

Deuterium (D) IDEAL GAS

Deuterium (D)

D<sub>1</sub>(g)

$\Delta_f H^\circ(298.15 \text{ K}) = 219.807 \pm 0.004 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{ion}} H^\circ = 221.720 \pm 0.004 \text{ kJ}\cdot\text{mol}^{-1}$

$S^\circ(298.15 \text{ K}) = 123.350 \pm 0.017 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

Electronic Level and Quantum Weight State	$\epsilon$ , $\text{cm}^{-1}$	g
$2^1S_{1/2}$	0.00	2

Enthalpy of Formation

The adopted value for  $\Delta_f H^\circ(\text{D}, \text{g}, 298.15 \text{ K})$  is derived using  $D_0 = 36748.9 \pm 0.4 \text{ cm}^{-1}$  from Herzberg<sup>1</sup> and auxiliary data for  $D_2$ .<sup>2</sup> An earlier value for the dissociation energy was reported by Herzberg and Monfils<sup>3</sup> as  $D_0 = 36743.6 \pm 0.5 \text{ cm}^{-1}$ . Two theoretical studies by Kolos and Wolniewicz<sup>4</sup> and Bunker<sup>5</sup> yielded a value of  $36748.2 \text{ cm}^{-1}$ . More recently, LeRoy and Barwell,<sup>6</sup> using a relationship involving the near-dissociation behavior of the rotational constants and the long range intermolecular potential, calculated  $D_0 = 36748.88 (\pm 0.3) \text{ cm}^{-1}$ .

Heat Capacity and Entropy

The electronic levels for D(g) are given in the compilation by Moore.<sup>7</sup> Our calculations indicate that the inclusion of levels up to  $n = 12$  has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of these levels; the first excited state lies at 82281  $\text{cm}^{-1}$  above the ground state. Since the inclusion of these upper levels has no effect on the thermodynamic functions (to 6000 K) we list only the ground state. The reported uncertainty in  $S^\circ(298.15 \text{ K})$  is due to uncertainties in the gram formula weight and the fundamental constants. The gram formula weight is that recommended by IUPAC.<sup>8</sup> Extension of these calculations above 6000 K may require consideration of the higher excited states and utilization of proper fill and cut off procedures.<sup>9</sup>

Reference

- <sup>1</sup>G. Herzberg, *J. Mol. Spectrosc.* **33**, 147 (1970).
- <sup>2</sup>JANAF Thermochemical Tables: D-(g), 3-31-77.
- <sup>3</sup>G. Herzberg and A. Monfils, *J. Mol. Spectrosc.* **5**, 482 (1960).
- <sup>4</sup>W. Kolos and L. Wolniewicz, *J. Mol. Spectrosc.* **54**, 303 (1975).
- <sup>5</sup>P. R. Bunker, private communication to G. Herzberg, *Phys. Rev. Letters* **23**, 1081 (1969).
- <sup>6</sup>R. J. LeRoy and M. G. Barwell, *Can. J. Phys.* **53**, 1983 (1975).
- <sup>7</sup>C. E. Moore, NSRDS-NBS 3, Section 6 (1972).
- <sup>8</sup>IUPAC Commission on Atomic Weights, *Pure Appl. Chem.* **37**, 589 (1974).
- <sup>9</sup>J. R. Downey, Dow Chemical Company, Thermal Research, AFOSR-TR-78-0960, Contract No. F 44620-75-0-0048, (1978).

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup>	H <sup>o</sup> - H <sup>o</sup> (T)	H <sup>o</sup> - H <sup>o</sup> (T)/T	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K <sub>c</sub>
Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa					
J·K <sup>-1</sup> ·mol <sup>-1</sup>		J·K <sup>-1</sup> ·mol <sup>-1</sup>		kJ·mol <sup>-1</sup>			
0	0	0	INFINITE	-6.197	219.807	219.807	INFINITE
100	20.786	100.643	141.830	-4.119	216.086	216.086	-112.872
200	20.786	115.051	125.251	-2.040	211.433	211.433	-55.221
250	20.786	119.689	123.692	-1.001	208.977	208.977	-43.663
298.15	20.786	123.350	123.350	0	206.553	206.553	-36.187
300	20.786	123.479	123.350	0.038	206.459	206.459	-35.948
350	20.786	126.683	123.603	1.078	203.889	203.889	-30.429
400	20.786	129.458	124.166	2.107	201.375	201.375	-26.234
450	20.786	131.907	124.892	3.156	198.627	198.627	-23.065
500	20.786	134.097	125.705	4.196	195.953	195.953	-20.469
600	20.786	137.886	127.429	6.274	192.473	192.473	-16.582
700	20.786	141.091	129.158	8.353	188.910	188.910	-13.798
800	20.786	143.866	130.827	10.431	185.265	185.265	-11.705
900	20.786	146.314	132.414	12.510	181.550	181.550	-10.073
1000	20.786	148.504	133.916	14.589	177.776	177.776	-8.764
1100	20.786	150.485	135.333	16.667	173.953	173.953	-7.690
1200	20.786	152.294	136.673	18.746	170.087	170.087	-6.794
1300	20.786	153.958	137.939	20.824	166.184	166.184	-6.034
1400	20.786	155.498	139.139	22.903	162.249	162.249	-5.382
1500	20.786	156.932	140.278	24.982	158.287	158.287	-4.816
1600	20.786	158.274	141.361	27.060	154.299	154.299	-4.319
1700	20.786	159.534	142.394	29.139	150.290	150.290	-3.880
1800	20.786	160.722	143.379	31.217	146.262	146.262	-3.490
1900	20.786	161.846	144.322	33.296	142.216	142.216	-3.140
2000	20.786	162.912	145.225	35.375	138.155	138.155	-2.825
2100	20.786	163.926	146.091	37.453	134.080	134.080	-2.539
2200	20.786	164.893	146.924	39.532	130.006	130.006	-2.279
2300	20.786	165.817	147.726	41.610	126.033	126.033	-2.042
2400	20.786	166.702	148.498	43.689	122.162	122.162	-1.823
2500	20.786	167.550	149.243	45.768	118.393	118.393	-1.623
2600	20.786	168.366	149.963	47.846	114.725	114.725	-1.437
2700	20.786	169.150	150.659	49.925	111.159	111.159	-1.265
2800	20.786	169.906	151.333	52.004	107.695	107.695	-1.105
2900	20.786	170.635	151.986	54.082	104.333	104.333	-0.957
3000	20.786	171.340	152.630	56.161	101.072	101.072	-0.817
3100	20.786	172.022	153.235	58.239	97.905	97.905	-0.687
3200	20.786	172.682	153.832	60.318	94.836	94.836	-0.565
3300	20.786	173.321	154.413	62.397	91.867	91.867	-0.450
3400	20.786	173.942	154.979	64.475	88.993	88.993	-0.342
3500	20.786	174.544	155.529	66.554	86.216	86.216	-0.240
3600	20.786	175.130	156.065	68.632	83.537	83.537	-0.144
3700	20.786	175.699	156.588	70.711	81.052	81.052	-0.052
3800	20.786	176.254	157.099	72.790	78.763	78.763	0.034
3900	20.786	176.794	157.597	74.868	76.567	76.567	0.116
4000	20.786	177.320	158.083	76.947	74.463	74.463	0.194
4100	20.786	177.833	158.559	79.025	72.451	72.451	0.268
4200	20.786	178.334	159.024	81.104	70.531	70.531	0.339
4300	20.786	178.823	159.478	83.183	68.702	68.702	0.407
4400	20.786	179.301	159.924	85.261	66.964	66.964	0.471
4500	20.786	179.768	160.359	87.340	65.317	65.317	0.532
4600	20.786	180.225	160.786	89.418	63.762	63.762	0.591
4700	20.786	180.672	161.205	91.497	62.296	62.296	0.648
4800	20.786	181.110	161.615	93.576	60.921	60.921	0.702
4900	20.786	181.538	162.017	95.654	59.635	59.635	0.754
5000	20.786	181.958	162.412	97.733	58.438	58.438	0.803
5100	20.786	182.370	162.799	99.811	57.331	57.331	0.851
5200	20.786	182.773	163.179	101.890	56.314	56.314	0.897
5300	20.786	183.169	163.553	103.969	55.387	55.387	0.942
5400	20.786	183.558	163.920	106.047	54.550	54.550	0.984
5500	20.786	183.939	164.280	108.126	53.795	53.795	1.025
5600	20.786	184.314	164.634	110.204	53.121	53.121	1.065
5700	20.786	184.682	164.983	112.283	52.528	52.528	1.103
5800	20.786	185.043	165.326	114.362	52.016	52.016	1.140
5900	20.786	185.399	165.663	116.440	51.584	51.584	1.176
6000	20.786	185.748	165.995	118.519	51.231	51.231	1.210

PREVIOUS: March 1977 (1 atm)

CURRENT: March 1982 (1 bar)

Deuterium (D)

D<sub>1</sub>(g)

**IDEAL GAS**

**Deuterium, Ion (D<sup>+</sup>)**  $M_r = 2.01355$  **Deuterium, Ion (D<sup>+</sup>)**  $D_1(g)$

$$S^\circ(298.15 \text{ K}) = 117.583 \pm 0.02 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1} \quad \Delta_f H^\circ(0 \text{ K}) = 1532.21 \pm 0.04 \text{ kJ} \cdot \text{mol}^{-1} \\ \Delta_f H^\circ(298.15 \text{ K}) = [1540.324] \text{ kJ} \cdot \text{mol}^{-1}$$

**Enthalpy of Formation**

$\Delta_f H^\circ(D^+, g, 0 \text{ K})$  is calculated from  $\Delta_f H^\circ(D, g, 0 \text{ K})^1$  using the spectroscopic value of  $IP(D) = 109708.608 \pm 0.005 \text{ cm}^{-1}$  (313.6727  $\pm$  0.0001  $\text{kJ} \cdot \text{mol}^{-1}$ ) from Moore.<sup>2</sup> The ionization limit is converted from  $\text{cm}^{-1}$  to  $\text{kJ} \cdot \text{mol}^{-1}$  using the factor,  $1 \text{ cm}^{-1} = 0.01196266 \text{ kJ} \cdot \text{mol}^{-1}$ , which is derived from the 1973 CODATA fundamental constants.<sup>3</sup> Rosenstock *et al.*<sup>4</sup> and Levin and Lias<sup>5</sup> have summarized additional ionization and appearance potential data.

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

**Heat Capacity and Entropy**

The thermodynamic functions of the proton gas are calculated using the recent CODAT fundamental constants (2) and assuming that the proton is an ideal monatomic gas. Since there is no electron associated with this species, there is only a translational contribution to the thermochemical function.

**References**

- <sup>1</sup>JANAF Thermochemical Tables:  $D(g)$ , 3-31-82;  $e^-(g)$ , 3-31-82.
- <sup>2</sup>C. E. Moore, U. S. Nat. Bur. Stand., NSRDS-NBS-3, Section 6, 1972.
- <sup>3</sup>E. R. Cohen and B. N. Taylor, J. Phys. Chem. Ref. Data 2, 663 (1973).
- <sup>4</sup>H. M. Rosenstock, K. Draxl *et al.*, J. Phys. Chem. Ref. Data 6, Supp. 1, 783 pp. (1977).
- <sup>5</sup>R. D. Levin and S. G. Lias, U. S. Nat. Bur. Stand., NSRDS-NBS-71, 634 pp. (1982).

