REFERENCE STATE

0	to	195.4	K crystal, white, beta
195.4	to	317.3	K crystal, white, alpha
317.3	to	1180.008	K liquid
above		1180.008	K ideal diatomic gas

Refer to the individual tables for details.

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	−5.360	0.	0.	0.
100	13.728	17.688	62.415	−4.473	0.	0.	0.
195.400	21.117	28.969	43.439	−2.827	ALPHA <--> BETA TRANSITION		
195.400	20.941	31.637	43.439	−2.306			
200	21.092	32.126	43.173	−2.209	0	0.	0.
298.15	23.825	41.077	41.077	0	0.	0.	0.
300	23.870	41.225	41.078	0.044	0	0.	0
317.300	24.351	42.574	41.123	0.460	BETA <--> LIQUID TRANSITION		
317.300	26.326	44.649	41.123	1.119			
400	26.326	50.747	42.507	3.296	0	0.	0.
500	26.326	56.621	44.764	5.929	0.	0.	0.
600	26.326	61.421	47.152	8.561	0.	0.	0
700	26.326	65.479	49.488	11.194	0.	0.	0.
800	26.326	68.995	51.711	13.826	0.	0.	0.
900	26.326	72.095	53.807	16.459	0.	0.	0.
1000	26.326	74.869	55.777	19.092	0.	0.	0.
1100	26.326	77.378	57.629	21.724	0.	0.	0.
1180.008	26.326	79.226	59.031	23.830	LIQUID <--> IDEAL GAS FUGACITY = 1 bar		
1180.008	18.540	133.233	59.031	87.558			
1200	18.551	133.544	60.270	87.929	0.	0.	0.
1300	18.604	135.031	65.964	89.787	0.	0.	0.
1400	18.648	136.412	70.948	91.649	0.	0	0.
1500	18.686	137.699	75.355	93.516	0.	0.	0.
1600	18.720	138.907	79.290	95.386	0.	0.	0.
1700	18.750	140.042	82.831	97.260	0.	0.	0.
1800	18.776	141.115	86.039	99 136	0.	0.	0.
1900	18.801	142.131	88.965	101.015	0.	0.	0.
2000	18.823	143.096	91.647	102.896	0.	0.	0.
2100	18.844	144.015	94.119	104.780	0.	0.	0.
2200	18.864	144.892	96.407	106.665	0.	0.	0.
2300	18.883	145.731	98.534	108.553	0.	0.	0.
2400	18.901	146.535	100.517	110.442	0.	0.	0.
2500	18.918	147.306	102.373	112.333	0.	0.	0.
2600	18.934	148.049	104.116	114.225	0.	0.	0.
2700	18.950	148.764	105.756	116.119	0	0.	0.
2800	18.965	149.453	107.305	118.015	0.	0	0.
2900	18.980	150.119	108.770	119.912	0.	0.	0.
3000	18.994	150.763	110.159	121.811	0.	0.	0.
3100	19.009	151.386	111.479	123.711	0.	0.	0.
3200	19.022	151.989	112.735	125.613	0.	0.	0.
3300	19.036	152.575	113.934	127.516	0.	0.	0.
3400	19.050	153.143	115.079	129.420	0.	0.	0.
3500	19.063	153.696	116.174	131.326	0.	0.	0.
3600	19.076	154.233	117.224	133.233	0.	0.	0.
3700	19.089	154.756	118.231	135.141	0	0.	0.
3800	19.102	155.265	119.199	137.050	0.	0.	0.
3900	19.114	155.761	120.130	138.961	0.	0	0.
4000	19.127	156.245	121.027	140.873	0.	0.	0.
4100	19.140	156.718	121.892	142.787	0.	0.	0.
4200	19.152	157.179	122.727	144.701	0.	0.	0.
4300	19.164	157.630	123.533	146.617	0	0.	0.
4400	19.176	158.071	124.313	148.534	0.	0.	0.
4500	19 189	158.502	125.068	150 452	0.	0	0.
4600	19.201	158.924	125.799	152.372	0.	0.	0.
4700	19.213	159.337	126.509	154.292	0.	0.	0.
4800	19.225	159.741	127.197	156.214	0.	0.	0.
4900	19.237	160.138	127.865	158.137	0.	0.	0.
5000	19.248	160.527	128.514	160.062	0.	0.	0.
5200	19.272	161.282	129.760	163.914	0.	0.	0.
5400	19.296	162.010	130.941	167.771	0.	0.	0.
5600	19.319	162.712	132.063	171.632	0.	0.	0.
5800	19.342	163.390	133.132	175.498	0.	0.	0.
6000	19.366	164.047	134.152	179.369	0.	0.	0.

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

$S°(298.15\ K) = 22.59 \pm 0.04\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = [-11.15]\ kJ \cdot mol^{-1}$

$\Delta_f H°(298.15\ K) = [-12.85]\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The enthalpy of formation is derived from $\Delta_r G°(820\ K) = 0$ for the process P(black)→P(red, IV). This calculation is based on the assumption that at 820 K the conversion of black to red phosphorus is known to occur.[1]

Heat Capacity and Entropy

The thermal functions are derived from the heat capacity measurments of Stephenson *et al.*[1] who reported measured values from 17.70 to 295.89 K.

Reference

[1]C. C. Stephenson, R. L. Potter, T. G. Maple and J. C. Morrow, J. Chem. Thermodynamics **1**, 59 (1969).

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⁻¹mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	−3.660	−11.151	−11.151	INFINITE
100	9.063	5.673	38.599	−3.293	−11.671	−10.469	5.469
200	17.343	14.800	24.438	−1.928	−12.569	−9.104	2.378
250	19.778	18.944	22.931	−0.997	−12.730	−8.218	1.717
298.15	21.547	22.586	22.586	0.	−12.851	−7.338	1.286
300	21.602	22.719	22.586	0.040	−12.855	−7.304	1.272
350	22.644	26.129	22.853	1.147	−13.684	−6.298	0.940
400	23.531	29.213	23.458	2.302	−13.845	−5.232	0.683
450	24.183	32.022	24.256	3.495	−13.969	−4.147	0.481
500	24.836	34.604	25.164	4.720	−14.060	−3.051	0.319
600	26.146	39.246	27.132	7.268	−14.144	−0.839	0.073
700	27.547	43.382	29.163	9.953	−14.092	1.376	−0.103
800	28.970	47.153	31.179	12.779	−13.899	3.575	−0.233
900	30.393	50.647	33.151	15.747	−13.563	5.740	−0.333
1000	31.815	53.923	35.066	18.857	−13.085	7.861	−0.411

PREVIOUS: CURRENT. June 1969

$S°(298.15\ K) = 23.197 \pm 0.08\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = [-10.71]\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = [-12.44]\ kJ·mol^{-1}$

Enthalpy of Formation

Stevenson *et al.*[1] have referenced the fluorine bomb calorimetry study of O'Hare and Hubbard[2] which yielded $\Delta_f H° = -1.2 \pm 1.0$ kcal·mol^{-1} for P(red, IV) → P(red, V).

Heat Capacity and Entropy

The thermal functions are derived from the heat capacity measurments of Stephenson *et al.*[1] who reported measured values from 16.15 to 304.93 K.

Reference

[1]C. C. Stephenson, R. L. Potter, T. G. Maple and J. C. Morrow, J. Chem. Thermodynamics 1, 59 (1969).
[2]P. A. G. O'Hare and W. N. Hubbard, Trans. Faraday Soc. 62, 2709 (1966).

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	−3.635	−10.714	−10.714	INFINITE
100	8.807	6.537	39.017	−3.248	−11.214	−10.099	5.275
200	17.175	15.494	25.028	−1.907	−12.136	−8.810	2.301
250	19.581	19.599	23.538	−0.985	−12.306	−7.958	1.663
298.15	21.263	23.197	23.197	0.	−12.439	−7.108	1.245
300	21.313	23.329	23.197	0.039	−12.444	−7.075	1.232
350	22.356	26.694	23.461	1.132	−13.287	−6.099	0.910
400	23.242	29.739	24.058	2.272	−13.463	−5.060	0.661
450	23.894	32.514	24.846	3.451	−13.601	−4.001	0.464
500	24.548	35.066	25.742	4.662	−13.706	−2.928	0.306
600	25.857	39.655	27.687	7.181	−13.819	−0.760	0.066
700	27.259	43.746	29.694	9.837	−13.796	1.417	−0.106
800	28.681	47.479	31.687	12.634	−13.632	3.581	−0.234
900	30.104	50.939	33.636	15.573	−13.325	5.715	−0.332
1000	31.526	54.185	35.530	18.655	−12.876	7.808	−0.408

PREVIOUS: CURRENT: June 1969

$S°(298.15\ K) = 22.85 \pm 0.08\ J \cdot K^{-1} \cdot mol^{-1}$
$T_{fus} = 870\ K$

$\Delta_f H°(0\ K) = -15.707\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -17.460\ kJ \cdot mol^{-1}$
$\Delta_{fus} H° = 18.8 \pm 0.8\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The enthalpy of formation is obtained from the enthalpies of sublimation represented by reaction I and II at 298.15 K.

(I) $4P(cr, white) \rightarrow P_4(g)$ 14.08 $kcal \cdot mol^{-1}$
(II) $4P(cr, red\ V) \rightarrow P_4(g)$ 30.771 $kcal \cdot mol^{-1}$

Of the calorimetric determinations only those of Giran[12] result in a reliable value for the enthalpy of formation, $4.4 \pm 0.4\ kcal \cdot mol^{-1}$. A comprehensive review is given by Rodewald.[13]

Heat Capacity and Entropy

The only reliable low temperature measurements, 15 to 305 K, are reported by Potter.[1] A value at 10 K was obtained by graphical extrapolation and a T^3 function was assumed from 0 to 10 K. High temperature heat capacities were obtained from a smooth curve joining the measurements of Kubashewski and Schrag[2] in the range 573 to 773 K and that of Regnault[3] at 331 K with those of Potter.[1] Measurements of Wigand[4] are too high. The uncertainty in the high temperature heat capacity is about 2%.

