434.628	−1319.346	−540.362	9.733
3000	177.335	693.899	543.114	452.356	−1318.271	−513.519	8.941
3100	177.426	699.716	548.072	470.095	−1317.131	−486.713	8.201
3200	177.511	705.350	552.900	487.841	−1315.923	−459.944	7.508
3300	177.590	710.814	557.602	505.597	−1314.640	−433.214	6.857
3400	177.662	716.116	562.187	523.359	−1313.279	−406.525	6.245
3500	177.728	721.267	566.659	541.129	−1311.838	−379.876	5.669
3600	177.783	726.275	571.024	558.904	−1310.315	−353.270	5.126
3700	177.834	731.146	575.286	576.685	−1308.708	−326.707	4.612
3800	177.881	735.890	579.450	594.471	−1307.017	−300.190	4.126
3900	177.924	740.511	583.521	612.261	−1305.242	−273.717	3.666
4000	177.962	745.016	587.502	630.056	−1303.384	−247.291	3.229
4100	177.994	749.411	591.398	647.853	−1301.442	−220.913	2.814
4200	178.022	753.700	595.211	665.654	−1299.419	−194.582	2.420
4300	178.048	757.889	598.946	683.458	−1297.316	−168.302	2.044
4400	178.071	761.983	602.605	701.264	−1295.134	−142.071	1.687
4500	178.092	765.985	606.191	719.072	−1292.875	−115.889	1.345
4600	178.108	769.899	609.708	736.882	−1290.542	−89.760	1.019
4700	178.122	773.730	613.157	754.693	−1288.136	−63.682	0.708
4800	178.135	777.480	616.541	772.506	−1285.661	−37.655	0.410
4900	178.146	781.153	619.863	790.320	−1283.117	−11.682	0.125
5000	178.155	784.752	623.125	808.135	−1280.509	14.239	−0.149
5100	178.159	788.280	626.329	825.951	−1277.837	40.108	−0.411
5200	178.163	791.740	629.477	843.767	−1275.105	65.924	−0.662
5300	178.167	795.134	632.571	861.584	−1272.314	91.687	−0.904
5400	178.171	798.464	635.612	879.401	−1269.468	117.396	−1.136
5500	178.176	801.733	638.603	897.218	−1266.568	143.051	−1.359
5600	178.180	804.944	641.545	915.036	−1263.617	168.655	−1.573
5700	178.184	808.098	644.439	932.854	−1260.616	194.203	−1.780
5800	178.188	811.197	647.288	950.673	−1257.568	219.699	−1.979
5900	178 192	814.243	650.092	968.492	−1254.475	245.145	−2.170
6000	178.197	817.238	652.852	986.311	−1251.339	270.535	−2.355

PREVIOUS. June 1969 (1 atm) CURRENT· June 1969 (1 bar)

Ethynyl (C_2H) IDEAL GAS $M_r = 25.02994$ Ethynyl (C_2H) $C_2H_1(g)$

$S°(298.15\ K) = [207.444 \pm 5.4]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [473.9 \pm 29]\ kJ{\cdot}mol^{-1}$

$\Delta_f H°(298.15\ K) = [477.0 \pm 29]\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights ϵ_i, cm^{-1}	g_i
0	[2]
[9000]	[4]

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[1920](1)
[640](2)
[3220](1)

Point Group: $[C_{\infty v}]$ $\sigma = 1$

Bond Distances: C–C = [1.207] Å; C–H = [1.061] Å

Bond Angle C–C–H = [180]°

Rotational Constant: B_0 = [1 474960] cm^{-1}

Enthalpy of Formation

The enthalpy of formation of $C_2H(g)$ is not well established; however, we can place reliable upper and lower limits on the value.

Cottrell,[1] gives an upper limit for the C–H bond dissociation energy in acetylene, $\Delta_a H°$(HCC–H) <121 kcal·mol^{-1}. This was obtained from the fact that ultra violet light of 121 kcal·mol^{-1} energy causes acetylene to from diacetylene and hydrogen; assuming that this process occurs through the CCH radical, the light energy is equated with $\Delta_a H°$(HCC–H). This value of $\Delta_a H°$ (HCC–H) gives an upper limit for $\Delta_f H°$(CCH, g, 298.15 K) <123 kcal·mol^{-1}.

A lower limit for $\Delta_a H°$(HCC–H) is obtained from a consideration of the C–H bond dissociation energies in ethylene and ethane, $\Delta_a H°(C_2H_3–H)$ = 103 kcal·mol^{-1} and $\Delta_a H°(C_2H_5–H)$ = 98 kcal·mol^{-1}. The heats of formation of the C_2H_3 and C_2H_5 radicals and their parent compounds are taken from Benson.[2] The vibrational frequency of the C–H stretch increases steadily form ethane to ethylene and acetylene. Similarly we expect the bond strength to increase, and so $\Delta_a H°$(HCC–H) >103 kcal·mol^{-1}; this yields $\Delta_f H°$(CCH, g, 298.15 K) >105 kcal·mol^{-1}.

Coats and Anderson,[3] obtained several values for $\Delta_f H°$(CCH, g, 298.15 K) from mass–spectroscopic measurements; their values range from 110 kcal·mol^{-1} to 153 kcal·mol^{-1}, but they chose to adopt 112 ± 3 kcal·mol^{-1}.

Our adopted value of $\Delta_f H°$(CCH, g, 298.15 K), 114 ± 7 kcal·mol^{-1}, (476.976 ± 29 kJ mol^{-1}), is 2 kcal·mol^{-1} smaller than that estimated by Tsang *et al.*[4]

Heat Capacity and Entropy

The molecule is assumed to be linear; the bond lengths are assumed to be the same as in acetylene and were taken from Sutton.[5]

The vibrational frequencies are those estimated by Plooster and Reed.[6] It should be noted that the values of the free energy function given by Plooster and Reed[6] are incorrect due to the neglect of the electronic contributions.

The electronic levels, $X^2\Sigma$ and $A^2\Pi$, were estimated by analogy with those of CN(g) which is isoelectronic, this assumption holds very well in the parent molecules HCCH and HCN.[7] The molecule $C_2H_2^+$, which is also isoelectronic with CCH, is predicted to have a $^2\Pi$ ground state by Herzberg.[7]

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ J·K^{-1}mol^{-1}	$S°$ J·K^{-1}mol^{-1}	$-[G°-H°(T_r)]/T$ J·K^{-1}mol^{-1}	$H°-H°(T_r)$ kJ·mol^{-1}	$\Delta_f H°$ kJ·mol^{-1}	$\Delta_f G°$ kJ·mol^{-1}	log K_f
0	0.	0.	INFINITE	−9.404	473.908	473.908	INFINITE
100	29.242	172.435	237.415	−6.498	475.195	463.178	−241.940
200	32.702	193.530	210.703	−3.435	476.258	450.726	−117.718
250	35.084	201.087	208.044	−1.739	476 664	444.295	−92.830
298.15	37.104	207.444	207.444	0.	476.976	438.031	−76.741
300	37.175	207.673	207.444	0.069	476.986	437.789	−76.226
350	38.922	213.539	207.904	1.972	477.224	431.236	−64.358
400	40.395	218.835	208.944	3.956	477.376	424.655	−55.454
450	41.675	223 669	210.316	6.009	477.441	418.060	−48.527
500	42.818	228.120	211.877	8.122	477.426	411.463	−42.985
600	44.837	236.109	215.265	12.507	477.190	398.288	−34.674
700	46.615	243.157	218.755	17.081	476.750	385.170	−28.742
800	48.212	249.487	222.208	21.824	476.174	372.125	−24.297
900	49.651	255.251	225.564	26.718	475.512	359.158	−20.845
1000	50.943	260.550	228.801	31.749	474.795	346.268	−18.087
1100	52.102	265.461	231.913	36.902	474.041	333.451	−15.834
1200	53.142	270.040	234.902	42.165	473.263	320.705	−13.960
1300	54.081	274.331	237.771	47.527	472.466	308.024	−12.377
1400	54.935	278.370	240.528	52.979	471.656	295.405	−11.022
1500	55.720	282.188	243.180	58.512	470.837	282.844	−9.849
1600	56.451	285.807	245.732	64.121	470.010	270.338	−8.826
1700	57.140	289.251	248.191	69.801	469.179	257.884	−7.924
1800	57.795	292.535	250.564	75.548	468.346	245.478	−7.124
1900	58.424	295.677	252.857	81.359	467.512	233.120	−6.409
2000	59.032	298.689	255.073	87.232	466.681	220.805	−5.767
2100	59.622	301.584	257.220	93.165	465.854	208.531	−5.187
2200	60.194	304.371	259.300	99.156	465.032	196.297	−4.661
2300	60 750	307 059	261.318	105.203	464.217	184.100	−4.181
2400	61.289	309.656	263.279	111.305	463.409	171.938	−3.742
2500	61.810	312.168	265.184	117.460	462.609	159.810	−3.339
2600	62.313	314.602	267.038	123.666	461.817	147.714	−2.968
2700	62.796	316.963	268.844	129.922	461.032	135.648	−2.624
2800	63.258	319.255	270.604	136.225	460.254	123.611	−2.306
2900	63.698	321.483	272.320	142.573	459.482	111.602	−2.010
3000	64.115	323.649	273.995	148.964	458.715	99.619	−1 735
3100	64.509	325.758	275.631	155.395	457.951	87.662	−1.477
3200	64.878	327.812	277.230	161.865	457.190	75.729	−1.236
3300	65.223	329.814	278.793	168.370	456.428	63.820	−1.010
3400	65.544	331.766	280.322	174.909	455.666	51.934	−0.798
3500	65.840	333.670	281.819	181.478	454 900	40.071	−0.598
3600	66.113	335.529	283.286	188.076	454.128	28.230	−0.410
3700	66.362	337.344	284.722	194.700	453.350	16.410	−0.232
3800	66.588	339.117	286.130	201.347	452.562	4 611	−0.063
3900	66.792	340.849	287.511	208.017	451.763	−7.166	0.096
4000	66.975	342.542	288.866	214.705	450.952	−18.924	0.247
4100	67.138	344.198	290.195	221.411	450.126	−30.660	0.391
4200	67.281	345.818	291.501	228.132	449.284	−42.376	0.527
4300	67.407	347.402	292.782	234.867	448.424	−54.073	0.657
4400	67.515	348.953	294.041	241.613	447.544	−65.748	0.781
4500	67.607	350.472	295.278	248.369	446.644	−77.404	0.898
4600	67.684	351.958	296.495	255.134	445.722	−89.040	1.011
4700	67.746	353.415	297.690	261.905	444.777	−100.655	1.119
4800	67.796	354.842	298.866	268.683	443.807	−112.249	1.222
4900	67.834	356.240	300.023	275.464	442.812	−123.824	1.320
5000	67.860	357.611	301.161	282.249	441.792	−135.377	1.414
5100	67.876	358.955	302.281	289.036	440.744	−146.910	1.505
5200	67.882	360.273	303.383	295.824	439.669	−158.422	1.591
5300	67.880	361.566	304.469	302.612	438.567	−169.914	1.675
5400	67.871	362.834	305.538	309.400	437.436	−181.384	1.755
5500	67.854	364.080	306.591	316.186	436.276	−192.833	1.831
5600	67.830	365.302	307.629	322.970	435.087	−204.261	1.905
5700	67.801	366.502	308.651	329.752	433.870	−215.667	1.976
5800	67.766	367.681	309.659	336.530	432.623	−227.051	2.045
5900	67.727	368.839	310.652	343.305	431.348	−238.414	2.111
6000	67.684	369.977	311.631	350.075	430.043	−249.755	2.174

PREVIOUS. March 1967 (1 atm) CURRENT: March 1967 (1 bar)

Ethynyl (C_2H) $C_2H_1(g)$

Chloroethyne (C_2HCl) IDEAL GAS M_r = 60.48294 Chloroethyne (C_2HCl) $C_2H_1Cl_1(g)$

$S°(298.15\ K) = 241.996\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [212.9 \pm 42]\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = [213.8 \pm 42]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	 ν, cm^{-1}
3340(1)	604(2)
2110(1)	326(2)
756(1)	

Ground State Quantum Weight: [1] $\sigma = 1$
Point Group: $C_{\infty v}$
Bond Distances: C–C = 1.204 Å; C–H = 1.055 Å; C–Cl = 1.637 Å
Bond Angles: Cl–C–C = 180°; C–C–H = 180°
Rotational Constant: $B_0 = 0.188645\ cm^{-1}$

Enthalpy of Formation

The value of $\Delta_f H°(298.15\ K) = 51.1\ kcal{\cdot}mol^{-1}$ is calculated from the estimated $\Delta_r H°(298.15\ K) = -53 \pm 10\ kcal{\cdot}mol^{-1}$ for $HCCCl(g) + Cl_2(g) \rightarrow CHCl{=}CCl_2(g)$, using $\Delta_f H°(CHCl{=}CCl_2, g, 298.15\ K) = -1.86\ kcal{\cdot}mol^{-1}$.[1] The value of $\Delta_r H°(298.15\ K)$ is assumed to be the same as that for the reaction $HCCH(g) + Cl\ (_2g) \rightarrow CHCl{=}CHCl(g)$, using $\Delta_f H°(C_2H_2, g, 298.15\ K) = 54.19\ kcal{\cdot}mol^{-1}$[1] and $\Delta_f H°(CHCl{=}CHCl, g, 298.15\ K) = 1.2\ kcal{\cdot}mol^{-1}$.[2]

Heat Capacity and Entropy

The linear molecular structure and bond distances were determined from the microwave spectrometrical studies by Tyler and Sheridan.[3] Their results are in good agreement with those of Westenberg *et al.*[4]

The vibrational frequencies were observed in the infrared spectra by Hunt and Wilson,[5] and Richardson and Goldstein.[6]

References

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[2] This is an average value of 0.9 and 1.47 $kcal{\cdot}mol^{-1}$ for cis– and trans– $CHCl = CHCl(g)$, respectively which are obtained from NBS.[1]
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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
0	0.	0.	INFINITE	−11.787	212.941	212.941	INFINITE
100	32.752	195.662	283.695	−8.803	212.851	207.961	−108.628
200	45.079	222.136	246.697	−4.912	213.223	202.966	−53.009
250	50.310	232.778	242.869	−2.523	213.513	200.369	−41.865
298.15	54.319	241.996	241.996	0.	213.802	197.811	−34.656
300	54.455	242.332	241.997	0.101	213.813	197.712	−34.425
350	57.682	250.979	242.672	2.907	214.094	195.006	−29.103
400	60.227	258.854	244.210	5.857	214.337	192.261	−25.107
450	62.290	266.071	246.244	8.922	214.527	189.490	−21.995
500	64.017	272.725	248.564	12.081	214.660	186.701	−19.504
600	66.824	284.655	253.608	18.629	214.771	181.095	−15.766
700	69.104	295.133	258.807	25.428	214.720	175.485	−13.095
800	71.050	304.491	263.943	32.438	214.562	169.889	−11.093
900	72.751	312.959	268.926	39.630	214.337	164.318	−9.537
1000	74.248	320.704	273.722	46.982	214.072	158.775	−8.294
1100	75.570	327.844	278.322	54.474	213.782	153.259	−7.278
1200	76.735	334.470	282.728	62.091	213.476	147.770	−6.432
1300	77.762	340.654	286.948	69.817	213.157	142.308	−5.718
1400	78.667	346.450	290.994	77.639	212.828	136.870	−5.107
1500	79.466	351.905	294.874	85.546	212.487	131.456	−4.578
1600	80.170	357.057	298.601	93.529	212.134	126.065	−4.116
1700	80.793	361.936	302.185	101.578	211.767	120.697	−3.709
1800	81.345	366.570	305.634	109.685	211.386	115.351	−3.347
1900	81.835	370.982	308.958	117.845	210.987	110.027	−3.025
2000	82.271	375.191	312.165	126.050	210.570	104.724	−2.735
2100	82.660	379.214	315.263	134.297	210.133	99.442	−2.473
2200	83.009	383.068	318.258	142.581	209.673	94.182	−2.236
2300	83.322	386.765	321.157	150.898	209.191	88.943	−2.020
2400	83.603	390.317	323.965	159.244	208.683	83.725	−1.822
2500	83.857	393.735	326.688	167.618	208.148	78.530	−1.641
2600	84.087	397.029	329.330	176.015	207.586	73.356	−1.474
2700	84.295	400.206	331.897	184 434	206.995	68.205	−1.319
2800	84.485	403.275	334.392	192.874	206.374	63.075	−1.177
2900	84.658	406.243	336.818	201.331	205.722	57.969	−1.044
3000	84.816	409.116	339.181	209.805	205.039	52.886	−0.921
3100	84.960	411.899	341.482	218.293	204.324	47.826	−0.806
3200	85.093	414.598	343.725	226.796	203.578	42.789	−0.698
3300	85.215	417.219	345.912	235.312	202.800	37.777	−0.598
3400	85.327	419.764	348.047	243.839	201.990	32.788	−0.504
3500	85.431	422.239	350.132	252.377	201.150	27.823	−0.415
3600	85.527	424.647	352.168	260.925	200.279	22.884	−0.332
3700	85.616	426.992	354.159	269.482	199.379	17.968	−0.254
3800	85.698	429.276	356.106	278.048	198.450	13.078	−0.180
3900	85.775	431.503	358.011	286.621	197.493	8.212	−0.110
4000	85.846	433.676	359.875	295.202	196.510	3.371	−0.044
4100	85.913	435.796	361.701	303.790	195.500	−1.445	0.018
4200	85.975	437.868	363.490	312.385	194.467	−6.236	0.078
4300	86.033	439.891	365.244	320.985	193.410	−11.002	0.134
4400	86.088	441.870	366.963	329.591	192.331	−15.744	0.187
4500	86.139	443.805	368.649	338.203	191.230	−20.460	0.237
4600	86.187	445.699	370.303	346.819	190.110	−25.152	0.286
4700	86.232	447.553	371.927	355.440	188.972	−29.820	0.331
4800	86.275	449.369	373.522	364.065	187.815	−34.463	0.375
4900	86.315	451.148	375.088	372.695	186 642	−39.081	0.417
5000	86.352	452.892	376.627	381.328	185.454	−43.676	0.456
5100	86.388	454.603	378.139	389.965	184.251	−48.247	0.494
5200	86.422	456.280	379.625	398.606	183.034	−52.793	0.530
5300	86.454	457.927	381.087	407.249	181.804	−57.317	0.565
5400	86.484	459.543	382.525	415.896	180.562	−61.817	0.598
5500	86.512	461.130	383.940	424.546	179.309	−66.294	0.630
5600	86.540	462.689	385.332	433.199	178.046	−70.748	0.660
5700	86.565	464.221	386.703	441.854	176.772	−75.180	0.689
5800	86.590	465.727	388.053	450.512	175.490	−79.588	0.717
5900	86.613	467.207	389.382	459.172	174.199	−83.975	0.743
6000	86.635	468.663	390.691	467.834	172.900	−88.341	0.769

PREVIOUS· December1968 (1 atm) CURRENT· December 1968 (1 bar)

Fluoroethyne (C_2HF) **IDEAL GAS** $M_r = 44.028343$ **Fluoroethyne (C_2HF)** **$C_2H_1F_1(g)$**

$S°(298.15\ K) = 231.611 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = [124.8 \pm 63]\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = [125.5 \pm 63]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
3360(1)
2250(1)
1060(1)
580(2)
367(2)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: $C_{\infty v}$
Bond Distances: C–F = 1.279 Å; C–C = 1.198 Å; C–H = 1.053 Å
Bond Angles: F–C–C = 180°; C–C–H = 180°
Rotational Constant: $B_0 = 0.323577\ cm^{-1}$

Enthalpy of Formation

The enthalpy of formation is estimated by assuming that the C–C bond strength is the average of those in C_2F_2(113 kcal·mol^{-1}) and C_2H_2(229 kcal·mol^{-1}). Combining the average value (171 kcal mol^{-1}) with the enthalpies of formation of CF and CH from the JANAF Tables, yields $\Delta_fH°(C_2HF, g, 298.15\ K) = 30 \pm 15$ kcal·mol^{-1}.

Heat Capacity and Entropy

Hunt and Wilson[1] and Brown and Tyler,[2] have reported the infrared spectrum and have assigned the fundamental frequencies. The frequencies used in the present table are median values of the two sets and are generally within 5 cm^{-1} of each set.

The molecule has been shown to be linear by Tyler and Sheridan,[3] who reported the rotational constant B_0.

The electronic ground is assumed to be $^1\Sigma$ by analogy with C_2H_2.

References

[1] G. R. Hunt and M. K. Wilson, J. Chem. Phys. 34, 1301 (1961).
[2] J. K. Brown and J. K. Tyler, Proc. Chem. Soc. (London) 1961, 13.
[3] J. K. Tyler an J. Sheridan, Trans. Faraday Soc. 59, 2661 (1963).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
0	0.	0.	INFINITE	−11.452	124.816	124.816	INFINITE
100	31.761	186.882	271.833	−8.495	124.701	119.758	−62.555
200	43.530	212.465	236.141	−4.735	124.996	114.742	−29.968
250	48.488	222.731	232.452	−2.430	125.261	112.149	−23.432
298.15	52.321	231.611	231.611	0.	125.520	109.600	−19.201
300	52.452	231.935	231.612	0.097	125.530	109.501	−19.066
350	55.619	240.268	232.263	2.802	125.774	106.810	−15.941
400	58.190	247.868	233.746	5.649	125.974	104.087	−13.592
450	60.324	254.849	235.708	8.613	126.118	101.342	−11.763
500	62.143	261.301	237.949	11.676	126.203	98.584	−10.299
600	65.147	272.907	242.830	18.046	126.216	93.055	−8.101
700	67.611	283.140	247.872	24.688	126.067	87.538	−6.532
800	69.723	292.309	252.863	31.557	125.813	82.051	−5.357
900	71.570	300.630	257.715	38.624	125.496	76.599	−4.446
1000	73.196	308.257	262.393	45.864	125.143	71.185	−3.718
1100	74.630	315.302	266.887	53.256	124.769	65.807	−3.125
1200	75.894	321.851	271.198	60.784	124.382	60.464	−2.632
1300	77.007	327.971	275.332	68.430	123.985	55.153	−2.216
1400	77.987	333.714	279.299	76.181	123.579	49.874	−1.861
1500	78.850	339.125	283.109	84.024	123.164	44.623	−1.554
1600	79.612	344.238	286.771	91.948	122.738	39.401	−1.286
1700	80.285	349.085	290.295	99.943	122.300	34.206	−1.051
1800	80.882	353.692	293.690	108.002	121.848	29.037	−0.843
1900	81.411	358.079	296.965	116.117	121.383	23.893	−0.657
2000	81.882	362.267	300.126	124.282	120.903	18.775	−0.490
2100	82.302	366.273	303.181	132.492	120.409	13.680	−0.340
2200	82.678	370.110	306.137	140.741	119.901	8.610	−0.204
2300	83.015	373.793	308.999	149.026	119.379	3.563	−0.081
2400	83.319	377.332	311.773	157.343	118.845	−1.461	0.032
2500	83.593	380.739	314.464	165.689	118.298	−6.463	0.135
2600	83.840	384.023	317.076	174.061	117.740	−11.442	0.230
2700	84.065	387.191	319.615	182.456	117.172	−16.400	0.317
2800	84.269	390.252	322.083	190.873	116.594	−21.337	0.398
2900	84.455	393.213	324.485	199.309	116.008	−26.252	0.473
3000	84.625	396.079	326.824	207.764	115.413	−31.148	0.542
3100	84.781	398.856	329.103	216.234	114.812	−36.024	0.607
3200	84.924	401.550	331.325	224.719	114.203	−40.879	0.667
3300	85.055	404.165	333.493	233.218	113.587	−45.716	0.724
3400	85.176	406.706	335.609	241.730	112.965	−50.534	0.776
3500	85.288	409.177	337.676	250.253	112.337	−55.334	0.826
3600	85.391	411.581	339.696	258.787	111.703	−60.115	0.872
3700	85.487	413.922	341.670	267.331	111.062	−64.879	0.916
3800	85.576	416.203	343.602	275.885	110.415	−69.626	0.957
3900	85.659	418.427	345.492	284.446	109.760	−74.355	0.996
4000	85.735	420.597	347.343	293.016	109.099	−79.068	1.033
4100	85.807	422.715	349.155	301.593	108.430	−83.764	1.067
4200	85.874	424.783	350.931	310.177	107.754	−88.443	1.100
4300	85.937	426.805	352.673	318.768	107.069	−93.107	1.131
4400	85.995	428.781	354.380	327.365	106.376	−97.754	1.160
4500	86.051	430.714	356.055	335.967	105.673	−102.385	1.188
4600	86.102	432.606	357.698	344.575	104.962	−107.001	1.215
4700	86.151	434.458	359.312	353.187	104.240	−111.601	1.240
4800	86.196	436.273	360.897	361.805	103.509	−116.186	1.264
4900	86.240	438.050	362.453	370.426	102.767	−120.755	1.287
5000	86.280	439.793	363.982	379.052	102.015	−125.309	1.309
5100	86.319	441.502	365.486	387.682	101.251	−129.848	1.330
5200	86.355	443.178	366.964	396.316	100.476	−134.372	1.350
5300	86.389	444.824	368.417	404.953	99.690	−138.881	1.369
5400	86.422	446.439	369.847	413.594	98.892	−143.374	1.387
5500	86.452	448.025	371.254	422.238	98.083	−147.854	1.404
5600	86.482	449.583	372.639	430.884	97.262	−152.318	1.421
5700	86.509	451.114	374.003	439.534	96.429	−156.767	1.437
5800	86.536	452.619	375.345	448.186	95.584	−161.202	1.452
5900	86.561	454.098	376.667	456.841	94.727	−165.622	1.466
6000	86.585	455.553	377.970	465.498	93.858	−170.027	1.480

PREVIOUS December 1967 (1 atm) CURRENT: December 1967 (1 bar)

Fluoroethyne (C_2HF) **$C_2H_1F_1(g)$**

Ethyne (C_2H_2) IDEAL GAS $M_r = 26.03788$ Ethyne (C_2H_2) $C_2H_2(g)$

$S°(298.15\ K) = 200.958\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 235.755 \pm 0.79\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 226.731 \pm 0.79\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
3373.7(1)
1973.8(1)
3281.9(1)
611.6(2)
729.3(2)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: $D_{\infty h}$
Rotational Constant $B_0 = 1.17684 \pm 0.00016\ cm^{-1}$

Spectroscopic constants used in calculating corrections to rigid rotator–harmonic oscillator approximation (cm^{-1}):

$x_{11} = -24.08$ $x_{22} = -7.92$ $x_{34} = -9.06$ $D_0 = 2.19 \times 10^{-6}$
$x_{12} = -16.94$ $x_{23} = -1.38$ $x_{35} = -5.73$ $g_{44} = 1.1$
$x_{13} = -99.01$ $x_{24} = -6.15$ $x_{44} = 5.38$ $g_{55} = 2.49$
$x_{14} = -16.46$ $x_{25} = -0.85$ $x_{45} = -12.65$
$x_{15} = -11.75$ $x_{33} = -25.69$ $x_{55} = -2.27$
Values of α, not available.