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T, = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>c</sub>
		S <sup>o</sup> - (G <sup>o</sup> - H <sup>o</sup> (T))/T	H <sup>o</sup> - H <sup>o</sup> (T)	KJ·mol <sup>-1</sup>	Δ <sub>f</sub> G <sup>o</sup>	
0	0	INFINITE	-6.197	1532.214		
100	20.786	94.876	-4.119			-266.407
200	20.786	109.284	-2.040			-264.743
250	20.786	113.922	-1.001			-226.412
298.15	20.786	117.583	0	1540.324		-197.639
300	20.786	117.712	0.038			-175.2305
350	20.786	120.916	1.078			-130.697
400	20.786	123.692	2.117			-111.096
450	20.786	126.140	3.156			-96.166
500	20.786	128.330	4.196			-83.334
600	20.786	132.120	6.274			-76.294
700	20.786	135.324	8.353			-68.885
800	20.786	138.100	10.431			-62.701
900	20.786	140.548	12.510			-57.460
1000	20.786	142.738	14.589			-52.960
1100	20.786	144.719	16.667			-49.055
1200	20.786	146.528	18.746			-46.081
1300	20.786	148.191	20.824			-43.750
1400	20.786	149.732	22.903			-41.959
1500	20.786	151.166	24.982			-40.681
1600	20.786	152.507	27.060			-39.532
1700	20.786	153.768	29.139			-38.560
1800	20.786	154.956	31.217			-37.751
1900	20.786	156.079	33.296			-37.051
2000	20.786	157.146	35.375			-36.453
2100	20.786	158.167	37.453			-35.953
2200	20.786	159.127	39.532			-35.551
2300	20.786	160.051	41.610			-35.245
2400	20.786	160.935	43.689			-34.999
2500	20.786	161.784	45.768			-34.804
2600	20.786	162.599	47.846			-34.653
2700	20.786	163.384	49.925			-34.544
2800	20.786	164.140	52.004			-34.468
2900	20.786	164.869	54.082			-34.417
3000	20.786	165.574	56.161			-34.377
3100	20.786	166.255	58.239			-34.344
3200	20.786	166.915	60.318			-34.317
3300	20.786	167.555	62.397			-34.295
3400	20.786	168.175	64.476			-34.277
3500	20.786	168.778	66.554			-34.262
3600	20.786	169.363	68.632			-34.250
3700	20.786	169.933	70.711			-34.241
3800	20.786	170.487	72.790			-34.234
3900	20.786	171.027	74.868			-34.229
4000	20.786	171.553	76.947			-34.226
4100	20.786	172.067	79.025			-34.224
4200	20.786	172.568	81.104			-34.223
4300	20.786	173.057	83.183			-34.222
4400	20.786	173.535	85.261			-34.221
4500	20.786	174.002	87.340			-34.220
4600	20.786	174.459	89.418			-34.219
4700	20.786	174.906	91.497			-34.218
4800	20.786	175.343	93.576			-34.217
4900	20.786	175.772	95.654			-34.216
5000	20.786	176.191	97.733			-34.215
5100	20.786	176.603	99.811			-34.214
5200	20.786	177.007	101.890			-34.213
5300	20.786	177.403	103.969			-34.212
5400	20.786	177.791	106.047			-34.211
5500	20.786	178.173	108.126			-34.210
5600	20.786	178.547	110.204			-34.209
5700	20.786	178.915	112.283			-34.208
5800	20.786	179.277	114.362			-34.207
5900	20.786	179.632	116.440			-34.206
6000	20.786	179.981	118.519			-34.205

PREVIOUS: March 1977 (1 atm)

CURRENT: March 1982 (1 bar)

Deuterium, Ion (D<sup>+</sup>)

EA(D, g) = 0.754209 ± 0.000003 eV  
 S°(298.15 K) = 117.590 ± 0.017 J·K<sup>-1</sup>·mol<sup>-1</sup>

IDEAL GAS

M<sub>r</sub> = 2.014651 Deuterium, Ion (D<sup>+</sup>)

ΔH<sup>o</sup>(0 K) = 147 038 ± 0.04 kJ·mol<sup>-1</sup>  
 ΔH<sup>o</sup>(298.15 K) = [142.753] kJ·mol<sup>-1</sup>

Electronic Level and Quantum State	Weight
ε <sub>v</sub> , cm <sup>-1</sup>	g <sub>v</sub>
<sup>1</sup> S <sub>0</sub>	1

Enthalpy of Formation

ΔH<sup>o</sup>(D<sup>+</sup>, g, 0 K) is calculated from ΔH<sup>o</sup>(D, g, 0 K)<sup>1</sup> using the adopted electron affinity of EA(D) = 0.754209 ± 0.000003 eV (72.7696 ± 0.0003 kJ·mol<sup>-1</sup>). This value is assumed to be the same as that recommended by Hotop and Lineberger<sup>2</sup> for H(g). Additional information on D<sup>+</sup>(g) and H<sup>+</sup>(g) may be obtained in the critical discussions of Hotop and Lineberger,<sup>2</sup> Rosenstock *et al.*,<sup>3</sup> and Massey.<sup>3</sup> ΔH<sup>o</sup>(D<sup>+</sup>, g, 298.15 K) is obtained from ΔH<sup>o</sup>(D, g, 0 K) by using EA(D) with JANAF<sup>4</sup> enthalpies, H<sup>o</sup>(0 K) - H<sup>o</sup>(298.15 K), for D<sup>+</sup>(g), D(g), and e<sup>-</sup>(ref). ΔH<sup>o</sup>(D<sup>+</sup> → D + e<sup>-</sup>, 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.*,<sup>3</sup> Δ<sub>t</sub>H<sup>o</sup>(298.15 K) should be changed by +6.197 kJ·mol<sup>-1</sup> if it is to be used in the convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The ground state electronic configuration for D<sup>+</sup>(g) is given by Hotop and Lineberger,<sup>2</sup> and Rosenstock *et al.*<sup>3</sup> A comparison of the isoelectronic sequence - H<sup>+</sup>(g), He(g), and Li<sup>+</sup>(g) - would suggest that stable electronic states may exist at 0.8 EA(H) or roughly 6400 cm<sup>-1</sup>. This would greatly affect the entropy. However, Pekeris<sup>5</sup> states that he was unable to find any bound states. In addition, Seman and Branscomb<sup>6</sup> state that theoretical and semiempirical evidence suggests that atomic negative ions have very few if any excited states below the continuum. We assume that the same arguments apply for D<sup>-</sup>(g) and that no stable excited states exist.

References

- <sup>1</sup>JANAF Thermochemical Tables: D(g), 3-31-82; e<sup>-</sup>(ref), 3-31-82.
- <sup>2</sup>H. Hotop and W. C. Lineberger, *J. Phys. Chem. Ref. Data*, **14**, 731, (1985).
- <sup>3</sup>H. Hotop and W. C. Lineberger, *J. Phys. Chem. Ref. Data*, **4**, 539 (1975).
- <sup>4</sup>H. M. Rosenstock, K. Draxl *et al.*, *J. Phys. Chem. Ref. Data*, **6**, Supp. 1, 783 pp. (1977).
- <sup>5</sup>H. S. W. Massey, "Negative Ions," 3rd ed., Cambridge University Press, Cambridge, 741 pp. (1976).
- <sup>6</sup>C. L. Pekeris, *Phys. Rev.* **126**, 1470 (1962).
- <sup>7</sup>M. L. Seman and L. M. Branscomb, *Phys. Rev.* **125**, 1602 (1962).

T/K	Enthalpy Reference Temperature = T, = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S° - (G° - H°(T))/T	H° - H°(T)	Δ <sub>f</sub> H°	
0	0.	INFINITE	-6.197	147.038	
100	20.786	94.883	-4.119		-23.749
200	20.786	109.291	-2.040		-23.595
250	20.786	113.929	-1.001		-23.514
298.15	20.786	117.590	0.		-23.514
300	20.786	117.719	0.038	142.753	-23.514
350	20.786	120.923	1.078	142.726	-23.514
400	20.786	123.699	2.117	141.996	-23.514
450	20.786	126.147	3.156	141.266	-23.514
500	20.786	128.337	4.196	140.534	-23.514
600	20.786	132.127	6.274	139.801	-23.514
700	20.786	135.331	8.353	138.327	-23.514
800	20.786	138.106	10.431	136.837	-23.514
900	20.786	140.555	12.510	135.324	-23.514
1000	20.786	142.745	14.589	133.785	-23.514
1100	20.786	144.726	16.667	132.218	-23.514
1200	20.786	146.534	18.746	130.622	-23.514
1300	20.786	148.198	20.824	129.098	-23.514
1400	20.786	149.739	22.903	127.546	-23.514
1500	20.786	151.173	24.982	125.970	-23.514
1600	20.786	152.514	27.060	124.374	-23.514
1700	20.786	153.774	29.139	122.749	-23.514
1800	20.786	154.962	31.217	121.088	-23.514
1900	20.786	156.086	33.296	119.494	-23.514
2000	20.786	157.152	35.375	117.861	-23.514
2100	20.786	158.167	37.453	116.182	-23.514
2200	20.786	159.134	39.532	114.466	-23.514
2300	20.786	160.058	41.610	112.713	-23.514
2400	20.786	160.942	43.689	110.922	-23.514
2500	20.786	161.791	45.768	109.097	-23.514
2600	20.786	162.606	47.846	107.236	-23.514
2700	20.786	163.390	49.925	105.336	-23.514
2800	20.786	164.146	52.004	103.399	-23.514
2900	20.786	164.876	54.082	101.426	-23.514
3000	20.786	165.580	56.161	99.416	-23.514
3100	20.786	166.262	58.239	97.371	-23.514
3200	20.786	166.922	60.318	95.292	-23.514
3300	20.786	167.562	62.397	93.178	-23.514
3400	20.786	168.182	64.475	91.029	-23.514
3500	20.786	168.785	66.554	88.845	-23.514
3600	20.786	169.370	68.632	86.626	-23.514
3700	20.786	169.940	70.711	84.372	-23.514
3800	20.786	170.494	72.790	82.084	-23.514
3900	20.786	171.034	74.868	79.762	-23.514
4000	20.786	171.560	76.947	77.406	-23.514
4100	20.786	172.073	79.025	75.119	-23.514
4200	20.786	172.574	81.104	72.802	-23.514
4300	20.786	173.063	83.183	70.456	-23.514
4400	20.786	173.541	85.261	68.081	-23.514
4500	20.786	174.008	87.340	65.676	-23.514
4600	20.786	174.465	89.418	63.241	-23.514
4700	20.786	174.912	91.497	60.776	-23.514
4800	20.786	175.350	93.576	58.281	-23.514
4900	20.786	175.779	95.654	55.756	-23.514
5000	20.786	176.198	97.733	53.201	-23.514
5100	20.786	176.610	99.811	50.616	-23.514
5200	20.786	177.014	101.890	48.001	-23.514
5300	20.786	177.410	103.969	45.356	-23.514
5400	20.786	177.798	106.047	42.681	-23.514
5500	20.786	178.180	108.126	40.000	-23.514
5600	20.786	178.554	110.204	37.313	-23.514
5700	20.786	178.922	112.283	34.620	-23.514
5800	20.786	179.284	114.362	31.921	-23.514
5900	20.786	179.639	116.440	29.216	-23.514
6000	20.786	179.988	118.519	26.506	-23.514