Fusion Data

The values of $\Delta_{fus}H$ and T_{fus} were calculated from the functions of the red (V) crystal and liquid. This may be compared with a reported triple point of 862.7 K by Smits and Bokhorst.[5]

Sublimation Data

Vapor pressure measurements on the triclinic allotrope, T. V. A designation V, are reported by Farr.[6] These data lead to a sublimation point of 704 K and $\Delta_{sub}H(298.15\ K)$ of $30.77 \pm 0.4\ kcal \cdot mol^{-1}$ of P_4. Smits and Bokhorst[7] measured the vapor pressure of a sample whose preparation indicates that is was probably P(cr, red, V). These results lead to $\Delta_{sub}H(298.15\ K) = 30.6 \pm 1\ kcal \cdot mol^{-1}$ of $P_4(g)$. An unpublished value of 30.84 $kcal \cdot mol^{-1}$ of P_4 by Stephenson[8] is quoted by Kane.

Stevenson and Yost[9] show that the vapor density measurements of Stock *et al.*[10] are best explained by a vapor essentially composed of only $P_4(g)$ below 800 K. This conclusion is supported by recent mass spectrometer measurements of Kane and Reynolds.[11]

References

[1] R. L. Potter, Dissertation, Massachusetts Institute of Technology (1946).
[2] O. Kubashewski and G. Schrag, Z. Elektrochem. 46, 675 (1940).
[3] V. Regnault, Ann. chim. phys. 9, 322 (1843).
[4] A. Wigan, Ann. Physik, 22, 64 (1907).
[5] A. Smits and S. C. Bokhorst, Verslag. Akad. Wetenschap. 23, 930 (1914).
[6] T. D. Farr, Tennessee Valley Authority Chemical Engineering Report No. 8 (1950).
[7] A. Smits and S. C. Bokhorst, Z. phys. Chem. 91, 248 (1916).
[8] C. C. Stephenson, quoted by J. S. Kane, Thesis Univ. of California (1955).
[9] D. P. Stevenson and D. M. Yost, J. Chem. Phys. 9, 403 (1941).
[10] A. Stock, G. E. Gibson and E. Stamm, Ber. 45, 3527 (1912).
[11] J. S. Kane and J. H. Reynolds, J. Chem. Phys. 25, 342 (1956).
[12] H. Giran, Ann. Chem. Phys. 30, 203 (1903).
[13] H. J. Rodewald, Helv. Chem. Acta 43, 878 (1960).

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
	$J \cdot K^{-1} \cdot mol^{-1}$			$kJ \cdot mol^{-1}$			
0	0.	0.	INFINITE	−3.607	−15.707	−15.707	INFINITE
100	8.724	6.303	38.578	−3.227	−16.215	−15.076	7.875
200	17.046	15.193	24.675	−1.896	−17.147	−13.760	3.594
250	19.464	19.270	23.192	−0.980	−17.323	−12.892	2.694
298.15	21.187	22.853	22.853	0.	−17.460	−12.026	2.107
300	21.251	22.984	22.853	0.039	−17.465	−11.992	2.088
350	22.293	26.340	23.116	1.128	−18.311	−10.999	1.642
400	23.179	29.376	23.711	2.266	−18.490	−9.942	1.298
450	23.832	32.144	24.497	3.441	−18.631	−8.864	1.029
500	24.485	34.689	25.390	4.649	−18.739	−7.773	0.812
600	25.794	39.267	27.330	7.162	−18.859	−5.566	0.485
700	27.196	43.241	29.324	9.742	−18.912	−3.345	0.250
800	36.987	47.698	31.335	13.091	−18.196	−1.158	0.076
900	30.041	51.571	33.380	16.372	−17.547	0.925	−0.054
1000	31.464	54.736	35.359	19.378	−17.174	2.959	−0.155

PREVIOUS: CURRENT: June 1961

$S°(298.15\ K) = 41.077 \pm 0.08\ J \cdot K^{-1} \cdot mol^{-1}$
$T_{trs} = 195.4 \pm 0.1$ K (white $\beta \rightarrow$ white α)
$T_{fus} = 317.30 \pm 0.05$ K

$\Delta_f H°(0\ K) = 0\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 0\ kJ \cdot mol^{-1}$
$\Delta_{trs} H° = 0.521 \pm 0.001\ kJ \cdot mol^{-1}$
$\Delta_{fus} H° = 0.659 \pm 0.002\ kJ \cdot mol^{-1}$

Enthalpy of Formation

Zero by definition. The enthalpies of white and red V phosphorus are tied together by the enthalpies of sublimation as determined by Giran.[1] A comprehensive review is given by Rodewald.[2]

Heat Capacity and Entropy

Low temperature measurements, 15–315 K, were made by Maples.[3] A Debye temperature, θ_D 124 K, was used to extrapolate to $T/K = 0$. Young and Hildenbrand[4] obtained heat capacities from enthalpy measurements that are 4% higher than those from the low Maples[3] temperature calorimeter which are preferred because of the proximity to the melting point.

Transition Data

Observed by Maples.[3]

Fusion Data

The selected enthalpy of fusion is that observed by Maples.[3] Young and Hildenbrand[4] obtain 125 cal·mol^{-1} for the same quantity. Maples'[3] value is consistent with vapor pressures and other thermochemical data; see the liquid and P_4(g) tables for details.

Sublimation Data

The vapor pressure measurements of Dainton and Kimberly[5] are the most precise and lead to $\Delta_{sub} H°(298.15\ K) = 14.08 \pm 0.2$ kcal·mol^{-1} of P_4(g). Measurements of Jolibois,[6] Smits and Bokhorst,[7] and Centzwer[8] lead to values that agree within the assigned uncertainty.

References

[1] H. Giran, Ann. Chim. Phys. 30, 203 (1903).
[2] H. J. Rodewald, Helv. Chim. Acta 43, 878 (1960).
[3] R. T. Maples, Dissertation, Massachusettes Institute of Technology (1949).
[4] F. E. Young and J. H. Hildenbrand, J. Am. Chem. Soc. 64, 839 (1942).
[5] F. S. Dainton and H. M. Kimberly, Trans. Faraday Soc. 46, 912 (1950).
[6] A. Jolibois, Compt. rend. 149, 287 (1908).
[7] A. Smits and S. C. Bokhorst, Z. phys. Chem. 91, 248 (1916).
[8] M. Centzwer, Z. phys. Chem. 85, 99 (1913).

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	−5.360	0.	0.	0.
100	13.728	17.688	62.415	−4.473	0.	0.	0.
195.400	21.117	28.969	43.439	−2.827	ALPHA <--> BETA		
195.400	20.941	31.637	43.439	−2.306	TRANSITION		
200	21.092	32.126	43.173	−2.209	0.	0.	0.
250	22.564	36.992	41.463	−1.118	0.	0.	0.
298.15	23.825	41.077	41.077	0.	0.	0.	0.
300	23.870	41.225	41.078	0.044	0.	0.	0.
317.300	24.351	42.574	41.123	0.460	---- BETA <--> LIQUID ----		
350	24.731	44.981	41.372	1.263	−0.717	0.071	−0.011
400	25.313	48.321	42.036	2.514	−0.782	0.188	−0.025
450	25.997	51.344	42.905	3.798	−0.815	0.312	−0.036
500	26.485	54.110	43.889	5.110	−0.818	0.437	−0.046
600	26.485	58.939	46.007	7.759	−0.802	0.687	−0.060
700	26.485	63.021	48.154	10.407	−0.786	0.934	−0.070
800	26.485	66.558	50.238	13.056	−0.771	1.179	−0.077
900	26.485	69.677	52.228	15.704	−0.755	1.422	−0.083
1000	26.485	72.468	54.115	18.353	−0.739	1.662	−0.087

PREVIOUS. CURRENT: June 1961

$S°(298.15\ K) = [43.011]\ J·K^{-1}·mol^{-1}$
$T_{fus}(white \rightarrow l) = 317.30 \pm 0.05\ K$
$T_{fus}(red, V \rightarrow l) = 870\ K$

$\Delta_f H°(298.15\ K) = [0.615]\ kJ·mol^{-1}$
$\Delta_{fus} H(white \rightarrow l) = 0.659\ kJ·mol^{-1}$
$\Delta_{fus} H(red, V \rightarrow l) = 18.8 \pm 0.002\ kJ·mol^{-1}$

Enthalpy of Formation

The enthalpy of formation for P(l) is calculated from that of P(white) by adding the enthalpy of fusion (white to liquid) and the difference in enthalpy, $H°(317.30\ K)–H°(298.15\ K)$, between the white crystal and liquid.

Heat Capacity and Entropy

Young and Hildenbrand[1] obtained an equation from enthalpy measurements which decreased with temperature. However, a better fit to the thermochemical data results if a constant heat capacity is assumed.

The entropy is derived from low temperature measurements on white phosphorus. See the white phosphorus table for details.

Vaporization Data

MacRae and Van Voorhis,[2] determinations of the vapor pressure, 44 to 150°C, are the most precise and lead to a $\Delta_{vap}H(298.15\ K)$ of $13.504 \pm 0.1\ kcal·mol^{-1}$ of P_4. A vapor pressure equation derived by Farr,[3] to fit the measurements reported in the literature leads to a value of $13.6 \pm 0.1\ kcal·mol^{-1}$ of P_4. The boiling point is calculated from the functions of P(l) and $P_4(g)$, and may be compared with the values of 552.7 and 553.7 resulting from Farr's[3] equation and observations of Smits and Bokhorst,[4] respectively.

References

[1]F. E. Young and J. H. Hildenbrand, J. Am. Chem. Sec. 64, 839 (1942).
[2]D. MacRae and C. C. Van Voorhis, J. Am. Chem. Soc. 43, 547 (1921).
[3]T. D. Farr, Tennessee Valley Authority Chemical Engineering Report No. 8(1950).
[4]A. Smits and S. C. Bokhorst, Proc. Akad. Wentenschop. 18, 106 (1915).