Enthalpy of Formation

Taken from Wagman *et al.*[1]

Heat Capacity and Entropy

Gordon[2] has used the constants listed above to calculate $C_p°$ from 298.15 K to 6000 K by the method of Pennington and Kobe.[3] The constants are from Bell and Nielsen[4] and Allen *et al.*[5] Heat capacities below 298.15 K have been calculated for a rigidly rotating harmonic oscillator.

References

[1]D. D. Wagman, J. E. Kilpatrick, K. S. Pitzer, and F. D. Rossini, J. Res. Nat. Bur. Stand. 35, 467 (1945).
2J. S. Gordon, personal communication, (February 1961).
[3]R. E. Pennington and K. A. Kobe, J. Chem. Phys. 22, 1442 (1954).
[4]E. E. Bell and H. H. Nielsen, J. Chem. Phys. 18, 1382 (1950).
[5]H. C. Allen, E. D. Tidewell and E. K. Plyler, J. Res. Nat. Bur. Stand. 57, 213 (1956).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.000	0.000	INFINITE	−10.012	227.288	227.288	INFINITE
100	29.347	163.294	234.338	−7.104	227.078	221.011	−115.444
200	35.585	185.097	204.720	−3.925	226.911	215.006	−56.154
298.15	44.095	200.958	200.958	0.000	226.731	209.200	−36.651
300	44.229	201.231	200.959	.082	226.728	209.092	−36.406
400	50.480	214.856	202.774	4.833	226.527	203.242	−26.541
500	54.869	226.610	206.393	10.108	226.227	197.452	−20.628
600	58.287	236.924	210.640	15.771	225.804	191.735	−16.692
700	61.149	246.127	215.064	21.745	225.294	186.097	−13.887
800	63.760	254.466	219.476	27.992	224.747	180.534	−11.788
900	66.111	262.113	223.794	34.487	224.198	175.041	−10.159
1000	68.275	269.192	227.984	41.208	223.669	169.607	−8.859
1100	70.245	275.793	232.034	48.136	223.170	164.226	−7.798
1200	72.053	281.984	235.941	55.252	222.705	158.888	−6.916
1300	73.693	287.817	239.709	62.540	222.275	153.588	−6.171
1400	75.178	293.334	243.344	69.985	221.877	148.319	−5.534
1500	76.530	298.567	246.853	77.572	221.506	143.078	−4.982
1600	77.747	303.546	250.242	85.286	221.160	137.861	−4.501
1700	78.847	308.293	253.518	93.117	220.833	132.665	−4.076
1800	79.852	312.829	256.688	101.053	220.521	127.487	−3.700
1900	80.760	317.171	259.758	109.084	220.222	122.327	−3.363
2000	81.605	321.335	262.733	117.203	219.931	117.182	−3.060
2100	82.362	325.335	265.620	125.401	219.647	112.052	−2.787
2200	83.065	329.183	268.422	133.673	219.367	106.935	−2.539
2300	83.712	332.890	271.145	142.012	219.088	101.830	−2.313
2400	84.312	336.465	273.793	150.414	218.809	96.738	−2.105
2500	84.858	339.918	276.369	158.873	218.527	91.658	−1.915
2600	85.370	343.256	278.878	167.384	218.242	86.589	−1.740
2700	85.846	346.487	281.322	175.945	217.950	81.530	−1.577
2800	86.295	349.618	283.706	184.553	217.652	76.483	−1.427
2900	86.713	352.653	286.031	193.203	217.346	71.447	−1.287
3000	87.111	355.600	288.301	201.895	217.030	66.421	−1.157
3100	87.474	358.462	290.519	210.624	216.705	61.406	−1.035
3200	87.825	361.245	292.686	219.389	216.368	56.402	−.921
3300	88.164	363.952	294.804	228.189	216.019	51.409	−.814
3400	88.491	366.589	296.877	237.022	215.658	46.426	−.713
3500	88.805	369.159	298.906	245.886	215.285	41.454	−.619
3600	89.101	371.665	300.892	254.782	214.899	36.493	−.529
3700	89.388	374.110	302.838	263.706	214.499	31.542	−.445
3800	89.666	376.498	304.745	272.659	214.084	26.603	−.366
3900	89.935	378.830	306.615	281.639	213.655	21.675	−.290
4000	90.194	381.110	308.449	290.646	213.210	16.758	−.219
4100	90.439	383.341	310.248	299.678	212.750	11.852	−.151
4200	90.678	385.523	312.015	308.733	212.273	6.958	−.087
4300	90.910	387.659	313.749	317.813	211.779	2.076	−.025
4400	91.137	389.752	315.453	326.915	211.268	−2.795	.033
4500	91.358	391.802	317.127	336.040	210.740	−7.655	.089
4600	91.563	393.813	318.772	345.186	210.194	−12.502	.142
4700	91.768	395.784	320.390	354.353	209.630	−17.337	.193
4800	91.970	397.718	321.981	363.540	209.049	−22.160	.241
4900	92.171	399.617	323.546	372.747	208.450	−26.971	.288
5000	92.370	401.481	325.086	381.974	207.833	−31.769	.332
5100	92.571	403.312	326.602	391.221	207.201	−36.555	.374
5200	92.768	405.111	328.094	400.488	206.553	−41.328	.415
5300	92.963	406.880	329.564	409.775	205.889	−46.089	.454
5400	93.153	408.620	331.012	419.080	205.211	−50.836	.492
5500	93.341	410.331	332.439	428.405	204.517	−55.572	.528
5600	93.525	412.014	333.845	437.748	203.810	−60.294	.562
5700	93.706	413.671	335.231	447.110	203.090	−65.004	.596
5800	93.883	415.302	336.597	456.489	202.356	−69.701	.628
5900	94.057	416.909	337.945	465.886	201.610	−74.386	.659
6000	94.228	418.491	339.274	475.301	200.853	−79.057	.688

PREVIOUS March 1961 (1 atm) CURRENT: March 1961 (1 bar

$\Delta_fH°$(0 K) = 60.986 ± 0.29 kJ·mol^{-1}
$S°$(298.15 K) = 219.330 J·K^{-1}·mol^{-1} $\Delta_fH°$(298.15 K) = 52.467 ± 0.29 kJ·mol^{-1}

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
3026.4(1)	3102.5(1)	3105.5(1)
1622.9(1)	1222.0(1)	826.0(1)
1342.2(1)	949.3(1)	2988.7(1)
1023.0(1)	943.0(1)	1443.5(1)

Ground State and Quantum Weight: 1 $\sigma = 4$
Point Group: D_{2h}
Bond Distances: H–C = 1.086 Å; C–C = 1.337 Å
Bond Angles: H–C–H = 117° 22'; H–C–C = 121° 19'
Product of the Moments of Inertia: $I_AI_BI_C = 5.4496 \times 10^{-117}$ g^3·cm^6

Enthalpy of Formation

The enthalpy of combustion of ethylene was measured by Rossini and Knowlton.[1] From the value, $\Delta_cH°$(298.15 K) = −337.28 ± 0.07 kcal·mol^{-1} for the reaction $C_2H_4(g) + 3\ O_2(g) = 2\ CO_2(g) + 2\ H_2O(l)$, the enthalpy of formation, $\Delta_fH°$(298.15 K), for C_2H_4(g) was derived to be 12.54 ± 0.07 kcal·mol^{-1}. The values of $\Delta_fH°$(298.15 K) for CO_2(g) and H_2O(l) used for calculation were obtained from Rossini *et al.*[2]

Heat Capacity and Entropy

The molecular structure, bond distances and angles were obtained from Allen and Plyler.[3] The vibrational frequencies were taken from Smith and Mills.[4] Eight of the twelve frequencies were reported by Arnett and Crawford,[5] Crawford *et al.*;[6] Stoicheff,[7] Feldman *et al.*,[8] and Allen and Plyler.[3] Herzberg[9] also reported the vibrational frequencies for ethylene as 3019.3 (1), 1623.3 (1), 1342.4 (1), 825.0 (1), 3272.3 (1), 1050 (1), 949.2 (1), 943 (1), 3105.5 (1), 995 (1), 298.5 (1) and 1443.5 (1) which are very close to the values adopted. The infrared and Raman spectra of ethylene before 1945 have been summarized by Herzberg.[9] The molecular structure of ethylene was also determined by Bartell and Bonham.[10] Their results, r(C–H) = 1.085 Å, r(C–C) = 1.334 Å principal moments of inertia are $I_A = 0.5763 \times 10^{-39}$, $I_B = 2.8004 \times 10^{-39}$, and $I_C = 3.3767 \times 10^{-39}$ g·cm^2.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−10.518	60.986	60.986	INFINITE
100	33.270	180.542	252.466	−7.192	58 194	60.476	−31.589
200	35.359	203.955	222.975	−3.804	55.542	63.749	−16.649
250	38.645	212.172	220.011	−1.960	54.002	65.976	−13.785
298.15	42.886	219.330	219.330	0.	52.467	68.421	−11.987
300	43.063	219.596	219.331	0.079	52.408	68.521	−11.930
350	48.013	226.602	219.873	2.355	50.844	71.330	−10.645
400	53.048	233.343	221.138	4.882	49.354	74.360	−9.710
450	57.907	239.874	222.858	7.657	47.951	77.571	−9.004
500	62.477	246.215	224.879	10.668	46.641	80.933	−8.455
600	70.663	258.348	229.456	17.335	44.294	88.017	−7.663
700	77.714	269.783	234.408	24.763	42.300	95.467	−7.124
800	83.840	280.570	239.511	32.847	40.637	103.180	−6.737
900	89.200	290.761	244.644	41.505	39.277	111.082	−6.447
1000	93.899	300.408	249.742	50.665	38.183	119.122	−6.222
1100	98.018	309.555	254.768	60.266	37.318	127.259	−6.043
1200	101.626	318.242	259.698	70.252	36.645	135.467	−5.897
1300	104.784	326.504	264.522	80.576	36.129	143.724	−5.775
1400	107.550	334.372	269.233	91.196	35.742	152.016	−5.672
1500	109.974	341.877	273.827	102.074	35.456	160.331	−5.583
1600	112.103	349.044	278.306	113.181	35.249	168.663	−5.506
1700	113.976	355.898	282.670	124.486	35.104	177.007	−5.439
1800	115.628	362.460	286.922	135.968	35.005	185.357	−5.379
1900	117.089	368.752	291.064	147.606	34.938	193.712	−5.326
2000	118.386	374 791	295.101	159.381	34.894	202.070	−5.278
2100	119.540	380.596	299.035	171.278	34 864	210.429	−5.234
2200	120.569	386.181	302.870	183.284	34.839	218.790	−5.195
2300	121.491	391.561	306.610	195.388	34 814	227.152	−5.159
2400	122.319	396.750	310.258	207.580	34.783	235.515	−5.126
2500	123.064	401.758	313.818	219.849	34 743	243.880	−5.096
2600	123.738	406.598	317.294	232.190	34 688	252.246	−5 068
2700	124.347	411.280	320.689	244.595	34.616	260.615	−5.042
2800	124.901	415.812	324.006	257.058	34.524	268.987	−5 018
2900	125.404	420.204	327.248	269.573	34.409	277.363	−4.996
3000	125.864	424.463	330.418	282.137	34.269	285 743	−4.975
3100	126.284	428.597	333.518	294.745	34.102	294.128	−4.956
3200	126.670	432.613	336.553	307.393	33.906	302.518	−4.938
3300	127.024	436.516	339.523	320.078	33.679	310.916	−4.921
3400	127.350	440.313	342.432	332.797	33.420	319.321	−4.906
3500	127.650	444.009	345.281	345.547	33.127	327.734	−4.891
3600	127.928	447.609	348.074	358.326	32.800	336.156	−4.877
3700	128.186	451.118	350.812	371.132	32.436	344.588	−4.865
3800	128.424	454.539	353.497	383.962	32.035	353.030	−4.853
3900	128.646	457.878	356.130	396.816	31.596	361.482	−4.842
4000	128.852	461.138	358.715	409 691	31.118	369.947	−4.831
4100	129.045	464.322	361.252	422.586	30.600	378.424	−4.821
4200	129.224	467.434	363.743	435.500	30.041	386.915	−4.812
4300	129.392	470.476	366.190	448.430	29.441	395.418	−4.803
4400	129.549	473.453	368.594	461.378	28.799	403.937	−4.795
4500	129.696	476.366	370.957	474.340	28.116	412.470	−4.788
4600	129.835	479.218	373.280	487.317	27.390	421.019	−4.781
4700	129.965	482.012	375.563	500.307	26.623	429.584	−4.774
4800	130.087	484.749	377.810	513.309	25.813	438.167	−4.768
4900	130.202	487.433	380.020	526.324	24.962	446.766	−4.763
5000	130.311	490.064	382.194	539.349	24.069	455.384	−4.757
5100	130.413	492.646	384.335	552.386	23.136	464.019	−4.753
5200	130.510	495.179	386.442	565.432	22.162	472.673	−4.748
5300	130.602	497.666	388.517	578.488	21.149	481.346	−4.744
5400	130.689	500.108	390.561	591.552	20.097	490.040	−4.740
5500	130.771	502.507	392.575	604.625	19.008	498.751	−4.737
5600	130.849	504.864	394.559	617.706	17.884	507.485	−4.734
5700	130.923	507.180	396.515	630.795	16.724	516.238	−4.731
5800	130.993	509.458	398.442	643.891	15.531	525.012	−4.728
5900	131.060	511.698	400.343	656.993	14.306	533.806	−4.726
6000	131.124	513.901	402.217	670.103	13.051	542.621	−4.724

PREVIOUS· September 1965 (1 atm) CURRENT September 1965 (1 bar)

Oxirane (C_2H_4O) IDEAL GAS $M_r = 44.05316$ Oxirane (C_2H_4O) $C_2H_4O_1(g)$

$S°(298.15\ K) = 243.012\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -40.119 \pm 0.63\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -52.635 \pm 0.63\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
3005(1)	3063 (1)	1153(1)
1490(1)	[1345] (1)	892(1)
1266(1)	807 (1)	3079(1)
1120(1)	3019 (1)	1143(1)
877(1)	1470 (1)	821(1)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: C_{2v}
Bond Distances: C–H = 1.0802 Å; C–O = 1.4363 Å; C–C = 1.4728 Å
Bond Angles: H–C–H = 116° 51'; H_2–C–C = 158° 5'; H_2–C–O = 142° 45.6'
Product of the Moments of Inertia: $I_AI_BI_C = 7.42728 \times 10^{-116}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The enthalpy of combustion of ethylene oxide (g) was determined by Pell and Pilcher[1] and Crog and Hunt[2] as −312.15 ± 0.14 and −312.55 ± 0.20 $kcal{\cdot}mol^{-1}$, respectively. The corresponding value of $\Delta_fH°(C_2H_4O, g, 298.15\ K)$ was evaluated to be −12.58 ± 0.15 and −12.19 ± 0.22 $kcal{\cdot}mol^{-1}$. The former value is adopted.

Heat Capacity and Entropy

The vibrational frequencies were taken from Lord and Nolin.[3] The infrared and Raman spectra of ethylene oxide have also been examined by Linnett[4] and Thompson and Cave.[5] The vibrational frequencies assigned were slightly different from the ones reported by Lord and Nolin.[3] As a result of analogies between ethylene oxide and ethylene imine, small changes of Lord and Nolin's assignment have been made by Potts.[6] The bond distances and angles were obtained from Cunningham *et al.*[7] The investigation of the structure of ethylene oxide by electron diffraction was reported by Ackermann and Mayer[8] and Igarashi.[9] The principal moments of inertia are: $I_A = 3.2793 \times 10^{-39}$, $I_B = 3.8059 \times 10^{-39}$, and $I_C = 5.9511 \times 10^{-39}\ g{\cdot}cm^2$.

The calculated heat capacities (307.2–371.2 K) are in good agreement with the experimentally measured ones reported by Kistiakowsky and Rice.[10]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−10.863	−40.119	−40.119	INFINITE
100	33.285	202.794	278.161	−7.537	−44.363	−35.641	18.617
200	36.701	226.467	246.985	−4.104	−48.426	−25.373	6.627
250	41.673	235.154	243.764	−2.153	−50.588	−19.360	4.045
298.15	47.901	243.012	243.012	0.	−52.635	−13.159	2.305
300	48.157	243.309	243.013	0.089	−52.711	−12.914	2.249
350	55.277	251.264	243.625	2.674	−54.705	−6.121	0.914
400	62.396	259.112	245.071	5.616	−56.527	0.946	−0.124
450	69.157	266.856	247.063	8.907	−58.172	8.230	−0.955
500	75.408	274.471	249.424	12.524	−59.648	15.689	−1.639
600	86.312	289.214	254.837	20.627	−62.139	31.000	−2.699
700	95.366	303.220	260.757	29.724	−64.090	46.685	−3.484
800	102.969	316.465	266.901	39.652	−65.578	62.616	−4.088
900	109.430	328.976	273.110	50.280	−66.671	78.710	−4.568
1000	114.963	340.800	279.293	61.507	−67.429	94.907	−4.957
1100	119.723	351.986	285.398	73.247	−67.909	111.166	−5.279
1200	123.832	362.584	291.392	85.430	−68.160	127.458	−5.548
1300	127.388	372.639	297.259	97.995	−68.226	143.763	−5.776
1400	130.472	382.195	302.987	110.892	−68.143	160.068	−5.972
1500	133.156	391.291	308.573	124 076	−67.944	176.362	−6.141
1600	135.498	399.961	314.016	137.511	−67.655	192.640	−6.289
1700	137.549	408.238	319.317	151.166	−67.297	208.898	−6.419
1800	139.350	416.152	324.478	165.013	−66.890	225.133	−6.533
1900	140.938	423.730	329.504	179.029	−66.447	241.344	−6.635
2000	142.342	430.996	334.398	193.194	−65.982	257.532	−6.726
2100	143.589	437.971	339.165	207.492	−65.505	273.696	−6.808
2200	144.699	444.677	343.810	221.908	−65.025	289.838	−6.882
2300	145.691	451.131	348.337	236.428	−64.549	305.957	−6.948
2400	146.580	457.351	352.750	251.042	−64.083	322.056	−7.009
2500	147.379	463.351	357.055	265.741	−63.632	338.136	−7.065
2600	148.101	469.146	361.255	280.516	−63.201	354.198	−7.116
2700	148.753	474.748	365.356	295.359	−62.793	370.243	−7.163
2800	149.344	480.168	369.360	310.264	−62.411	386.275	−7.206
2900	149.882	485.419	373.272	325.226	−62.059	402.293	−7.246
3000	150.373	490.508	377.095	340.239	−61.738	418.300	−7.283
3100	150.821	495.446	380.834	355.299	−61.451	434.296	−7.318
3200	151.232	500.241	384.491	370.402	−61.199	450.283	−7.350
3300	151.609	504.901	388.069	385.544	−60.984	466.264	−7.380
3400	151.956	509.432	391.572	400.723	−60.807	482.239	−7.409
3500	152.275	513.842	395.003	415.934	−60.670	498.208	−7.435
3600	152.571	518.135	398.364	431.177	−60.574	514.175	−7.460
3700	152.844	522.320	401.658	446.448	−60.519	530.139	−7.484
3800	153.098	526.399	404.887	461.745	−60.508	546.103	−7.507
3900	153.333	530.379	408.054	477.067	−60.540	562.067	−7.528
4000	153.553	534.264	411.161	492.411	−60.616	578.032	−7.548
4100	153.757	538.058	414.210	507.777	−60.738	593.999	−7.568
4200	153.947	541.765	417.203	523.162	−60.906	609.971	−7.586
4300	154.125	545.390	420.142	538.566	−61.120	625.947	−7.604
4400	154.292	548.935	423.029	553.987	−61.381	641.927	−7.621
4500	154.448	552.404	425.866	569.424	−61.688	657.915	−7.637
4600	154.595	555.801	428.654	584.876	−62.043	673.909	−7.652
4700	154.732	559.127	431.394	600.343	−62.446	689.913	−7.668
4800	154.862	562.386	434.089	615.822	−62.896	705.926	−7.682
4900	154.984	565.580	436.740	631.315	−63.393	721.948	−7.696
5000	155.099	568.712	439.349	646.819	−63.938	737.981	−7.710
5100	155.207	571.785	441.915	662.334	−64.530	754.025	−7.723
5200	155.310	574.800	444.442	677.860	−65.168	770.081	−7.736
5300	155.407	577.759	446.930	693.396	−65.852	786.150	−7.748
5400	155.499	580.665	449.379	708.941	−66.582	802.233	−7.760
5500	155.586	583.519	451.792	724.496	−67.357	818.328	−7.772
5600	155.669	586.323	454.170	740.058	−68.175	834.439	−7.783
5700	155.747	589.079	456.512	755.629	−69.037	850.565	−7.795
5800	155.821	591.788	458.822	771.208	−69.942	866.707	−7.806
5900	155.892	594.453	461.098	786.793	−70.887	882.862	−7.816
6000	155 960	597.073	463.342	802.386	−71.873	899.036	−7.827

PREVIOUS September 1965 (1 atm) CURRENT: September 1965 (1 bar)

Potassium Cyanide ((KCN)$_2$) IDEAL GAS M_r = 130.2320 Potassium Cyanide ((KCN)$_2$) $C_2K_2N_2(g)$

$S°(298.15 \text{ K}) = [373.129] \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = [-8.2 \pm 42] \text{ kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = [-8.4 \pm 42] \text{ kJ·mol}^{-1}$

Vibratonal Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
[240](1)	[220](1)	[2158](1)
[130](1)	[225](1)	[2158](1)
[205](1)	[207](1)	[2158](1)
[130](1)	[207](1)	[2158](1)

Ground State Quantum Weight: [1] $\sigma = 4$
Point Group: [D_{2h}]
Bond Distances: K–C = [2.75] Å; C–N = [1.16] Å
Bond Angles: N–C–K = [140]°; C–K–C = [100]°; K–C–K = [80]°
Product of the Moments of Inertia: $I_A I_B I_C = [2.948540 \times 10^{-112}] \text{ g}^3\text{·cm}^6$

Enthalpy of Formation

$\Delta_f H°((KCN)_2$, g, 298.15 K) was calculated based on an estimated enthalpy of dissociation, 40 kcal·mol^{-1} for the reaction $(KCN)_2(g) \rightarrow 2\,KCN(g)$, which was obtained by comparison with that for $(NaCN)_2(g)$.