PREVIOUS: March 1977 (1 atm)

CURRENT: March 1982 (1 bar)

Deuterium, Ion (D<sup>+</sup>)

D<sub>r</sub>(g)

Hydrofluoric Acid-d<sub>1</sub> (DF)

IDEAL GAS

M<sub>r</sub> = 21.012505

D<sub>1</sub>F<sub>1</sub>(g)

S°(298.15 K) = 179.702 J·K<sup>-1</sup>·mol<sup>-1</sup> ΔH<sup>0</sup>(0 K) = -275.458 ± 0.8 kJ·mol<sup>-1</sup>  
 ΔH<sup>0</sup>(298.15 K) = -275.516 ± 0.8 kJ·mol<sup>-1</sup>

State	ε, cm <sup>-1</sup>	g	ω <sub>e</sub> , cm <sup>-1</sup>	ω <sub>e</sub> x <sub>e</sub> , cm <sup>-1</sup>	B <sub>e</sub> , cm <sup>-1</sup>	σ = I	α <sub>e</sub> , cm <sup>-1</sup>	r <sub>e</sub> , Å
X <sup>1</sup> Σ <sup>+</sup>	0	1	2998.19	45.76	11.000		0.2907	0.9187
V <sup>1</sup> Σ <sup>+</sup>	83755	1	839.4	8.90	2.121		0.00712	2.088

Enthalpy of Formation

The enthalpy of formation was calculated from ΔH<sup>0</sup>(298.15 K) of HF(g), -65.13 ± 0.2 kcal·mol<sup>-1</sup>, given in JANAF Thermochemical Tables<sup>1</sup> the appropriate thermal functions (see tables for H<sub>2</sub>, D<sub>2</sub>, DF and HF<sup>1</sup> and the estimated zero point energies. The energies for H<sub>2</sub>(g) and D<sub>2</sub>(g) are those given by Herzberg and Monfils.<sup>2</sup> The energies for HF(g) and DF(g) include the Dunham correction and were calculated from the data given by Mann *et al.*,<sup>3</sup> and Spanbauer *et al.*<sup>4</sup>

Heat Capacity and Entropy

The vibrational and rotational constants of the respective electronic levels were taken from Rosen.<sup>5</sup> The National Bureau of Standards prepared this table<sup>6</sup> by critical analysis of data existing in 1972. Using molecular constants and ΔH<sup>0</sup> selected by NBS,<sup>6</sup> we recalculate the table in terms of 1973 fundamental constants,<sup>7</sup> 1975 atomic weights,<sup>8</sup> and current JANAF reference states for the elements.

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T/K	C <sub>p</sub> <sup>o</sup>	S° - [G° - F°(T)]/T	H° - H°(T)	ΔH <sup>o</sup>	Standard State Pressure = p° = 0.1 MPa	log K <sub>r</sub>
0	0	0	0	0	INFINITE	INFINITE
100	29.117	147.887	-8.638	-275.458	-275.458	144.194
200	29.125	168.071	-5.771	-276.050	-276.050	144.194
250	29.130	174.571	-4.859	-276.667	-276.667	144.194
298.15	29.137	179.702	-4.103	-277.473	-277.473	144.194
300	29.137	179.882	0	-277.516	-277.516	144.194
350	29.150	184.375	0.054	-277.518	-277.518	144.194
400	29.174	188.268	1.511	-277.586	-277.586	144.194
450	29.221	191.707	2.969	-277.674	-277.674	144.194
500	29.290	194.790	4.429	-277.779	-277.779	144.194
600	29.561	200.152	5.892	-277.899	-277.899	144.194
700	29.962	206.738	8.333	-278.002	-278.002	144.194
800	30.463	213.990	11.809	-278.438	-278.438	144.194
900	31.016	221.990	14.879	-279.218	-279.218	144.194
1000	31.585	230.687	17.503	-279.992	-279.992	144.194
1100	32.137	239.706	21.033	-280.747	-280.747	144.194
1200	32.661	249.174	24.219	-281.511	-281.511	144.194
1300	33.148	259.053	27.459	-282.264	-282.264	144.194
1400	33.594	269.290	30.750	-283.011	-283.011	144.194
1500	34.001	279.931	34.087	-283.753	-283.753	144.194
1600	34.370	290.981	37.468	-284.491	-284.491	144.194
1700	34.705	302.422	40.886	-285.224	-285.224	144.194
1800	35.008	314.247	44.340	-285.954	-285.954	144.194
1900	35.284	326.464	47.736	-286.681	-286.681	144.194
2000	35.534	339.071	51.041	-287.404	-287.404	144.194
2100	35.762	352.073	54.259	-288.124	-288.124	144.194
2200	35.970	365.473	57.398	-288.841	-288.841	144.194
2300	36.162	379.273	60.462	-289.554	-289.554	144.194
2400	36.339	393.473	63.454	-290.264	-290.264	144.194
2500	36.501	408.073	66.381	-290.971	-290.971	144.194
2600	36.652	423.073	69.250	-291.674	-291.674	144.194
2700	36.792	438.473	72.068	-292.374	-292.374	144.194
2800	36.923	454.273	74.834	-293.071	-293.071	144.194
2900	37.045	470.473	77.550	-293.764	-293.764	144.194
3000	37.160	487.073	80.216	-294.454	-294.454	144.194
3100	37.269	504.073	82.834	-295.141	-295.141	144.194
3200	37.371	521.473	85.404	-295.824	-295.824	144.194
3300	37.468	539.273	87.926	-296.504	-296.504	144.194
3400	37.560	557.473	90.401	-297.181	-297.181	144.194
3500	37.647	576.073	92.830	-297.854	-297.854	144.194
3600	37.731	595.073	95.214	-298.524	-298.524	144.194
3700	37.811	614.473	97.554	-299.191	-299.191	144.194
3800	37.888	634.273	99.850	-299.854	-299.854	144.194
3900	37.961	654.473	102.104	-300.514	-300.514	144.194
4000	38.033	675.073	104.316	-301.171	-301.171	144.194
4100	38.101	696.073	106.486	-301.824	-301.824	144.194
4200	38.168	717.473	108.614	-302.474	-302.474	144.194
4300	38.232	739.273	110.700	-303.121	-303.121	144.194
4400	38.295	761.473	112.744	-303.764	-303.764	144.194
4500	38.355	784.073	114.746	-304.404	-304.404	144.194
4600	38.414	807.073	116.706	-305.041	-305.041	144.194
4700	38.472	830.473	118.624	-305.674	-305.674	144.194
4800	38.528	854.273	120.500	-306.304	-306.304	144.194
4900	38.583	878.473	122.334	-306.931	-306.931	144.194
5000	38.637	903.073	124.126	-307.554	-307.554	144.194
5100	38.690	928.073	125.876	-308.174	-308.174	144.194
5200	38.742	953.473	127.584	-308.791	-308.791	144.194
5300	38.795	979.273	129.250	-309.404	-309.404	144.194
5400	38.843	1005.473	130.874	-310.014	-310.014	144.194
5500	38.892	1032.073	132.456	-310.621	-310.621	144.194
5600	38.940	1059.073	133.996	-311.224	-311.224	144.194
5700	38.988	1086.473	135.494	-311.824	-311.824	144.194
5800	39.035	1114.273	136.950	-312.421	-312.421	144.194
5900	39.081	1142.473	138.364	-313.014	-313.014	144.194
6000	39.127	1171.073	139.736	-313.604	-313.604	144.194

PREVIOUS: June 1977 (1 atm)

CURRENT: June 1977 (1 bar)

Hydrofluoric Acid - D<sub>1</sub> (DF)

D<sub>1</sub>F<sub>1</sub>(g)

Hydrogen-d<sub>1</sub> (HD, or <sup>1</sup>H<sup>2</sup>H) IDEAL GAS

$S^{\circ}(298.15\text{ K}) = 143.803 \pm 0.033 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   $M_r = 3.022042$  Hydrogen - D<sub>1</sub>(HD)  $\Delta H_f^{\circ}(0\text{ K}) = 0.330 \pm 0.008 \text{ kJ}\cdot\text{mol}^{-1}$   $\Delta H_f^{\circ}(298.15\text{ K}) = 0.321 \pm 0.013 \text{ kJ}\cdot\text{mol}^{-1}$

Vibrational and Rotational Levels (cm<sup>-1</sup>)  
 Direction Summation of Electronic Ground State:  
 $E = G - G_0 + F = G - G_0 + BZ - DZ^2 + HZ^3 + H^2Z^4/(H+LZ)$ ,  
 where  $Z = J(J+1)$ ,  $Y = v+1/2$ , and we omit subscript  $v$  on  $G, F, B, D, H$ , and  $L$   
 $G = 3815.403Y - 93.61504Y^2 + 1.39630Y^3 - 0.118666Y^4 + 5.97675 \times 10^{-5}Y^5 - 2.08092 \times 10^{-6}Y^6$   
 $B = 45.66910 - 2.031845Y + 7.27360 \times 10^{-4}Y^2 - 1.82824 \times 10^{-5}Y^3 + 3.06318 \times 10^{-7}Y^4$   
 $D = 2.6527 \times 10^{-2} - 1.1534 \times 10^{-3}Y + 1.7075 \times 10^{-4}Y^2 - 2.1142 \times 10^{-5}Y^3 + 9.9570 \times 10^{-7}Y^4$   
 $H = 2.206 \times 10^{-3} - 2.648 \times 10^{-4}Y + 3.047 \times 10^{-5}Y^2 - 1.327 \times 10^{-6}Y^3$   
 $L = 2.122 \times 10^{-8} - 3.912 \times 10^{-9}Y + 3.298 \times 10^{-10}Y^2$   
 $v_{\text{max}} = 17, J_{\text{max}} = 46 - 42 v/v_{\text{max}}$

Ground State Configuration:  $1\Sigma^+$  Symmetry Number = 1

Enthalpy of Formation

$\Delta H_f^{\circ}(0\text{ K})$  is derived from  $D_0^{\circ} = 36406.0 \pm 0.4 \text{ cm}^{-1}$  (104.090 ± 0.001 kcal·mol<sup>-1</sup>) based on absorption limits analyzed by Herzberg.<sup>1</sup> He derived  $D_0^{\circ}$  values of 36406.6 and 36405.8 cm<sup>-1</sup> from lower and upper absorption edges. Thorson,<sup>2</sup> by theoretical treatment of absorption-edge doubling, concluded that the value from the upper edge is more accurate. We adopt a value closer to that from the upper edge and essentially the same as that selected by the National Bureau of Standards.<sup>3</sup>

Heat Capacity and Entropy

These are calculated by direct summation<sup>4</sup> over vibrational-rotational energy levels of the electronic ground state. We performed the direct summation with an extended version of a program written by W. H. Evans and provided through cooperation of D. D. Wagman, both of the U. S. National Bureau of Standards. Contributions of excited states ( $T_0 > 9000 \text{ cm}^{-1}$ ) are negligible at 6000 K.