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	26.326	43.011	43.011	0.	0.615	0.038	−0.007
300	26.326	43.173	43.011	0.049	0.619	0.035	−0.006
317.300	26.326	44.649	43.061	0.504	---- BETA <---> LIQUID ----		
350	26.326	47.232	43.332	1.365	0.	0.	0.
400	26.326	50.747	44.044	2.681	0.	0.	0.
450	26.326	53.848	44.964	3.998	0.	0.	0.
500	26.326	56.621	45.994	5.314	0.	0.	0.
600	26.326	61.421	48.177	7.946	0.	0.	0.
700	26.326	65.479	50.366	10.579	0.	0.	0.
800	26.326	68.995	52.480	13.212	0.	0.	0.
900	26.326	72.095	54.491	15.844	0.	0.	0.
1000	26.326	74.869	56.392	18.477	0.	0.	0.
1100	26.326	77.378	58.188	21.109	0.	0.	0.
1180.008	26.326	79.226	59.552	23.216	----- FUGACITY = 1 bar -----		
1200	26.326	79.669	59.884	23.742	−63.572	1.078	−0.047
1300	26.326	81.776	61.488	26.374	−62.797	6.434	−0.259
1400	26.326	83.727	63.008	29.007	−62.027	11.731	−0.438
1500	26.326	85.543	64.450	31.640	−61.262	16.973	−0.591
1600	26.326	87.242	65.822	34.272	−60.499	22.164	−0.724
1700	26.326	88.838	67.129	36.905	−59.740	27.307	−0.839
1800	26.326	90.343	68.378	39.537	−58.984	32.405	−0.940
1900	26.326	91.766	69.572	42.170	−58.230	37.462	−1.030
2000	26.326	93.117	70.715	44.802	−57.479	42.479	−1.109

PREVIOUS· CURRENT June 1961

0 to 195.4K crystal, white, beta
195.4 to 317.3K crystal, white, alpha
above 317.3K 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⁻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	−5.360	0.	0.	0.
100	13.728	17.688	62.415	−4.473	0.	0.	0.
195.400	21.117	28.969	43.439	−2.827	ALPHA <--> BETA TRANSITION		
195.400	20.941	31.637	43.439	−2.306			
200	21.092	32.126	43.173	−2.209	0.	0.	0.
250	22.564	36.992	41.463	−1.118	0.	0.	0.
298.15	23.825	41.077	41.077	0.	0.	0.	0.
300	23.870	41.225	41.078	0.044	0.	0.	0.
317.300	24.351	42.574	41.123	0.460	BETA <--> LIQUID TRANSITION		
317.300	26.326	44.649	41.123	1.119			
350	26.326	47.232	41.575	1.980	0.	0.	0.
400	26.326	50.747	42.507	3.296	0.	0.	0.
450	26.326	53.848	43.598	4.612	0.	0.	0.
500	26.326	56.621	44.764	5.929	0.	0.	0.
600	26.326	61.421	47.152	8.561	0.	0.	0.
700	26.326	65.479	49.488	11.194	0.	0.	0.
800	26.326	68.995	51.711	13.826	0.	0.	0.
900	26.326	72.095	53.807	16.459	0.	0.	0.
1000	26.326	74.869	55.777	19.092	0.	0.	0.
1100	26.326	77.378	57.629	21.724	0.	0.	0.
1180.008	26.326	79.226	59.031	23.830	----- FUGACITY = 1 bar -----		
1200	26.326	79.669	59.371	24.357	−63.572	1.078	−0.047
1300	26.326	81.776	61.015	26.989	−62.797	6.434	−0.259
1400	26.326	83.727	62.568	29.622	−62.027	11.731	−0.438
1500	26.326	85.543	64.040	32.254	−61.262	16.973	−0.591
1600	26.326	87.242	65.438	34.887	−60.499	22.164	−0.724
1700	26.326	88.838	66.768	37.520	−59.740	27.307	−0.839
1800	26.326	90.343	68.036	40.152	−58.984	32.405	−0.940
1900	26.326	91.766	69.248	42.785	−58.230	37.462	−1.030
2000	26.326	93.117	70.408	45.417	−57.479	42.479	−1.109

PREVIOUS: CURRENT June 1961

IP(P, g) = 84580 ± 10 cm^{-1}
$S°$(298.15 K) = 163.198 ± 0.02 $J·K^{-1}·mol^{-1}$

$\Delta_f H°$(0 K) = 315.55 ± 1.0 $kJ·mol^{-1}$
$\Delta_f H°$(298.15 K) = 316.39 ± 1.0 $kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^4S_{3/2}$	0.0	4
$^2D_{3/2}$	11360.80	4
$^2D_{5/2}$	11376.40	6
$^2P_{1/2}$	18722.65	2
$^2P_{3/2}$	18747.95	4

Enthalpy of Formation

The value adopted for the enthalpy of formation, $\Delta_f H°$(298.15 K) = 316.39 ± 1.0 $kJ·mol^{-1}$, of the monatomic gas is that recommended by CODATA.[1] It is derived from $\Delta_f H°(P_2, g, 298.15\ K)$,[1,2] and the dissociation energy $D_0°(P_2)$ = 40596 ± 20 cm^{-1} obtained by Herzberg.[3]

Heat Capacity and Entropy

The electronic energy levels are given in the compilations by Moore.[4,5] There are 2.45 levels observed below the ionization potential. Only the ground state and the four lowest lying levels are used in the calculation. These are the contributions of the levels arising from three terms $^4S°$, $^2D°$, and $^2P°$– of the $3s^2 3p^3$ configuration. The remaining levels lie above 55000 cm^{-1} and do not contribute significantly even at 6000 K. The reported uncertainty in $S°$(298.15 K) is due to uncertainties in the relative atomic mass and the fundamental constants. Extension of these calculations beyond 6000 K may require consideration of higher excited states, estimation of missing levels, and utilization of proper cut off procedures.[6]

CODATA[1] used a slightly different values for the relative atomic mass and the fundamental constants. This causes a difference in the $S°$(298.15 K) value of 0.004 $J·K^{-1}·mol^{-1}$.

References

[1] J. D. Cox, chairman, CODATA Task Group on Key Values for Thermodynamics, J. Chem. Thermodynamics 10, 903 (1978).
[2] JANAF Thermochemical Tables: P_2(g), 12–30–82.
[3] G. Herzberg, Ann. Phys. 15, 677 (1932).
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[6] J. R. Downey, Jr., The Dow Chemical Company, Report AFOSR–TR–78–0960, 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	−6.197	315.553	315.553	INFINITE
100	20.786	140.490	181.678	−4.119	316.744	304.464	−159.036
200	20.786	154.898	165.099	−2.040	316.559	292.005	−76.264
250	20.786	159.536	163.540	−1.001	316.507	285.871	−59.729
298.15	20.786	163.198	163.198	0.	316.390	279.980	−49.051
300	20.786	163.326	163.198	0.038	316.384	279.754	−48.709
350	20.786	166.530	163.451	1.078	315.488	273.733	−40.852
400	20.786	169.306	164.013	2.117	315.211	267.787	−34.969
450	20.786	171.754	164.740	3.156	314.934	261.876	−30.398
500	20.786	173.944	165.553	4.196	314.657	255.996	−26.744
600	20.786	177.734	167.277	6.274	314.103	244.315	−21.270
700	20.786	180.938	169.005	8.353	313.549	232.728	−17.366
800	20.786	183.714	170.674	10.431	312.995	221.220	−14.444
900	20.786	186.162	172.262	12.510	312.441	209.781	−12.175
1000	20.786	188.352	173.763	14.589	311.887	198.404	−10.364
1100	20.788	190.333	175.181	16.667	311.333	187.083	−8.884
1200	20.791	192.142	176.520	18.746	247.207	176.890	−7.700
1300	20.797	193.806	177.787	20.826	247.429	171.021	−6.872
1400	20.810	195.348	178.987	22.906	247.647	165.135	−6.161
1500	20.831	196.785	180.126	24.988	247.862	159.234	−5.545
1600	20.865	198.130	181.210	27.073	248.076	153.319	−5.005
1700	20.914	199.396	182.242	29.161	248.291	147.390	−4.529
1800	20.981	200.593	183.229	31.256	248.510	141.448	−4.105
1900	21.068	201.730	184.173	33.358	248.733	135.494	−3.725
2000	21.178	202.813	185.078	35.470	248.964	129.528	−3.383
2100	21.312	203.850	185.948	37.595	249.205	123.551	−3.073
2200	21.471	204.845	186.784	39.734	249.458	117.561	−2.791
2300	21.653	205.803	187.590	41.890	249.727	111.560	−2.534
2400	21.859	206.729	188.369	44.065	250.013	105.547	−2.297
2500	22.088	207.626	189.121	46.262	250.320	99.521	−2.079
2600	22.337	208.497	189.850	48.483	250.648	93.483	−1.878
2700	22.605	209.345	190.556	50.730	251.001	87.431	−1.691
2800	22.890	210.172	191.242	53.005	251.380	81.366	−1.518
2900	23.189	210.981	191.909	55.309	251.786	75.287	−1.356
3000	23.500	211.772	192.558	57.643	252.222	69.194	−1.205
3100	23.821	212.548	193.190	60.009	252.688	63.085	−1.063
3200	24.148	213.309	193.807	62.407	253.185	56.961	−0.930
3300	24.480	214.057	194.409	64.839	253.713	50.821	−0.804
3400	24.814	214.793	194.998	67.303	254.273	44.664	−0.686
3500	25.148	215.517	195.574	69.802	254.866	38.491	−0.574
3600	25.480	216.230	196.138	72.333	255.490	32.300	−0.469
3700	25.808	216.933	196.690	74.897	256.146	26.091	−0.368
3800	26.129	217.625	197.232	77.494	256.834	19.864	−0.273
3900	26.444	218.308	197.764	80.123	257.552	13.619	−0.182
4000	26.749	218.982	198.286	82.783	258.299	7.355	−0.096
4100	27.045	219.646	198.799	85.473	259.076	1.072	−0.014
4200	27.329	220.301	199.303	88.191	259.880	−5.231	0.065
4300	27.601	220.947	199.799	90.938	260.711	−11.553	0.140
4400	27.860	221.585	200.287	93.711	261.567	−17.894	0.212
4500	28.106	222.214	200.767	96.510	262.447	−24.255	0.282
4600	28.338	222.834	201.240	99.332	263.350	−30.637	0.348
4700	28.555	223.446	201.706	102.177	264.274	−37.037	0.412
4800	28.758	224.049	202.165	105.042	265.218	−43.458	0.473
4900	28.947	224.644	202.618	107.928	266.180	−49.899	0.532
5000	29.121	225.231	203.064	110.831	267.160	−56.360	0.589
5100	29.281	225.809	203.505	113.752	268.154	−62.840	0.644
5200	29.426	226.379	203.939	116.687	269.163	−69.340	0.697
5300	29.557	226.941	204.368	119.636	270.185	−75.859	0.748
5400	29.675	227.494	204.791	122.598	271.218	−82.398	0.797
5500	29.779	228.040	205.209	125.571	272.260	−88.956	0.845
5600	29.871	228.577	205.621	128.553	273.311	−95.533	0.891
5700	29.950	229.107	206.029	131.545	274.370	−102.129	0.936
5800	30.016	229.628	206.431	134.543	275.435	−108.743	0.979
5900	30.072	230.142	206.828	137.547	276.505	−115.376	1.021
6000	30.116	230.647	207.221	140.557	277.578	−122.027	1.062