Heat Capacity and Entropy

The molecular structure and bond angles were assumed to be the same as those for KCN(cr) reported by Bijvoet and Lely.[1] The C–N bond distance was assumed to be the same as that for KCN(g), and the K–C bond distance was assumed to be 10% longer than that in KCN(g). The vibrational frequencies were estimated by comparison with those for $K_2F_2(g)$. The last six frequencies were adopted from the bending and asymmetric stretching frequencies for KCN(g). The three principal moments of inertia are $I_A = 40.5737 \times 10^{-39}$, $I_B = 67.3413 \times 10^{-39}$, and $I_C = 107.9149 \times 10^{-39}$ g·cm^2.

Reference

[1] J. M. Bijvoet and J. A. Lely, Rec. Trav. Chim. 59, 908 (1940).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−24.786	−8.217	−8.217	INFINITE
100	77.547	266.448	465.521	−19.907	−9.825	−13.178	6.883
200	103.437	330.321	383.046	−10.545	−9.215	−16.652	4.349
250	107.785	353.916	374.932	−5.254	−8.720	−18.570	3.880
298.15	110.262	373.129	373.129	0.	−8.368	−20.502	3.592
300	110.337	373.812	373.132	0.204	−8.359	−20.578	3.583
350	112.029	390.955	374.482	5.766	−12.978	−22.435	3.348
400	113.310	406.001	377.500	11.400	−13.082	−23.779	3.105
450	114.405	419.411	381.425	17.094	−13.238	−25.107	2.914
500	115.421	431.518	385.839	22.839	−13.451	−26.415	2.760
600	117.361	452.734	395.269	34.479	−14.030	−28.957	2.521
700	119.200	470.965	404.811	46.308	−14.781	−31.388	2.342
800	120.890	486.995	414.102	58.314	−15.680	−33.700	2.200
900	122.393	501.322	423.011	70.480	−16.725	−35.892	2.083
1000	123.702	514.287	431.500	82.786	−17.931	−37.958	1.983
1100	124.828	526.131	439.573	95.214	−177.226	−30.675	1.457
1200	125.791	537.035	447.246	107.747	−176.702	−17.376	0.756
1300	126.614	547.137	454.546	120.368	−176.230	−4.118	0.165
1400	127.317	556.547	461.500	133.065	−175.804	9.105	−0.340
1500	127.920	565.352	468.133	145.828	−175.417	22.299	−0.777
1600	128.439	573.624	474.470	158.647	−175.069	35.468	−1.158
1700	128.888	581.425	480.534	171.514	−174.757	48.617	−1.494
1800	129.277	588.803	486.346	184.422	−174.481	61.749	−1.792
1900	129.616	595.802	491.924	197.367	−174.241	74.866	−2.058
2000	129.913	602.458	497.286	210.344	−174.041	87.971	−2.298
2100	130.175	608.803	502.447	223.349	−173.881	101.068	−2.514
2200	130.405	614.864	507.420	236.378	−173.766	114.158	−2.710
2300	130.610	620.666	512.218	249.429	−173.699	127.244	−2.890
2400	130.793	626.228	516.854	262.499	−173.684	140.328	−3.054
2500	130.956	631.571	521.336	275.587	−173.726	153.412	−3.205
2600	131.102	636.710	525.675	288.690	−173.831	166.499	−3.345
2700	131.234	641.660	529.880	301.807	−174.002	179.592	−3.474
2800	131.353	646.435	533.958	314.936	−174.248	192.692	−3.595
2900	131.460	651.046	537.916	328.077	−174.573	205.803	−3.707
3000	131.558	655.505	541.762	341.228	−174.984	218.926	−3.812
3100	131.647	659.820	545.501	354.388	−175.488	232.064	−3.910
3200	131.729	664.001	549.139	367.557	−176.094	245.221	−4.003
3300	131.803	668.056	552.682	380.734	−176.789	258.396	−4.090
3400	131.871	671.991	556.133	393.917	−177.609	271.596	−4.173
3500	131.934	675.815	559.498	407.108	−178.547	284.820	−4.251
3600	131.992	679.532	562.781	420.304	−179.619	298.074	−4.325
3700	132.046	683.150	565.986	433.506	−180.830	311.360	−4.396
3800	132.095	686.672	569.116	446.713	−182.188	324.680	−4.463
3900	132.141	690.104	572.174	459.925	−183.704	338.038	−4.528
4000	132.184	693.450	575.164	473.141	−185.374	351.436	−4.589
4100	132.224	696.714	578.089	486.362	−187.220	364.878	−4.649
4200	132.261	699.901	580.952	499.586	−189.258	378.368	−4.706
4300	132.295	703.013	583.754	512.814	−191.491	391.909	−4.761
4400	132.327	706.055	586.499	526.045	−193.373	405.450	−4.813
4500	132.358	709.029	589.189	539.279	−195.885	419.087	−4.865
4600	132.386	711.939	591.826	552.516	−198.594	432.783	−4.914
4700	132.413	714.786	594.412	565.756	−201.465	446.535	−4.963
4800	132.438	717.574	596.949	578.999	−204.323	460.327	−5.009
4900	132.461	720.305	599.439	592.244	−207.595	474.208	−5.055
5000	132.483	722.981	601.883	605.491	−211.075	488.157	−5.100
5100	132.504	725.605	604.283	618.740	−214.766	502.178	−5.143
5200	132.524	728.178	606.641	631.992	−218.669	516.273	−5.186
5300	132.542	730.703	608.958	645.245	−222.784	530.446	−5.228
5400	132.560	733.180	611.236	658.500	−227.113	544.698	−5.269
5500	132.577	735.613	613.475	671.757	−231.652	559.032	−5.309
5600	132.593	738.002	615.678	685.016	−236.402	573.451	−5.349
5700	132.608	740.349	617.844	698.276	−240.670	587.861	−5.387
5800	132.622	742.655	619.976	711.537	−245.745	602.440	−5.426
5900	132.635	744.922	622.075	724.800	−251.012	617.109	−5.463
6000	132.648	747.152	624.141	738.064	−256.468	631.869	−5.501

PREVIOUS: March 1966 (1 atm) CURRENT. March 1966 (1 bar)

Potassium Cyanide ((KCN)$_2$) $C_2K_2N_2(g)$

Lithium Carbide (Li_2C_2) CRYSTAL M_r = 37.904f Lithium Carbide (Li_2C_2) $C_2Li_2(cr)$

$S°(298.15\ K) = 58.6 \pm 4\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K)$ = Unknown

$\Delta_f H°(298.15\ K) = -59.4 \pm 8\ kJ \cdot mol^{-1}$

Enthalpy of Formation

Data from the U. S Nat. Bur. of Stand.[1]

Heat Capacity and Entropy

Data from the U. S. Nat. Bur. of Stand.[1]

Reference

[1] G. T. Fursukawa, M L. Reilly *et al.*, U S. Nat. Bur. Stand. Report 6928, Appendix B, (1960).

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
0							
100							
200							
298.15	71.546	58.576	58.576	0.000	−59.413	−56.111	9.830
300	71 965	59.020	58.577	.133	−59.403	−56.090	9.766
400	87.404	82.023	61.608	8.166	−58.616	−55.096	7.195
500	95.060	102.405	67.777	17.314	−63.987	−53.685	5.608
600	99.705	120.169	75.062	27.064	−63.360	−51.682	4.499
700	102.926	135.791	82.644	37.203	−62.618	−49.793	3.716
800	105.353	149.698	90.173	47.620	−61.835	−48.014	3.135
900	107.361	162.225	97.494	58.258	−61.048	−46.333	2.689
1000	109.077	173.628	104.546	69.082	−60.243	−44.741	2.337
1100	110.583	184.095	111.308	80.066	−59.409	−43.231	2.053
1200	112.006	193.779	117.782	91.196	−58.533	−41.799	1.819
1300	113.345	202.797	123 979	102.464	−57.608	−40.442	1.625
1400	114.600	211.243	129.914	113.862	−56.621	−39.158	1.461
1500	115.813	219.191	135.603	125.383	−55.564	−37.947	1.321
1600	116.985	226.703	141.064	137.022	−54.433	−36.809	1.202
1700	118.156	233.831	146.313	148 780	−343.695	−21.392	.657
1800	119.286	240.616	151.365	160.652	−340.897	−2.513	.073
1900	120.416	247.096	156.234	172.637	−338.033	16.208	−.446
2000	121.503	253.301	160.934	184.734	−335.103	34.777	−.908

PREVIOUS: CURRENT: December 1960

Magnesium Carbide (MgC_2) CRYSTAL $M_r = 48.327$ Magnesium Carbide (MgC_2) $C_2Mg_1(cr)$

$S°(298.15\ K) = 54.4 \pm 8\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = \text{Unknown}$
$\Delta_f H°(298.15\ K) = 87.9 \pm 21\ kJ \cdot mol^{-1}$

Enthalpy of Formation

Data from.[1]

Heat Capacity and Entropy

Data from Furukawa, *et al.*[1]

Reference

[1] G. T. Furukawa, M. L. Reilly *et al.*, U. S. Nat. Bur. Stand. Report 6928, Appendix B, (1960).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
0							
100							
200							
298.15	56.233	54.392	54.392	0.000	87.864	84.811	−14.859
300	56.442	54.740	54.393	.104	87.891	84.792	−14.764
400	64.392	72.161	56.714	6.179	89.364	83.538	−10.909
500	68.408	86.989	61.326	12.832	90.697	81.921	−8.558
600	70.877	99.691	66.688	19.802	91.744	80.063	−6.970
700	72.634	110.753	72.210	26.981	92.505	78.052	−5.824
800	74.015	120.545	77.651	34.315	93.009	75.950	−4.959
900	75.145	129.329	82.914	41.774	93.280	73.799	−4.283
1000	76.149	137.300	87.960	49.340	84.744	72.342	−3.779
1100	77.027	144.599	92.782	56.999	84.584	71.109	−3.377
1200	77.864	151.337	97.384	64.744	84.396	69.892	−3.042
1300	78.701	157.603	101.778	72.573	84.196	68.692	−2.760
1400	79.454	163.463	105.977	80.480	−43.416	70.674	−2.637
1500	80.207	168.971	109.995	88.464	−42.260	78.783	−2.743
1600	80.919	174.170	113.845	96.520	−41.092	86.814	−2.834
1700	81.630	179.097	117.540	104.647	−39.908	94.772	−2.912
1800	82.341	183.783	121.091	112.846	−38.701	102.660	−2.979
1900	83.011	188.253	124.509	121.114	−37.470	110.480	−3.037
2000	83.722	192.529	127.804	129.450	−36.211	118.234	−3.088
2100	84.391	196.630	130.984	137.856	−34.922	125.925	−3.132
2200	85.061	200.571	134.058	146.329	−33.602	133.553	−3.171
2300	85.730	204.367	137.033	154.868	−32.249	141.121	−3.205
2400	86.400	208.030	139.916	163.475	−30.863	148.629	−3.235
2500	87.069	211.571	142.711	172.148	−29.442	156.079	−3.261

PREVIOUS: CURRENT: December 1960

Magnesium Carbide (MgC_2) $C_2Mg_1(cr)$

CNC Radical (CNC) IDEAL GAS $M_r = 38.0287$ CNC Radical (C_2N) $C_2N_1(g)$

$S°(298.15 \text{ K}) = [230 \pm 8]$ J·K^{-1}·mol^{-1}

$\Delta_f H°(0 \text{ K}) = [552 \pm 126]$ kJ·mol^{-1}
$\Delta_f H°(298.15 \text{ K}) = [556 \pm 126]$ kJ·mol^{-1}

Electronic Levels and Quantum Weights ϵ_i, cm^{-1}	g_i
0	2
26.41	2
30338.53	4
34802.33	2

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[1200] (1)
321 (2)
[900] (1)

Point Group: $D_{\infty h}$ $\sigma = 2$
Bond Distance: C–N = 1.245 Å
Bond Angle: C–N–C = 180°
Rotational Constant: $B_0 = 0.452740$ cm^{-1}

Enthalpy of Formation

Merer and Travis[1] stated that the observed bond length in CNC(g) indicated double–bonded CN links. The value of the C = N dissociation energy is derived as 147 kcal·mol^{-1} from the enthalpy of combustion of n–butyl–isobutylidine amine determined by Coates and Sutton.[2] However, due to possible extra binding energy from the unpaired electron, we assume here a slightly higher value of 160 kcal·mol^{-1}. This yields a $\Delta_f H°$(CNC, g, 298.15 K) = 133 kcal·mol^{-1}. It is also possible to calculate another value by assuming that the ratio of the enthalpy of atomization of Si_2N to that of $C_2N(g)$ is equal to the ratio of the dissociation energies of SiN(g) and CN(g); by this method $\Delta_f H°$(CNC, g, 298.15 K) = 144 kcal·mol^{-1}.

Heat Capacity and Entropy

Merer and Travis[1] have observed the ultraviolet absorption sectrum of the CNC radical. They ave assigned the configuration, bond distance, and the electronic levels. In addition, they have derived ν_2; the remaining frequencies are estimated by comparison with the $^1\Pi$ state of $C_3(g)$, which has been assigned by Weltner and McLeod.[3]

References

[1] A. J. Merer and D. N. Travis, Can. J. Phys. 44, 353 (1956).
[2] G. E. Coates and L. E. Sutton, J. Chem. Soc. 1187 (1948).
[3] W. Weltner and D. J. McLeod, J. Chem. Phys. 40, 1305 (1964); 45, 3096 (1966).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−11.080	551.829	551.829	INFINITE
100	32.963	188.237	267.905	−7.967	553.372	542.729	−283.493
200	40.683	213.673	234.935	−4.252	554.978	531.475	−138.807
250	43.425	223.053	231.645	−2.148	555.764	525.507	−109.799
298.15	45.751	230.905	230.905	0.	556.472	519.615	−91.034
300	45.835	231.188	230.906	0.085	556.498	519.386	−90.433
350	47.975	238.418	231.472	2.431	557.174	513.147	−76.583
400	49.849	244.949	232.755	4.878	557.787	506.814	−66.183
450	51.465	250.916	234.446	7.412	558.332	500.409	−58.086
500	52.844	256.412	236.371	10.020	558.807	493.947	−51.602
600	55.010	266.249	240.550	15.419	559.557	480.901	−41.866
700	56.572	274.852	244.849	21.002	560.073	467.748	−34.904
800	57.713	282.485	249.086	26.719	560.394	454.534	−29.678
900	58.563	289.334	253.184	32.535	560.552	441.291	−25.612
1000	59.208	295.539	257.114	38.425	560.576	428.037	−22.358
1100	59.706	301.206	260.868	44.372	560.486	414.786	−19.697
1200	60.097	306.419	264.450	50.363	560.300	401.549	−17.479
1300	60.410	311.242	267.866	56.389	560.031	388.330	−15.603
1400	60.663	315.728	271.126	62.443	559.689	375.134	−13.996
1500	60.871	319.921	274.241	68.520	559.283	361.966	−12.605
1600	61.043	323.855	277.220	74.616	558.820	348.826	−11.388
1700	61.187	327.560	280.074	80.728	558.305	335.717	−10.315
1800	61.309	331.061	282.810	86.853	557.742	322.639	−9.363
1900	61.414	334.379	285.438	92.989	557.135	309.594	−8.511
2000	61.503	337.532	287.964	99.135	556.488	296.583	−7.746
2100	61.580	340.534	290.397	105.289	555.802	283.604	−7.054
2200	61.648	343.400	292.741	111.450	555.080	270.659	−6.426
2300	61.707	346.142	295.004	117.618	554.324	257.748	−5.854
2400	61.759	348.770	297.190	123.792	553.536	244.870	−5.329
2500	61.805	351.292	299.304	129.970	552.716	232.025	−4.848
2600	61.846	353.716	301.350	136.153	551.865	219.214	−4.404
2700	61.883	356.051	303.333	142.339	550.985	206.437	−3.994
2800	61.916	358.302	305.256	148.529	550.077	193.692	−3.613
2900	61.946	360.476	307.123	154.722	549.141	180.981	−3.260
3000	61.973	362.576	308.937	160.918	548.178	168.302	−2.930
3100	61.998	364.609	310.700	167.117	547.188	155.656	−2.623
3200	62.020	366.577	312.416	173.318	546.173	143.042	−2.335
3300	62.041	368.486	314.086	179.521	545.132	130.460	−2.065
3400	62.061	370.339	315.713	185.726	544.065	117.910	−1.811
3500	62.079	372.138	317.300	191.933	542.974	105.392	−1.573
3600	62.096	373.887	318.848	198.141	541.859	92.905	−1.348
3700	62.113	375.588	320.358	204.352	540.719	80.450	−1.136
3800	62.129	377.245	321.834	210.564	539.556	68.026	−0.935
3900	62.145	378.859	323.275	216.778	538.369	55.632	−0.745
4000	62.160	380.433	324.685	222.993	537.159	43.270	−0.565
4100	62.176	381.968	326.063	229.210	535.926	30.938	−0.394
4200	62.191	383.466	327.412	235.428	534.670	18.636	−0.232
4300	62.207	384.930	328.733	241.648	533.392	6.365	−0.077
4400	62.224	386.360	330.026	247.870	532.092	−5.877	0.070
4500	62.241	387.759	331.294	254.093	530.769	−18.088	0.210
4600	62.259	389.127	332.536	260.318	529.425	−30.271	0.344
4700	62.277	390.466	333.754	266.545	528.059	−42.423	0.471
4800	62.297	391.777	334.950	272.773	526.671	−54.546	0.594
4900	62.318	393.062	336.123	279.004	525.262	−66.641	0.710
5000	62.339	394.321	337.274	285.237	523.833	−78.706	0.822
5100	62.362	395.556	338.405	291.472	522.382	−90.742	0.929
5200	62.387	396.767	339.515	297.709	520.911	−102.750	1.032
5300	62.412	397.956	340.607	303.949	519.419	−114.729	1.131
5400	62.439	399.123	341.680	310.192	517.907	−126.680	1.225
5500	62.468	400.269	342.735	316.437	516.376	−138.603	1.316
5600	62.498	401.395	343.772	322.686	514.824	−150.498	1.404
5700	62.530	402.501	344.793	328.937	513.253	−162.364	1.488
5800	62.563	403.589	345.797	335.192	511.662	−174.204	1.569
5900	62.598	404.659	346.786	341.450	510.051	−186.015	1.647
6000	62.634	405.711	347.759	347.711	508.421	−197.799	1.722

PREVIOUS. March 1967 (1 atm) CURRENT March 1967 (1 bar)

CNC Radical (C_2N) $C_2N_1(g)$

Ethanedinitrile ((CN)$_2$) IDEAL GAS M_r = 52.0354 Ethanedinitrile ((CN)$_2$) C$_2$N$_2$(g)

$S°$(298.15 K) = 241.565 J·K^{-1}·mol^{-1}

$\Delta_f H°$(0 K) = 307.219 ± 1.80 kJ·mol^{-1}
$\Delta_f H°$(298.15 K) = 309.072 ± 1.80 kJ·mol^{-1}

Vibrational Frequencies and Degeneracies ν, cm^{-1}
2328.5 (1)
850.6 (1)
2149 (1)
507.2 (2)
240 (2)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: $D_{\infty h}$
Bond Distances: C–N = 1.157 Å; C–C = 1.380 Å
Bond Angle: N–C–C–N = 180°
Rotational Constant: B_0 = 0.157545 ± 0.00015 cm^{-1}

Enthalpy of Formation

Knowlton and Prosen[1] reported $\Delta_f H°$(298.15 K) = −261.94 ± 0.43 kcal·mol^{-1} for the reaction $C_2N_2(g) + 2O_2(g) \rightarrow CO_2(g) + N_2(g)$. When corrected for a change in the atomic weight of carbon, this becomes $\Delta_f H°$(298.15 K) = −261.95 ± 0.43 kcal, whence $\Delta_f H°$(298.15 K) for C_2N_2(g) is found to be 73.87 ± 0.43 kcal·mol^{-1}.

Heat Capacity and Entropy

Langseth and Moller[2] determined the vibrational frequencies by Raman spectroscopy. Moller and Stoicheff[3] determined B_0 by Raman spectroscopy and calculated the bond lengths listed above. These agree with lengths found from electron-diffraction measurements by Langseth and Moller[2] (C–N distance = 1.15 Å, C–C distance = 1.38 Å) and Pauling *et al.*[4] (C–N distance = 1.16 ± 0.02 Å, C–C distance = 1.37 ± 0.02 Å). From measurements reported by Ruehrwein and Giauque,[5] $S°$(298.15 K) is calculated by the 3rd law to be 57.63 cal·K^{-1}·mol^{-1}, in satisfactory agreement with the value calculated here.