Vibrational-rotational levels are represented by the polynomials given above.  $G, B,$  and  $D$  are our fits of data from Dabrowski and Herzberg.<sup>5</sup> Data from Durie and Herzberg,<sup>6</sup> McKellar *et al.*,<sup>7</sup> Brannon *et al.*,<sup>8</sup> and Stoicheff<sup>9</sup> were also used where appropriate. Observed HD data extend to  $v_{\text{max}} = 17$  for  $G$  and  $B,$  but only  $v = 1$  for  $H.$  We estimate polynomials  $H$  and  $L$  by isotopic relations from those of  $H_2$  in order to provide a similar extrapolation to high  $J$  values. Our  $H$  polynomial differs from  $H_0$  and  $H_1$ <sup>8,9</sup> by less than the experimental uncertainty. Our combination of  $H$  and  $L$  should be consistent with our adopted approximation for the infinite series (F) of rotational levels. We assume that  $F$  has the form proposed by Khachikuzov<sup>10</sup> and Woolley *et al.*<sup>11</sup> We assume a linear approximation<sup>10</sup> for the limiting values ( $J_{\text{max}}$ ) of rotational quantum number. Values in the  $J_{\text{max}}$  equation are estimated by comparison with  $H_2$  and  $D_2$  so that  $J_{\text{max}}$  is consistent with observation for HD<sup>7</sup> of a rovibrational level at  $J = 6, v = 16.$

Thermodynamic functions are calculated using 1973 fundamental constants,<sup>12</sup> 1975 atomic weight of H, and 1973 isotopic mass of D.<sup>13</sup> Results apply either to <sup>1</sup>H<sup>2</sup>H or to HD containing H of natural abundance, even though the vibrational-rotational constants are for <sup>1</sup>H<sup>2</sup>H. Maximum difference between thermodynamic functions for <sup>1</sup>H<sup>2</sup>H and HD is 0.0002 cal·K<sup>-1</sup>·mol<sup>-1</sup> in  $S^{\circ}(298.15\text{ K}).$  Our calculations agree to within 0.002 cal·K<sup>-1</sup>·mol<sup>-1</sup> (or kcal·mol<sup>-1</sup>) with those of Woolley *et al.*<sup>11</sup> up to 2000 K. The more approximate  $C_p^{\circ}$  values of NBS<sup>3</sup> differ by less than 0.04 cal·K<sup>-1</sup>·mol<sup>-1</sup> in the range 3000 to 6000 K. We omit the nuclear-spin contribution (R in 6) to entropy and Gibbs-energy function.

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T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (G <sup>o</sup> - H <sup>o</sup> (T))/T	H <sup>o</sup> - H <sup>o</sup> (T)/T	ΔH <sup>o</sup>	log K <sub>r</sub>
0	0	INFINITE	INFINITE	-8.509	INFINITE
100	29.288	111.898	169.759	-5.786	0.330
200	29.188	132.147	146.473	-2.865	0.176
298.15	29.200	143.803	0	-1.463	0.231
300	29.202	143.803	0.054	-1.474	0.257
400	29.231	152.988	2.976	-2.074	0.271
500	29.283	158.915	4.711	-2.675	0.279
600	29.395	168.808	6.329	-3.275	0.285
700	29.594	178.728	7.834	-3.874	0.289
800	29.890	188.683	9.232	-4.471	0.292
900	30.269	198.670	10.526	-5.066	0.294
1000	30.708	208.682	11.719	-5.659	0.296
1100	31.183	218.719	12.812	-6.250	0.297
1200	31.674	228.778	13.806	-6.838	0.298
1300	32.164	238.857	14.702	-7.415	0.298
1400	32.641	248.951	15.502	-8.011	0.299
1500	33.101	259.058	16.206	-8.595	0.299
1600	33.539	269.175	16.816	-9.179	0.300
1700	33.951	279.299	17.332	-9.761	0.300
1800	34.341	289.428	17.756	-10.343	0.300
1900	34.706	299.558	18.087	-10.924	0.300
2000	35.050	309.682	18.326	-11.505	0.300
2100	35.371	319.806	18.472	-12.085	0.301
2200	35.676	329.925	18.528	-12.665	0.301
2300	35.962	339.997	18.497	-13.245	0.301
2400	36.234	349.994	18.374	-13.824	0.301
2500	36.491	359.902	18.153	-14.403	0.301
2600	36.738	369.721	17.832	-14.983	0.301
2700	36.972	379.451	17.411	-15.562	0.301
2800	37.198	389.094	16.891	-16.141	0.301
2900	37.414	398.651	16.276	-16.720	0.301
3000	37.625	408.126	15.572	-17.299	0.301
3100	37.829	417.519	14.782	-17.878	0.301
3200	38.028	426.832	13.907	-18.457	0.301
3300	38.223	436.067	12.947	-19.036	0.301
3400	38.414	445.224	11.902	-19.616	0.301
3500	38.602	454.307	10.771	-20.195	0.301
3600	38.788	463.316	9.556	-20.774	0.301
3700	38.971	472.251	8.258	-21.354	0.301
3800	39.153	481.114	6.877	-21.933	0.301
3900	39.334	489.907	5.414	-22.513	0.302
4000	39.513	498.632	3.869	-23.093	0.302
4100	39.690	507.291	2.244	-23.673	0.302
4200	39.866	515.884	0.556	-24.253	0.302
4300	40.041	524.411	-1.197	-24.834	0.302
4400	40.213	532.874	-2.926	-25.414	0.302
4500	40.384	541.276	-4.741	-25.995	0.302
4600	40.551	549.616	-6.644	-26.576	0.302
4700	40.715	557.899	-8.626	-27.157	0.302
4800	40.876	566.124	-10.687	-27.739	0.302
4900	41.033	574.291	-12.828	-28.321	0.302
5000	41.185	582.407	-15.049	-28.902	0.302
5100	41.333	590.472	-17.350	-29.485	0.302
5200	41.474	598.487	-20.731	-30.067	0.302
5300	41.610	606.451	-24.192	-30.650	0.302
5400	41.738	614.364	-28.733	-31.233	0.302
5500	41.859	622.226	-34.354	-31.817	0.302
5600	41.972	630.041	-41.065	-32.400	0.302
5700	42.078	637.809	-48.466	-32.985	0.302
5800	42.174	645.532	-56.567	-33.570	0.302
5900	42.261	653.211	-65.368	-34.155	0.302
6000	42.339	660.846	-74.869	-34.740	0.302

PREVIOUS: June 1977 (1 atm)

CURRENT: June 1977 (1 bar)

Hydrogen - D<sub>1</sub>(HD)

D<sub>1</sub>H<sub>2</sub>(g)

Hydrogen-D<sub>1</sub> Ion (HD\*)

M<sub>r</sub> = 3.021493

IDEAL GAS

Hydrogen-D<sub>1</sub> Ion (HD\*)

$S^\circ(298.15\text{ K}) = 155.552 \pm 0.04\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $\Delta H^\circ(0\text{ K}) = 1490.499 \pm 0.021\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta H^\circ(298.15\text{ K}) = [1496.793]\text{ kJ}\cdot\text{mol}^{-1}$

Vibrational and Rotational Levels (cm<sup>-1</sup>)  
 Direct Summation using Energy-Level Equations for the Σ<sub>g</sub><sup>+</sup> Electronic Ground State.  
 $E = G - G_0 + F = G - G_0 + BZ - DZ^2 + LZ^3 + \dots = G - G_0 + BZ - DZ^2 + HZ^3 + I(H+L)Z^4$   
 where Z = N(N+1), Y = v+1/2, and we omit subscript v on G, F, B, D, H, and L.  
 $G = 202.19\text{ Y} - 50.5532\text{ Y}^2 + 0.0604244\text{ Y}^3 - 0.0163194\text{ Y}^4$   
 $B = 22.4643 - 103566\text{ Y} + 0.01800076\text{ Y}^2 - 0.000633016\text{ Y}^3$   
 $D = 1.12041 \times 10^{-2} - 4.24035 \times 10^{-4}\text{ Y} + 1.26643 \times 10^{-9}\text{ Y}^2$   
 $H = 7.26086 \times 10^{-6} - 2.19375 \times 10^{-7}\text{ Y}$  and  $L = 5.06679 \times 10^{-9}$   
 $v_{\text{max}} = 21$  and  $N_{\text{max}} = 47 - 38v/v_{\text{max}}$   
 Electronic statistical weight = 2 and rotational statistical weights = l(even and odd M)

Enthalpy of Formation

$\Delta H^\circ(0\text{ K}) = 356.238 \pm 0.005\text{ kcal}\cdot\text{mol}^{-1}$  is obtained from that of HD(g) using IP(HD) = 124568.5 ± 12 cm<sup>-1</sup> (356159 ± 0.004 kcal·mol<sup>-1</sup>). Takekawa and Tanaka<sup>3</sup> determined IP = 124569.5 ± 0.6 cm<sup>-1</sup> from Rydberg spectra of HD. Similar studies on H<sub>2</sub> by Herzberg and Jungen<sup>4</sup> revealed a bias of ~10 cm<sup>-1</sup> attributed to a pressure shift in the spectra. We assume an equal shift for HD, adjust IP by -1.0 cm<sup>-1</sup> and increase the uncertainty due to this adjustment.  $\Delta H^\circ(0\text{ K})$  is converted to  $\Delta H^\circ(298.15\text{ K})$  by use of JANAF<sup>1</sup> enthalpies,  $H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})$ , for H<sub>2</sub>, D<sub>2</sub>, HD\*, and e<sup>-</sup>(g). The difference in  $\Delta H^\circ(298.15\text{ K})$  between HD\* and HD should not be interpreted as a room-temperature ionization threshold due to inclusion of these enthalpies and to threshold effects noted by Rosenstock *et al.*<sup>5</sup>  
 The adopted spectroscopic IP(HD) receives strong support from a value calculated indirectly from experimental values<sup>6</sup> of  $D_0^0(\text{HD})$  and IP(H) combined with the theoretical value<sup>7</sup> of  $D_0^0(\text{HD}^+)$ , this indirect value differs by only 0.3 cm<sup>-1</sup>. Furthermore, IP(HD) can be predicted<sup>8</sup> approximately from that of H<sub>2</sub> (or D<sub>2</sub>) using differences in zero-point energies<sup>9</sup> of the diatomic molecules and their ions. Predicted values of IP(HD) deviate from the observed value by -16 cm<sup>-1</sup> (based on H<sub>2</sub>) and +16 cm<sup>-1</sup> (based on D<sub>2</sub>) inclusion of an empirical adjustment for the difference IP(D<sub>2</sub>)-IP(H) overcorrects the predictions, giving deviations of +14 cm<sup>-1</sup> (based on H<sub>2</sub>) and -14 cm<sup>-1</sup> (based on D<sub>2</sub>). The average of deviations derived from H<sub>2</sub> and D<sub>2</sub> is zero, suggesting that the slight discrepancies are due to the approximate nature of the prediction. An approximate photoionization result, reviewed by Rosenstock *et al.*,<sup>5</sup> deviates from the spectroscopic result by ~130 cm<sup>-1</sup>.