PREVIOUS: June 1961 (1 atm) CURRENT: December 1982 (1 bar)

$IP(P^+, g) = 159100 \pm 100\ cm^{-1}$
$S°(298.15\ K) = 166.970 \pm 0.02\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 1327.35 \pm 0.42\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [1336.333]\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^3P_0$	0.0	1
$^3P_1$	164.8	3
$^3P_2$	469.0	5
$^1D_2$	8882.6	5
$^1S_0$	21576.2	1

Enthalpy of Formation

$\Delta_f H°(P^+, g, 0\ K)$ is calculated from $\Delta_f H°(P, g, 0\ K)$[1] using the spectroscopic value of $IP(P) = 84580 \pm 10\ cm^{-1}$ ($1011.80 \pm 1\ 0.12\ kJ \cdot mol^{-1}$) from Moore.[2] The ionization limit is converted from cm^{-1} to $kJ \cdot mol^{-1}$ using the factor, $1\ cm^{-1} = 0.01196266\ kJ \cdot mol^{-1}$, 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.

$\Delta_f H°(P^+, g, 298.15\ K)$ is calculated from $\Delta_f H°(P, g, 0\ K)$ by using IP(P) with JANAF[1] enthalpies, $H°(0\ K) - H°(298.15\ K)$, for P(g), $P^+(g)$, and e^-(ref). $\Delta_f H°(P \rightarrow P^+ + e^-, 298.15\ K)$ 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 $-6.197\ kJ \cdot mol^{-1}$ 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,[2,6] is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels and cutting off the summation in the partition function[7] 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 approximately $52000\ cm^{-1}$ 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.[7]

References

[1]JANAF Thermochemical Tables: P (g), 6-30-62; 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, 783 pp. (1977).
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[7]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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	$J \cdot K^{-1} \cdot mol^{-1}$			$kJ \cdot mol^{-1}$			
0	0.	0.	INFINITE	−8.141	1327.354		
100	30.205	135.606	191.683	−5.608			
200	28.395	156.122	169.413	−2.658			
250	27.038	162.312	167.402	−1.273			
298.15	25.856	166.970	166.970	0.	1336.333	1292.543	−226.448
300	25.815	167.130	166.971	0.048	1336.375	1292.272	−225.004
350	24.826	171.032	167.281	1.313	1336.744	1284.905	−191.762
400	24.058	174.295	167.959	2.534	1337.688	1277.434	−166.816
450	23.466	177.093	168.822	3.722	1338.599	1269.848	−147.400
500	23.010	179.540	169.774	4.883	1339.483	1262.161	−131.857
600	22.372	183.675	171.759	7.150	1341.196	1246.535	−108.520
700	21.966	187.091	173.712	9.365	1342.857	1230.626	−91.830
800	21.694	190.005	175.571	11.547	1344.485	1214.481	−79.297
900	21.505	192.548	177.319	13.707	1346.091	1198.134	−69.538
1000	21.371	194.807	178.957	15.850	1347.680	1181.609	−61.721
1100	21.274	196.839	180.492	17.982	1349.258	1164.926	−55.318
1200	21.206	198.687	181.932	20.106	1287.256	1149.177	−50.022
1300	21.160	200.382	183.287	22.224	1289.595	1137.576	−45.708
1400	21.134	201.949	184.565	24.338	1291.925	1125.795	−42.004
1500	21.126	203.407	185.773	26.451	1294.250	1113.847	−38.788
1600	21.134	204.771	186.918	28.564	1296.571	1101.744	−35.968
1700	21.156	206.053	188.006	30.679	1298.891	1089.497	−33.476
1800	21.192	207.263	189.043	32.796	1301.210	1077.112	−31.257
1900	21.239	208.410	190.032	34.917	1303.531	1064.599	−29.268
2000	21.296	209.501	190.979	37.044	1305.855	1051.964	−27.474
2100	21.362	210.541	191.886	39.177	1308.183	1039.212	−25.849
2200	21.435	211.537	192.756	41.317	1310.516	1026.349	−24.369
2300	21.514	212.491	193.594	43.464	1312.855	1013.380	−23.015
2400	21.596	213.409	194.400	45.619	1315.200	1000.309	−21.771
2500	21.681	214.292	195.179	47.783	1317.551	987.140	−20.625
2600	21.768	215.144	195.930	49.956	1319.910	973.877	−19.565
2700	21.855	215.967	196.657	52.137	1322.275	960.524	−18.582
2800	21.941	216.763	197.361	54.327	1324.648	947.082	−17.668
2900	22.026	217.535	198.043	56.525	1327.028	933.556	−16.815
3000	22.110	218.283	198.706	58.732	1329.414	919.947	−16.018
3100	22.190	219.009	199.349	60.947	1331.808	906.259	−15.270
3200	22.268	219.715	199.974	63.170	1334.208	892.493	−14.568
3300	22.343	220.401	200.583	65.400	1336.614	878.652	−13.908
3400	22.414	221.069	201.176	67.638	1339.026	864.738	−13.285
3500	22.481	221.720	201.754	69.883	1341.444	850.753	−12.697
3600	22.545	222.354	202.317	72.134	1343.867	836.699	−12.140
3700	22.605	222.973	202.867	74.392	1346.295	822.578	−11.613
3800	22.660	223.576	203.404	76.655	1348.727	808.391	−11.112
3900	22.712	224.166	203.929	78.924	1351.164	794.140	−10.636
4000	22.760	224.741	204.442	81.197	1353.604	779.826	−10.183
4100	22.804	225.304	204.944	83.476	1356.048	765.451	−9.752
4200	22.845	225.854	205.435	85.758	1358.494	751.017	−9.340
4300	22.882	226.392	205.916	88.045	1360.943	736.524	−8.947
4400	22.916	226.918	206.388	90.334	1363.395	721.975	−8.571
4500	22.946	227.434	206.850	92.628	1365.848	707.369	−8.211
4600	22.973	227.938	207.303	94.924	1368.303	692.709	−7.866
4700	22.998	228.433	207.747	97.222	1370.760	677.996	−7.535
4800	23.019	228.917	208.183	99.523	1373.217	663.230	−7.217
4900	23.038	229.392	208.611	101.826	1375.676	648.414	−6.912
5000	23.054	229.858	209.031	104.131	1378.135	633.546	−6.619
5100	23.068	230.314	209.444	106.437	1380.594	618.630	−6.336
5200	23.080	230.762	209.850	108.744	1383.054	603.666	−6.064
5300	23.090	231.202	210.249	111.053	1385.513	588.654	−5.802
5400	23.097	231.634	210.641	113.362	1387.972	573.596	−5.548
5500	23.103	232.058	211.026	115.672	1390.430	558.492	−5.304
5600	23.107	232.474	211.406	117.983	1392.888	543.344	−5.068
5700	23.110	232.883	211.779	120.294	1395.345	528.152	−4.840
5800	23.111	233.285	212.146	122.605	1397.801	512.916	−4.619
5900	23.110	233.680	212.508	124.916	1400.256	497.639	−4.406
6000	23.108	234.068	212.864	127.227	1402.710	482.319	−4.199

PREVIOUS: CURRENT: December 1982 (1 bar)

Phosphorus, Ion (P^-) IDEAL GAS $M_r = 30.97431$

EA(P, g) = 0.7465 ± 0.0003 eV
$S°(298.15\ K) = 169.124 \pm 0.001\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 243.527 \pm 1.0\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [238.717]\ kJ \cdot mol^{-1}$

Electonic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^3P_2$	0	5
$^3P_1$	181	3
$^3P_0$	263	1
$^1D_2$	6675	5
$^1S_0$	16131	1

Enthalpy of Formation

$\Delta_f H°(P^-, g, 0\ K)$ is calculated from $\Delta_f H°(P, g, 0\ K)$[1] using the adopted electron affinity of EA(P) = 0.7465 ± 0.0003 eV (72.026 ± 0.029 $kJ \cdot mol^{-1}$). This value, recommended by Hotop and Lineberger,[2] is based on tunable laser photodetachment threshold studies.[3,4] Additional information on $P^-(g)$ may be obtained in the critical discussions of Hotop and Lineberger,[2,5] Rosenstock *et al.*[6] and Massey.[7]

$\Delta_f H°(P^-, g, 298.15\ K)$ is obtained from $\Delta_f H°(P, g, 0\ K)$ by using EA(P) with JANAF[1] enthalpies, $H°(0\ K)-H°(298\ 15\ K)$, for $P^-(g)$, P(g), and e^-(ref). $\Delta_f H°(P^- \rightarrow P + e^-, 298.15\ K)$ differs from a room-temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[6] $\Delta_f H°(298.15\ K)$ should be changed by + 6.197 $kJ \cdot mol^{-1}$ if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The ground state electronic configuration for $P^-(g)$ is given by Hotop and Lineberger,[2,5] Rosenstock,[6] and Massey.[7] The fine sturcture seperation has been measured experimentally via a tunetable laser photodetachment threshold technique[3,4] and is that recommended by Hotop and Lineberger.[2]

References

[1]JANAF Thermochemical Tables: P(g), 12-31-82; e^-(ref), 3-31-82.
[2]H. Hotop and W. C. Lineberger, J. Phys. Chem. Ref. Data, 14, 731 (1985).
[3]D. Feldmann, Z. Physik A 277, 19 (1976).
[4]J. Slater and W. C. Lineberger, Phys. Rev. A 15, 2277 (1977).
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[6]H. M. Rosenstock, K. Draxl *et al.*, J. Phys. Chem. Ref. Data 6, Supp. 1, 783 pp. (1977).
[7]H. S. W. Massey, "Negative Ions", 3rd ed., Cambridge University Press, Cambridge, 741 pp. (1976).