References

[1] J. W. Knowlton and E. J. Prosen, J. Res. Nat. Bur. Stand. 46, 489 (1951).
[2] A. Langseth and C. K. Moller, Acta Chem. Scand. 4, 725 (1950).
[3] C. K. Moller and B. P. Stoicheff, Can. J. Phys. 32, 625 (1954).
[4] L. Pauling, H. D. Springall, and K. J. Palmer, J. Amer. Chem. Soc. 61, 927 (1939).
[5] R. A. Ruehrwein and W. F. Giauque, J. Amer. Chem. Soc. 61, 2940 (1939).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−12.626	307.219	307.219	INFINITE
100	36.399	191.121	286.323	−9.520	307.303	304.362	−158.982
200	48.910	220.447	246.531	−5.217	308.042	301.183	−78.661
250	53.388	231.863	242.482	−2.655	308.558	299.409	−62.558
298.15	56.746	241.565	241.565	0.	309.072	297.601	−52.138
300	56.859	241.917	241.566	0.105	309.092	297.529	−51.804
350	59.585	250.894	242.269	3.019	309.606	295.561	−44.110
400	61.799	259.000	243.862	6.055	310.079	293.522	−38.330
450	63.677	266.390	245.961	9.193	310.495	291.427	−33.828
500	65.332	273.186	248.348	12.419	310.850	289.288	−30.222
600	68.218	285.360	253.526	19.101	311.392	284.922	−24.805
700	70.704	296.067	258.853	26.050	311.752	280.479	−20.930
800	72.861	305.652	264.114	33.230	311.982	275.995	−18.021
900	74.717	314.344	269.220	40.612	312.117	271.487	−15.757
1000	76.302	322.301	274.136	48.165	312.184	266.969	−13.945
1100	77.650	329.638	278.852	55.864	312.199	262.446	−12.463
1200	78.795	336.445	283.371	63.688	312.171	257.924	−11.227
1300	79.769	342.791	287.701	71.618	312.109	253.406	−10.182
1400	80.598	348.734	291.850	79.637	312.015	248.894	−9.286
1500	81.308	354.320	295.831	87.733	311.895	244.389	−8.510
1600	81.918	359.587	299.652	95.895	311.748	239.893	−7.832
1700	82.445	364.569	303.326	104.114	311.577	235.407	−7.233
1800	82.901	369.295	306.861	112.382	311.382	230.932	−6.701
1900	83.299	373.788	310.266	120.692	311.165	226.469	−6.226
2000	83.648	378.070	313.550	129.040	310.925	222.017	−5.798
2100	83.954	382.159	316.720	137.421	310.663	217.578	−5.412
2200	84.225	386.071	319.784	145.830	310.379	213.152	−5.061
2300	84.465	389.820	322.748	154.265	310.073	208.740	−4.741
2400	84.679	393.419	325.619	162.722	309.746	204.341	−4.447
2500	84.870	396.880	328.400	171.199	309.397	199.956	−4.178
2600	85.041	400.212	331.099	179.695	309.026	195.586	−3.929
2700	85.195	403.425	333.718	188.207	308.634	191.230	−3.700
2800	85.335	406.525	336.263	196.734	308.220	186.889	−3.486
2900	85.461	409.522	338.738	205.274	307.785	182.563	−3.288
3000	85.576	412.421	341.146	213.826	307.328	178.253	−3.104
3100	85.680	415.229	343.491	222.388	306.850	173.958	−2.931
3200	85.775	417.951	345.776	230.961	306.350	169.680	−2.770
3300	85.863	420.592	348.003	239.543	305.828	165.417	−2.618
3400	85.943	423.156	350.176	248.134	305.285	161.170	−2.476
3500	86.016	425.649	352.297	256.732	304.720	156.939	−2.342
3600	86.084	428.073	354.368	265.337	304.134	152.725	−2.216
3700	86.147	430.432	356.392	273.948	303.526	148.528	−2.097
3800	86.205	432.730	358.371	282.566	302.896	144.347	−1.984
3900	86.259	434.970	360.306	291.189	302.244	140.183	−1.878
4000	86.309	437.155	362.200	299.818	301.571	136.036	−1.776
4100	86.356	439.287	364.055	308.451	300.876	131.906	−1.681
4200	86.399	441.368	365.871	317.089	300.159	127.794	−1.589
4300	86.439	443.402	367.650	325.731	299.420	123.699	−1.503
4400	86.477	445.389	369.395	334.376	298.659	119.621	−1.420
4500	86.513	447.333	371.105	343.026	297.877	115.561	−1.341
4600	86.546	449.235	372.783	351.679	297.073	111.518	−1.266
4700	86.577	451.096	374.429	360.335	296.247	107.493	−1.195
4800	86.606	452.919	376.046	368.994	295.398	103.486	−1.126
4900	86.634	454.705	377.633	377.656	294.528	99.497	−1.061
5000	86.660	456.456	379.192	386.321	293.635	95.525	−0.998
5100	86.684	458.172	380.724	394.988	292.720	91.572	−0.938
5200	86.707	459.856	382.229	403.658	291.783	87.637	−0.880
5300	86.729	461.508	383.710	412.329	290.824	83.720	−0.825
5400	86.750	463.129	385.165	421.003	289.842	79.822	−0.772
5500	86.769	464.721	386.597	429.679	288.837	75.942	−0.721
5600	86.788	466.285	388.006	438.357	287.811	72.080	−0.672
5700	86.805	467.821	389.393	447.037	286.761	68.237	−0.625
5800	86.822	469.331	390.759	455.718	285.688	64.413	−0.580
5900	86.838	470.815	392.103	464.401	284.592	60.607	−0.537
6000	86.853	472.275	393.427	473.086	283.472	56.820	−0.495

PREVIOUS: March 1961 (1 atm) CURRENT: March 1961 (1 bar)

Ethanedinitrile ((CN)$_2$) C$_2$N$_2$(g)

Sodium Cyanide ((NaCN)$_2$) IDEAL GAS $M_r = 98.01494$ Sodium Cyanide ((NaCN)$_2$) $C_2N_2Na_2(g)$

$S°(298.15\ K) = [347.102]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [-8.3 \pm 13]\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = [-8.8 \pm 13]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	 ν, cm^{-1}	 ν, cm^{-1}
[295](1)	[250](1)	[239](1)
[175](1)	[290](1)	[239](1)
[250](1)	[239](1)	[2176](1)
[170](1)	[239](1)	[2176](1)

Ground State Quantum Weight: 1 $\sigma = [4]$
Point Group: [D_{2h}]
Bond Distances: N–C = [1.16] Å; C–Na = [2.19] Å
Bond Angles: C–Na–C = [105]°; Na–C–Na = [75]°; N–C–Na = [142.5]°
Product of the Moments of Inertia: $I_A I_B I_C = [4.483815 \times 10^{-113}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The mass spectra of vapors from samples of NaCN have been observed by Porter[1] at temperatures around 1000 K. The results indicate that the compound evaporates as NaCN(g) and $Na_2(CN)_2(g)$. A comparison of relative ion currents produced by electron bombardment of NaCN vapors effusing from single–and double–oven–type Knudsen cells, yielded information on the partial pressures of monomer and dimer. Based on the partial pressures for NaCN(g) and $(NaCN)_2(g)$ reported at temperatures, 903–1049 K, the vapor pressures of $(NaCN)_2(g)$ over NaCN(l), 1078.2–1626.2 K, were calculated from the total vapor pressure measurements reported by Ingold.[2] By the 2nd and 3rd law methods, the values of $\Delta_{vap}H°(298.15\ K)$ (l → dimer) were evaluated to be 38.89 and 38.21 kcal·mol^{-1}, respectively. Using the 3rd law value, the enthalpy of formation for $(NaCN)_2(g)$ was evaluated.

Heat Capacity and Entropy

The molecular structure, bond distances and C–Na–C bond angle were estimated by Porter.[1] The vibrational frequencies were estimated by comparison with those for NaCl(g). The last six frequencies were the bending and asymmetric stretching frequencies for NaCN(g). The principal moments of inertia are: $I_A = 13.5707 \times 10^{-39}$, $I_B = 51.0944 \times 10^{-39}$, and $I_C = 64.6652 \times 10^{-39}\ g{\cdot}cm^2$.

References

[1] R. F. Porter, J. Chem. Phys. 35, 318 (1961).
[2] C. K. Ingold, J. Chem. Soc. 123, 885 (1923).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−23.178	−8.299	−8.299	INFINITE
100	67.677	247.172	435.395	−18.822	−9.644	−13 427	7.013
200	98.488	305.757	356.722	−10.193	−9.489	−17 132	4.474
250	104.306	328 419	348.858	−5.110	−9.102	−19.087	3.988
298.15	107.686	347.102	347.102	0.	−8.786	−21.041	3.686
300	107.789	347.768	347.104	0.199	−8.777	−21.117	3.677
350	110.089	364.568	348.426	5.650	−8 631	−23.189	3 461
400	111.781	379.383	351.387	11.198	−13.984	−24.854	3.246
450	113.163	392.631	355.247	16.823	−14.207	−26.200	3.041
500	114.386	404.618	359.594	22.512	−14 466	−27.519	2.875
600	116.596	425.672	368.900	34.063	−15.087	−30.073	2.618
700	118.601	443.798	378.335	45.824	−15.818	−32.514	2.426
800	120.401	459.755	387.535	57.776	−16.636	−34 844	2.275
900	121.985	474.030	396.366	69.897	−17.535	−37.067	2.151
1000	123.355	486.955	404.789	82.166	−18.527	−39.185	2.047
1100	124.529	498.769	412.803	94.562	−19.633	−41.199	1.956
1200	125.531	509.648	420.426	107.066	−214.401	−38.226	1 664
1300	126.385	519.731	427.682	119.663	−213.953	−23.563	0.947
1400	127.115	529.124	434.596	132.339	−213.547	−8.933	0.333
1500	127.740	537.916	441.194	145.083	−213.178	5.669	−0 197
1600	128.278	546.178	447.500	157.884	−212.842	20.248	−0.661
1700	128.743	553.969	453.536	170.736	−212.538	34.807	−1.069
1800	129.146	561.339	459.322	183.631	−212.264	49.348	−1.432
1900	129.497	568.332	464.877	196.563	−212.018	63.875	−1.756
2000	129.805	574.982	470.218	209.529	−211.801	78.390	−2.047
2100	130.075	581.322	475.358	222.523	−211.611	92.895	−2.311
2200	130.314	587.379	480.314	235.543	−211.449	107.391	−2.550
2300	130.526	593.176	485.096	248.585	−211.316	121.881	−2.768
2400	130.715	598.735	489.716	261.647	−211.212	136.366	−2.968
2500	130.884	604.075	494 184	274.727	−211.139	150.846	−3.152
2600	131.035	609.211	498.510	287.823	−211.099	165.325	−3.321
2700	131.171	614.159	502.702	300.934	−211.093	179.803	−3.478
2800	131.294	618.932	506.768	314.057	−211.124	194.281	−3.624
2900	131.406	623.541	510.716	327.192	−211.193	208.760	−3.760
3000	131.507	627.998	514.552	340.338	−211.303	223.243	−3.887
3100	131.599	632.311	518.281	353.493	−211.458	237.731	−4.006
3200	131.683	636.491	521.910	366.658	−211.660	252.224	−4.117
3300	131.761	640.544	525.444	379.830	−211.912	266.724	−4.222
3400	131.831	644.478	528.887	393.010	−212.218	281.232	−4.321
3500	131.896	648.301	532.245	406.196	−212.581	295.751	−4.414
3600	131.956	652.017	535.521	419.389	−213.006	310.280	−4.502
3700	132.012	655.634	538.718	432.587	−213.497	324.823	−4.586
3800	132.063	659.155	541.841	445.791	−214.057	339.379	−4.665
3900	132.111	662.586	544.894	459.000	−214.692	353.951	−4.741
4000	132.155	665.931	547.878	472.213	−215.406	368.541	−4.813
4100	132.196	669.195	550.797	485.430	−216.204	383.149	−4.881
4200	132.234	672.381	553.654	498.652	−217.087	397.778	−4.947
4300	132.270	675.493	556.452	511.877	−218.069	412.429	−5.010
4400	132.303	678.534	559.192	525.106	−219.066	427.097	−5.070
4500	132.334	681.508	561.877	538.338	−220.208	441.794	−5.128
4600	132.364	684.417	564.510	551.573	−221.471	456.519	−5.184
4700	132.391	687.264	567.091	564.810	−222.845	471.272	−5.238
4800	132.417	690.051	569.624	578.051	−224.335	486.056	−5.289
4900	132.441	692.782	572.110	591.294	−225.947	500.872	−5.339
5000	132.464	695.458	574.550	604.539	−227.670	515.722	−5.388
5100	132.486	698.081	576.946	617.786	−229.538	530.608	−5.435
5200	132.506	700.654	579.301	631.036	−231.543	545.532	−5.480
5300	132.526	703.178	581.614	644.288	−233.691	560.496	−5.524
5400	132.544	705.655	583.888	657.541	−235.987	575.502	−5.567
5500	132.561	708.088	586.125	670.796	−238.436	590.552	−5.609
5600	132.577	710.476	588.324	684.053	−241.043	605.647	−5.649
5700	132.593	712.823	590.488	697.312	−243.813	620.791	−5.689
5800	132.608	715.129	592.617	710.572	−246.750	635.985	−5.728
5900	132.622	717.396	594.712	723.833	−249.859	651.231	−5.766
6000	132.635	719.625	596.776	737.096	−252.828	666.495	−5.802

PREVIOUS· March 1966 (1 atm) CURRENT March 1966 (1 bar)

Sodium Cyanide ((NaCN)$_2$) $C_2N_2Na_2(g)$

CCO Radical (CCO) IDEAL GAS $M_r = 40.0214$ CCO Radical (C_2O) $C_2O_1(g)$

$S°(298.15\ K) = 233.07\ J{\cdot}K^{-1}\ mol^{-1}$

$\Delta_f H°(0\ K) = 282.6 \pm 63\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 286.6 \pm 63\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights	
ϵ_i, cm^{-1}	g_i
0	3
[4050]	[2]
[6450]	[1]

Vibrational Frequencies and Degeneracies ν, cm^{-1}
1074 (1)
381 (2)
1978 (1)

Point Group: $C_{\infty v}$ $\sigma = 1$
Bond Distance: C–C = [1.160] Å
Bond Angle: C–C–O = 180°
Rotational Constant: B_0 = [0.408483] cm^{-1}

Enthalpy of Formation

The adopted enthalpy of formation, $\Delta_f H°(C_2O,\ g,\ 298.15\ K) = 68.5\ kcal{\cdot}mol^{-1}$, was calculated from the enthalpy of reaction $\Delta_r H°(298.15\ K) = 65.5\ kcal{\cdot}mol^{-1}$ for $C_3O_2(g) = C_2O(g) + CO(g)$ using all JANAF functions (dated Sept. 30, 1965). The value of $\Delta_r H°$ was obtained from the 3rd law calculation of the equilibrium constant ($K_p = 3.3 \times 10^{-6}$ atm at 1060 K) which was determined in the studies of decomposition rate of $C_3O_2(g)$ by Palmer and Cross.[1]

Jacox *et al.*[2] observed the photodissociation of C_2O near 5000 Å which corresponds to a minimum of 57 kcal·mol^{-1} for $C_2O(g) \rightarrow C(g) + CO(g)$. This yields $\Delta_f H°(C_2O,\ g,\ 298.15\ K) \leq 87\ kcal{\cdot}mol^{-1}$ which was not adopted because the irradiation was not monochromatic and thus possibly contained all wavelengths below 5000 Å.

Heat Capacity and Entropy

Jacox *et al.*[2] have observed three vibrational fundamentals in the infrared spectrum by matrix isolation, and suggested a linear structure with $^3\Sigma$ ground state for the CCO radical (g). They also estimated the bond distances C–C = 1.160 Å and C–O = 1.279 Å based on the structural analogy between the carbon suboxide and the CCO radical. Bayes[3] has predicted that the ^1Z and $^1\Sigma$ states lie respectively 0.5 and 0.8 eV above the ground state. These two elctronic states have been included in the tabulation.

References

[1] H. B. Palmer and W. D Cross, Carbon 3, 475 (1966).
[2] M. E. Jacox, D. E. Milligan, N. G. Moll, and W. E. Thompson, J. Chem. Phys. 43, 3745 (1965).
[3] K. D. Bayes, J. Amer. Chem. Soc. 85, 1730 (1963).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.473	282.575	282.575	INFINITE
100	31.198	192.768	268.031	−7.526	283.950	273.529	−142.877
200	38.530	216.773	236.873	−4.020	285.348	262.574	−68.577
250	41.079	225.656	233.764	−2.027	286.020	256.802	−53.656
298.15	43.064	233.066	233.066	0.	286.604	251.121	−43.995
300	43.133	233.333	233.067	0.080	286.625	250.900	−43.686
350	44.880	240.116	233.599	2.281	287.146	244.904	−36.550
400	46.416	246.211	234.801	4.564	287.578	238.839	−31.189
450	47.795	251.759	236.381	6.920	287.919	232.725	−27.014
500	49.044	256.861	238.178	9.342	288.173	226.578	−23.670
600	51.227	266.001	242.071	14.358	288.454	214.228	−18.650
700	53.064	274.040	246.075	19.576	288.498	201.851	−15.062
800	54.626	281.230	250.028	24.962	288.374	189.479	−12.372
900	55.971	287.744	253.862	30.494	288.133	177.131	−10.280
1000	57.142	293.703	257.553	36.150	287.813	164.814	−8.609
1100	58.173	299.199	261.092	41.917	287.438	152.532	−7.243
1200	59.086	304.300	264.483	47.781	287.025	140.286	−6.106
1300	59.896	309.062	267.731	53.731	286.585	128.075	−5.146
1400	60.617	313.528	270.844	59.757	286.125	115.899	−4.324
1500	61.258	317.732	273.831	65.852	285.650	103.756	−3.613
1600	61.825	321.704	276.700	72.006	285.161	91.646	−2.992
1700	62.325	325.468	279.459	78.214	284.659	79.567	−2.445
1800	62.764	329.043	282.115	84.469	284.143	67.517	−1.959
1900	63.148	332.447	284.676	90.765	283.611	55.497	−1.526
2000	63.481	335.695	287.146	97.097	283.063	43.505	−1.136
2100	63.769	338.799	289.532	103.460	282.495	31.541	−0.785
2200	64.016	341.771	291.840	109.850	281.908	19.605	−0.465
2300	64.226	344.622	294.073	116.262	281.298	7.695	−0.175
2400	64.402	347.359	296.237	122.694	280.663	−4.187	0.091
2500	64.550	349.991	298.335	129.142	280.004	−16.043	0.335
2600	64.671	352.525	300.370	135.603	279.317	−27.871	0.560
2700	64.769	354.968	302.348	142.075	278.602	−39.672	0.768
2800	64.847	357.325	304.269	148.556	277.858	−51.447	0.960
2900	64.907	359.602	306.138	155.044	277.084	−63.194	1.138
3000	64.952	361.803	307.957	161.537	276.280	−74.914	1.304
3100	64.983	363.933	309.729	168.034	275.444	−86.607	1.459
3200	65.002	365.997	311.455	174.533	274.576	−98.273	1.604
3300	65.012	367.997	313.138	181.034	273.676	−109.910	1.740
3400	65.012	369.938	314.780	187.535	272.745	−121.520	1.867
3500	65.005	371.822	316.383	194.036	271.780	−133.102	1.986
3600	64.991	373.653	317.949	200.536	270.784	−144.656	2.099
3700	64.972	375.434	319.479	207.034	269.755	−156.182	2.205
3800	64.948	377.166	320.974	213.530	268.693	−167.680	2.305
3900	64 921	378.853	322.437	220.024	267.600	−179.149	2.399
4000	64.890	380.496	323.868	226.514	266.474	−190.590	2.489
4100	64.856	382.098	325.268	233.002	265.315	−202.002	2.574
4200	64.821	383.661	326.640	239.486	264.125	−213.386	2.654
4300	64.784	385.185	327.984	245.966	262.902	−224.741	2.730
4400	64.745	386.674	329.301	252.442	261.648	−236.067	2.802
4500	64.705	388.129	330.592	258.915	260.362	−247.364	2.871
4600	64.665	389.551	331.859	265.383	259.043	−258.633	2.937
4700	64.624	390.941	333.101	271.848	257.693	−269.872	2.999
4800	64.583	392.301	334.320	278.308	256.311	−281.082	3.059
4900	64.542	393.632	335.517	284.764	254.897	−292.263	3.116
5000	64.500	394.936	336.692	291.216	253.451	−303.415	3.170
5100	64.459	396.213	337.847	297.664	251.973	−314.537	3.222
5200	64.418	397 464	338.981	304.108	250.462	−325.631	3.271
5300	64.378	398.690	340.097	310.548	248.919	−336.695	3.318
5400	64.338	399.893	341.193	316.984	247.342	−347.730	3.364
5500	64.299	401.074	342.271	323.416	245.733	−358.735	3.407
5600	64.260	402.232	343.331	329.844	244.090	−369.710	3.449
5700	64.222	403.369	344.375	336.268	242.414	−380.656	3.488
5800	64.184	404.486	345.401	342.688	240.703	−391.572	3.526
5900	64.147	405.582	346.412	349.105	238.959	−402.459	3.563
6000	64.111	406.660	347 407	355.517	237.179	−413.315	3.598

PREVIOUS. September 1966 (1 atm) CURRENT: September 1966 (1 bar)

$S°(298.15\ K) = 236.731\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 609.3 \pm 29\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 615.0 \pm 29\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights

ϵ_i, cm^{-1}	g_i
0	1
[13000]	[6]
20085	2

Vibrational Frequencies and Degeneracies

ν, cm^{-1}
853 (1)
300 (2)
1742 (1)

Point Group: $C_{\infty v}$ $\sigma = 1$
Bond Distances: C–C = [128] Å; C–Si = [1.75] Å
Bond Angle: C–C–Si = 180°
Rotational Constant: B_0 = [0.201171] cm^{-1}

Enthalpy of Formation

The selected value is an average based on the equilibrium data summarized below. Drowart and co-workers have used the Knudsen effusion–mass spectrometric technique to determine the vapor equilibria over the systems SiC–graphite,[1] SiC–silison[2] and boron–carbon–silicon.[3] 3rd law analysis of the partial pressures of C_2Si and Si lead to the concordant values 146.7, 149.0 and 146.0 kcal·mol^{-1}. Although the drifts all suggest that the entropy of C_2Si may be about 3.5 less than tabulated, this is of doubtful significance because the uncertainty bands are so large. The low condensation coefficient suggested by Drowart[2] may also be involved. Rates of free evaporation reported by Voronin[4] lead to apparent pressures which are smaller by a factor of 1/30, thus confirming the existence of a low evaporation coefficient. The adopted value of $\Delta_f H°(298.15\ K) = 147 \pm 7$ kcal·mol^{-1} includes allowance for the unlikely possibility that the entropy may be in error by up to 3.5 cal·K^{-1}·mol^{-1}.

Source	Method	Reaction*	T/K	Dat Points	$\Delta_r H°$(298.15 K) kcal·mol^{-1} 2nd law	$\Delta_r H°$(298.15 K) kcal·mol^{-1} 3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°$(298.15 K) kcal·mol^{-1}
Drowart	Mass Spec.	A	2149–2316	7	31 ± 9	38.98	3.5 ± 4.1	146.7
Drowart	Mass Spec.	B	1935–2160	4	188 ± 10	194.8	3.3 ± 4.9	149.0
Verhaegen	Mass Spec.	A	2166–2344	5	30 ± 16	38.31	3.9 ± 7.2	146.0

*Reactions: (A) $2\ C(graph) + Si(g) = C_2Si(g)$ (B) $2\ SiC(\alpha) = Si(l) + C_2Si(g)$

Heat Capacity and Entropy

The known molecular constants are from the assignments of Weltner and McLeod.[5] These authors observed the infrared spectrum, emission spectrum and visible absorption spectrum of C_2Si in matrix isolation. The matrix data allowed more certain assignment of the A–X band system of the gas as observed by Kleman[6] and McKellar.[7] Weltner concluded that this system probably involves transitions between a $^1\Sigma^+$ ground state and a $^1\Pi$ excited state. The two stretching frequencies were observed in the matrix infrared spectrum, whereas the bending mode, 300 cm^{-1}, was derived solely from the analysis of the A–X band system. The analysis presumed a linear unsymmetrical structure for the molecule.

A $^3\pi$ excited state is assumed to lie 7000 cm^{-1} below the $^1\pi$ state, which presumably arises from the same molecular orbital configuration. The effect of the estimated level is to increase the entropy by about 0.2 and 1.8 cal·K^{-1}·mol^{-1} at 3000 and 6000 K. Bond distances are estimated by comparison with those in Si_2, C_2 and C_3.