Heat Capacity and Entropy

Thermodynamic functions for ortho-para "equilibrium" HD\* are calculated by direct summation using the energy-level equations listed above. We use 1973 fundamental constants<sup>7</sup> in an extended version of a computer program written by W. H. Evans and provided by D. D. Wagman of the U. S. National Bureau of Standards. Excited electronic states are neglected because they do not contribute significantly. The electronic statistical weight is taken equal to the multiplicity since we neglect the very small rotational splitting.<sup>5</sup>  
 Coefficients of the energy-level polynomials are calculated from the theoretical values of H<sub>2</sub><sup>1</sup> using rho = 0.86617 n isotopic equations. These polynomials are confirmed by six rotation-vibration transitions (v=3, N=52) observed between 1642 and 1869 cm<sup>-1</sup> by an infrared laser-resonance method.<sup>8</sup> Our polynomials predict these transitions within 0.1 cm<sup>-1</sup>. We give the polynomial coefficients, especially higher order ones, to many more digits than are justified by their accuracy. The equations are very approximate near N<sub>max</sub> but, judging by H<sub>2</sub><sup>1</sup>, this should have little effect on the thermodynamic functions even at 6000 K. The approximate v<sub>max</sub> is derived from the G polynomial.  
 The thermodynamic functions include contributions from quasi-bound levels lying above  $D_0^0(\text{HD}^+ - \text{H}^+ + \text{D}) = 21516\text{ cm}^{-1}$ . At 6000 K these levels contribute 0.39 cal·K<sup>-1</sup>·mol<sup>-1</sup> to C<sub>p</sub> and 0.048 cal·K<sup>-1</sup>·mol<sup>-1</sup> to the Gibbs-energy function. Their contribution is negligible below 3000 K. Limiting rotational quantum numbers N<sub>max</sub> are estimated from H<sub>2</sub>, H<sub>2</sub>, and HD<sup>1</sup> by comparing energy increments and rotational quanta found above the respective values of D<sup>0</sup>. The crudity of these estimates makes C<sub>p</sub><sup>0</sup> at 6000 K somewhat more uncertain than in the case of H<sub>2</sub><sup>1</sup>.

References

- <sup>1</sup>JANAF Thermochemical Tables: H<sub>2</sub>(g), D<sub>2</sub>(g), H\*(g), e<sup>-</sup>(g), 3-31-77; HD(g), 6-30-77; H<sub>2</sub>(g), HD\*(g), D<sub>2</sub>(g), 9-30-77.
- <sup>2</sup>S. Takekawa and Y. Tanaka, *J. Chem. Phys.*, **56**, 6125 (1972).
- <sup>3</sup>G. Herzberg and Ch. Jungen, *J. Mol. Spectrosc.*, **41**, 425 (1972).
- <sup>4</sup>H. M. Rosenstock, K. Drazl, B. W. Steiner and J. T. Herron, *J. Phys. Chem. Ref. Data*, **6**, Supp. 1 (1977).
- <sup>5</sup>G. Hunter and H. O. Pritchard, *J. Chem. Phys.*, **46**, 2153 (1967).
- <sup>6</sup>D. Villarejo, *J. Chem. Phys.*, **48**, 4014 (1968).
- <sup>7</sup>E. R. Cohen and B. N. Taylor, *J. Phys. Chem. Ref. Data*, **2**, 633 (1973).
- <sup>8</sup>W. H. Wing, G. A. Ruff, W. E. Lamb and J. J. Spezeski, *Phys. Rev. Lett.*, **36**, 1488 (1976).

T/K	C <sub>p</sub> <sup>0</sup>	S <sup>0</sup>	H <sup>0</sup> -F <sup>0</sup> (T)	ΔH <sup>0</sup>	ΔG <sup>0</sup>	log K <sub>r</sub>
0	0	0	0	1490.499		
100	29.179	123.637	-8.614			-260.210
200	29.213	143.870	-5.791			-258.593
298.15	29.334	155.552	0	1496.793	1485.251	-193.396
300	29.339	155.733	0.054	1496.872	1485.179	-193.366
400	29.742	164.221	3.005	1498.848	1480.777	-184.221
500	30.461	170.950	6.014	1501.108	1476.235	-178.057
600	31.354	176.561	9.104	1503.338	1471.052	-173.356
700	32.281	181.464	12.286	1505.640	1465.491	-169.300
800	33.161	185.833	15.558	1508.002	1459.594	-165.325
900	33.960	189.786	18.915	1510.412	1453.399	-161.428
1000	34.672	193.402	22.347	1512.853	1446.934	-157.580
1100	35.304	196.737	25.847	1515.316	1440.223	-153.890
1200	35.865	199.833	29.406	1517.790	1433.387	-150.329
1300	36.369	202.724	33.018	1520.269	1426.414	-146.889
1400	36.825	205.436	36.678	1522.749	1419.311	-143.563
1500	37.244	207.991	40.382	1525.228	1412.070	-140.346
1600	37.633	210.407	44.126	1527.704	1404.724	-137.234
1700	38.001	212.700	47.900	1530.177	1397.274	-134.236
1800	38.351	214.882	51.705	1532.647	1389.721	-131.344
1900	38.692	216.965	55.571	1535.115	1382.074	-128.561
2000	39.024	218.958	59.463	1537.584	1374.431	-125.889
2100	39.353	220.870	63.382	1540.053	1366.794	-123.326
2200	39.681	222.708	67.334	1542.524	1359.169	-120.873
2300	40.008	224.479	71.318	1545.002	1351.552	-118.528
2400	40.335	226.189	75.335	1547.482	1343.945	-116.290
2500	40.661	227.842	79.387	1550.000	1336.353	-114.158
2600	40.984	229.443	83.476	1552.567	1328.789	-112.139
2700	41.303	230.996	87.592	1555.189	1321.258	-110.231
2800	41.614	232.503	91.728	1557.868	1313.764	-108.434
2900	41.914	233.969	95.900	1560.512	1306.312	-106.746
3000	42.199	235.395	100.110	1563.222	1298.917	-105.164
3100	42.466	236.783	104.344	1565.984	1291.584	-103.692
3200	42.710	238.135	108.603	1568.800	1284.317	-102.334
3300	42.929	239.453	112.885	1571.674	1277.121	-101.085
3400	43.119	240.737	117.187	1574.608	1270.000	-100.000
3500	43.278	241.990	121.507	1577.601	1263.000	-99.000
3600	43.403	243.211	125.842	1580.654	1256.121	-98.121
3700	43.494	244.401	130.187	1583.769	1249.369	-97.369
3800	43.549	245.562	134.539	1586.948	1242.741	-96.741
3900	43.568	246.693	138.896	1590.192	1236.241	-96.241
4000	43.551	247.796	143.252	1593.504	1230.000	-95.900
4100	43.499	248.871	147.607	1596.884	1224.000	-95.645
4200	43.412	249.918	151.950	1599.344	1218.284	-95.501
4300	43.292	250.938	156.286	1601.800	1212.834	-95.558
4400	43.140	251.930	160.608	1604.355	1207.648	-95.767
4500	42.959	252.899	164.913	1607.000	1202.812	-96.113
4600	42.751	253.841	169.199	1609.744	1198.326	-96.600
4700	42.517	254.758	173.462	1612.588	1194.190	-97.234
4800	42.260	255.651	177.705	1615.532	1190.304	-98.000
4900	41.983	256.519	181.914	1618.576	1186.668	-98.900
5000	41.687	257.365	186.097	1621.720	1183.292	-100.000
5100	41.375	258.187	190.250	1624.964	1180.166	-101.312
5200	41.049	258.987	194.372	1628.308	1177.181	-102.839
5300	40.711	259.766	198.466	1631.752	1174.337	-104.577
5400	40.363	260.524	202.514	1635.296	1171.624	-106.528
5500	40.008	261.261	206.532	1638.940	1169.140	-108.692
5600	39.645	261.979	210.515	1642.684	1166.876	-111.071
5700	39.279	262.677	214.461	1646.528	1164.832	-113.678
5800	38.909	263.357	218.371	1650.472	1162.908	-116.515
5900	38.538	264.019	222.243	1654.516	1161.194	-119.592
6000	38.166	264.664	226.078	1658.760	1159.690	-122.919

PREVIOUS: September, 1977 (1 am) CURRENT: September, 1977 (1 bar)

Hydrogen-d, Ion (HD<sup>+</sup>)

$S^\circ(298.15\text{ K}) = [151.206 \pm 0.4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

$M_r = 3.022591$  Hydrogen - D<sub>1</sub>, Ion (HD<sup>+</sup>)

$\Delta H_f^\circ(0\text{ K}) = [241.543 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta H_f^\circ(298.15\text{ K}) = [235.484] \text{ kJ}\cdot\text{mol}^{-1}$

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T)]/T	Standard State Pressure = p <sup>o</sup> = 0.1 MPa	D <sub>1</sub> H <sub>1</sub> (g)
			kJ·mol <sup>-1</sup>	log K <sub>t</sub>
0	0	INFINITE	241.543	-1.652
100	29.198	119.174	-8.656	-41.398
200	29.364	139.437	-5.818	-35.533
250	29.471	145.992	-7.895	-31.188
298.15	29.771	151.206	-1.426	-27.807
300	29.786	151.207	0	-25.113
400	30.239	156.015	0.055	-21.095
500	30.787	160.077	1.553	-18.246
600	31.383	163.748	3.081	-16.125
700	31.983	167.086	4.635	-14.487
800	32.583	170.000	6.219	-13.186
900	33.121	172.510	7.827	-12.128
1000	33.652	174.723	9.475	-11.253
1100	34.102	176.662	11.160	-10.518
1200	34.571	178.350	12.890	-9.892
1300	35.063	180.000	14.660	-9.354
1400	35.572	181.510	16.475	-8.887
1500	36.100	182.980	18.330	-8.477
1600	36.655	184.420	20.230	-8.116
1700	37.235	185.830	22.170	-7.796
1800	37.838	187.210	24.150	-7.509
1900	38.462	188.570	26.170	-7.252
2000	39.105	189.910	28.230	-7.021
2100	39.765	191.230	30.330	-6.811
2200	40.440	192.540	32.470	-6.620
2300	41.130	193.840	34.650	-6.446
2400	41.835	195.130	36.870	-6.287
2500	42.555	196.410	39.130	-6.141
2600	43.290	197.680	41.430	-6.007
2700	44.040	198.940	43.770	-5.883
2800	44.805	200.190	46.150	-5.768
2900	45.585	201.430	48.570	-5.662
3000	46.380	202.660	51.030	-5.563
3100	47.190	203.880	53.530	-5.471
3200	48.015	205.090	56.070	-5.386
3300	48.855	206.290	58.650	-5.306
3400	49.710	207.480	61.270	-5.231
3500	50.580	208.660	63.930	-5.161
3600	51.465	209.830	66.630	-5.095
3700	52.365	210.990	69.370	-5.033
3800	53.280	212.140	72.150	-4.975
3900	54.210	213.280	74.970	-4.921
4000	55.155	214.410	77.830	-4.869
4100	56.115	215.530	80.730	-4.821
4200	57.090	216.640	83.670	-4.775
4300	58.080	217.740	86.650	-4.732
4400	59.085	218.830	89.670	-4.691
4500	60.105	219.910	92.730	-4.652
4600	61.140	220.980	95.830	-4.615
4700	62.190	222.040	98.970	-4.580
4800	63.255	223.090	102.150	-4.547
4900	64.335	224.130	105.370	-4.516
5000	65.430	225.160	108.630	-4.486
5100	66.540	226.180	111.930	-4.458
5200	67.665	227.190	115.270	-4.431
5300	68.805	228.190	118.650	-4.405
5400	69.960	229.180	122.070	-4.381
5500	71.130	230.160	125.530	-4.357
5600	72.315	231.130	129.030	-4.335
5700	73.515	232.090	132.570	-4.314
5800	74.730	233.040	136.150	-4.294
5900	75.960	233.980	139.770	
6000	77.210	234.910	143.430	