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
	$J \cdot K^{-1} \cdot mol^{-1}$			$kJ \cdot mol^{-1}$			
0	0.	0.	INFINITE	−6.748	243.527		
100	23.554	143.795	189.435	−4.564			
200	23.042	160.101	171.176	−2.215			
250	22.540	165.187	169.490	−1.076			
298.15	22.168	169.124	169.124	0.	238.717	206.795	−36.230
300	22.156	169.261	169.124	0.041	238.676	206.597	−35.972
350	21.873	172.654	169.393	1.141	236.801	201.412	−30.059
400	21.664	175.560	169.986	2.230	235.534	196.443	−25.653
450	21.508	178.102	170.750	3.309	234.257	191.634	−22.244
500	21.388	180.362	171.600	4.381	232.974	186.966	−19.532
600	21.222	184.245	173.394	6.511	230.393	178.007	−15.497
700	21.116	187.508	175.184	8.627	227.798	169.481	−12.647
800	21.047	190.323	176.904	10.735	225.195	161.328	−10.534
900	21.004	192.799	178.535	12.838	222.586	153.501	−8.909
1000	20.983	195.011	180.074	14.937	219.974	145.965	−7.624
1100	20.982	197.011	181.525	17.035	217.361	138.690	−6.586
1200	21.002	198.837	182.892	19.134	151.176	132.732	−5.778
1300	21.042	200.520	184.184	21.236	149.342	131.269	−5.274
1400	21.100	202.081	185.408	23.343	147.508	129.948	−4.848
1500	21.174	203.539	186.568	25.456	145.676	128.758	−4.484
1600	21.261	204.909	187.672	27.578	143.849	127.689	−4.169
1700	21.360	206.200	188.725	29.709	142.028	126.735	−3.894
1800	21.467	207.424	189.730	31.850	140.214	125.888	−3.653
1900	21.579	208.588	190.692	34.003	138.409	125.142	−3.440
2000	21.694	209.698	191.615	36.166	136.612	124.490	−3.251
2100	21.810	210.759	192.501	38.341	134.826	123.928	−3.083
2200	21.924	211.776	193.354	40.528	133.048	123.450	−2.931
2300	22.036	212.753	194.177	42.726	131.280	123.054	−2.795
2400	22.144	213.693	194.970	44.935	129.522	122.734	−2.671
2500	22.246	214.599	195.738	47.155	127.772	122.487	−2.559
2600	22.344	215.474	196.480	49.384	126.030	122.310	−2.457
2700	22.435	216.319	197.199	51.623	124.296	122.200	−2.364
2800	22.520	217.136	197.897	53.871	122.570	122.154	−2.279
2900	22.598	217.928	198.574	56.127	120.850	122.169	−2.201
3000	22.670	218.695	199.232	58.390	119.136	122.244	−2.128
3100	22.735	219.440	199.872	60.661	117.427	122.376	−2.062
3200	22.794	220.162	200.495	62.937	115.724	122.563	−2.001
3300	22.847	220.865	201.101	65.219	114.024	122.803	−1.944
3400	22.894	221.547	201.693	67.506	112.328	123.094	−1.891
3500	22.936	222.212	202.269	69.798	110.636	123.435	−1.842
3600	22.972	222.858	202.832	72.093	108.946	123.825	−1.797
3700	23.004	223.488	203.382	74.392	107.258	124.262	−1.754
3800	23.030	224.102	203.919	76.694	105.571	124.744	−1.715
3900	23.053	224.700	204.445	78.998	103.886	125.270	−1.678
4000	23.072	225.284	204.958	81.304	102.201	125.840	−1.643
4100	23.087	225.854	205.461	83.612	100.517	126.452	−1.611
4200	23.098	226.411	205.953	85.921	98.834	127.105	−1.581
4300	23.106	226.954	206.435	88.232	97.149	127.798	−1.552
4400	23.112	227.486	206.908	90.543	95.465	128.530	−1.526
4500	23.115	228.005	207.371	92.854	93.779	129.301	−1.501
4600	23.115	228.513	207.825	95.165	92.093	130.108	−1.477
4700	23.113	229.010	208.270	97.477	90.405	130.953	−1.455
4800	23.109	229.497	208.708	99.788	88.716	131.834	−1.435
4900	23.104	229.973	209.137	102.099	87.025	132.749	−1.415
5000	23.096	230.440	209.558	104.409	85.332	133.700	−1.397
5100	23.088	230.897	209.972	106.718	83.637	134.684	−1.379
5200	23.077	231.345	210.379	109.026	81.940	135.701	−1.363
5300	23.066	231.785	210.779	111.333	80.241	136.752	−1.348
5400	23.053	232.216	211.172	113.639	78.539	137.834	−1.333
5500	23.040	232.639	211.558	115.944	76.835	138.947	−1.320
5600	23.025	233.054	211.938	118.247	75.128	140.092	−1.307
5700	23.010	233.461	212.312	120.549	73.419	141.267	−1.295
5800	22.994	233.861	212.680	122.849	71.707	142.473	−1.283
5900	22.977	234.254	213.043	125.148	69.992	143.707	−1.272
6000	22.960	234.640	213.399	127.445	68.274	144.971	−1.262

PREVIOUS: CURRENT: December 1982 (1 bar)

$S°(298.15\ K) = 234.241\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 138.8 \pm 41.8\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 138.6 \pm 41.8\ kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^2\Pi$	0	2
$A^2\Sigma$	324	2
$B^2\Pi$	[20000]	2
$C^2\Sigma$	22000	4
	34594	2

$\omega_e = 743.5 \pm 3.8\ cm^{-1}$ $\omega_e x_e = 3.8 \pm 0.9\ cm^{-1}$ $\sigma = 1$
$B_e = [0.29]\ cm^{-1}$ $\alpha_e = [0.0016]\ cm^{-1}$ $r_e = [1.92]$ Å

Enthalpy of Formation

The dissociation energy, $D_0°$, of PS(g) is estimated to be 140 ± 25 kcal·mol^{-1} by comparison with the corresponding quantity for PO(g) and from a linear Birge-Sponer extrapolation of the third excited ($C^2\Sigma$) electronic state potential function. It is assumed that the ($C^2\Sigma$) state dissociates to S(g) in its ground (^{3}P) state and P(g) in its first excited (^{2}D) state. The fundamental vibrational frequency in the $C^2\Sigma$ state (ω_e') is 531.8 ± 2.5 cm^{-1} and the corresponding anharmonic term ($\omega_e x_e$) is 2.6 ± 0.5 cm^{-1}. These constants are calculated from a reanalysis of the spectral data of Dressler.[1] The corresponding enthalpy of formation of PS(g) is 37.3 ± 25 kcal·mol^{-1}. The excited state ($C^2\Sigma$) data are used to calculate $D_0°$ instead of the ground state ($X^2\Pi$) data because the vibrational constants of the upper level are known more accurately and because the extrapolation is 50 kcal·mol^{-1} smaller for this level.

Heat Capacity and Entropy

The spectra of PS(g) have been studied by Dressler[1] in the near UV and visible regions. He reported the above electronic levels which correspond to the doublet pi ground state and two of the excited levels ($B^2\Pi$, $C^2\Sigma$). The level of the first excited electronic state ($A^2\Sigma$) is estimated by analogy with NO(g).

Dressler[1] estimated the value of the rotational constant B_e. The value of α_e is calculated from the Morse potential function. The bond distance is calculated from B_e. The fundamental vibrational frequency ω_e and the anharmonic vibrational term $\omega_e x_e$ are calculated from a reanalysis of the spectral data reported by Dressler.[1]

References

[1] K. Dressler, Helv. Phys. Scta. 28, 563 (1955).