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	$\Delta_f G°$ (kJ·mol^{-1})	log K_f
0	0.	0.	INFINITE	−11.055	609.313	609.313	INFINITE
100	33.354	193.558	274.049	−8.049	611.934	593.151	−309.831
200	41.224	219.393	240.775	−4.276	613.875	573.562	−149.799
250	43.686	228.867	237.472	−2.151	614.559	563.400	−117.716
298.15	45.611	236.731	236.731	0.	615.048	553.501	−96.971
300	45.678	237.014	236.732	0.084	615.064	553.119	−96.307
350	47.364	244.185	237.295	2.412	615.414	542.765	−81.003
400	48.832	250.607	238.564	4.817	615.630	532.370	−69.520
450	50.132	256.435	240.231	7.292	615.724	521.956	−60.587
500	51.292	261.779	242.122	9.828	615.709	511.537	−53.440
600	53.260	271.311	246.212	15.059	615.408	490.725	−42.721
700	54.831	279.643	250.405	20.467	614.822	469.988	−35.071
800	56.080	287.050	254.531	26.015	614.019	449.350	−29.340
900	57.074	293.715	258.521	31.674	613.047	428.823	−24.888
1000	57.869	299.771	262.348	37.423	611.939	408.412	−21.333
1100	58.510	305.317	266.006	43.243	610.715	388.118	−18.430
1200	59.031	310.431	269.497	49.121	609.392	367.939	−16.016
1300	59.462	315.174	272.831	55.046	607.979	347.875	−13.978
1400	59.823	319.594	276.015	61.011	606.482	327.922	−12.235
1500	60.133	323.732	279.060	67.009	604.907	308.080	−10.728
1600	60.409	327.622	281.974	73.036	603.258	288.345	−9.413
1700	60.662	331.292	284.769	79.090	551.363	269.162	−8.270
1800	60.907	334.766	287.451	85.169	549.808	252.606	−7.330
1900	61.153	338.066	290.028	91.272	548.234	236.138	−6.492
2000	61.410	341.209	292.509	97.400	546.643	219.753	−5.739
2100	61.685	344.212	294.901	103.554	545.041	203.448	−5.060
2200	61.985	347.088	297.208	109.737	543.431	187.219	−4.445
2300	62.314	349.851	299.437	115.952	541.819	171.064	−3.885
2400	62.676	352.511	301.593	122.201	540.209	154.979	−3.373
2500	63.073	355.077	303.682	128.488	538.607	138.960	−2.903
2600	63.504	357.559	305.706	134.817	537.016	123.006	−2.471
2700	63.971	359.964	307.672	141.191	535.441	107.112	−2.072
2800	64.471	362.300	309.581	147.612	533.887	91.277	−1.703
2900	65.001	364.571	311.438	154.086	532.358	75.496	−1.360
3000	65.558	366.784	313.246	160.613	530.857	59.768	−1.041
3100	66.140	368.943	315.008	167.198	529.387	44.090	−0.743
3200	66.740	371.053	316.727	173.842	527.951	28.458	−0.465
3300	67.355	373.116	318.405	180.547	526.551	12.870	−0.204
3400	67.980	375.136	320.044	187.313	525.189	−2.675	0.041
3500	68.609	377.115	321.646	194.143	523.866	−18.181	0.271
3600	69.239	379.057	323.214	201.035	138.430	−23.189	0.336
3700	69.864	380.963	324.749	207.990	137.600	−27.667	0.391
3800	70.480	382.834	326.253	215.008	136.806	−32.123	0.442
3900	71.083	384.673	327.727	222.086	136.050	−36.559	0.490
4000	71.669	386.480	329.174	229.224	135.329	−40.975	0.535
4100	72.234	388.256	330.593	236.419	134.642	−45.374	0.578
4200	72.775	390.004	331.987	243.670	133.988	−49.757	0.619
4300	73.290	391.722	333.356	250.973	133.365	−54.124	0.657
4400	73.776	393.413	334.702	258.327	132.769	−58.478	0.694
4500	74.232	395.076	336.025	265.727	132.199	−62.818	0.729
4600	74.656	396.712	337.327	273.172	131.651	−67.145	0.762
4700	75.047	398.322	338.607	280.657	131.122	−71.461	0.794
4800	75.404	399.905	339.868	288.180	130.610	−75.766	0.825
4900	75.728	401.464	341.109	295.737	130.111	−80.060	0.853
5000	76.018	402.997	342.332	303.325	129.621	−84.345	0.881
5100	76.274	404.504	343.536	310.939	129.138	−88.619	0.908
5200	76.498	405.988	344.723	318.578	128.657	−92.884	0.933
5300	76.689	407.447	345.892	326.238	128.177	−97.140	0.957
5400	76.850	408.882	347.046	333.915	127.692	−101.387	0.981
5500	76.980	410.293	348.183	341.607	127.202	−105.625	1.003
5600	77.082	411.681	349.304	349.310	126.702	−109.853	1.025
5700	77.156	413.046	350.411	357.022	126.188	−114.073	1.045
5800	77.204	414.389	351.502	364.740	125.659	−118.283	1.065
5900	77.228	415.709	352.579	372.462	125.112	−122.485	1.084
6000	77.229	417.007	353.642	380.185	124.544	−126.677	1.103

PREVIOUS: March 1967 (1 atm) CURRENT: March 1967 (1 bar)

$S^\circ(298.15\ K) = 237.2 \pm 13\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH^\circ(0\ K) = 811 \pm 17\ kJ{\cdot}mol^{-1}$
$\Delta_fH^\circ(298.15\ K) = 820 \pm 17\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
1225 (1)
63.5 (2)
2040 (1)

Ground State Quantum Weight: [1] $\sigma = 2$
Point Group: $D_{\infty h}$
Bond Distances: C–C = 1.277 Å
Bond Angle: C–C–C = 180°
Rotational Constant: $B_0 = 0.430334$ cm^{-1}

Enthalpy of Formation

Drowart *et al.*[1] have measured mass spectrometrically the ion intensity ratio C_3^+/C^+ as a function of temperature from 1800 to 2700 K. We derive from a 2nd law analysis of their data $\Delta_fH^\circ(2200\ K) = 185.2 \pm 3.3\ kcal{\cdot}mol^{-1}$, and $S^\circ(2200\ K) = 74.9 \pm 2.8\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ by calculation of the absolute pressure from the vapor pressure of monatomic carbon and a relative ionization cross–section ratio of 2.3. The entropy uncertainty includes 1.3 cal·K^{-1}·mol^{-1} for uncertainty in the absolute pressure. Several earlier mass–spectrometric determinations[2–4] are in reasonable agreement. The absolute magnitude of the pressure is also confirmed by the work of Thorn and Winslow[5] who measured the total pressure of all species over graphite as 1.2 to 4.8×10^{-7} atm at 2400 K. Subtracting the JANAF values for C and C_2 we obtain $C_3 = 5.4 \times 10^{-8}$ to 2.2×10^{-7} atm, which compares with Drowart's value of 3.3×10^{-8} to 1.3×10^{-7} atm. The 2nd law enthalpy of formation is reported[5] to be $\Delta_fH^\circ(2400\ K) = 184.4\ kcal{\cdot}mol^{-1}$ but the range is only 80 K. It does, however, confirm the magnitude of the mass–spectrometric values for both enthalpy and entropy. We have adopted a enthalpy of formation within the uncertainty limits of Dowart's measurements which with the adopted functions yields pressures in the 2000–3000 K range consistent with the measurements. We were not able to generate functions which agree exactly with the 2nd law entropies, since even direct summation over only the observed levels of the bending frequency gives an entropy which is already too large.

Heat Capacity and Entropy

The stretching frequencies are from Merer,[6] Weltner *et al.*[7] and Weltner and McLeod.[8] The bending frequency and its harmonics are from Gausset *et al.*[9] and Merer.[6] The rotational constant and bond distance are from Gausset *et al.*[9]

As indicated briefly above, the calculated entropy of C_3 gas is higher than the experimental value even when a summation is performed only over the observed first six levels of the bending frequency. Treatment of the vibration as a harmonic oscillator or as a anharmonic oscillator gives values considerably higher. Strauss and Thiele[10] have also calculated functions based on a quartic potential function which still yields values several units higher than the experiments. In order to reduce the entropy to the approximate range of the measurements we have made the assumption that the potential function is of an unusual form above the sixth vibrational level. We assume that the large amplitude of the bending vibration causes a drastic change in the function, possibly due to the increasing repulsion between end carbons, as the amplitude increases. Thus, we assume a very steeply rising potential above the sixth vibrational level. We have chosen to represent this part of the potential by a harmonic oscillator of 650 cm^{-1}. The choice of 650 cm^{-1} is arbitrary, but is not unreasonable for a bending vibration, and yields functions which approximate the experimental data.

In order to explain the observed spectrum of C_3O_2, a molecule with a bending frequency of 63 cm^{-1}, Smith and Barrett[11] have proposed that potential maxima occur in the bending potential away from linearity. Thus, the adoption of an unusual potential function for C_3 bending may be justifiable. We do not claim that our functions are necessarily correct but only that they include all known facts and satisfy the experimental equilibrium observations. Further investigation of the carbon vapor pressure and of the higher vibrational levels of C_3 is desirable.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	Δ_fH°	Δ_fG°	log K_f
0	0.	0.	INFINITE	−11.761	811.456	811.456	INFINITE
100	42.459	193.021	272.308	−7.929	815.110	796.093	−415.836
200	39.861	221.795	240.748	−3.791	818.268	775.758	−202.607
298.15	37.740	237.246	237.246	0.	820.064	754.464	−132.179
300	37.719	237.479	237.247	0.070	820.086	754.057	−131.293
400	37.497	248.274	238.720	3.821	820.770	731.916	−95.578
500	38.380	256.727	241.504	7.612	820.580	709.709	−74.143
600	39.706	263.841	244.649	11.515	819.749	687.604	−59.861
700	41.125	270.069	247.844	15.557	818.472	665.676	−49.673
800	42.480	275.650	250.977	19.738	816.891	643.953	−42.046
900	43.714	280.726	254.005	24.049	815.098	622.441	−36.126
1000	44.815	285.390	256.913	28.477	813.156	601.138	−31.400
1100	45.786	289.708	259.701	33.008	811.105	580.035	−27.544
1200	46.647	293.729	262.371	37.630	808.974	559.122	−24.338
1300	47.413	297.494	264.929	42.334	806.781	538.389	−21.633
1400	48.095	301.033	267.383	47.110	804.538	517.828	−19.320
1500	48.710	304.372	269.739	51.951	802.255	497.428	−17.322
1600	49.267	307.534	272.003	56.850	799.940	477.181	−15.578
1700	49.773	310.536	274.182	61.802	797.595	457.081	−14.044
1800	50.233	313.394	276.282	66.803	795.226	437.119	−12.685
1900	50.660	316.122	278.307	71.848	792.834	417.289	−11.472
2000	51.053	318.731	280.264	76.934	790.421	397.586	−10.384
2100	51.417	321.230	282.155	82.057	787.989	378.004	−9.402
2200	51.760	323.630	283.986	87.216	785.538	358.538	−8.513
2300	52.081	325.938	285.761	92.408	783.069	339.184	−7.703
2400	52.384	328.161	287.481	97.632	780.584	319.938	−6.963
2500	52.667	330.305	289.152	102.885	778.081	300.796	−6.285
2600	52.936	332.376	290.775	108.165	775.562	281.754	−5.661
2700	53.189	334.379	292.353	113.471	773.025	262.809	−5.084
2800	53.430	336.318	293.888	118.802	770.472	243.959	−4.551
2900	53.659	338.197	295.384	124.157	767.902	225.200	−4.056
3000	53.877	340.019	296.842	129.534	765.315	206.531	−3.596
3100	54.084	341.789	298.263	134.932	762.711	187.947	−3.167
3200	54.283	343.510	299.650	140.350	760.089	169.448	−2.766
3300	54.476	345.183	301.005	145.788	757.450	151.031	−2.391
3400	54.660	346.812	302.328	151.245	754.793	132.695	−2.039
3500	54.834	348.399	303.622	156.720	752.118	114.437	−1.708
3600	55.003	349.946	304.887	162.212	749.425	96.256	−1.397
3700	55.164	351.455	306.126	167.720	746.713	78.149	−1.103
3800	55.321	352.929	307.338	173.244	743.982	60.116	−0.826
3900	55.472	354.368	308.526	178.784	741.233	42.156	−0.565
4000	55.618	355.774	309.689	184.339	738.464	24.266	−0.317
4100	55.757	357.149	310.830	189.907	735.676	6.445	−0.082
4200	55.893	358.494	311.949	195.490	732.868	−11.307	0.141
4300	56.024	359.811	313.047	201.086	730.040	−28.992	0.352
4400	56.151	361.100	314.124	206.695	727.192	−46.611	0.553
4500	56.275	362.364	315.182	212.316	724.324	−64.165	0.745
4600	56.392	363.602	316.222	217.949	721.434	−81.655	0.927
4700	56.506	364.816	317.243	223.594	718.524	−99.082	1.101
4800	56.618	366.007	318.246	229.250	715.593	−116.447	1.267
4900	56.726	367.175	319.233	234.918	712.641	−133.751	1.426
5000	56.831	368.322	320.203	240.596	709.667	−150.994	1.577
5100	56.932	369.449	321.158	246.284	706.672	−168.178	1.722
5200	57.031	370.555	322.097	251.982	703.654	−185.302	1.861
5300	57 127	371.642	323.022	257.690	700.614	−202.368	1.994
5400	57.221	372.711	323.932	263.407	697.552	−219.377	2.122
5500	57.312	373.762	324.828	269.134	694.468	−236.329	2.244
5600	57.402	374.795	325.712	274.870	691.361	−253.225	2.362
5700	57.488	375.812	326.582	280.614	688.232	−270.064	2.475
5800	57.573	376.813	327.439	286.367	685.080	−286.849	2.583
5900	57.655	377 798	328.284	292.129	681.904	−303.579	2.688
6000	57.735	378.767	329.118	297.898	678.706	−320.256	2.788

PREVIOUS December 1969 (1 atm) CURRENT: December 1969 (1 bar)

Aluminum Carbide (Al_4C_3) CRYSTAL M_r = 143.95916 Aluminum Carbide (Al_4C_3) C_3Al_4(cr)

$\Delta_f H°(0\ K) = -210.84 \pm 6.7\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = 88.969 \pm 1.26\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = -215.69 \pm 6.7\ kJ \cdot mol^{-1}$

T_{fus} = [2500] K $\Delta_{fus}H°$ = Unknown

Enthalpy of Formation

The $\Delta_f H°(298.15\ K) = -51.55 \pm 1.6\ kcal \cdot mol^{-1}$ is the average value of $\Delta_f H°(298.15\ K) = -49.7 \pm 1.2\ kcal \cdot mol^{-1}$ by King and Armstrong[1] and that of $\Delta_f H°(298.15\ K) = -53.4 \pm 2.0\ kcal \cdot mol^{-1}$ by Mah.[2] Both measured the enthalpy of reaction $Al_4C_3(cr) + 6O_2(g) \rightarrow 2Al_2O_3(cr, \alpha) + 3CO_2(g)$ and used their $\Delta_r H°(298.15\ K)$ and the $\Delta_f H°(298.15\ K)$ of Al_2O_3(cr) and CO_2(g) to calculate the $\Delta_f H°(298.15\ K)$ of Al_4C_3(cr). The $\Delta_r H°(298.15\ K)$ measured by King and Armstrong was $-1033.3 \pm 1.1\ kcal \cdot mol^{-1}$, the $\Delta_r H°(298.15\ K)$ measured by Mah[2] was $-1029.6 \pm 1.9\ kcal \cdot mol^{-1}$.

Heat Capacity and Entropy

The low temperature heat capacities, 18–390 K, were measured by Saba and Furukawa.[3] The high temperature heat capacities, 273–1173 K, were measured by Victor *et al.*[4] These two sets of heat capacity data were joined smoothly and extrapolated to 2000 K by Saba and Furukawa.[3] The values of $C_p°$ above 2000 K were estimated by extrapolation graphically. $S°(298.15\ K)$ was reported by Saba and Furukawa,[3] using $S°(\text{extrap. } 20\ K) = 0.013\ cal \cdot K^{-1} \cdot mol^{-1}$.

Fusion Data

T_{fus} was estimated by Ruff and Jellinek.[5]

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[2] A. D Mah, U. S. Bur. Mines Report 6415, (1964).

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[4] A. C. Victor, W. R. Thurber, and T. B. Douglas, U. S Nat. Bur. Stand. Report 7437, (1962).

[5] O. Ruff and E. Jellinek, Z. Anorg. Allg. Chem. 97, 312 (1916).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−16.468	−210.843	−210.843	INFINITE
100	29.702	11.749	167.728	−15.598	−212.086	−210.181	109.787
200	82.098	49.200	98.655	−9.891	−214.566	−207.241	54.126
298.15	116.784	88.969	88.969	0.	−215.685	−203.356	35.627
300	117.298	89.693	88.971	0.217	−215.695	−203.279	35.394
400	138.507	126.645	93.865	13.112	−215.901	−199.095	25.999
500	150.892	158.981	103.729	27.626	−215.898	−194.894	20.360
600	159.201	187.262	115.345	43.150	−216.050	−190.683	16.600
700	165.180	212.270	127.440	59.381	−216.527	−186.423	13.911
800	169.707	234.633	139.466	76.134	−217.461	−182.065	11.888
900	173.264	254.834	151.181	93.288	−218.975	−177.557	10.305
1000	176.142	273.243	162.480	110.762	−263.532	−169.804	8.870
1100	178.527	290.146	173.328	128.499	−265.077	−160.356	7.615
1200	180.540	305.768	183.722	146.455	−266.575	−150.769	6.563
1300	182.268	320.288	193.675	164.597	−268.030	−141.059	5.668
1400	183.770	333.852	203.209	182.900	−269.446	−131.239	4.897
1500	185.096	346.577	212.347	201.345	−270.825	−121.318	4.225
1600	186.276	358.561	221.114	219.914	−272.171	−111.307	3.634
1700	187.334	369.886	229.536	238.596	−273.486	−101.213	3.110
1800	188.297	380.621	237.634	257.378	−274.774	−91.042	2.642
1900	189.171	390.826	245.430	276.252	−276.037	−80.800	2.221
2000	189.979	400.550	252.945	295.210	−277.278	−70.492	1.841
2100	190.631	409.835	260.196	314.241	−278.504	−60.123	1.495
2200	191.251	418.718	267.202	333.335	−279.719	−49.695	1.180
2300	191.836	427.232	273.976	352.490	−280.926	−39.212	0.891
2400	192.389	435.408	280.533	371.701	−282.124	−28.677	0.624
2500	192.907	443.273	286.886	390.966	−283.314	−18.093	0.378
2600	193.393	450.848	293.047	410.282	−284.499	−7.460	0.150
2700	193.845	458.155	299.028	429.644	−285.679	3.217	−0.062
2800	194.263	465.213	304.838	449.050	−1462.462	17.810	−0.332
2900	194.648	472.037	310.486	468.495	−1459.259	70.620	−1.272
3000	194.999	478.641	315.982	487.978	−1456.059	123.320	−2.147

PREVIOUS: June 1963 CURRENT: September 1965

Chromium Carbide (Cr_7C_3) CRYSTAL $M_r = 400.005$

$\Delta_f H°(0\ K) = -163.51 \pm 16.7\ kJ\cdot mol^{-1}$

$S°(298.15\ K) = 200.983 \pm 1.26\ J\cdot K^{-1}\cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = -160.67 \pm 16.7\ kJ\cdot mol^{-1}$

Enthalpy of Formation

Mah[1] determined the heat of combustion of Cr_7C_3(cr) using oxygen bomb calorimetry She reported $\Delta_c H°(298.15\ K) = -1193.0 \pm 0.9$ kcal·mol^{-1} based on the reaction $Cr_7C_3(cr) + 33/4O_2(g) = 7/2\ Cr_2O_3(cr) + 3CO_2(g)$. Using JANAF auxiliary data,[2] we calculate $\Delta_f H°(298.15\ K) = -38.4$ kcal·mol^{-1} for Cr_7C_3(cr). Mah[1] reported that the six combustion runs gave 99.90 to 99.84% completion of combustion. Corrections for incomplete combustion, formation of small amounts of CO(g), and impurities were made by Mah.[1] These corrections amount to no more than 1.04% of the $\Delta_c E$ value.

The pressures of CO(g) in equilibrium with a Cr_2O_3–Cr_7C_3–$Cr_{23}C_6$ mixture have been measured by Kelley *et al.*[3] and Kulkarni and Worrell.[4] Kelley *et al.*[3] also examined the Cr_2O_3–Cr_3C_2–Cr_7C_3 system. Kulkarni and Worrell[4] measured the CO pressure using a torsion effusion technique while Kelley *et al.*[3] measured the pressure manometrically. The results of our analyses are tabulated in the following table. In all cases we have assumed unit activity for the condensed species.

Source	T/K	Data Points	Reaction	$\Delta_r H°$(298.15 K), kcal·mol^{-1} 2nd law	$\Delta_r H°$(298.15 K), kcal·mol^{-1} 3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°$(298.15 K) kcal·mol^{-1}
[3]	1307–1497	9	A	994.44	970.74	−16.9 ± 4.3	−41.53
[4]	1111–1250	11[b]	B	220.48	218.99	−1.3 ± 0.6	−35.18
[3]	1505–1723	15[c]	B	211.34	220.89	5.8 ± 2.0	−35.81

[a] Reactions: (A) $5Cr_2O_3(cr) + 27Cr_3C_2(cr) = 13Cr_7C_3(cr) + 15CO(g)$ (B) $Cr_2O_3(cr) + 3Cr_7C_3(cr) = Cr_{23}C_6(cr) + 3CO(g)$.

[b] 1234 6, 1250.0 K points deleted due to statistical test, effective range is now 1111–1220 K.

[c] 1524 K point deleted due to statistical test.

We adopt $\Delta_f H°(298.15\ K) = -38.4 \pm 4.0$ kcal·mol^{-1} for Cr_7C_3(cr) based on the combustion data of Mah.[1] The equilibrium studies by Kulkarni and Worrell[4] and Kelley *et al.*[3] are in reasonable agreement with the adopted value. Equilibrium studies involving Cr_7C_3(cr) by Hancock and Pidgeon,[5] Alekseev and Shvartsman,[6] and Bolgar *et al.*[7] are not considered.[2]

Heat Capacity and Entropy

The heat capacity (54–295 K, 29 pts.) and enthalpy (480–1580 K, 15 pts.) have been measured by Kelley *et al.*[3] Using the Debye function suggested,[3] we calculate $S°(50\ K) = 1.679$ cal·K^{-1}·mol^{-1} and $H°(50;0) = 62.66$ cal·K^{-1}·mol^{-1}. The adopted heat capacity curve is based solely on the above mentioned study with the constraint that the heat capacity values derived from the enthalpy data join smoothly with the low temperature heat capacity values near 298.15 K. The observed $C_p°$ values deviate from the adopted values within ±0.2% for $T < 298.15$ K. The enthalpy data agrees within ±0.35% with the tabulated values except for the 1263.4 K data (1.66% or ~1.0 kcal·mol^{-1} too low) and the two points at 1545.1 and 1578.1 K which were not included in the polynomial curve fit.[3] The polynomial is used to extrapolate $C_p°$ values above 1500 K.

Phase Data

Storms[8] has summarized much of the phase data for the chromium carbides and reported a hexagonal structure for Cr_7C_3. The homogeneity range for Cr_7C_3 is not known.[8]

Decomposition Data

The tentative phase diagram for the Cr–Cr_3C_2 system as proposed by Storms[8] indicated an incongruent melting at 2053 K.