Enthalpy Reference Temperature = T<sub>r</sub> = 298.15 K

Standard State Pressure = p<sup>o</sup> = 0.1 MPa

log K<sub>t</sub>

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1977 (1 bar)

Hydrogen - d<sub>1</sub>, Ion (HD<sup>+</sup>)

$S^\circ(298.15\text{ K}) = [151.206 \pm 0.4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

$M_r = 3.022591$  Hydrogen - D<sub>1</sub>, Ion (HD<sup>+</sup>)

$\Delta H_f^\circ(0\text{ K}) = [241.543 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta H_f^\circ(298.15\text{ K}) = [235.484] \text{ kJ}\cdot\text{mol}^{-1}$

Electronic Level and Quantum State	Weight
X <sup>2</sup> Σ <sup>+</sup>	2
ω <sub>x</sub> X <sub>v</sub> = [1473] cm <sup>-1</sup>	
B <sub>v</sub> = [19.0] cm <sup>-1</sup>	
ω <sub>2</sub> X <sub>v</sub> = [26.3] cm <sup>-1</sup>	
α <sub>x</sub> = [0.259]	
σ = 2	
r <sub>e</sub> = [1.15] Å	

IDEAL GAS

Heat Capacity and Entropy

The vibrational constants for H<sub>2</sub><sup>+</sup>(g) are estimated to be the same as in the isoelectronic species He<sub>2</sub><sup>+</sup>. The vibrational constants for HD<sub>2</sub><sup>+</sup>(g) are calculated from those for H<sub>2</sub><sup>+</sup>(g) using isotopic relations. The internuclear distance is estimated to be ~8% larger than that for He<sub>2</sub><sup>+</sup>(g). The same relationship appeared to exist for the (N<sub>2</sub>, NO, O<sub>2</sub>) isoelectronic series. B<sub>v</sub> is calculated from r<sub>e</sub> whereas α<sub>x</sub> is calculated assuming a Morse function for the ground state.

The ground and excited electronic states are discussed in detail by Massey.<sup>4</sup> No excited state contributions are included in this calculation.

References

- <sup>1</sup>T. E. Sharpe, Lockheed Report LMSC 5-10-69-9 (1969).
- <sup>2</sup>JANAF Thermochemical Tables: H(g), H<sup>+</sup>(g), D<sub>1</sub>(g), H<sub>2</sub>(g), and e<sup>-</sup>(g), 3-31-77; H<sub>2</sub><sup>+</sup>(g), 9-30-77; HD(g), 6-30-77.
- <sup>3</sup>H. M. Rosenstock, K. Draxl, B. W. Steiner, and J. T. Herron, J. Phys. Chem. Ref. Data 6, Supp. 1, 783 pp. (1977).
- <sup>4</sup>H. S. W. Massey, "Negative Ions," 3rd ed., Cambridge University Press, Cambridge, 741 pp. (1976).
- <sup>5</sup>B. Rosen, Ed., Spectroscopic Data Relative to Diatomic Molecules, Pergamon Press, New York, (1970).

Enthalpy of Formation

The enthalpy of formation at 0 K for HD<sup>+</sup>(g) is based on the electron affinity value from a Rydberg-Klein-Rees configuration-interaction calculation for H<sub>2</sub><sup>+</sup>. This study by Sharpe<sup>1</sup> led to EA(H<sub>2</sub><sup>+</sup>) = -2.5 eV. Assuming this value is valid for HD<sup>+</sup>(g) and using auxiliary data,<sup>2</sup> we calculate ΔH<sub>f</sub><sup>o</sup>(0 K) = 57.73 ± 10 kcal·mol<sup>-1</sup> and D<sup>o</sup>(HD<sup>+</sup>) = 29.0 ± 10 kcal·mol<sup>-1</sup>; the latter value is calculated for dissociation into ground state D(g) and H<sup>+</sup>(g) or D<sup>+</sup>(g) and H(g). The adopted EA (H<sub>2</sub><sup>+</sup>) value is suggested to be the more reliable value of eight studies considered by Rosenstock *et al.*<sup>3</sup>

In terms of molecular orbitals, the ground state for HD<sup>+</sup>(g) is the (1σ<sub>g</sub>)<sup>2</sup> (2pσ<sub>g</sub>)<sup>2</sup> Σ<sub>g</sub><sup>+</sup> state involving two bonding electrons and one antibonding electron. We would expect, however, the ground state to be (1σ<sub>g</sub>)<sup>2</sup> (1σ<sub>u</sub>)<sup>2</sup>. As stated by Massey,<sup>4</sup> we should expect only a weakly-bound molecule as compared with HD(g) for which the ground state has no electron in an antibonding orbital. Our adopted calculated EA (HD) value is consistent with this viewpoint. Further discussion of the HD<sup>+</sup>(g) ion may be found in Massey.<sup>4</sup>

ΔH<sub>f</sub><sup>o</sup>(0 K) is converted to ΔH<sub>f</sub><sup>o</sup>(298.15 K) by use of JANAF<sup>2</sup> enthalpies, H<sup>o</sup>(0 K)-H<sup>o</sup>(298.15 K), for D<sub>1</sub>(g), H<sub>2</sub>(g), DH<sup>+</sup>(g), and e<sup>-</sup>(g). ΔH<sub>f</sub><sup>o</sup>(298.15 K) should not be interpreted as a room temperature electron affinity due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*<sup>3</sup>

Heat Capacity and Entropy

The vibrational constants for H<sub>2</sub><sup>+</sup>(g) are estimated to be the same as in the isoelectronic species He<sub>2</sub><sup>+</sup>. The vibrational constants for HD<sub>2</sub><sup>+</sup>(g) are calculated from those for H<sub>2</sub><sup>+</sup>(g) using isotopic relations. The internuclear distance is estimated to be ~8% larger than that for He<sub>2</sub><sup>+</sup>(g). The same relationship appeared to exist for the (N<sub>2</sub>, NO, O<sub>2</sub>) isoelectronic series. B<sub>v</sub> is calculated from r<sub>e</sub> whereas α<sub>x</sub> is calculated assuming a Morse function for the ground state.

The ground and excited electronic states are discussed in detail by Massey.<sup>4</sup> No excited state contributions are included in this calculation.

References

- <sup>1</sup>T. E. Sharpe, Lockheed Report LMSC 5-10-69-9 (1969).
- <sup>2</sup>JANAF Thermochemical Tables: H(g), H<sup>+</sup>(g), D<sub>1</sub>(g), H<sub>2</sub>(g), and e<sup>-</sup>(g), 3-31-77; H<sub>2</sub><sup>+</sup>(g), 9-30-77; HD(g), 6-30-77.
- <sup>3</sup>H. M. Rosenstock, K. Draxl, B. W. Steiner, and J. T. Herron, J. Phys. Chem. Ref. Data 6, Supp. 1, 783 pp. (1977).
- <sup>4</sup>H. S. W. Massey, "Negative Ions," 3rd ed., Cambridge University Press, Cambridge, 741 pp. (1976).
- <sup>5</sup>B. Rosen, Ed., Spectroscopic Data Relative to Diatomic Molecules, Pergamon Press, New York, (1970).

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1977 (1 bar)

Hydrogen - d<sub>1</sub>, Ion (HD<sup>+</sup>)

D<sub>1</sub>H<sub>1</sub>(g)

Water-d<sub>1</sub>(HDO)

IDEAL GAS

Water-D<sub>1</sub>(HDO)

D<sub>1</sub>H<sub>2</sub>O(g)

S°(298.15 K) = 199.512 J·K⁻¹·mol⁻¹
ΔHf°(0 K) = -242.435 ± 0.063 kJ·mol⁻¹
ΔHf°(298.15 K) = -245.371 ± 0.063 kJ·mol⁻¹

Vibrational Frequencies and Degeneracies

Table with 2 columns: ν, cm⁻¹; 2723.66(1), 1402.80(1), 3707.47(1)

Ground State Quantum Weight: 1
Point Group: C<sub>s</sub>

Bond Distances: O-H = 0.9584 Å; O-D = 0.9854 Å
Bond Angle: H-O-D = 104.45°
Product of the Moments of Inertia: IaIbIc = 1.59584 × 10⁻¹¹⁹ g³·cm⁶

Enthalpy of Formation

3rd and 2nd law (where possible) analyses of the more recent determinations... of the reaction (A) H2O(g) + HD(g) = HDO(g) + H2(g), and (B) H2O(g) + D2O(g) = HDO(g) + H2(g)...

Heat Capacity and Entropy

Table with 3 columns: Source, Reaction, T/K; Cerrai et al., Suez², Hulston⁶, Wolfsberg⁷, Pyper, Newbury and Barton³, Friedman and Shiner⁴

\*Second law: ΔHf°(298.15 K), S°(298.15 K) (obs.-calc.); bKeq at temperature cited.

References

1I. Cerrai, C. Marchetti, R. Renzoni, L. Rosso, M. Silvestri, and S. Villani, Chem. Eng. Prog. Symp. Ser. 50, (11), 271 (1954).
2H. Suez, Z. Naturforsch. 4a, 328 (1949).