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	−9.610	138.765	138.765	INFINITE
100	30.805	197.931	264.579	−6.665	140.134	123.361	−64.437
200	33.947	220.417	237.429	−3.402	139.491	106.560	−27.831
250	34.711	228.080	234.819	−1.685	139.097	98.370	−20.553
298.15	35.243	234.241	234.241	0.	138.603	90.569	−15.867
300	35.260	234.459	234.242	0.065	138.582	90.271	−15.718
350	35.679	239.928	234.673	1.839	137.254	82.337	−12.288
400	36.008	244.714	235.635	3.632	134.300	74.630	−9.746
450	36.268	248.971	236.885	5.439	132.865	67.248	−7.806
500	36.478	252.803	238.288	7.258	131.365	60.040	−6.272
600	36.790	259.484	241.280	10.922	128.812	46.022	−4.007
700	37.008	265.172	244.297	14.613	126.523	32.407	−2.418
800	37.169	270.125	247.223	18.322	124.389	19.108	−1.248
900	37.292	274.510	250.016	22.045	69.223	7.153	−0.415
1000	37.392	278.445	252.665	25.779	68.468	0.296	−0.015
1100	37.474	282.012	255.173	29.523	67.708	−6.484	0.308
1200	37.544	285.276	257.548	33.274	3.367	−12.117	0.527
1300	37.606	288.284	259.798	37.031	3.364	−13.407	0.539
1400	37.662	291.073	261.934	40.795	3.347	−14.697	0.548
1500	37.712	293.673	263.964	44.564	3.316	−15.984	0.557
1600	37.759	296.108	265.898	48.337	3.271	−17.270	0.564
1700	37.803	298.399	267.743	52.115	3.213	−18.552	0.570
1800	37.845	300.561	269.506	55.898	3.142	−19.830	0.575
1900	37.885	302.608	271.195	59.684	3.061	−21.104	0.580
2000	37.924	304.552	272.815	63.475	2.968	−22.373	0.584
2100	37.962	306.403	274.371	67.269	2.867	−23.638	0.588
2200	38.000	308.170	275.867	71.067	2.757	−24.898	0.591
2300	38.037	309.860	277.309	74.869	2.639	−26.152	0.594
2400	38.074	311.480	278.699	78.675	2.515	−27.401	0.596
2500	38.112	313.035	280.041	82.484	2.385	−28.645	0.599
2600	38.150	314.530	281.339	86.297	2.250	−29.884	0.600
2700	38.190	315.971	282.595	90.114	2.110	−31.117	0.602
2800	38.231	317.361	283.812	93.935	1.968	−32.345	0.603
2900	38.274	318.703	284.993	97.760	1.822	−33.568	0.605
3000	38.319	320.001	286.138	101.590	1.675	−34.786	0.606
3100	38.367	321.259	287.251	105.424	1.525	−35.999	0.607
3200	38.418	322.477	288.333	109.263	1.375	−37.207	0.607
3300	38.471	323.660	289.385	113.108	1.225	−38.410	0.608
3400	38.528	324.810	290.410	116.958	1.074	−39.609	0.609
3500	38.588	325.927	291.409	120.814	0.924	−40.803	0.609
3600	38.652	327.015	292.383	124.676	0.775	−41.993	0.609
3700	38.720	328.075	293.334	128.544	0.626	−43.179	0.610
3800	38.792	329.109	294.262	132.420	0.480	−44.361	0.610
3900	38.868	330.117	295.168	136.303	0.335	−45.539	0.610
4000	38.948	331.103	296.054	140.193	0.192	−46.714	0.610
4100	39.032	332.065	296.921	144.092	0.051	−47.885	0.610
4200	39.120	333.007	297.769	148.000	−0.087	−49.052	0.610
4300	39.212	333.928	298.599	151.916	−0.223	−50.216	0.610
4400	39.307	334.831	299.412	155.842	−0.356	−51.377	0.610
4500	39.407	335.715	300.209	159.778	−0.485	−52.536	0.610
4600	39.510	336.583	300.991	163.724	−0.612	−53.691	0.610
4700	39.617	337.434	301.757	167.680	−0.735	−54.843	0.610
4800	39.727	338.269	302.509	171.647	−0.854	−55.993	0.609
4900	39.840	339.089	303.247	175.626	−0.970	−57.141	0.609
5000	39.957	339.895	303.972	179.615	−1.082	−58.286	0.609
5100	40.076	340.688	304.684	183.617	−1.191	−59.429	0.609
5200	40.197	341.467	305.384	187.631	−1.295	−60.570	0.608
5300	40.321	342.234	306.072	191.657	−1.395	−61.709	0.608
5400	40.447	342.989	306.749	195.695	−1.491	−62.846	0.608
5500	40.575	343.732	307.414	199.746	−1.583	−63.981	0.608
5600	40.705	344.464	308.070	203.810	−1.670	−65.115	0.607
5700	40.836	345.186	308.714	207.887	−1.753	−66.247	0.607
5800	40.968	345.897	309.349	211.977	−1.831	−67.378	0.607
5900	41.102	346.599	309.975	216.081	−1.905	−68.508	0.607
6000	41.236	347.291	310.591	220.198	−1.974	−69.636	0.606

PREVIOUS: June 1967 (1 atm) CURRENT: June 1967 (1 bar)

Phosphorus (P_2) IDEAL GAS $M_r = 61.94752$ Phosphorus (P_2) $P_2(g)$

$S°(298.15\ K) = 218.13 \pm 0.4\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 145.47 \pm 2.1\ kJ \cdot mol^{-1}$

$\Delta_f H°(298.15\ K) = 143.65 \pm 2.1\ kJ \cdot mol^{-1}$

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

$\omega_e = 780.43\ cm^{-1}$ $\omega_e x_e = 2.804\ cm^{-1}$ $\sigma = 2$

$B_e = 0.30327\ cm^{-1}$ $\alpha_e = 0.00142\ cm^{-1}$ $r_e = 1.8943\ Å$

Enthalpy of Formation

Stevenson and Yost[1] have shown that the vapor density measurements of Stock *et al.*[2] best fit a vapor composed of $P_2(g)$ and $P_4(g)$. From these data, Farr[3] calculated the equilibrium constants which lead to $\Delta_r H°(298.15\ K) = 54.59 \pm 0.01\ kcal \cdot mol^{-1}$ for the process $P_4(g) \rightarrow P_2(g)$, from which the value for $\Delta_f H°(P_2, g, 298.15\ K)$ is calculated using $\Delta_f H°(P_4, g, 298.15\ K) = 30.77\ kcal \cdot mol^{-1}$.

Heat Capacity and Entropy

Molecular and spectroscopic constants are those listed by Herzberg.[4] More recent measurements of Dressler[5] are in agreement with the values selected by Herzberg.[4]

The dissociation energy, $D_0° = 116 \pm 1\ kcal \cdot mol^{-1}$, is given by Gaydon.[6]

References

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[5] K. Dressler, Helv. Phys. Acta 28, 563 (1955).
[6] A. G. Gaydon, "Dissociation Energies and Spectra of Diatomic Molecules," 2nd ed., Chapman and Hall, Ltd., London, 261 pp. (1953).

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	−8.904	145.469	145.469	INFINITE
100	29.120	185.370	245.321	−5.995	146.604	131.604	−68.743
200	30.103	205.754	220.998	−3.049	145.023	116.723	−30.485
250	31.082	212.574	218.653	−1.520	144.369	109.721	−22.925
298.15	32.034	218.131	218.131	0.	143.653	103.112	−18.065
300	32.069	218.329	218.132	0.059	143.625	102.861	−17.910
350	32.945	223.340	218.525	1.685	141.379	96.272	−14.368
400	33.679	227.789	219.410	3.351	140.413	89.894	−11.739
450	34.280	231.792	220.568	5.051	139.479	83.636	−9.708
500	34.770	235.430	221.875	6.778	138.574	77.480	−8.094
600	35.499	241.838	224.682	10.293	136.824	65.427	−5.696
700	36.000	247.350	227.536	13.870	135.136	53.661	−4.004
800	36.356	252.182	230.321	17.489	133.489	42.135	−2.751
900	36.618	256.480	232.993	21.138	131.873	30.813	−1.788
1000	36.819	260.348	235.538	24.810	130.280	19.670	−1.027
1100	36.976	263.865	237.956	28.500	128.705	8.685	−0.412
1180.008	37.079	266.465	239.802	31.463	----- FUGACITY = 1 bar -----		
1200	37.103	267.088	240.251	32.204	0.	0.	0.
1300	37.208	270.062	242.432	35.920	0.	0.	0.
1400	37.296	272.823	244.505	39.645	0.	0.	0.
1500	37.373	275.399	246.480	43.379	0.	0.	0.
1600	37.440	277.813	248.363	47.120	0.	0.	0.
1700	37.499	280.085	250.163	50.867	0.	0.	0.
1800	37.553	282.230	251.886	54.619	0.	0.	0.
1900	37.602	284.261	253.537	58.377	0.	0.	0.
2000	37.647	286.191	255.121	62.139	0.	0.	0.
2100	37.689	288.029	256.645	65.906	0.	0.	0.
2200	37.728	289.783	258.112	69.677	0.	0.	0.
2300	37.766	291.461	259.526	73.452	0.	0.	0.
2400	37.801	293.069	260.890	77.230	0.	0.	0.
2500	37.835	294.613	262.208	81.012	0.	0.	0.
2600	37.868	296.098	263.483	84.797	0.	0.	0.
2700	37.899	297.527	264.718	88.586	0.	0.	0.
2800	37.930	298.906	265.914	92.377	0.	0.	0.
2900	37.960	300.238	267.075	96.171	0.	0.	0.
3000	37.989	301.525	268.202	99.969	0.	0.	0.
3100	38.017	302.771	269.297	103.769	0.	0.	0.
3200	38.045	303.979	270.362	107.572	0.	0.	0.
3300	38.072	305.150	271.399	111.378	0.	0.	0.
3400	38.099	306.287	272.408	115.187	0.	0.	0.
3500	38.126	307.392	273.392	118.998	0.	0.	0.
3600	38.152	308.466	274.351	122.812	0.	0.	0.
3700	38.178	309.512	275.288	126.628	0.	0.	0.
3800	38.204	310.530	276.202	130.448	0.	0.	0.
3900	38.229	311.523	277.095	134.269	0.	0.	0.
4000	38.254	312.491	277.968	138.093	0.	0.	0.
4100	38.279	313.436	278.821	141.920	0.	0.	0.
4200	38.304	314.359	279.656	145.749	0.	0.	0.
4300	38.328	315.260	280.474	149.581	0.	0.	0.
4400	38.353	316.142	281.275	153.415	0.	0.	0.
4500	38.377	317.004	282.059	157.251	0.	0.	0.
4600	38.401	317.848	282.828	161.090	0.	0.	0.
4700	38.425	318.674	283.582	164.932	0.	0.	0.
4800	38.449	319.483	284.321	168.775	0.	0.	0.
4900	38.473	320.276	285.047	172.621	0.	0.	0.
5000	38.497	321.053	285.759	176.470	0.	0.	0.
5100	38.521	321.816	286.459	180.321	0.	0.	0.
5200	38.544	322.564	287.146	184.174	0.	0.	0.
5300	38.568	323.299	287.821	188.030	0.	0.	0.
5400	38.591	324.020	288.485	191.888	0.	0.	0.
5500	38.615	324.728	289.138	195.748	0.	0.	0.
5600	38.638	325.424	289.779	199.611	0.	0.	0.
5700	38.661	326.108	290.411	203.476	0.	0.	0.
5800	38.685	326.781	291.032	207.343	0.	0.	0.
5900	38.708	327.442	291.644	211.212	0.	0.	0.
6000	38.731	328.093	292.246	215.084	0.	0.	0.