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[7] A. S. Bolgar, V. V. Fesenko, and G. P. Gordinko, Poroshk. Met. 38, 100 (1966).
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Chromium Carbide (Cr_7C_3) C_3Cr_7(cr)

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−34.397	−163.508	−163.508	INFINITE
100	80.414	39.481	355.684	−31.620	−163.089	−163.752	85.535
200	167.414	125.392	218.991	−18.720	−162.255	−164.668	43.007
298.15	209 748	200.983	200.983	0.	−160.666	−166.161	29.111
300	210.372	202.282	200.987	0.389	−160.628	−166.195	28.937
400	236.714	266.701	209.591	22.844	−159.033	−168.182	21.962
500	252.873	321.361	226.622	47.369	−156.663	−170.748	17.838
600	263.504	368.438	246.427	73.206	−154.596	−173.765	15.128
700	271.956	409.702	266.865	99.986	−152.839	−177.103	13.216
800	279.608	446.519	287.061	127.566	−151.313	−180.676	11.797
900	287.006	479.880	306.660	155.897	−150.046	−184.425	10.704
1000	294.369	510.499	325.534	184.966	−149.159	−188.297	9.836
1100	301.779	538.903	343.655	214.773	−148.794	−192.233	9.128
1200	309.269	565.481	361.045	245.324	−149.015	−196.177	8.539
1300	316.842	590.535	377.743	276.629	−149.909	−200.076	8.039
1400	324.494	614.295	393.798	308.695	−151.542	−203.879	7.607
1500	332.214	636.945	409.259	341.530	−153.940	−207.538	7.227
1600	339.992	658.634	424.171	375.140	−157.128	−211.012	6.889
1700	347.824	679.481	438.580	409.531	−161.123	−214.261	6.583
1800	355.703	699.585	452.525	444.707	−165.938	−217.252	6.304
1900	363.619	719.028	466.043	480.672	−171.585	−219.953	6.047
2000	371.568	737.882	479.166	517.431	−178.075	−222.334	5.807
2100	379.552	756.204	491.924	554.987	−185.417	−224.370	5.581
2200	387.543	774.045	504.344	593.342	−328.970	−221.450	5.258
2300	395.530	791.448	516.450	632.496	−325.008	−216.649	4.920
2400	403.526	808.451	528.264	672.449	−320.295	−212.036	4 615
2500	411.517	825.085	539.805	713.201	−314.828	−207.635	4.338

PREVIOUS: CURRENT: December 1973

Magnesium Carbide (Mg_2C_3) CRYSTAL M_r = 84.643 Magnesium Carbide (Mg_2C_3) $C_3Mg_2(cr)$

$\Delta_f H°(0\ K)$ = Unknown

$S°(298.15\ K) = 100.41 \pm 13\ J\cdot K^{-1}\cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = 79.5 \pm 33\ kJ\cdot mol^{-1}$

Enthalpy of Formation

Data from Furukawa *et al.*[1]

Heat Capacity and Entropy

Data from Furukawa *et al.*[1]

References

[1] G. T. Furukawa, M. L. Reilly *et al.*, U. S. Nat. Bur. Stand. Report 6928, Appendix B, (1960).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J\cdot K^{-1}mol^{-1}$			$kJ\cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	93.763	100.416	100.416	0.	79.496	74.173	−12.995
300	94.140	100.997	100.418	0.174	79.530	74.140	−12.909
400	107.361	130.046	104.288	10.303	81.481	72.052	−9.409
500	114.056	154.770	111.979	21.395	83.260	69.481	−7.259
600	118.198	175.949	120.919	33.018	84.614	66.591	−5.797
700	121.127	194.398	130.127	44.990	85.523	63.509	−4.739
800	123.386	210.724	139.200	57.219	86.012	60.326	−3.939
900	125.269	225.368	147.975	69.653	86.106	57.106	−3.314
1000	126.943	238.654	156.389	82.265	68.636	55.320	−2.890
1100	128.449	250.825	164.428	95.036	67.964	54.021	−2.565
1200	129.830	262.061	172.102	107.950	67.262	52.784	−2.298
1300	131.168	272.506	179.428	121.001	66.554	51.606	−2.074
1400	132.424	282.272	186.429	134.180	−188.965	56.817	−2.120
1500	133.679	291.452	193.128	147.486	−186.940	74.303	−2.587
1600	134.892	300.118	199.547	160.915	−184.884	91.652	−2.992
1700	136.064	308.331	205.706	174.463	−182.790	108.871	−3.345
1800	137.235	316.142	211.626	188.128	−180.652	125.967	−3.655
1900	138.365	323.592	217.325	201.907	−178.466	142.942	−3.930
2000	139.536	330.719	222.817	215.803	−176.227	159.800	−4.174
2100	140.666	337.554	228.119	229.813	−173.931	176.545	−4.391
2200	141.754	344.123	233.244	243.934	−171.579	193.180	−4.587
2300	142.884	350.449	238.203	258.166	−169.167	209.706	−4.763
2400	144.013	356.554	243.008	272.511	−166.692	226.126	−4.921
2500	145.101	362.455	247.669	286.967	−164.155	242.441	−5.066

PREVIOUS. CURRENT: December 1960

Carbon Suboxide (C_3O_2) IDEAL GAS M_r = 68.0318

$S°(298.15\ K) = 276.07 \pm 0.8\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -96.819 \pm 1.84\ kJ{\cdot}mol^{-1}$

$\Delta_fH°(298.15\ K) = -93.638 \pm 1.84\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies		
ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
2200(1)	2258(1)	550(2)
830(1)	1573(1)	63(2)
	577(2)	

Ground State Quantum Weight: 1 $\sigma = 2$

Point Group: $D_{\infty h}$

Bond Distances: C–C = 1.28 Å; C–O = 1.16 Å

Bond Angles: C–C–C = 180°; O–C–C = 180°

Rotational Constant: $B_0 = 0.073337\ cm^{-1}$

Enthalpy of Formation

Kybett *et al.*[1] have determined the enthalpy of combustion of the liquid form under its own pressure using the sample from the heat capacity determinations.[2]

The average of four determinations gave $\Delta_fH°(l, 298.15\ K) = -28.03 \pm 0.24\ kcal\ mol^{-1}$; the authors report −29.03 due to an arithmetic error. The sample was 99.98 mol % pure. McDougall and Kilpatrick[2] measured $\Delta_{vap}H°(230\ K) = 6.421 \pm 0.012\ kcal{\cdot}mol^{-}$ from which we calculate $\Delta_{vap}H°(298.15\ K) = 5.65 \pm 0.2\ kcal{\cdot}mol^{-1}$. Thus the enthalpy of formation of the gas is found to be $22.38 \pm 0.44\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

There has been considerable controversy as to the configuration of this molecule and the assignment of its vibrational frequencies. However, the evidence seems fairly conclusive for the linearity of the molecule from the work of Lafferty *et al.*[3] and Miller and Fateley.[4] The rotational constant adopted here is that found by Lafferty *et al.*[3] and the vibrational frequencies are those reported by Miller and Fateley,[4] except for ν_7 which is taken from Miller *et al.*[5] and Borgers.[7] The low frequency Π_u mode is confirmed by the work of McDougall and Kilpatrick,[2] who measured the low temperature entropy of C_3O_2(cr) and (l) and also the enthalpy of vaporization. From a comparison of the entropy calculated statistically and that measured, they conclude $\nu_7 = 63.2\ cm^{-1}$. The values adopted are confirmed by 3rd law analysis of the vapor pressure data of McDougall *et al.*[5] which indicates a enthalpy of vaporization in fair agreement with their calorimetric value. The drift in the 3rd law analysis indicates that the entropy of the solid is too low or that of the gas is too high by $1\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$. Alternatively as systematic error in the pressure measurements could have caused this deviation.

The bond distances are taken from the electron diffraction experiments of Livingston and Rao[6] and are in good accord with the adopted rotational constant.

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Carbon Suboxide (C_3O_2) $C_3O_2(g)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−15.018	−96.819	−96.819	INFINITE
100	45.309	217.230	328.013	−11.078	−95.963	−100.070	52.271
200	56.055	251.539	281.870	−6.066	−94.842	−104.603	27.320
250	62.055	264.706	277.147	−3.110	−94.230	−107.114	22.380
298.15	66.989	276.071	276.071	0.	−93.638	−109.649	19.210
300	67.161	276.486	276.072	0.124	−93.616	−109.749	19.109
350	71.401	287.167	276.906	3.591	−93.038	−112.484	16.787
400	74.976	296.941	278.808	7.253	−92.526	−115.298	15.056
450	78.069	305.955	281.330	11.081	−92.100	−118.171	13.717
500	80.806	314.324	284.216	15.054	−91.764	−121.087	12.650
600	85.504	329.486	290.524	23.377	−91.335	−126.996	11.056
700	89.406	342.969	297.071	32.129	−91.157	−132.957	9.921
800	92.664	355.126	303.580	41.237	−91.148	−138.931	9 071
900	95.380	366.202	309.932	50.643	−91.251	−144.898	8.410
1000	97.642	376.372	316.075	60.298	−91.428	−150.850	7.880
1100	99.527	385.770	321.989	70.159	−91.657	−156.781	7.445
1200	101.103	394.499	327.672	80.193	−91.926	−162.690	7.082
1300	102.426	402.646	333.129	90.371	−92.228	−168.575	6.773
1400	103.542	410.278	338.370	100.671	−92.560	−174.436	6.508
1500	104.490	417.455	343.406	111.074	−92.921	−180.272	6.278
1600	105.298	424.225	348.247	121.565	−93.313	−186.083	6.075
1700	105.993	430.630	352.907	132.130	−93.736	−191.868	5.895
1800	106.592	436.706	357.395	142.760	−94.192	−197.628	5.735
1900	107.112	442.483	361.722	153.446	−94.683	−203.361	5.591
2000	107.566	447.989	365.899	164.180	−95.209	−209.067	5.460
2100	107.964	453.247	369.934	174.957	−95.774	−214.746	5.342
2200	108.314	458.278	373.837	185.771	−96.378	−220.397	5.233
2300	108.625	463.100	377.613	196.619	−97.022	−226.020	5.133
2400	108.900	467.729	381.272	207.495	−97.708	−231.615	5.041
2500	109.146	472.179	384.820	218.398	−98.435	−237.179	4.956
2600	109.367	476.465	388.263	229.324	−99.205	−242 714	4.876
2700	109.565	480.596	391.607	240.270	−100.018	−248.218	4.802
2800	109.744	484.584	394.857	251.236	−100.875	−253.691	4.733
2900	109.905	488.438	398.018	262.218	−101.774	−259.134	4.668
3000	110.052	492.166	401.094	273.216	−102.717	−264.544	4.606
3100	110.185	495.777	404.090	284.228	−103.703	−269.921	4.548
3200	110.307	499.277	407.011	295.253	−104.733	−275.268	4.493
3300	110 419	502.673	409.858	306.290	−105.805	−280.581	4.441
3400	110.521	505 971	412.637	317.337	−106.919	−285.860	4.392
3500	110.615	509.176	415.349	328.393	−108.076	−291.106	4.345
3600	110.701	512.294	417.999	339.459	−109.274	−296.319	4.299
3700	110.781	515.328	420.589	350.533	−110.514	−301.498	4.256
3800	110.855	518.283	423.121	361.615	−111.796	−306.642	4.215
3900	110.924	521.163	425.598	372.704	−113.118	−311.752	4.175
4000	110.987	523.973	428.023	383.800	−114.481	−316.828	4.137
4100	111.046	526.714	430.396	394.902	−115.885	−321.870	4.101
4200	111.102	529.391	432.722	406.009	−117.329	−326.876	4.065
4300	111.153	532.005	435.000	417.122	−118.814	−331.848	4.031
4400	111.201	534.561	437.234	428.240	−120.339	−336.785	3.998
4500	111.246	537.061	439 425	439.362	−121.905	−341.687	3.966
4600	111.288	539.506	441.574	450.489	−123.511	−346.554	3.935
4700	111.328	541.900	443.683	461.620	−125.157	−351.384	3.905
4800	111.365	544.244	445.754	472.754	−126.845	−356.180	3.876
4900	111.400	546.541	447 788	483.892	−128.574	−360.939	3.848
5000	111.433	548.792	449.785	495.034	−130.345	−365.663	3.820
5100	111.464	550.999	451.748	506 179	−132.158	−370.351	3.793
5200	111 493	553.164	453.678	517.327	−134.015	−375.005	3.767
5300	111.521	555.288	455.575	528.477	−135 914	−379.620	3.741
5400	111.547	557.372	457.441	539.631	−137 859	−384.201	3.716
5500	111.572	559.419	459.276	550.787	−139.848	−388.745	3 692
5600	111.595	561.430	461.083	561.945	−141.883	−393.251	3 668
5700	111.618	563.405	462.861	573.106	−143.966	−397.722	3 645
5800	111.639	565.347	464.611	584.269	−146.096	−402.155	3.622
5900	111.659	567.255	466.334	595.434	−148.275	−406.552	3.599
6000	111.678	569.132	468.032	606.600	−150.504	−410 911	3.577

PREVIOUS June 1968 (1 atm) CURRENT June 1968 (1 bar)

Carbon Suboxide (C_3O_2) $C_3O_2(g)$

Carbon (C_4) **IDEAL GAS** $M_r = 48.044$ **Carbon (C_4)** **C_4(g)**

$S°(298.15\ K) = 228.3 \pm 16.7\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 964 \pm 33\ kJ \cdot mol^{-1}$

$\Delta_f H°(298.15\ K) = 971 \pm 33\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[2150] (1)
[950] (1)
[1700] (1)
[550] (2)
[550] (2)

Ground State Configuration: $[^1\Sigma]$

$\sigma = 2$

Point Group: $[D_{\infty h}]$

Bond Distances: C–C = [1.28] Å

Bond Angle: C–C–C = [180°]

Rotational Constant: B_0 = [0.171328] cm^{-1}

Enthalpy of Formation

The enthalpy of formation is obtained from the mass-spectrometric results of Drowart *et al* [1] who obtained $\Delta_f H°(2400\ K) = 226 \pm 7$ $kcal \cdot mol^{-1}$. This was obtained from a 2nd law analysis of the ion intensity ratio C_4^+/C^+ over a temperature range of 2200–2700 K. the absolute pressure, obtained from a knowledge of the monatomic carbon vapor pressure and an estimated ionization cross-section ratio of 4.96, yields a 2nd law entropy at 2400 K of 90.5 ± 3 $cal \cdot K^{-1} \cdot mol^{-1}$. The uncertainty in the ionization cross-section ratio is probably no more than a factor of two which gives an overall entropy uncertainty of ±4.5 $cal \cdot K^{-1} \cdot mol^{-1}$. The enthalpy of formation at temperatures other than 2400 K depend on the functions adopted, for a discussion of these see below.

Heat Capacity and Entropy

The molecular properties of C_4 are all estimated. We have chosen a set of functions which is consistent with the mass- spectrometric observations of Drowart *et al.*[1] The thermodynamic functions of C_4 were first estimated by Pitzer and Clementi[2] but the basis for this estimate has completely changed. Originally they were calculated by analogy with C_3, C_3O_2 and CO_2, but the discovery of very low bending frequencies in C_3 and C_3O_2 complicated the picture by raising the calculated entropies significantly. Sandborn[3] has correlated the bending force constants in several related triatomics and has estimated the vibrational frequencies in C_4 and C_5. These vibrational frequencies yield high entropies outside the limits of the 2nd law determination. Since these frequencies are estimates based on a basically triatomic correlation we have chosen to adopt two bending frequencies of 550 cm^{-1} rather than the 200 cm^{-1} and 440 cm^{-1} estimated by Sandborn. In addition we have assumed that the ground state arising from a π^2 term is Σ^1 and not Σ^3 as assumed by Pitzer and Clementi. The basis for both these changes is to make the functions conform to the only available measured data. Use of the present table will yield values for the vapor pressure of C_4 in excellent agreement with the measurements in the 2000–3000 K range. Outside this range they provide only a general indication of the variation since they may not correspond to the real situation.

The stretching frequencies are from Sandborn[3] and the bond length is estimated from C_3.

References

[1] J. Drowart, R. P. Burns, G. DeMaria and M. G. Inghram, J. Chem. Phys. 31, 1131 (1959).
[2] K. S. Pitzer and E. Clementi, J. Am. Chem. Soc. 81, 4477 (1959).
[3] R. H. Sandborn, J. Chem. Phys. 49, 4219 (1968).

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.791	964.101	964.101	INFINITE
100	29.865	187.031	265.752	−7.872	966.782	948.459	−495.424
200	39.876	210.373	232.603	−4.446	968.902	929.293	−242.706
250	45.537	219.893	229.123	−2.308	969.858	919.279	−192.073
298.15	50.176	228.322	228.322	0.	970.688	909.460	−159.334
300	50.338	228.633	228.323	0.093	970.718	909.080	−158.285
350	54.319	236.701	228.951	2.712	971.454	898.747	−134.131
400	57.657	244.179	230.393	5.514	972.048	888.318	−116.002
450	60.512	251.139	232.316	8.470	972.491	877.823	−101.895
500	62.998	257.646	234.527	11.559	972.786	867.287	−90.605
600	67.134	269.512	239.389	18.074	972.988	846.161	−73.665
700	70.424	280.117	244.463	24.958	972.781	825.034	−61.565
800	73.067	289.700	249.528	32.137	972.276	803.959	−52.493
900	75.201	298.434	254.484	39.554	971.555	782.961	−45.442
1000	76.933	306.450	259.285	47.164	970.672	762.052	−39.806
1100	78.348	313.851	263.914	54.930	969.663	741.238	−35.198
1200	79.511	320.719	268.365	62.825	968.553	720.520	−31.363
1300	80.475	327.123	272.641	70.826	967.358	699.899	−28.122
1400	81.279	333.117	276.749	78.915	966.088	679.372	−25.348
1500	81.955	338.748	280.697	87.078	964.753	658.939	−22.946
1600	82.528	344.056	284.492	95.303	963.358	638.596	−20.848
1700	83.017	349.075	288.145	103.580	961.907	618.343	−18.999
1800	83.437	353.832	291.663	111.904	960.404	598.176	−17.359
1900	83.800	358.353	295.055	120.266	958.850	578.095	−15.893
2000	84.115	362.660	298.329	128.662	957.248	558.096	−14.576
2100	84.390	366.770	301.491	137.088	955.599	538.179	−13.386
2200	84.632	370.702	304.548	145.539	953.904	518.341	−12.307
2300	84.846	374.469	307.507	154.013	952.164	498.582	−11.323
2400	85.035	378.084	310.373	162.507	950.379	478.899	−10.423
2500	85.204	381.559	313.151	171.019	948.551	459.291	−9.596
2600	85.355	384.903	315.847	179.548	946.679	439.758	−8.835
2700	85.490	388.127	318.464	188.090	944.765	420.297	−8.131
2800	85.612	391.239	321.008	196.645	942.808	400.908	−7.479
2900	85.722	394.245	323.482	205.212	940.809	381.590	−6.873
3000	85.822	397.153	325.890	213.789	938.768	362.341	−6.309
3100	85.913	399.968	328.234	222.376	936.684	343.161	−5 782
3200	85.996	402.697	330.519	230.971	934.560	324.049	−5.290
3300	86.071	405.345	332.746	239.575	932.393	305.004	−4.828
3400	86.140	407.915	334.919	248.186	930.186	286.025	−4.394
3500	86.204	410.413	337.041	256.803	927.937	267.112	−3 986
3600	86.263	412.842	339.113	265.426	925.646	248.263	−3.602
3700	86.317	415.207	341.138	274.055	923.315	229.479	−3.240
3800	86.367	417.509	343.117	282.689	920.943	210.758	−2.897
3900	86.413	419.753	345.054	291.328	918.530	192.101	−2.573
4000	86.456	421.942	346.949	299.972	916.075	173.505	−2.266
4100	86.496	424.077	348.804	308.620	913.580	154.972	−1.974
4200	86.533	426.162	350.621	317.271	911.044	136.500	−1.698
4300	86.568	428.198	352.402	325.926	908.468	118.089	−1.434
4400	86.600	430.189	354.147	334.584	905.850	99.738	−1.184
4500	86.631	432.135	355.858	343.246	903.192	81.447	−0.945
4600	86.659	434.040	357.537	351.911	900.493	63.216	−0.718
4700	86.686	435.904	359.185	360.578	897.754	45.044	−0.501
4800	86.711	437.729	360.802	369.248	894.974	26.930	−0.293
4900	86.734	439.517	362.391	377.920	892.154	8.875	−0.095
5000	86.756	441.270	363.951	386.594	889.293	−9.122	0.095
5100	86.777	442.988	365.484	395.271	886.391	−27.062	0.277
5200	86.797	444.673	366.990	403.950	883.449	−44.944	0.451
5300	86.816	446.327	368.472	412.630	880.466	−62.769	0.619
5400	86.833	447.950	369.929	421.313	877.443	−80.538	0.779
5500	86.850	449.543	371.362	429.997	874.379	−98.250	0.933
5600	86.866	451.108	372.772	438.683	871.275	−115.906	1.081
5700	86.881	452.646	374.160	447.370	868.130	−133.507	1.223
5800	86.895	454.157	375.526	456.059	864.945	−151.052	1.360
5900	86.908	455.642	376.871	464.749	861.719	−168.541	1.492
6000	86.921	457.103	378.196	473.441	858.453	−185.976	1.619

PREVIOUS: December 1969 (1 atm)   CURRENT December 1969 (1 bar)

Carbon (C_4) **C_4(g)**

Tetramethylsilane ($Si(CH_3)_4$) IDEAL GAS M_r = 88.22478

$S°(298.15\ K) = 361.189\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K)$ = Unknown

$\Delta_f H°(298.15\ K) = [-286.604]\ kJ \cdot mol^{-1}$

Enthalpy of Formation

Source unknown.

Heat Capacity and Entropy

$C_p°$ taken from Janz *et al.*[1]

Reference

[1] G. J. Janz, Y. Mikawa, and F. Behnke, Rensseler Polytechnic Institute, personal communication, (March 16, 1960).

Tetramethylsilane ($Si(CH_3)_4$) $C_4H_{12}Si_1(g)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	138.574	361.189	361.189	0.	−286.604	−148.063	25.940
300	139.076	362.047	361.191	0.257	−286.768	−147.202	25.630
400	167.695	406.038	366.996	15.617	−295.056	−99.399	12.980
500	193.761	446.324	378.886	33.719	−302.074	−49.646	5.186
600	216.271	483.685	393.276	54.245	−307.811	1.399	−0.122
700	235.852	518.525	408.708	76.871	−312.352	53.310	−3.978
800	253.006	551.160	424.497	101.331	−315.801	105.794	−6.908
900	268.153	581.853	440.292	127.405	−318.275	158.652	−9.208
1000	281.416	610.807	455.910	154.897	−319.909	211.739	−11.060
1100	293.047	638.185	471.247	183.632	−320.839	264.954	−12.582
1200	303.256	664.131	486.249	213.457	−321.187	318.227	−13.852
1300	312.210	688.765	500.888	244.241	−321.064	371.510	−14.927
1400	319.992	712.196	515.152	275.862	−320.568	424.768	−15.848
1500	326.352	734.499	529.037	308.192	−319.809	477.981	−16.645

PREVIOUS December 1960 (1 atm) CURRENT· December 1960 (1 bar)

2–Butynedinitrile (C_4N_2) IDEAL GAS $M_r = 76.0574$ 2–Butynedinitrile (C_4N_2) $C_4N_2(g)$

$S°(298.15\ K) = 290.11 \pm 0.8\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 528.60 \pm 0.8\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 533.46 \pm 0.8\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies		
ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
2290(1)	2241(1)	263(2)
2119(1)	1154(1)	472(2)
692(1)	504(2)	107(2]

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: $D_{\infty h}$
Bond Distances: CN = 1.14 Å; C–C = 1.37 Å; C–C = 1.19 Å
Rotational Constant: $B_0 = 0.045397\ cm^{-1}$

Enthalpy of Formation

Armstrong and Marantz,[1] measured the enthalpy of combustion of the liquid for which they obtain a $\Delta_f H°(298.15\ K)$ of 120.6 kcal·mol^{-1} using 94.05 kcal·mol^{-1} for $\Delta_f H°(CO_2, g, 298.15\ K)$. They calculate the $\Delta_f H°(C_4N_2, g, 298.15\ K)$ with a $\Delta_{vap}H$ taken from Saggiomo.[2]

Heat Capacity and Entropy

Bond lengths determined by Miller and Hannan[3] from X-ray diffraction measurements on the solid. The vibrational frequencies were observed in the infrared and Raman by Miller *et al.*[4]