Continued on page 1048

Water-D<sub>1</sub>(HDO)

D<sub>1</sub>H<sub>2</sub>O(g)

Table with 8 columns: T/K, Cp, S°, [S°-H°(T₂)]/T, H°-H°(T₁)/T, ΔHf°, ΔG°, log Kf; includes data for T/K from 0 to 6000

PREVIOUS: June 1977 (1 am)

CURRENT: June 1977 (1 bar)



D<sub>1</sub>N<sub>1</sub>(g)

Imidogen - D<sub>1</sub>(ND)

IDEAL GAS

Imidogen-d<sub>1</sub> (ND)

$S^\circ(298.15\text{ K}) = 187.234\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   $\Delta H^\circ(0\text{ K}) = 375.276 \pm 20.9\text{ kJ}\cdot\text{mol}^{-1}$   $\Delta H^\circ(298.15\text{ K}) = 375.305 \pm 20.9\text{ kJ}\cdot\text{mol}^{-1}$

State	$\epsilon_e, \text{cm}^{-1}$	$g_e$	$\omega_e, \text{cm}^{-1}$	$\omega_e x_e, \text{cm}^{-1}$	$B_e, \text{cm}^{-1}$	$\alpha_e, \text{cm}^{-1}$	$r_e, \text{Å}$
X <sup>2Σ<sup>+</sup></sup>	0	3	2422	50.6	8.993	0.252	1.040

**Enthalpy of Formation**

$\Delta H_f^\circ(298.15\text{ K})$  of ND(g) minus NH(g) was calculated from the JANAF thermal functions and the zero point energies of H<sub>2</sub>(g), D<sub>2</sub>(g) [given by Herzberg and Monfils],<sup>1</sup> NH(g), and ND(g) [given by Haar, *et al.*],<sup>2</sup>  $\Delta H_f^\circ(298.15\text{ K})$  of ND(g) was calculated from this value and the JANAF selection for  $\Delta H_f^\circ(298.15\text{ K})$  of NH(g).<sup>3</sup>

**Heat Capacity and Entropy**

The molecular constants which are given for NH in the JANAF Thermochemical Tables<sup>3</sup> were adjusted for the isotope effect. The National Bureau of Standards prepared this table<sup>4</sup> by critical analysis of data existing in 1972. Using molecular constants and  $\Delta H_f^\circ$  selected by NBS,<sup>4</sup> we recalculate the table in terms of 1973 fundamental constants,<sup>5</sup> 1975 atomic weights,<sup>6</sup> and current JANAF reference states for the elements.

**References**

- <sup>1</sup>G. Herzberg and A. Monfils, *J. Mol. Spectrosc.* **5**, 482 (1960).
- <sup>2</sup>L. Haar, A. S. Friedman, and C. W. Beckett, *NBS Monograph* **20**, (1961).
- <sup>3</sup>JANAF Thermochemical Tables, 2nd Edition, NSRDS-NBS 37, (June 1971).
- <sup>4</sup>S. Abramowitz *et al.*, *U. S. Nat. Bur. Stand., Rept. 10904*, 239, (July 1972).
- <sup>5</sup>CODATA Task Group on Fundamental Constants, *CODATA Bulletin* **11**, (December 1973).
- <sup>6</sup>IUPAC Commission on Atomic Weights, *Pure Appl. Chem.* **47**, 75 (1976); **37**, 589 (1974).

T/K	Enthalpy Reference Temperature - T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	ΔG <sup>o</sup>	
	J·K <sup>-1</sup> ·mol <sup>-1</sup>	J·K <sup>-1</sup> ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	
0	0	INFINITE	0	375.276	INFINITE
100	29.118	155.412	-8.648	375.276	-195.052
200	29.131	175.599	-5.773	375.325	-97.030
250	29.140	182.100	-2.860	375.306	-77.426
298.15	29.159	187.234	-1.403	375.305	-64.762
300	29.160	187.414	0	375.305	-64.655
350	29.208	191.912	0.054	375.305	-64.357
400	29.300	195.818	1.513	375.305	-55.021
450	29.449	199.277	2.975	375.307	-38.020
500	29.655	202.900	4.444	375.311	-42.574
600	30.213	207.844	5.921	375.318	-38.218
700	30.801	212.551	8.913	375.348	-31.683
800	31.604	216.722	11.968	375.385	-27.014
900	32.298	220.485	15.003	375.445	-23.513
1000	32.943	223.922	18.288	375.514	-20.769
			21.551	375.589	-18.609
1100	33.528	227.090	24.875	375.668	-16.825
1200	34.050	230.030	28.254	375.749	-15.239
1300	34.514	232.774	31.683	375.829	-14.080
1400	34.925	235.347	35.155	375.908	-13.002
1500	35.290	237.770	38.666	375.986	-12.066
1600	35.615	240.058	42.212	376.061	-11.248
1700	35.903	242.226	45.788	376.134	-10.576
1800	36.166	244.286	49.392	376.204	-9.884
1900	36.401	246.247	53.020	376.271	-9.309
2000	36.614	248.120	56.671	376.337	-8.792
2100	36.809	249.911	60.343	376.400	-8.324
2200	36.987	251.628	64.033	376.461	-7.898
2300	37.152	253.276	67.740	376.519	-7.509
2400	37.304	254.860	71.463	376.576	-7.153
2500	37.446	256.386	75.200	376.631	-6.825
2600	37.579	257.857	78.952	376.684	-6.523
2700	37.703	259.278	82.716	376.735	-6.242
2800	37.821	260.651	86.492	376.784	-5.982
2900	37.932	261.980	90.280	376.831	-5.740
3000	38.038	263.268	94.078	376.877	-5.513
3100	38.139	264.517	97.887	376.920	-5.302
3200	38.235	265.729	101.706	376.962	-5.103
3300	38.328	266.907	105.534	377.001	-4.917
3400	38.417	268.053	109.371	377.039	-4.741
3500	38.503	269.167	113.217	377.075	-4.576
3600	38.586	270.253	117.072	377.108	-4.419
3700	38.667	271.312	120.934	377.140	-4.271
3800	38.745	272.344	124.805	377.169	-4.131
3900	38.822	273.351	128.683	377.195	-3.998
4000	38.896	274.335	132.569	377.219	-3.872
4100	38.969	275.296	136.463	377.241	-3.752
4200	39.040	276.236	140.363	377.260	-3.637
4300	39.110	277.156	144.271	377.276	-3.528
4400	39.178	278.056	148.185	377.290	-3.424
4500	39.246	278.937	152.106	377.302	-3.325
4600	39.312	279.800	156.034	377.310	-3.229
4700	39.377	280.646	159.969	377.316	-3.138
4800	39.441	281.476	163.910	377.320	-3.051
4900	39.505	282.290	167.857	377.322	-2.967
5000	39.567	283.089	171.810	377.321	-2.887
5100	39.629	283.873	175.770	377.318	-2.809
5200	39.690	284.643	179.736	377.313	-2.735
5300	39.751	285.400	183.708	377.306	-2.664
5400	39.811	286.143	187.686	377.298	-2.595
5500	39.870	286.874	191.670	377.289	-2.528
5600	39.929	287.593	195.660	377.279	-2.464
5700	39.987	288.300	199.656	377.269	-2.403
5800	40.045	288.996	203.658	377.258	-2.343
5900	40.103	289.681	207.665	377.247	-2.285
6000	40.160	290.356	211.678	377.236	-2.230

PREVIOUS: June 1977 (1 atm)

CURRENT: June 1977 (1 bar)

Imidogen - D<sub>1</sub>(ND)

D<sub>1</sub>N<sub>1</sub>(g)

IDEAL GAS

Hydroxyl-d<sub>1</sub>(OD)

Hydroxyl-D<sub>1</sub>(OD)

D<sub>1</sub>O<sub>1</sub>(g)

$S^{\circ}(298.15\text{ K}) = 189.651\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   $\Delta H^{\circ}(0\text{ K}) = 36.021 \pm 1.3\text{ kJ}\cdot\text{mol}^{-1}$   $\Delta H^{\circ}(298.15\text{ K}) = 36.602 \pm 1.21\text{ kJ}\cdot\text{mol}^{-1}$   $M_r = 18.013502$

State	$\epsilon_c\text{ cm}^{-1}$	$g$	Electronic States and Molecular Constants			$r_e\text{ \AA}$
			$\omega_e\text{ cm}^{-1}$	$\omega_e x_e\text{ cm}^{-1}$	$B_e\text{ cm}^{-1}$	
X <sup>2</sup> T <sub>1</sub>	0	2	2720.9	44.2	10.02	0.970
A <sup>2</sup> Σ <sup>+</sup>	139.7	2	2320.6	55.4	9.198	1.012
B <sup>2</sup> Σ <sup>+</sup>	35474	2	684.3	55.6	2.91	1.80
	68769	2	Symmetry Number = 1			

Enthalpy of Formation

The enthalpy of formation was calculated from the selected value for  $\Delta H^{\circ}(298.15\text{ K})$  of OH(g),  $-0.27 \pm 3\text{ kcal}\cdot\text{mol}^{-1}$ ,<sup>18</sup> the appropriate thermal functions, and zero point energies of H<sub>2</sub>(g), D<sub>2</sub>(g), OH(g), and OD(g). The zero point energies of H<sub>2</sub>(g) and D<sub>2</sub>(g) were taken from Herzberg and Monfils.<sup>1</sup> The zero point energies of OH and OD include the Dunham correction (see Herzberg and Monfils).<sup>1</sup> The molecular constants are those given by Rosen<sup>2</sup> with the exception of the spin-coupling constants taken from Herzberg.<sup>3</sup>

Heat Capacity and Entropy

The vibrational and rotational constants of the respective electronic levels were taken from Rosen.<sup>2</sup> Comparison of the results with those from a more exact treatment given by Haar *et al.*<sup>4</sup> indicates errors in the table above 400 K are negligible. Below this, they may be appreciable. In particular, it is recommended that  $H^{\circ}(0\text{ K})-H^{\circ}(298.15\text{ K})$ ,  $S^{\circ}(298.15\text{ K})$  and  $C_p^{\circ}(298.15\text{ K})$  be taken as  $-2.151\text{ kcal}\cdot\text{mol}^{-1}$ , 45.307 cal·K<sup>-1</sup>·mol<sup>-1</sup>, and 7.156 cal·K<sup>-1</sup>·mol<sup>-1</sup>, respectively. These errors result from dealing with the ground state (X<sup>2</sup>T<sub>1</sub>) as two different electronic states separated by 139.7 cm<sup>-1</sup>.

The National Bureau of Standards prepared this table<sup>5</sup> by critical analysis of data existing in 1972. Using molecular constants and  $\Delta H^{\circ}$  selected by NBS,<sup>5</sup> we recalculate the table in terms of 1973 fundamental constants,<sup>6</sup> 1975 atomic weights,<sup>7</sup> and current JANAF reference states for the elements.

References

- <sup>1</sup>G. Herzberg and A. Monfils, *J Mol Spectrosc.* **5**, 482 (1960).
- <sup>2</sup>B. Rosen, Ed., "Spectroscopic Data Relative to Diatomic Molecules," D. Van Nostrand Co., Inc., New York, pp. 232, 561, (1950).
- <sup>3</sup>G. Herzberg, "Spectra of Diatomic Molecules," U. S. Nat. Bur. Stand. Monograph 20, (1961).
- <sup>4</sup>L. Haar, A. S. Friedman, and C. W. Beckett, *U. S. Nat. Bur. Stand., Rept. 10904*, 239, (July 1972).
- <sup>5</sup>S. Abramowitz *et al.*, *U. S. Nat. Bur. Stand., Rept. 10904*, 239, (July 1972).
- <sup>6</sup>CODATA Task Group on Fundamental Constants, *CODATA Bulletin II*, (December 1973).
- <sup>7</sup>IUPAC Commission on Atomic Weights, *Pure Appl. Chem.* **47**, 75 (1976); **37**, 589 (1974).
- <sup>8</sup>JANAF Thermochemical Tables: OH(g), 6-30-77.