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

$S°(298.15\ K) = 280.0 \pm 0.4\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 66.2 \pm 2.1\ kJ \cdot mol^{-1}$

$\Delta_f H°(298.15\ K) = 58.9 \pm 2.1\ kJ \cdot mol^{-1}$

Vibrational Levels and Degeneracies ν, cm^{-1}
606 (1)
363 (2)
464.5(3)

Ground State QuantumWeight: 1 $\sigma = 12$
Point Group: T_d
Bond Length: P–P = 2.21 ± 0.2 Å
Bond Angle: P–P–P = 109.4712°
Product of the Principal Moments of Inertia: $I_A I_B I_C = 15.8528 \times 10^{-114}\ g^3 \cdot cm^6$

Enthalpy of Formation

Taken as the enthalpy of formation of white phosphorus.

Heat Capacity and Entropy

The frequencies and degeneracies are those assigned by Gutowsky and Hoffman.[1] Molecular parameters of the gas were determined from electron diffraction measurements by Maxwell *et al.*[2] Thomas and Gingrich[3] obtained a P–P distance of 2.25 Å from X-ray studies on the liquid. On the basis of the selected values for P(white), a 3rd law entropy of 66.89 $cal \cdot K^{-1} \cdot mol^{-1}$ (for p=1 atm) is derived for P_4(g). The principal moments of inertia are: $I_A = I_B = I_C = 25.1209 \times 10^{-39} g\ cm^2$.

References

[1]H. S. Gutowsky and G. S. Hoffman, J. Am. Chem. Soc. 72, 5751(1950).
[2]L. R. Maxwell, S. B. Hendricks, and V. M. Moseley, J. Chem. Phys. 3, 699(1935).
[3]C. D. Thomas and N. S. Gingrich, J. Chem. Phys. 6, 659(1938).

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	−14.133	66.214	66.214	INFINITE
100	37.232	223.901	331.278	−10.738	66.060	50.745	−26.506
200	55.620	255.381	285.819	−6.087	61.657	36.281	−9.476
250	62.447	268.567	281.073	−3.127	60.250	30.101	−6.289
298.15	67.158	279.992	279.992	0.	58.907	24.416	−4.278
300	67.309	280.408	279.993	0.124	58.854	24.202	−4.214
350	70.765	291.058	280.827	3.581	54.568	18.822	−2.809
400	73.260	300.679	282.717	7.185	52.907	13.830	−1.806
450	75.100	309.419	285.206	10.896	51.353	9.040	−1.049
500	76.486	317.407	288.032	14.687	49.879	4.418	−0.462
600	78.386	331.534	294.136	22.439	47.100	−4.410	0.384
700	79.586	343.714	300.369	30.341	44.472	−12.785	0.954
800	80.388	354.397	306.468	38.343	41.943	−20.791	1.358
900	80.949	363.899	312.331	46.411	39.482	−28.485	1.653
1000	81.356	372.450	317.923	54.527	37.068	−35.907	1.876
1100	81.660	380.219	323.238	62.679	34.689	−43.089	2.046
1200	81.893	387.335	328.287	70.857	−221.952	−45.742	1.991
1300	82.075	393.897	333.085	79.056	−221.184	−31.089	1.249
1400	82.221	399.985	337.649	87.271	−220.420	−16.495	0.615
1500	82.338	405.662	341.996	95.499	−219.659	−1.956	0.068
1600	82.435	410.979	346.143	103.738	−218.902	12.533	−0.409
1700	82.515	415.979	350.106	111.985	−218.148	26.975	−0.829
1800	82.583	420.698	353.898	120.240	−217.398	41.372	−1.201
1900	82.640	425.164	357.532	128.502	−216.653	55.728	−1.532
2000	82.689	429.405	361.020	136.768	−215.911	70.045	−1.829
2100	82.731	433.440	364.374	145.039	−215.174	84.324	−2.097
2200	82.767	437.289	367.601	153.314	−214.440	98.569	−2.340
2300	82.799	440.969	370.712	161.592	−213.711	112.780	−2.561
2400	82.827	444.494	373.713	169.874	−212.987	126.960	−2.763
2500	82.852	447.876	376.612	178.158	−212.266	141.110	−2.948
2600	82.874	451.126	379.416	186.444	−211.550	155.230	−3.119
2700	82.893	454.254	382.130	194.733	−210.839	169.324	−3.276
2800	82.911	457.269	384.760	203.023	−210.131	183.391	−3.421
2900	82.927	460.178	387.311	211.315	−209.429	197.433	−3.556
3000	82.941	462.990	389.787	219.608	−208.730	211.451	−3.682
3100	82.954	465.710	392.193	227.903	−208.036	225.445	−3.799
3200	82.966	468.344	394.531	236.199	−207.346	239.418	−3.908
3300	82.976	470.897	396.807	244.496	−206.661	253.368	−4.010
3400	82.986	473.374	399.023	252.794	−205.980	267.298	−4.107
3500	82.995	475.780	401.182	261.093	−205.303	281.208	−4.197
3600	83.003	478.118	403.286	269.393	−204.631	295.099	−4.282
3700	83.010	480.392	405.340	277.694	−203.964	308.972	−4.362
3800	83.017	482.606	407.344	285.995	−203.300	322.826	−4.438
3900	83.024	484.762	409.302	294.297	−202.641	336.663	−4.509
4000	83.030	486.864	411.215	302.600	−201.987	350.483	−4.577
4100	83.035	488.915	413.085	310.903	−201.337	364.286	−4.641
4200	83.040	490.916	414.914	319.207	−200.692	378.074	−4.702
4300	83.045	492.870	416.704	327.511	−200 051	391.847	−4.760
4400	83.050	494.779	418.457	335.816	−199.414	405.604	−4.815
4500	83.054	496.645	420.174	344.121	−198.782	419.348	−4.868
4600	83.058	498.471	421.856	352.426	−198.154	433.077	−4.918
4700	83.061	500.257	423.506	360.732	−197.531	446.793	−4.966
4800	83.065	502.006	425.123	369.039	−196.912	460.495	−5.011
4900	83.068	503.719	426.709	377.345	−196.298	474.185	−5.055
5000	83.071	505.397	428.266	385.652	−195.688	487.862	−5.097
5100	83.074	507.042	429.795	393.960	−195.082	501.527	−5.137
5200	83.076	508.655	431.296	402.267	−194.481	515.180	−5.175
5300	83.079	510.238	432.771	410.575	−193.885	528.822	−5.212
5400	83.081	511.791	434.220	418.883	−193.293	542.452	−5.247
5500	83.084	513.315	435.644	427.191	−192.705	556.071	−5.281
5600	83.086	514.812	437.044	435.500	−192.122	569.680	−5.314
5700	83.088	516.283	438.422	443.808	−191.543	583.279	−5.345
5800	83.090	517.728	439.777	452.117	−190.969	596.867	−5.375
5900	83.091	519.148	441.110	460.426	−190.399	610.446	−5.404
6000	83.093	520.545	442.422	468.735	−189.834	624.014	−5.433

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

Phosphorus Sulfide (P_4S_3) CRYSTAL $M_r = 220.07504$

$S°(298.15\ K) = [200.832]\ J·K^{-1}·mol^{-1}$
$T_{fus} = 440\ K$

$\Delta_f H°(298.15\ K) = [-224.647]\ kJ·mol^{-1}$
$\Delta_{fus} H° = [9.204]\ kJ·mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(298.15\ K)$ is estimated from vapor density reported by Yost and Russell.[1] T_{fus} is from Yost and Russell.[1] Other data estimated.

Reference

[1]D. M. Yost and H. Russell, "Systematic Inorganic Chemistry of the Fifth and Sixth Group Nonmetallic Elements," Prentice Hall, New York (1944).

Phosphorus Sulfide (P_4S_3) P_4S_3(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							
100							
200							
250							
298.15	146.440	200.832	200.832	0.	−224.647	−206.864	36.242
300	146.440	201.738	200.835	0.271	−224.679	−206.754	35.999
400	146.440	243.866	206.579	14.915	−236.834	−199.434	26.043
440.000	146.440	257.823	210.613	20.773	--- CRYSTAL <--> LIQUID ---		
500	146.440	276.543	217.425	29.559	−244.505	−189.235	19.769
600	146.440	303.242	229.571	44.203	−251.145	−177.539	15.456
700	146.440	325.816	241.749	58.847	−257.072	−164.797	12.297
800	146.440	345.370	253.507	73.491	−262.592	−151.234	9.875
900	146.440	362.619	264.691	88.135	−427.249	−133.753	7.763
1000	146.440	378.048	275.269	102.779	−428.703	−101.065	5.279
1100	146.440	392.005	285.257	117.423	−430.204	−68.228	3.240
1200	146.440	404.747	294.691	132.067	−686.040	−30.940	1.347
1300	146.440	416.468	303.614	146.711	−684.535	23.590	−0.948
1400	146.440	427.321	312.067	161.355	−683.095	78.007	−2.910
1500	146.440	437.424	320.091	175.999	−681.718	132.323	−4.608
1600	146.440	446.875	327.723	190.643	−680.401	186.549	−6.090
1700	146.440	455.753	334.996	205.287	−679.139	240.694	−7.396
1800	146.440	464.123	341.939	219.931	−677.929	294.767	−8.554
1900	146.440	472.041	348.580	234.575	−676.769	348.774	−9.588
2000	146.440	479.552	354.943	249.219	−675.654	402.721	−10.518

PREVIOUS: CURRENT: December 1960

Phosphorus Sulfide (P_4S_3) P_4S_3(cr)

$S°$(298.15 K) = [207.097] J·K^{-1}·mol^{-1}
T_{fus} = 440 K

$\Delta_f H°$(298.15 K) = [−220.784] kJ·mol^{-1}
$\Delta_{fus} H°$ = [9.204] kJ·mol^{-1}

Enthalpy of Formation

$\Delta_f H°(P_4S_3, l, 298.15\ K)$ is calculated from that of the crystal by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(440\ K) - H°(298\ 15\ K)$, between the crystal and liquid.

Fusion Data

T_{fus} is from Yost and Russell.[1]

Vaporization Data

T_{vap}(1 atm) = 680 K is given by Yost and Russell.[1]

Reference

[1]D. M. Yost and H. Russell, "Systematic Inorganic Chemistry of the Fifth and Sixth Group Nonmetallic Elements," Prentice Hall, New York (1944).