References

[1] G. T. Armstrong and S. Marantz, J. Phys. Chem. **64**, 1776 (1960).
[2] A. J. Saggiomo, J. Org. Chem. **22**, 1171 (1957).
[3] F. A. Miller and R. B. Hannan Jr., J. Chem. Phys. **21**, 110 (1953).
[4] F. A. Miller, R. B. Hannan Jr., and L. R. Cousins, J. Chem. Phys. **23**, 2127 (1955).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
0	0.	0.	INFINITE	−17.734	528.600	528.600	INFINITE
100	49.991	216.793	356.363	−13.957	529.237	523.919	−273.667
200	71.983	258.541	297.572	−7.806	531.171	517.925	−135.268
250	79.961	275.500	291.495	−3.999	532.341	514.480	−107.495
298.15	85.888	290.112	290.112	0.	533.460	510.937	−89.514
300	86.088	290.644	290.114	0.159	533.502	510.797	−88.938
350	90.899	304.290	291.181	4.588	534.590	506.926	−75.655
400	94.823	316.692	293.606	9.234	535.569	502.906	−65.673
450	98.158	328.058	296.811	14.061	536.417	498.770	−57.896
500	101.091	338.554	300.467	19.043	537.132	494.548	−51.665
600	106.147	357.446	308.425	29.413	538.205	485.923	−42.303
700	110.417	374 138	316.643	40.247	538.905	477.150	−35.605
800	114.050	389.126	324.782	51.475	539.340	468.295	−30.577
900	117.130	402.742	332.699	63.038	539.588	459.398	−26.663
1000	119.730	415.222	340.336	74.885	539.703	450.481	−23.531
1100	121.921	426.739	347.674	86.971	539.716	441.557	−20.968
1200	123.768	437.429	354.714	99.258	539.649	432.636	−18.832
1300	125.329	447.399	361.464	111.715	539.516	423.724	−17.025
1400	126.654	456.737	367.940	124.316	539.325	414.823	−15.477
1500	127.784	465.514	374.155	137.039	539.082	405.938	−14.136
1600	128.751	473.793	380.126	149.867	538.791	397.071	−12.963
1700	129.584	481.624	385.868	162.785	538.455	388.224	−11.929
1800	130.305	489.052	391.396	175.780	538.075	379.398	−11.010
1900	130.933	496.114	396.723	188.843	537.651	370.594	−10.188
2000	131.481	502.844	401.862	201.964	537.186	361.813	−9.450
2100	131.963	509.271	406.825	215.137	536.679	353.057	−8.782
2200	132.388	515.420	411.623	228.355	536.130	344.325	−8.175
2300	132.764	521.314	416.265	241.613	535.541	335.620	−7.622
2400	133.099	526.971	420.760	254.906	534.910	326.941	−7.116
2500	133.398	532.411	425.118	268.231	534.239	318.290	−6.650
2600	133.667	537.648	429.346	281.585	533.526	309.666	−6.221
2700	133.908	542.697	433.451	294.964	532.772	301.070	−5.825
2800	134.126	547.571	437.441	308.366	531.978	292.503	−5.457
2900	134.323	552.281	441.320	321.788	531.142	283.964	−5 115
3000	134.502	556.838	445.095	335.230	530.265	275.456	−4.796
3100	134.665	561.251	448.771	348.688	529.348	266.977	−4.499
3200	134.813	565.529	452.353	362.162	528.389	258.529	−4.220
3300	134.950	569.679	455.846	375.650	527.388	250.111	−3.959
3400	135.075	573.710	459.254	389.152	526.347	241.724	−3.714
3500	135.189	577.627	462.580	402.665	525.264	233.369	−3.483
3600	135.295	581.437	465.829	416.189	524.140	225.045	−3.265
3700	135.393	585.145	469.004	429.724	522.975	216.752	−3.060
3800	135 484	588.757	472.108	443.268	521.768	208.492	−2.866
3900	135.567	592.278	475.144	456.820	520.519	200.264	−2.682
4000	135.645	595.711	478.116	470.381	519.230	192.069	−2.508
4100	135.718	599.061	481.025	483.949	517.898	183.906	−2.343
4200	135.785	602.333	483.874	497.524	516.525	175.777	−2.186
4300	135.848	605.528	486.667	511.106	515.110	167.680	−2.037
4400	135.907	608.652	489.404	524.694	513.654	159.617	−1.895
4500	135.962	611.707	492.088	538.287	512.155	151.588	−1.760
4600	136.014	614.696	494.721	551.886	510.615	143.592	−1.631
4700	136.062	617.621	497.305	565.490	509.034	135.630	−1.507
4800	136.108	620.487	499.841	579.098	507.410	127.703	−1.390
4900	136.151	623.293	502.332	592.711	505.744	119.809	−1.277
5000	136.191	626.044	504.779	606.328	504.036	111.950	−1.170
5100	136.229	628.742	507.183	619.949	502.285	104.126	−1.066
5200	136.265	631.387	509.546	633.574	500.493	96.336	−0.968
5300	136.299	633.983	511.870	647.202	498.658	88.581	−0.873
5400	136.331	636.531	514.155	660.834	496.781	80.862	−0.782
5500	136.361	639.033	516.403	674.468	494.861	73.177	−0.695
5600	136.390	641.490	518.614	688.106	492.899	65.528	−0.611
5700	136.418	643.905	520.791	701.746	490.894	57.914	−0.531
5800	136.444	646.278	522.935	715.389	488.846	50.335	−0.453
5900	136.468	648 610	525.045	729.035	486.754	42.793	−0.379
6000	136.492	650.904	527.124	742.683	484.619	35.286	−0.307

PREVIOUS: March 1961 (1 atm) CURRENT March 1961 (1 bar)

Nickel Carbonyl (Ni(CO)$_4$) LIQUID M_r = 170.7416 Nickel Carbonyl (Ni(CO)$_4$) $C_4Ni_1O_4(l)$

$S°(298.15\ K) = [319.56 \pm 12.6]\ J \cdot K^{-1} \cdot mol^{-1}$
$T_{fus} = 253.86 \pm 0.1\ K$

$\Delta_f H°(298.15\ K) = -631.78 \pm 8.4\ kJ \cdot mol^{-1}$
$\Delta_{fus} H° = 13.832 \pm 0.021\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The adopted enthalpy of formation is a weighted average based on enthalpy of combustion data of Smagina and Ormont[1] and Fischer *et al.*[2] The results of Smagina and Ormont[1] have been recalculated along the lines indicated by Sykes,[3] using recent values of $\Delta_f H°$(NiO, cr)[4] and other auxiliary data.[5] Their corrected value of $\Delta_f H°$(Ni(CO)$_4$, l, 298.15 K) is −150 3 ± 3.0 kcal mol^{-1} (average of 3 determinations using Pt fuse). Fischer *et al.*[2] made two sets of determinations yielding the following values of $\Delta_f H°$(Ni(CO)$_4$, l, 298.15 K); −150.3 ± 0.5 kcal·mol^{-1} (average of 5 determinations using benzoic acid fuse) and −152.3 ± 0.5 kcal·mol^{-1} (average of 4 determinations using Pt fuse). Fischer *et al.*[2] mention that the difference in their two sets of values may be due to hydration effects but a more likely explanation is higher uncertainties in the percentage combustion, as suggested by Sykes.[3] Therefore, we adopt an uncertainty of ±2.0 kcal·mol^{-1}.

Heat Capacity and Entropy

We adopt the smooth values of $C_p°$ (90–270 K) reported by Spice *et al.*[6] Values above 270 K are based on a linear extrapolation of liquid $C_p°$ values from 255–270 K. The $C_p°$ data reported by Duncan and Murray[7] were calculated from gas phase $C_p°$ data via a poorly defined procedure and show large deviations from the adopted $C_p°$.

The value of $S°$(298.15 K) is difficult to assess because of the lack of $C_p°$ data below 90 K. The adopted value of $S°$(298.15 K) is chosen so as to get the best agreement between second and third law analysis of the consistent vapor pressure data of Suginuma and Satozaki,[8] Walsh,[9] and Baev.[10] This treatment results in a value of $S°$(cr, 90 K) = 23.95 cal·K^{-1}·mol^{-1}. Spice *et al.*[6] had estimated a value of $S°$(cr, 90 K) = 20.6 cal·K^{-1}·mol^{-1} based on comparisons (at 90 and 120 K) with a "standard" heat capacity curve.

Fusion Data

The adopted values of T_{fus} and $\Delta_{fus}H°$ are those reported by Spice *et al.*[6] The value of $\Delta_{fus}H°$ is the mean of three calorimetrically determined values. Walsh[9] reported a value of T_{fus} approximately 2 K higher than the adopted value and also reported that T_{fus} is very sensitive to purity of the Ni(CO)$_4$. However, we find the purity determinations of Spice *et al.*[6] more than compelling than those of Walsh.[9]

Vaporization Data

The normal boiling point at 1 atm, T_{vap} = 315.4 ± 0.2 K, is based on the vapor pressure measurements of Suginuma and Satozaki,[8] Walsh[9] and Baev;[10] fugacity corrections have not been made. See Ni(CO)$_4$(g) table[5] for analysis of $\Delta_{vap}H°$.

References

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[6] J. E. Spice, L. A. K. Staveley and G. A. Harrow, J. Chem. Soc., 100 (1955).
[7] A. B. F. Duncan and J. W. Murray, J. Chem. Phys. 2, 636 (1934).
[8] B. Suginuma and K. Satozaki, Bull. Inst. Phys. Chem. Research (Tokyo) 21, 432 (1942).
[9] K. A. Walsh, U. S. Atomic Energy Commission Report LA–1649, (1953).
[10] A. K. Baev, Obshch. Prikl. Khim. 2, 146 (1970).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0							
100	98.031	145.316	484.659	−33.934	−645.917	−624.661	326.289
170.000	138.490	207.499	358.113	−25.604	GLASS <– –> LIQUID TRANSITION		
170.000	196.230	207 499	358.113	−25.604			
200	197.903	239.525	337.985	−19.692	−640.692	−604.698	157.931
298.15	203.342	319.560	319.560	0.	−631.784	−588.980	103.187
300	203.426	320.818	319.564	0.376	−631.628	−588.715	102.504
400	208.949	380.097	327.609	20.995	−623.770	−575.626	75.169
500	214.472	427.315	342.983	42.166	−616.991	−564.395	58.962
600	219.995	466.906	360.424	63.889	−611.178	−554.437	48.268
700	225.518	501.234	378.141	86.165	−605.825	−545.398	40.698

PREVIOUS· CURRENT: March 1978

$S°(298.15\ K) = 415.51 \pm 8.4\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -605.71 \pm 10.5\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -601.58 \pm 10.5\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies, Degeneracies, and Anharmonicities

ν, cm^{-1}	ν, cm^{-1}	x_{ij}, cm^{-1}
2132.4(1)	458.9(3)	$x_{11} = -2.6$
370.8(1)	423.1(3)	$x_{15} = -11.0$
380 (2)	79 (3)	$x_{55} = -5.0$
62 (2)	300 (3)	$g_{55} = -4.5$
2057.8(3)		All others = 0

Ground State Quantum Weight: 1 $\sigma = 12$
Point Group: T_d
Bond Distances: Ni–C = 1.82 ± 0.03 Å; C–O = 1.15 ± 0.02 Å
Bond Angles: C–Ni–C = 109.4712°; Ni–C–O = 180°
Product of the Moments of Inertia: $I_A I_B I_C = 5.14154 \times 10^{-112}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The value of $\Delta_f H°$(g, 298.15 K) is obtained from $\Delta_f H°$(l, 298.15 K)[1] by addition of the enthalpy of vaporization, $\Delta_{vap}H°(298.15\ K) = 7.22 \pm 1.5\ kcal{\cdot}mol^{-1}$. The adopted value of the enthalpy of vaporization is selected from our 3rd law analysis of the vaporization data given below and is based primarily on the data of Suginuma and Satozaki,[2] Baev[3] and Walsh.[4] The uncertainty has been increased above that indicated in the table below to account for uncertainties in the free energy functions of the liquid and gas. Fugacity corrections have not been applied but they are expected to be within the stated uncertainty. The enthalpy of vaporization at the boiling point, $\Delta_{vap}H°$, is the difference between $\Delta_f H°$(g) and $\Delta_f H°$(l) at the boiling point.

Data for the equilibrium $Ni(cr) + 4CO(g) = Ni(CO)_4(g)$ have been reviewed by Kipnis.[7] The data show considerable scatter and this has been attributed to differences in chemical potential of nickel (sheet or powder) used in the reaction.[7,8] Values of $\Delta_f H°$(298.15 K) derived from these studies are less negative than the adopted value by several kcal·mol^{-1} and are less reliable due to uncertainty in the chemical potential of nickel.

Source	Data Points	T/K	$\Delta_{vap}H°$(298.15 K), kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°$(298.15 K) kcal·mol^{-1}
[2]	20	273–298	7.209 ± 0.024	7.217 ± 0.005	0.026 ± 0.084	143.78 ± 2.5
[2]	18	273–307	7.285 ± 0.015	7.224 ± 0.005	−0.208 ± 0.052	143.78 ± 2.5
[3]	33*	285–312	7.146 ± 0.013	7.216 ± 0.006	0.231 ± 0.043	143.78 ± 2.5
[4]	5	273–308	7.233 ± 0.031	7.222 ± 0.005	−0.037 ± 0.105	143.78 ± 2.5
[5]	9	253–316	6.933 ± 0.025	7.209 ± 0.043	0.961 ± 0.086	143.79 ± 2.5
[6]	8	275–313	7.284 ± 0.075	7.264 ± 0.016	−0.068 ± 0.255	143.74 ± 2.5

*Point at 281.94 K rejected by statistical test.

Heat Capacity and Entropy

The adopted vibrational data, including anharmonicity, are from Jones *et al.*[9] The largest uncertainty in these assignments is in the frequency of the MCO bending vibration, ν_3. Jones *et al.*[9] chose 380 cm^{-1} based on a study of the spectra of substituted carbonyls by Bigorgne and Bouquet.[10] Ross *et al.*[11] summarized values of $S°$(298.15 K) (96.2 to 99.8 cal·K^{-1}·mol^{-1}) obtained from various frequency assignments; most of this variation is due to alternate assignments for ν_3. The adopted molecular structure data are from the electron diffraction study of Brockway and Cross[12] which conclusively indicates a tetrahedral structure. Moment of inertia calculations based on the adopted bond distances and angles yield $I_A = I_B = I_C = 8.01120 \times 10^{-38}\ g{\cdot}cm^2$.

The thermodynamic functions, including the effects of available vibrational anharmonicities, are calculated using the computer program of McDowell.[13] Compared to a harmonic oscillator calculation using the same data the present results are identical at 298.15 K, while at 6000 K the entropy is 0.333 cal·K^{-1}·mol^{-1} higher.

References

[1] JANAF Thermochemical Tables: Ni(CO)$_4$(l), 3–31–78.
[2] B. Suginuma and K. Satozaki, Bull. Inst. Phys. Chem. Research (Tokyo) 21, 432 (1942).
[3] A. K. Baev, Obshch Prikl. Khim. 2, 146 (1970).
[4] K. A. Walsh, U. S. Atomic Energy Commission Report LA-1649, (1953).

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−30.495	−605.714	−605.714	INFINITE
100	84.479	286.831	532.198	−24.537	−606.311	−599.206	312.993
200	127.972	359.892	428.595	−13.741	−604.533	−592.611	154.774
298.15	149.289	415.507	415.507	0.	−601.576	−587.378	102.906
300	149.557	416.431	415.510	0.276	−601.519	−587.290	102.256
400	160.377	461.081	421.524	15.823	−598.734	−582.983	76.130
500	167.490	497.670	433.204	32.233	−596.716	−579.297	60.519
600	173.167	528.724	446.600	49.274	−595.585	−575.934	50.140
700	178.000	555.790	460.306	66.839	−594.943	−572.706	42.736
800	182.138	579.836	473.772	84.851	−594.376	−569.571	37.189
900	185.652	601.497	486.781	103.245	−594.059	−566.492	32.878
1000	188.623	621.216	499.253	121.963	−593.948	−563.436	29.431
1100	191.125	639.314	511.174	140.954	−594.007	−560.383	26.610
1200	193.238	656.037	522.558	160.175	−594.219	−557.319	24.259
1300	195.025	671.577	533.431	179.590	−594.575	−554.230	22.269
1400	196.543	686.087	543.822	199.171	−595.076	−551.109	20.562
1500	197.836	699.692	553.765	218.891	−595.721	−547.947	19.081
1600	198.949	712.496	563.289	238.731	−596.514	−544.737	17.784
1700	199.902	724.587	572.425	258.675	−597.462	−541.473	16.637
1800	200.748	736.037	581.199	278.708	−615.719	−537.434	15.596
1900	201.472	746.911	589.637	298.820	−616.893	−533.053	14.655
2000	202.121	757.262	597.762	319.000	−618.127	−528.608	13.806
2100	202.683	767.137	605.594	339.241	−619.424	−524.101	13.036
2200	203.192	776.578	613.153	359.535	−620.783	−519.529	12.335
2300	203.641	785.620	620.456	379.877	−622.208	−514.895	11.694
2400	204.049	794.296	627.520	400.262	−623.699	−510.199	11.104
2500	204.412	802.633	634.359	420.685	−625.257	−505.437	10.561
2600	204.744	810.657	640.986	441.143	−626.882	−500.613	10.057
2700	205.042	818.390	647.415	461.633	−628.575	−495.724	9.590
2800	205.317	825.852	653.655	482.151	−630.336	−490.771	9.155
2900	205.566	833.061	659.718	502.695	−632.164	−485.756	8.749
3000	205.798	840.034	665.613	523.264	−634.059	−480.674	8.369
3100	206.013	846.785	671.349	543.854	−636.021	−475.528	8.013
3200	206.213	853.329	676.934	564.466	−1014.883	−465.132	7.592
3300	206.396	859.678	682.376	585.096	−1015.322	−447.946	7.090
3400	206.568	865.842	687.682	605.745	−1015.825	−430.744	6.618
3500	206.730	871.832	692.858	626.409	−1016.390	−413.529	6.172
3600	206.882	877.658	697.911	647.090	−1017.019	−396.295	5.750
3700	207.024	883.328	702.846	667.786	−1017.711	−379.044	5.351
3800	207.158	888.851	707.668	688.495	−1018.466	−361.771	4.973
3900	207.284	894.234	712.383	709.217	−1019.284	−344.479	4.614
4000	207.405	899.483	716.995	729.951	−1020.166	−327.166	4.272
4100	207.521	904.606	721.509	750.698	−1021.112	−309.829	3.947
4200	207.631	909.608	725.928	771.455	−1022.122	−292.469	3.637
4300	207.736	914.495	730.257	792.224	−1023.197	−275.083	3.342
4400	207.836	919.272	734.499	813.002	−1024.338	−257.673	3.059
4500	207.932	923.944	738.657	833.791	−1025.546	−240.236	2.789
4600	208.024	928.515	742.735	854.589	−1026.822	−222.772	2.530
4700	208.113	932.989	746.735	875.395	−1028.167	−205.277	2.281
4800	208.200	937.372	750.661	896.211	−1029.583	−187.754	2.043
4900	208.285	941.666	754.516	917.035	−1031.071	−170.199	1.814
5000	208.367	945.874	758.301	937.868	−1032.634	−152.615	1.594
5100	208.446	950.001	762.019	958.709	−1034.273	−134.997	1.383
5200	208.522	954.050	765.673	979.557	−1035.991	−117.350	1.179
5300	208.596	958.022	769.265	1000.413	−1037.789	−99.665	0.982
5400	208.669	961.922	772.797	1021.276	−1039.673	−81.948	0.793
5500	208.738	965.752	776.271	1042.147	−1041.642	−64.195	0.610
5600	208.807	969.514	779.688	1063.024	−1043.702	−46.404	0.433
5700	208.874	973.210	783.051	1083.908	−1045.855	−28.577	0.262
5800	208.941	976.843	786.361	1104.799	−1048.103	−10.709	0.096
5900	209.006	980.416	789.620	1125.696	−1050.452	7.194	−0.064
6000	209.070	983.929	792.829	1146.600	−1052.904	25.143	−0.219

PREVIOUS: March 1978 (1 atm) CURRENT. March 1978 (1 bar)

Carbon (C_5) IDEAL GAS $M_r = 60.055$ Carbon (C_5) $C_5(g)$

$S°(298.15\ K) = 242.0 \pm 16.7\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 972 \pm 25\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 979 \pm 25\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}
[1920] (1)	[550] (2)
[770] (1)	[550] (2)
[2210] (1)	[550] (2)
[1430] (1)	

Ground State Configuration: $[^1\Sigma]$ $\sigma = 2$
Point Group: $[D_{\infty h}]$
Bond Distance: C–C = [1.28] Å
Bond Angle: C–C–C = [180°]
Rotational Constant: $B_0 = [0.085664]\ cm^{-1}$

Enthalpy of Formation

The enthalpy of formation is obtained from the mass–spectrometric results of Drowart *et al* [1] who obtained $\Delta_f H°(2400\ K) = 230 \pm 5\ kcal{\cdot}mol^{-1}$. This was obtained from a 2nd law analysis of the ion intensity ration C_5^+/C^+ over a temperature range of 2200–2700 K. The absolute pressure, obtained from a knowledge of the monatomic carbon vapor pressure and an estimated ionization cross–section ratio of 6.3, yields a 2nd law entropy at 2400 K of $103.7 \pm 2\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$. The uncertainty in the ionization cross–section ratio is probably no more than a factor of two which gives an overall entropy uncertainty of $\pm 3.5\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$. The enthalpy of formation at temperatures other than 2400 K depend on the functions adopted, for a discussion of these see below.

Heat Capacity and Entropy

The molecular properties of C_5 are all estimated. We have chosen a set of functions which is consistent with the mass–spectrometric observations of Drowart *et al.*[1] The thermodynamic functions of C_5 were first estimated by Pitzer and Clementi[2] but the basis for this estimate has completely changed. Originally they were calculated by analogy with C_3, C_3O_2 and CO_2, but the discovery of very low bending frequencies in C_3 and C_3O_2 complicated the picture by raising the calculated entropies significantly. Sandborn[3] has correlated the bending force constants in several related triatomics and has estimated the vibrational frequencies in C_4 and C_5. These vibrational frequencies yield high entropies outside the limits of the 2nd law determination. Since these frequencies are estimates, based on a basically triatomic correlation we have chosen to adopt three doubly degenerate bending frequencies of 550 cm^{-1} in place of the 130 cm^{-1}, 330 cm^{-1} and 520 cm^{-1} frequencies estimated by Sandborn.[3] The basis for this change is to make the functions conform to the only available measured data. Use of the present tables will yield values for the vapor pressure of C_4 is excellent agreement with the measurements in the 2000–3000 K range. Outside this range they provide only a general indication of the variation since they may not correspond to the real situation.

The stretching frequencies are from Sandborn[3] and the bond length is estimated equal to that in C_3.

References

[1] J. Drowart, R. P. Burns, G. DeMaria, M. G. Inghram, J. Chem. Phys. 31, 1131 (1959).
[2] K. S. Pitzer and E. Clementi, J. Am. Chem. Soc. 81, 4477 (1959).
[3] R. H. Sandborn, J. Chem. Phys. 49, 4219 (1968).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−11.914	972.398	972.398	INFINITE
100	30.260	195.633	285.525	−8.989	975.024	955.937	−499.330
200	45.669	220.670	247.105	−5.287	977.094	936.042	−244.469
250	54.253	231.807	242.941	−2.784	978.119	925.660	−193.406
298.15	61.135	241.972	241.972	0.	979.056	915.470	−160.387
300	61.372	242.350	241.973	0.113	979.090	915.075	−159.329
350	67.147	252.260	242.742	3.331	979.954	904.336	−134.965
400	71.899	261.546	244.519	6.811	980.674	893.482	−116.677
450	75.903	270.252	246.899	10.509	981.231	882.548	−102.444
500	79.347	278.432	249.648	14.392	981.622	871.561	−91.051
600	85.013	293.421	255.718	22.622	981.961	849.508	−73.956
700	89.478	306.874	262.081	31.355	981.829	827.437	−61.744
800	93.049	319.064	268.454	40.488	981.357	805.410	−52.588
900	95.926	330.195	274.705	49.942	980.638	783.458	−45.471
1000	98.259	340.427	280.772	59.655	979.736	761.595	−39.782
1100	100.164	349.885	286.631	69.579	978.691	739.831	−35.132
1200	101.731	358.670	292.273	79.676	977.532	718.167	−31.261
1300	103.029	366.865	297.699	89.916	976.277	696.603	−27.990
1400	104.113	374.541	302.916	100.275	974.938	675.140	−25.190
1500	105.025	381.756	307.934	110.733	973.524	653.774	−22.766
1600	105.798	388.560	312.763	121.276	972.041	632.506	−20.649
1700	106.457	394.994	317.412	131.889	970.494	611.332	−18.784
1800	107.023	401.096	321.893	142.564	968.885	590.251	−17.129
1900	107.513	406.895	326.216	153.291	967.218	569.261	−15.650
2000	107.938	412.421	330.389	164.064	965.493	548.360	−14.322
2100	108.310	417.697	334.422	174.877	963.713	527.547	−13.122
2200	108.637	422.743	338.323	185.725	961.877	506.820	−12.033
2300	108.925	427.579	342.099	196.603	959.988	486.177	−11.041
2400	109.181	432.220	345.758	207.509	958.045	465.618	−10.134
2500	109.409	436.682	349.306	218 439	956.049	445.142	−9.301
2600	109.613	440.977	352.750	229.390	954.001	424.745	−8.533
2700	109.796	445.117	356.095	240.360	951.900	404.429	−7.824
2800	109.960	449.113	359.346	251.348	949.748	384.192	−7.167
2900	110.109	452.974	362.508	262.352	947.544	364.032	−6.557
3000	110.244	456.710	365.586	273.370	945.289	343.949	−5.989
3100	110.367	460.327	368.584	284.400	942.982	323.942	−5.458
3200	110.479	463.832	371.506	295.443	940.624	304.011	−4.962
3300	110.581	467.234	374.356	306.496	938.215	284.154	−4.498
3400	110.675	470.536	377.137	317.559	935.755	264.371	−4.062
3500	110.761	473.746	379.851	328.631	933.244	244.660	−3.651
3600	110.840	476.867	382.503	339.711	930.682	225.023	−3.265
3700	110.913	479.905	385.094	350.798	928.069	205.457	−2.901
3800	110.981	482.864	387.629	361.893	925.406	185.962	−2.556
3900	111.043	485.747	390.108	372.994	922.692	166.539	−2.231
4000	111.101	488.559	392.534	384.101	919.927	147.185	−1.922
4100	111.155	491.303	394.910	395.214	917.111	127.901	−1.629
4200	111.206	493.983	397.237	406.332	914.245	108.687	−1.352
4300	111.252	496.600	399.517	417.455	911.328	89.541	−1.088
4400	111.296	499.158	401.753	428.583	908.361	70.464	−0.837
4500	111.337	501.660	403.945	439.714	905.343	51.455	−0.597
4600	111.376	504.107	406 096	450.850	902.275	32.513	−0.369
4700	111.412	506.503	408.207	461.990	899.156	13.639	−0.152
4800	111.446	508.849	410.279	473.132	895.987	−5.168	0.056
4900	111.477	511.147	412.315	484.279	892.767	−23.909	0.255
5000	111.507	513.399	414.314	495.428	889.496	−42.584	0 445
5100	111.536	515.608	416.278	506.580	886.176	−61.192	0.627
5200	111.562	517.774	418.209	517.735	882.804	−79.735	0.801
5300	111.587	519.899	420.108	528.892	879.383	−98.213	0.968
5400	111.611	521.985	421.976	540.052	875.910	−116.626	1.128
5500	111.634	524.033	423.813	551.215	872.388	−134.974	1.282
5600	111.655	526.045	425.620	562.379	868.815	−153.257	1.430
5700	111.676	528.021	427.399	573.546	865.191	−171.477	1.571
5800	111.695	529.964	429.151	584.714	861.517	−189.632	1.708
5900	111.713	531.873	430.876	595.885	857.793	−207.723	1.839
6000	111.730	533.751	432.575	607.057	854.018	−225.751	1.965

PREVIOUS: December 1969 (1 atm) CURRENT. December 1969 (1 bar)

Iron Carbonyl ($Fe(CO)_5$) LIQUID M_r = 195.8990 Iron Carbonyl ($Fe(CO)_5$) $C_5Fe_1O_5(l)$

$S°(298.15\ K) = 337.08 \pm 4\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{fus} = 253.1 \pm 0.1\ K$

$\Delta_fH°(298.15\ K) = -766.09 \pm 7.1\ kJ{\cdot}mol^{-1}$
$\Delta_{fus}H° = 13.226 \pm 0.013\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

The adopted enthalpy of formation is based on the enthalpy of combustion measurements of Cotton *et al.*[1] The average energy of combustion reported by these authors is $-386.86 \pm 1.7\ kcal{\cdot}mol^{-1}$ which yields a value of $\Delta_cH°(298.15\ K) = -385.82 \pm 1.7\ kcal{\cdot}mol^{-1}$. Using auxiliary JANAF data[2] we calculate the adopted value of $\Delta_fH°(298.15\ K) = -183.1 \pm 1.7\ kcal{\cdot}mol^{-1}$. Earlier combustion work by Roth[3] and Mittasch[4] appears less reliable due to incomplete characterization of products.

Heat Capacity and Entropy

The adopted heat capacity is derived by merging the $C_p°$ data of Leadbetter and Spice[5] (22–287 K) with $C_p°$ data derived from the enthalpy measurements of Welty *et al.*[6] (302–387 K). Leadbetter and Spice report a small anomaly in $C_p°(cr)$ near 230 K which they attribute to the presence of a small amount of impurity; therefore we have smoothed through this anomaly. The heat capacity[5] and enthalpy data[6] of the liquid merge smoothly and yield a constant $C_p° = 55.876\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ from the melting point to 387 K. We assume $C_p°$ remains constant at this value above this temperature.

The adopted value of $S°(298.15\ K)$ is obtained by the appropriate integration of $C_p°$ data assuming $S°(25\ K) = 3.49 \pm 1.0\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$. $S°(25\ K)$ is obtained by using a single Debye function with 18 degrees of freedom and $\theta_D = 155$ K as suggested by Leadbetter and Spice.[5] The uncertainty in this procedure is rather large since a single Debye function fits the observed $C_p°$ data quite poorly.

Fusion Data

The adopted values of T_{fus} and $\Delta_{fus}H°$ are those reported by Leadbetter and Spice.[5] The value of T_{fus} agrees well with that listed by Brynestad.[7] For $\Delta_{fus}H°$ the only other value is $\Delta_{fus}H° = 3250 \pm 40\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ reported by Mittasch.[4] This is much less precise than the adopted value which is an average of two determinations.

Vaporization Data

The adopted boiling point, $T_{vap}(1\ atm) = \sim 377$ K, is based on the vapor pressure data of Trautz and Badstubner[8] and Baev;[9] fugacity corrections have not been made. See the enthalpy of formation section of the $Fe(CO)_5(g)$ table[2] for details of the selected value of $\Delta_{vap}H°$.

References

[1] F. A. Cotton, A. K. Fischer and G. Wilkinson, J Amer. Chem. Soc. 81, 800 (1959).
[2] JANAF Thermochemical Tables: $Fe_2O_3(cr)$, 6–30–65; $CO_2(g)$, 9–20–65, $Fe(CO)_5(g)$, 3–31–78.
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[5] A. J. Leadbetter and J. E. Spice, Can. J. Chem. 37, 1923 (1959).
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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−52.934	−787.554	−787.554	INFINITE
100	105.240	113.401	580.650	−46.725	−789.327	−756.258	395.029
200	164.163	204.889	370.766	−33.175	−786.457	−724.021	189.095
253.100	191.020	246.527	340.393	−23.758		CRYSTAL <--> LIQUID	
253.100	233.785	298.781	340.393	−10.532		TRANSITION	
298.15	233.785	337.078	337.078	0.	−766.090	−696.975	122.107
300	233 785	338.524	337.083	0.432	−765.919	−696.547	121.280
400	233.785	405.780	346.253	23.811	−757.710	−674.716	88.109
500	233.785	457.948	363.569	47.190	−751.465	−654.729	68.399
600	233.785	500.572	382.958	70.568	−746.962	−635.831	55.354
700	233.785	536.610	402.401	93.947	−743.911	−617.569	46.084

PREVIOUS: CURRENT: March 1978

Iron Carbonyl ($Fe(CO)_5$) IDEAL GAS M_r = 195.8990 Iron Carbonyl ($Fe(CO)_5$) $C_5Fe_1O_5(g)$

$S°(298.15\ K) = 439.3 \pm 12.6\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -729.52 \pm 7.1\ kJ{\cdot}mol^{-1}$

$\Delta_fH°(298.15\ K) = -727.85 \pm 7.1\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies, Degeneracies, and Anharmonicities

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}	x_{ij}, cm^{-1}	x_{ij}, cm^{-1}
2120.7 (1)	618.8 (1)	474.3 (2)	$x_{1,1} = -2.2$	$x_{1,6} = -11.9$
2041.7 (1)	429.0 (1)	104.9 (2)	$x_{2,10} = -6.9$	$x_{1,10} = -7.2$
442.8 (1)	100 (1)	74.3 (2)	$x_{6,6} = -7.7$	$x_{2,6} = -14.1$
413.4 (1)	2013.3 (2)	488 (2)	$x_{10,10} = -5.6$	$x_{2,2} = x_{6,10} = -2.0$
383 (1)	645.0 (2)	375 (2)	$x_{1,2} = -9.3$	all others = 0
2034.0 (1)	542.5 (2)	97.3 (2)		

Point Group: D_{3h} $\sigma = 6$

Bond Distances: $Fe\text{–}C_{eq} = 1.833 \pm 0.004$ Å; $Fe\text{–}C_{ax} = 1.806 \pm 0.005$ Å; $C\text{–}O = 1.145 \pm 0.003$ Å

Bond Angles: Fe–C–O = 180°; $C_{ax}\text{–}Fe\text{–}C_{ax}$ = 180°; $C_{eq}\text{–}Fe\text{–}C_{eq}$ = 120°; $C_{ax}\text{–}Fe\text{–}C_{eq}$ = 90°

Product of the Moments of Inertia: $I_AI_BI_C = 9.94833 \times 10^{-112}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The adopted value of $\Delta_fH°$(g, 298.15 K) is obtained from $\Delta_fH°$(l, 298.15 K)[1] by addition of the enthalpy of vaporization, $\Delta_{vap}H°(298.15\ K) = 9.14 \pm 1.2\ kcal{\cdot}mol^{-1}$. The adopted value of the enthalpy of vaporization is selected from our 3rd law analysis of the vaporization data below and is based primarily on the data of Trautz and Badstubner[2] and Baev.[3] The uncertainty has been increased above that indicated in the table below to account for uncertainties in the free functions of the liquid and gas. Fugacity corrections have not been made but they are expected to be well within the stated uncertainty. The enthalpy of vaporization at the boiling point, $\Delta_{vap}H°$, is calculated from the difference between $\Delta_fH°$(g) and $\Delta_fH°$(l) at the boiling point.

Source	Data Points	T/K	$\Delta_{vap}H°$(298.15 K), kcal·mol⁻¹ 2nd law	3rd law	Drift cal⁻¹·K⁻¹·mol⁻¹	$\Delta_fH°$(298.15 K) kcal·mol⁻¹
2	69	320–377	9.727 ± 0.004	9.138 ± 0.49	−1.688 ± 0.011	173.96 ± 1.7
3	28	266–353	9.215 ± 0.041	9.141 ± 0.036	−0.224 ± 0.125	173.96 ± 1.7
4	16	293–306	9.754 ± 0.095	9.219 ± 0.017	−1.780 ± 0.317	173.88 ± 1.7
5	12	254–306	9.207 ± 0.106	9.241 ± 0.042	0.121 ± 0.381	173.86 ± 1.7
6	13	258–293	9.505 ± 0.014	9.247 ± 0.025	−0.936 ± 0.052	173.85 ± 1.7
7	7	266–351	7.195 ± 0.550	8.977 ± 0.440	5.915 ± 1.816	174.12 ± 1.8

Heat Capacity and Entropy

The selected vibrational data, including anharmonicity, are from Jones *et al.*[8] The largest uncertainty in these assignments is for ν_9; Jones estimates it to lie at $100 \pm 15\ cm^{-1}$. The uncertainty in this assignment coupled with unknown anharmonicities for the low frequency vibrational modes lead to rather large uncertainties in the thermal functions. Following the arguments of Jones we estimate an uncertainty at $\pm 3.0\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ in S°(298.15 K).

The adopted molecular structure data are from the electron diffraction data of Beagley *et al.*[9] which clearly indicate that the Fe–C axial bond is shorter than the Fe–C equatorial bond. Moment of inertia calculations based on the adopted bond distances and angles yield $I_A = 9\ 078946 \times 10^{-38}\ g{\cdot}cm^2$ and $I_B = I_C = 1.046785 \times 10^{-37}\ g{\cdot}cm^2$. The electron diffraction study of Almenningen *et al.*[10] is in excellent agreement with the adopted data although a slightly smaller difference between the axial and equatorial Fe–C bond lengths is indicated. This would lead to an insignificant difference in S°(298.15 K).

The thermodynamic functions, including the effects of available vibrational anharmonicities, are calculated using the computer program of McDowell.[11] Compared to a harmonic oscillator calculation using the same data the present results are identical at 298.15 K, while at 6000 K the entropy is $0.407\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ higher.

References

[1] JANAF Thermochemical Tables: $Fe(CO)_5(l)$, 3–31–78.

[2] M. Trautz and W. Badstubner, Z. Electrokhem. 35, 799 (1929).

[3] A. K. Baev, Obshch. Prikl. Khim. #2, 146 (1970).

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[10] A. Almenningen, A. Haaland and K. Wahl, Acta Chem. Scand. 23, 2245 (1969).

[11] R. E. McDowell, QCPE #269, Quantum Chemistry Program Exchange, Indiana University, (1974).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	S° (J·K⁻¹mol⁻¹)	−[G°−H°(T_r)]/T (J·K⁻¹mol⁻¹)	H°−H°(T_r) (kJ·mol⁻¹)	$\Delta_fH°$ (kJ·mol⁻¹)	$\Delta_fG°$ (kJ·mol⁻¹)	log K_f
0	0.	0.	INFINITE	−33.145	−729.524	−729.524	INFINITE
100	90.843	299.071	568.282	−26.921	−731.282	−716.779	374.407
200	139.336	377.190	454.024	−15.367	−730.407	−702.431	183.456
298.15	170.703	439.286	439.286	0.	−727.849	−689.207	120.746
300	171.134	440.344	439.290	0.316	−727.794	−688.968	119.960
400	189.027	492.243	446.244	18.399	−724.880	−676.471	88.338
500	200.830	535.762	459.914	37.924	−722.489	−664.660	69.437
600	209.820	573.204	475.747	58.474	−720.815	−653.263	56.872
700	217.105	606.113	492.067	79.832	−719.784	−642.094	47.914
800	223.115	635.508	508.193	101.852	−719.325	−631.034	41.202
900	228.088	662.084	523.839	124.420	−719.472	−619.996	35.984
1000	232.209	686.335	538.894	147.442	−720.469	−608.900	31.806
1100	235.633	708.633	553.325	170.839	−722.455	−597.633	28.379
1200	238 490	729.261	567.137	194.549	−723.964	−586.239	25.518
1300	240.887	748.448	580.355	218.521	−723.888	−574.766	23.094
1400	242.910	766.375	593.009	242.713	−723.955	−563.293	21.017
1500	244.628	783.194	605.133	267.092	−724.162	−551.811	19.216
1600	246.097	799.030	616.761	291.630	−724.511	−540.311	17.639
1700	247.362	813.989	627.927	316.305	−725.955	−528.765	16.247
1800	248.458	828.159	638.661	341.097	−726.933	−517.139	15.007
1900	249.413	841.619	648.992	365.991	−742.160	−504.751	13 877
2000	250.250	854.434	658.946	390.975	−743.682	−492.217	12.855
2100	250.989	866.662	668.548	416.038	−745.279	−479.605	11.930
2200	251.644	878.353	677.821	441.170	−746.953	−466.913	11.086
2300	252.227	889.552	686.785	466.364	−748.706	−454.146	10.314
2400	252.751	900.298	695.459	491.614	−750.540	−441.301	9.605
2500	253.222	910.626	703.861	516.913	−752.456	−428.377	8.950
2600	253.647	920.566	712.005	542.256	−754.454	−415.374	8.345
2700	254.032	930.146	719.908	567.640	−756.537	−402.293	7.783
2800	254.387	939.391	727.583	593.062	−758.702	−389.133	7.259
2900	254.708	948.323	735.041	618.517	−760.951	−375.896	6.771
3000	255.006	956.963	742.296	644.003	−763.284	−362.578	6.313
3100	255.279	965.329	749.356	669.517	−765.698	−349.180	5.884
3200	255.534	973.438	756.233	695.058	−1116.495	−328.282	5.359
3300	255.768	981.305	762.934	720.623	−1117.171	−303.641	4.806
3400	255.988	988.944	769.470	746.211	−1117.960	−278.976	4.286
3500	256.193	996.367	775.847	771.820	−1118.861	−254.288	3.795
3600	256.386	1003.587	782.073	797.449	−1119.874	−229.571	3.331
3700	256.566	1010.614	788.156	823.097	−1120.999	−204.827	2.892
3800	256.737	1017.459	794.100	848.762	−1122.235	−180.047	2.475
3900	256.898	1024.130	799.913	874.444	−1123.583	−155.234	2.079
4000	257.051	1030.636	805.600	900.141	−1125.043	−130.388	1.703
4100	257.196	1036.985	811.167	925.854	−1126.615	−105.502	1.344
4200	257.335	1043.184	816.617	951.580	−1128.299	−80.577	1.002
4300	257.466	1049.241	821.957	977.320	−1130.098	−55.609	0.676
4400	257.593	1055.161	827.190	1003.073	−1132.010	−30.601	0.363
4500	257.714	1060.952	832.321	1028.839	−1134.038	−5.547	0.064
4600	257.831	1066.617	837.353	1054.616	−1136.182	19.553	−0.222
4700	257.942	1072.163	842.290	1080.405	−1138.445	44.703	−0.497
4800	258.050	1077.595	847.136	1106.204	−1140.828	69.902	−0.761
4900	258.155	1082.917	851.894	1132.015	−1143.332	95.152	−1.014
5000	258.256	1088.133	856.566	1157.835	−1145.961	120.454	−1.258
5100	258.353	1093.249	861.157	1183.666	−1148.717	145.811	−1.493
5200	258.449	1098.266	865.669	1209.506	−1151.602	171.219	−1.720
5300	258.541	1103.190	870.104	1235.355	−1154 619	196.688	−1.938
5400	258.631	1108.024	874.465	1261.214	−1157.773	222.213	−2.149
5500	258.719	1112.770	878.755	1287.081	−1161.066	247.797	−2.353
5600	258.804	1117.433	882.976	1312.958	−1164.504	273.445	−2.551
5700	258.888	1122.014	887.129	1338.842	−1168.089	299.153	−2.741
5800	258.970	1126.517	891.218	1364.735	−1171.827	324.929	−2.926
5900	259.050	1130.945	895.244	1390.636	−1175.723	350.764	−3.105
6000	259.129	1135.299	899.209	1416.545	−1179.782	376.673	−3.279

PREVIOUS: March 1978 (1 atm) CURRENT: March 1978 (1 bar)

$\Delta_fH°(0\ K) = -333.57 \pm 41.9\ kJ{\cdot}mol^{-1}$

$S°(298.15\ K) = 612.044 \pm 4.2\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_fH°(298.15\ K) = -328.44 \pm 41.9\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

Mah[1] determined the enthalpy of combustion of $Cr_{23}C_6(cr)$ using oxygen bomb calorimetry. Using auxiliary JANAF data[2] and the value $\Delta_cH°(303.15\ K) = -3604.2 \pm 1.5\ kcal{\cdot}mol^{-1}$ reported by Mah[1] for the combustion of $Cr_{23}C_6$, we calculate $\Delta_fH°(298.15\ K) = -78.5\ kcal{\cdot}mol^{-1}$ for $Cr_{23}C_6(cr)$. The combustion equation is $Cr_{23}C_6(cr) + 93/4\ O_2(g) = 23/2\ Cr_2O_3(cr) + 6\ CO_2(g)$. The factor (23/2) makes the Δ_fH value for $Cr_{23}C_6$ extremely sensitive to the corresponding value for $Cr_2O_3(cr)$. Of the nine combustion runs, Mah[1] reported complete combustion in three runs and 99.40 to 99.85% completion in the remaining six. Corrections for incomplete combustion, formation of small amounts of CO(g) and impurities were made by Mah.[1] These corrections amount to no more than 0.7% of the $\Delta_cE°$ value.

The pressures of CO(g) in equilibrium with a $Cr_{23}C_6$–Cr_2O_3–Cr mixture have been measured by Kelley *et al.*[3] and Kulkarni and Worrell.[4] Our analysis of their data is tabulated below. Kulkarni and Worrell[4] measured the CO pressure using a torsion effusion technique while Kelley *et al.*[3] measured the pressure manometrically. In all cases unit activity is assumed for the condensed species.

Source	TK	Comments[a]	Reaction[c]	$\Delta_fH°$(298.15 K), kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_fH°$(298.15 K) kcal·mol^{-1}
4	1170–1307	1/4 mm	A(15 pts.)	466.37	462.43	−3.2 ± 2.5	−78.53
4	1158–1286	1/3 mm	A(8 pts.)	450.14	462.31	9.9 ± 7.2	−78.41
4	1156–1283	1/2 mm	A(9 pts.)	451.46	467.72	13.3 ± 3.3	−83.82
3	1571–1772		A(18 pts.)[b]	459.47	467.19	4.6 ± 4.0	−83.29

[a] effusion orifice diameter

[b] 1725, 1775 K points rejected due to statistical test.

[c] Reaction: (A)$Cr_{23}C_6$ (cr) + 2 Cr_2O_3(cr) = 27Cr(cr)

We adopt $\Delta_fH°(298.15\ K) = -78.5 \pm 10.0\ kcal{\cdot}mol^{-1}$ for $Cr_{23}C_6(cr)$ based on the combustion data of Mah,[1] with excellent support in the equilibrium studies by Kulkarni and Worrell[4] for orifice diameters of 1/4 and 1/3 mm. Kulkarni and Worrell[4] concluded that equilibrium was not obtained in the cell with the 1/2 mm orifice in order to provide an explanation for the low pressures observed. Equilibrium studies involving $Cr_{23}C_6(cr)$ by Hancock and Pidgeon,[5] Alekseev and Shvartsman,[6] and Bolgar *et al.*[7] are not considered.[2]

Heat Capacity and Entropy

The heat capacity (55–295 K, 29 pts.) and enthalpy (467–1697 K, 26 pts.) have been measured by Kelley *et al.*[3] When the research was performed, Kelley *et al.*[3] considered the sample to be Cr_4C. All the data are corrected to the composition $Cr_{23}C_6$, assuming that the sample actually contained excess Cr. The contribution of the assumed free Cr was subtracted from the reported heat capacity and enthalpy values using JANAF data for Cr.[2] These corrections amount to 0.6 cal·K^{-1}·mol^{-1} at 55 K and 5.0 cal·K^{-1}·mol^{-1} at 295 K for the heat capacity data and are in a range of 1.00–1.85 kcal·mol^{-1} for the enthalpy data. We adopt $S°(50\ K) = 4.861\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ and $H°(50;0) = 181.6\ cal{\cdot}mol^{-1}$. The enthalpy data are fit to a six term polynomial with a constraint to join smoothly in the 298.15 K region with the enthalpy derived from the heat capacity data. There is considerable scatter in the enthalpy data. Deviations of the observed data from the tabulated data are within ±0.6% except for the 486.5 K data point which is approximately 1% (500 cal·mol^{-1}) too high. The enthalpy polynomial is used to extrapolate the results to 2000 K.

Phase Data

Storms[8] has summarized the phase information in the Cr–C system and reported that $Cr_{23}C_6$ has a complex face-centered-cubic structure. The range of homogeneity for $Cr_{23}C_6$ is unknown.[8]

Decomposition Data

The tentative phase diagram of the Cr–Cr_3C_2 system proposed by Storms[8] indicated that $Cr_{23}C_6$ has an incongruent melting point at 1793 K.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−104.755	−333.575	−333.575	INFINITE
100	250.316	117.835	1081.808	−96.397	−332.734	−334.089	174.510
200	509.447	383.581	666.329	−56.550	−331.274	−335.894	87.726
298.15	628.152	612.044	612.044	0.	−328.444	−338.693	59.338
300	629.692	615.935	612.056	1.164	−328.373	−338.757	58.983
400	704.376	808.005	637.736	68.108	−326.027	−342.211	44.688
500	753.538	970.840	688.496	141.172	−320.639	−346.880	36.238
600	785.751	1111.290	747.532	218.255	−315.571	−352.615	30.698
700	808.114	1234.112	808.454	297.960	−311.244	−359.142	26.799
800	829.072	1343.386	868.614	379.818	−307.585	−366.242	23.913
900	850.247	1442.252	926.944	463.778	−304.702	−373.756	21.692
1000	872.142	1532.961	983.070	549.890	−302.997	−381.534	19.929
1100	894.857	1617.144	1036.931	638.234	−302.930	−389.406	18.491
1200	918.329	1696.008	1088.602	728.888	−304.701	−397.203	17.290
1300	942.471	1770.464	1138.215	821.923	−308.594	−404.770	16.264
1400	967.178	1841.209	1185.923	917.402	−314.817	−411.950	15.370
1500	992.361	1908.794	1231.877	1015.375	−323.452	−418.601	14.577
1600	1017.946	1973.655	1276.225	1115.888	−334.571	−424.596	13.862
1700	1043.862	2036.143	1319.099	1218.976	−348.224	−429.817	13.207
1800	1070.058	2096.549	1360.622	1324.670	−364.452	−434.162	12.599
1900	1096.488	2155.112	1400.903	1432.996	−383.294	−437.533	12.029
2000	1123.115	2212.030	1440.043	1543.974	−404.778	−439.843	11.488

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The structure of CF_2 has been reported by Powell and Lide[16] from microwave measurements and has been confirmed by Mathews[17] from the fine structure of the 2500 Å absorption band. Mathews also reported ν_2, and Herr and Pimentel[18] reported ν_3, both from gas phase studies. Milligan *et al.*[19] have observed all three vibrations in matrix-isolated CF_2 as 1222, 668 and 1102 cm^{-1}. The electronic levels are from Mathews[17] with the triplet level estimated by Simons[20] to explain the low $C = C$ bond energy of 70 kcal in C_2F_4.

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