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	184 096	207.097	207 097	0.	−220.784	−204.869	35.892
300	184.096	208.236	207.101	0.341	−220.746	−204.770	35.654
400	184.096	261.197	214.322	18.750	−229.136	−198.668	25.943
440.000	184.096	278.743	219.393	26.114	--- CRYSTAL <---> LIQUID ---		
500	184.096	302.277	227.957	37.160	−233 041	−190.638	19.916
600	184.096	335.842	243.226	55.569	−235.916	−181.869	15.833
700	184.096	364.220	258.536	73.979	−238.077	−172.684	12.886
800	184.096	388.803	273.317	92.389	−239.831	−163.219	10.657
900	184.096	410.486	287.377	110.798	−400.722	−150.307	8.724
1000	184.096	429.882	300.675	129.208	−398.411	−122.607	6.404
1100	184.096	447.429	313.231	147.617	−396.146	−95.137	4.518
1200	184.096	463.447	325.091	166.027	−648.216	−63.557	2.767
1300	184.096	478.183	336.308	184.437	−642.946	−15.050	0.605
1400	184.096	491.826	346.936	202.846	−637.741	33.054	−1.233
1500	184.096	504.527	357.023	221.256	−632.598	80.788	−2.813
1600	184.096	516.408	366.617	239.665	−627.515	128.181	−4.185
1700	184.096	527.569	375.760	258.075	−622.487	175.258	−5.385
1800	184.096	538.092	384.489	276.485	−617.512	222.041	−6.443
1900	184.096	548.045	392.838	294.894	−612.586	268.548	−7.383
2000	184.096	557.488	400.836	313.304	−607.706	314.797	−8.222
2100	184.096	566.470	408.511	331.713	−602.867	360.803	−8.974
2200	184.096	575.034	415.887	350.123	−598.067	406.579	−9.653
2300	184.096	583.218	422.986	368.533	−593.303	452.138	−10.268
2400	184.096	591.053	429.827	386.942	−588.572	497.491	−10.828
2500	184.096	598.568	436.427	405.352	−583.872	542.647	−11.338
2600	184.096	605.788	442.803	423.761	−579.201	587.615	−11.805
2700	184.096	612.736	448.969	442.171	−574.554	632.404	−12.235
2800	184.096	619.431	454.938	460.581	−569.931	677.022	−12.630
2900	184.096	625.891	460.722	478.990	−565.330	721.474	−12.995
3000	184.096	632.133	466.333	497.400	−560.752	765.769	−13.333

PREVIOUS: CURRENT: December 1960

0 to 440 K crystal
above 440 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°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0							
100							
200							
250							
298.15	146.440	200.832	200.832	0.	−224.647	−206.864	36.242
300	146.440	201.738	200.835	0.271	−224.679	−206.754	35.999
400	146.440	243.866	206.579	14.915	−236.834	−199.434	26.043
440.000	146.440	257.823	210.613	20.773	CRYSTAL <--> LIQUID		
440.000	184.096	278.743	210.613	29.977	TRANSITION		
500	184.096	302.277	220.231	41.023	−233.041	−190.638	19.916
600	184.096	335.842	236.787	59.433	−235.916	−181.869	15.833
700	184.096	364.220	253.017	77.842	−238.077	−172.684	12.886
800	184.096	388.803	268.488	96.252	−239.831	−163.219	10.657
900	184.096	410.486	283.084	114.661	−400.722	−150.307	8.724
1000	184.096	429.882	296.811	133.071	−398.411	−122.607	6.404
1100	184.096	447.429	309.719	151.481	−396.146	−95.137	4.518
1200	184.096	463.447	321.872	169.890	−648.216	−63.557	2.767
1300	184.096	478.183	333.337	188.300	−642.946	−15.050	0.605
1400	184.096	491.826	344.176	206.709	−637.741	33.054	−1.233
1500	184.096	504.527	354.448	225.119	−632.598	80.788	−2.813
1600	184.096	516.408	364.203	243.529	−627.515	128.181	−4.185
1700	184.096	527.569	373.488	261.938	−622.487	175.258	−5.385
1800	184.096	538.092	382.343	280.348	−617.512	222.040	−6.443
1900	184.096	548.045	390.804	298.757	−612.586	268.548	−7.383
2000	184.096	557.488	398.905	317.167	−607.706	314.797	−8.222
2100	184.096	566.470	406.672	335.577	−602.867	360.803	−8.974
2200	184.096	575.034	414.131	353.986	−598.067	406.579	−9.653
2300	184.096	583.218	421.306	372.396	−593.303	452.138	−10.268
2400	184.096	591.053	428.217	390.805	−588.572	497.491	−10.828
2500	184.096	598.568	434.882	409.215	−583.872	542.647	−11.338
2600	184.096	605.788	441.317	427.625	−579.201	587.615	−11.805
2700	184.096	612.736	447.538	446.034	−574.554	632.404	−12.235
2800	184.096	619.431	453.558	464.444	−569.931	677.022	−12.630
2900	184.096	625.891	459.390	482.853	−565.330	721.474	−12.995
3000	184.096	632.133	465.045	501.263	−560.752	765.769	−13.333

PREVIOUS: CURRENT: December 1960

$S°(298.15\ K)$ = [319.265] $J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(298.15\ K)$ = [−151.042] $kJ \cdot mol^{-1}$

Enthalpy of Formation
All data estimated.

Heat Capacity and Entropy
All data estimated.

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	154.808	319.265	319.265	0.	−151.042	−168.570	29.533
300	154.808	320.223	319.268	0.286	−151.059	−168.679	29.370
400	154.808	364.758	325.340	15.767	−162.377	−173.334	22.635
500	154.808	399.302	336.806	31.248	−169.211	−175.321	18.316
600	154.808	427.527	349.646	46.729	−175.015	−175.979	15.320
700	154.808	451.391	362.520	62.210	−180.105	−175.731	13.113
800	154.808	472.063	374.950	77.690	−184.788	−174.783	11.412
900	154.808	490.297	386.773	93.171	−348.607	−170.022	9.868
1000	154.808	506.607	397.955	108.652	−349.225	−150.146	7.843
1100	154.808	521.362	408.514	124.133	−349.889	−130.206	6.183
1200	154.808	534.832	418.487	139.614	−604.888	−105.891	4.609
1300	154.808	547.223	427.920	155.094	−602.546	−64.403	2.588
1400	154.808	558.696	436.856	170.575	−600.270	−23.093	0.862
1500	154.808	569.376	445.339	186.056	−598.056	18.056	−0.629
1600	154.808	579.368	453.407	201.537	−595.902	59.060	−1.928
1700	154.808	588.753	461.095	217.018	−593.803	99.930	−3.070
1800	154.808	597.601	468.435	232.498	−591.757	140.679	−4.082
1900	154.808	605.971	475.456	247.979	−589.760	181.315	−4.985
2000	154.808	613.912	482.182	263.460	−587.808	221.847	−5.794
2100	154.808	621.465	488.636	278.941	−585.898	262.283	−6.524
2200	154.808	628.667	494.839	294.422	−584.027	302.628	−7.185
2300	154.808	635.548	500.808	309.902	−582.191	342.889	−7.787
2400	154.808	642.137	506.560	325.383	−580.389	383.072	−8.337
2500	154.808	648.456	512.111	340.864	−578.619	423.179	−8.842
2600	154.808	654.528	517.472	356.345	−576.875	463.217	−9.306
2700	154.808	660.371	522.657	371.826	−575.157	503.188	−9.735
2800	154.808	666.001	527.677	387.306	−573.463	543.095	−10.132
2900	154.808	671.433	532.541	402.787	−571.792	582.943	−10.500
3000	154.808	676.681	537.258	418.268	−570.142	622.733	−10.843
3100	154.808	681.757	541.838	433.749	−568.512	662.469	−11.163
3200	154.808	686.672	546.288	449.230	−566.900	702.152	−11.461
3300	154.808	691.436	550.615	464.710	−565.307	741.785	−11.741
3400	154.808	696.057	554.825	480.191	−563.732	781.370	−12.004
3500	154.808	700.545	558.924	495.672	−562.175	820.909	−12.251
3600	154.808	704.906	562.919	511.153	−560.635	860.404	−12.484
3700	154.808	709.148	566.814	526.634	−559.113	899.857	−12.704
3800	154.808	713.276	570.614	542.114	−557.609	939.268	−12.911
3900	154.808	717.297	574.324	557.595	−556.123	978.640	−13.107
4000	154.808	721.217	577.948	573.076	−554.655	1017.974	−13.293
4100	154.808	725.039	581.489	588.557	−553.207	1057.272	−13.470
4200	154.808	728.770	584.951	604.038	−551.778	1096.535	−13.637
4300	154.808	732.412	588.338	619.518	−550.369	1135.764	−13.797
4400	154.808	735.971	591.653	634.999	−548.981	1174.960	−13.949
4500	154.808	739.450	594.899	650.480	−547.615	1214.125	−14.093
4600	154.808	742.853	598.079	665.961	−546.270	1253.260	−14.231
4700	154.808	746.182	601.195	681.442	−544.948	1292.366	−14.363
4800	154.808	749.441	604.249	696.922	−543.650	1331.444	−14.489
4900	154.808	752.634	607.245	712.403	−542.375	1370.495	−14.610
5000	154.808	755.761	610.184	727.884	−541.124	1409.520	−14.725
5100	154.808	758.827	613.069	743.365	−539.898	1448.521	−14.836
5200	154.808	761.833	615.901	758.846	−538.698	1487.498	−14.942
5300	154.808	764.782	618.682	774.326	−537.523	1526.452	−15.044
5400	154.808	767.675	621.415	789.807	−536.375	1565.384	−15.142
5500	154.808	770.516	624.100	805.288	−535.253	1604.295	−15.236
5600	154.808	773.305	626.739	820.769	−534.157	1643.186	−15.327
5700	154.808	776.045	629.335	836.250	−533.088	1682.058	−15.414
5800	154.808	778.738	631.888	851.730	−532.046	1720.911	−15.498
5900	154.808	781.384	634.399	867.211	−531.031	1759.746	−15.580
6000	154.808	783.986	636.871	882.692	−530.044	1798.564	−15.658

PREVIOUS: CURRENT: December 1960