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> ))/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	ΔG <sup>o</sup>	
	J·K <sup>-1</sup> ·mol <sup>-1</sup>	J·K <sup>-1</sup> ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	
0	0	INFINITE	-9.207	36.021	INFINITE
100	32.617	155.537	-6.138	36.021	35.013
200	30.775	177.535	-2.976	36.492	33.664
250	30.282	184.345	-1.450	36.559	32.949
298.15	29.989	189.651	0	36.602	32.249
300	29.980	189.652	0.055	36.603	32.222
350	29.798	190.016	1.549	36.629	31.470
400	29.705	196.415	3.037	36.638	30.755
450	29.688	201.912	4.521	36.632	30.020
500	29.740	205.042	6.007	36.614	29.286
600	30.076	210.487	8.993	36.546	27.826
700	30.491	215.148	12.018	36.454	26.380
800	31.056	219.256	15.095	36.330	24.948
900	31.657	222.949	18.230	36.244	23.529
1000	32.252	226.315	20.426	36.141	22.122
1100	32.815	229.416	24.680	36.044	20.725
1200	33.335	232.293	27.983	35.953	19.342
1300	33.809	234.981	31.345	35.868	17.955
1400	34.237	237.502	34.748	35.787	16.580
1500	34.622	239.878	38.191	35.710	15.211
1600	34.968	242.123	41.671	35.635	13.847
1700	35.279	244.253	45.183	35.561	12.487
1800	35.559	246.277	48.726	35.486	11.132
1900	35.813	248.207	52.294	35.410	9.781
2000	36.043	250.050	55.887	35.330	8.434
2100	36.252	251.813	59.502	35.246	7.092
2200	36.444	253.504	63.137	35.158	5.753
2300	36.619	255.128	66.790	35.064	4.419
2400	36.782	256.690	70.461	34.965	3.088
2500	36.932	258.195	74.146	34.858	1.762
2600	37.071	259.646	77.846	34.745	0.440
2700	37.201	261.047	81.560	34.625	-0.877
2800	37.323	262.403	85.286	34.497	-2.189
2900	37.438	263.714	89.025	34.362	-3.497
3000	37.546	264.985	92.774	34.219	-4.800
3100	37.648	266.218	96.534	34.069	-6.098
3200	37.745	267.415	100.303	33.911	-7.392
3300	37.838	268.578	104.082	33.746	-8.680
3400	37.926	269.709	107.871	33.573	-9.963
3500	38.011	270.809	111.668	33.392	-11.241
3600	38.092	271.881	115.473	33.204	-12.513
3700	38.171	272.926	119.286	33.009	-13.781
3800	38.246	273.945	123.107	32.806	-15.042
3900	38.320	274.940	126.935	32.596	-16.299
4000	38.391	275.911	130.771	32.378	-17.550
4100	38.460	276.859	134.613	32.153	-18.795
4200	38.528	277.787	138.463	31.921	-20.035
4300	38.594	278.694	142.319	31.682	-21.269
4400	38.659	279.582	146.181	31.435	-22.498
4500	38.722	280.452	150.050	31.181	-23.721
4600	38.784	281.304	153.926	30.920	-24.938
4700	38.846	282.138	157.807	30.652	-26.150
4800	38.907	282.957	161.695	30.379	-27.355
4900	38.967	283.760	165.589	30.093	-28.555
5000	39.026	284.548	169.488	29.802	-29.749
5100	39.085	285.321	173.394	29.504	-30.937
5200	39.144	286.081	177.305	29.199	-32.119
5300	39.202	286.827	181.223	28.886	-33.295
5400	39.261	287.560	185.146	28.565	-34.466
5500	39.319	288.281	189.075	28.237	-35.630
5600	39.378	288.990	193.010	27.902	-36.788
5700	39.437	289.687	196.950	27.558	-37.940
5800	39.496	290.374	200.897	27.207	-39.086
5900	39.555	291.049	204.849	26.849	-40.227
6000	39.613	291.715	208.808	26.482	-41.360

PREVIOUS: June 1977 (1 atm)

CURRENT: June 1977 (1 bar)

Hydroxyl-D<sub>1</sub>(OD)

D<sub>1</sub>O<sub>1</sub>(g)

Mercapto-d<sub>1</sub> (SD)

M<sub>r</sub> = 34.074102 Mercapto-D<sub>1</sub> (SD)

D<sub>1</sub>S<sub>1</sub>(g)

S°(298.15 K) = 201.484 J·K<sup>-1</sup>·mol<sup>-1</sup> Δ<sub>f</sub>H°(0 K) = 137.893 ± 5.0 kJ·mol<sup>-1</sup>  
 Δ<sub>f</sub>H°(298.15 K) = 138.490 ± 5.0 kJ·mol<sup>-1</sup>

State	ε <sub>i</sub> , cm <sup>-1</sup>	g <sub>i</sub>	Electronic States and Molecular Constants (σ = 1) ω <sub>e</sub> , cm <sup>-1</sup>	B <sub>e</sub> , cm <sup>-1</sup>	α <sub>e</sub> , cm <sup>-1</sup>	r <sub>e</sub> , Å
X <sup>2</sup> Π <sub>g</sub>	0	2				
A <sup>2</sup> Σ <sup>+</sup>	376.8	2				
B <sup>2</sup> Σ <sup>+</sup>	30769	2	1417	4.392	0.172	1.423
C <sup>2</sup> Δ	59566	2	1917.7	4.532	0.105	1.405
D <sup>2</sup> Δ	63872	4				
E <sup>2</sup> Σ <sup>+</sup>	71205	4				
E <sup>2</sup> Σ <sup>-</sup>	71328	2	[1930.4]	[4.949]	[0.101]	
F <sup>2</sup> Δ	76717	4				
G <sup>2</sup> Δ	79320	4				
H <sup>2</sup> Δ	80858	4				

Enthalpy of Formation

The enthalpy of formation was calculated from the appropriate thermal functions (see tables for HS, DS, H<sub>2</sub>, D<sub>2</sub>)<sup>1</sup> the selected value for Δ<sub>f</sub>H°(298.15 K) of HS(g) (33.3 ± 1.2 kcal·mol<sup>-1</sup>, refer to table for HS(g)<sup>1</sup>, and the zero point energies of H<sub>2</sub>(g),<sup>2</sup> D<sub>2</sub>(g),<sup>2</sup> HS(g),<sup>2</sup> and DS(g).<sup>2</sup> The Dunham corrections were made in Herzberg and Monfils,<sup>2</sup> for H<sub>2</sub>(g) and D<sub>2</sub>(g). Spectroscopic constants tabulated in Rosen,<sup>3</sup> were used to calculate the zero point energies of HS and DS including Dunham corrections.

Heat Capacity and Entropy

The vibrational and rotational constants of the respective electronic levels were taken from Rosen.<sup>3</sup> From a comparison of this approximate calculation with more exact methods (see HS(g) table), it is concluded that the errors are negligible above 400 K. Below this, they may be appreciable. In particular, it is recommended that H°(0 K) - H°(298.15 K), S°(298.15 K) and C<sub>p</sub>°(298.15 K) be taken as -2.171 kcal·mol<sup>-1</sup>, 48.138 cal·K<sup>-1</sup>·mol<sup>-1</sup>, and 7.760 cal·K<sup>-1</sup>·mol<sup>-1</sup>, respectively. These errors result from dealing with the ground state (1L) as two different electronic states separated by 376.8 cm<sup>-1</sup>.

The National Bureau of Standards prepared this table<sup>4</sup> by critical analysis of data existing in 1972. Using molecular constants and Δ<sub>f</sub>H° selected by NBS,<sup>4</sup> we recalculate the table in terms of 1973 fundamental constants,<sup>5</sup> 1975 atomic weights,<sup>6</sup> and current JANAF reference states for the elements. Our calculated C<sub>p</sub>° values agree with the NBS table up to 4000 K; above 4000 K our values trend slightly higher and at 6000 K the difference from the original NBS table is 0.017 cal·K<sup>-1</sup>·mol<sup>-1</sup>.

References

- <sup>1</sup>JANAF Thermochemical Tables: HS(g), DS(g), 6-30-77; H<sub>2</sub>(g), D<sub>2</sub>(g), 3-31-77.
- <sup>2</sup>G. Herzberg and A. Monfils, J. Mol. Spectrosc. 5, 482 (1960).
- <sup>3</sup>B. Rosen, "Spectroscopic Data Relative to Diatomic Molecules," Pergamon Press, New York, (1970). For spin-coupling constants, refer to L. Haar, A. S. Friedman, and C. W. Beckett, U. S. Nat. Bur. Stand. Monograph 20, (1961).
- <sup>4</sup>S. Abramowitz et al., U. S. Nat. Bur. Stand., Rept. 10904, 239, (July 1972).
- <sup>5</sup>CODATA Task Group on Fundamental Constants, CODATA Bulletin 11, (December 1973).
- <sup>6</sup>IUPAC Commission on Atomic Weights, Pure Appl. Chem. 47, 75 (1976); 37, 589 (1974).

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (C <sub>p</sub> <sup>o</sup> - H°(T))/T	H° - H°(T)	Δ <sub>f</sub> H <sup>o</sup>	log K <sub>r</sub>
Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K					
Standard State Pressure = P° = 0.1 MPa					
0	0	INFINITE	-9.294	137.893	INFINITE
100	30.185	166.532	230.567	138.738	17.371
200	32.699	188.421	204.473	138.793	19.167
250	32.752	195.733	202.021	138.682	23.876
298.15	32.520	201.484	0	138.490	19.199
300	32.509	201.685	0.060	109.406	-19.049
350	32.249	206.676	1.679	138.204	-15.608
400	32.086	210.970	3.287	104.581	-13.044
450	32.049	214.746	4.893	134.596	-11.082
500	32.125	218.126	6.490	133.464	-9.526
600	32.510	224.013	9.723	131.635	-8.218
700	33.047	229.064	13.000	130.075	-7.190
800	33.613	233.514	16.334	128.685	-6.383
900	34.148	237.504	19.721	127.428	-5.737
1000	34.650	241.127	23.161	126.294	-5.199
1100	35.055	244.448	26.646	125.273	-4.733
1200	35.425	247.515	30.171	124.324	-4.339
1300	35.747	250.363	33.730	123.439	-3.990
1400	36.029	253.023	37.319	122.614	-3.681
1500	36.276	255.517	40.934	121.847	-3.407
1600	36.493	257.866	44.573	121.132	-3.163
1700	36.687	260.084	48.232	120.464	-2.944
1800	36.860	262.186	51.909	119.841	-2.746
1900	37.016	264.183	55.603	119.258	-2.566
2000	37.157	266.085	59.312	118.711	-2.401
2100	37.286	267.901	63.034	118.200	-2.249
2200	37.405	269.630	66.769	117.722	-2.108
2300	37.514	271.304	70.515	117.277	-1.976
2400	37.616	272.903	74.272	116.864	-1.852
2500	37.712	274.440	78.038	116.481	-1.735
2600	37.802	275.921	81.814	116.127	-1.624
2700	37.886	277.349	85.598	115.800	-1.518
2800	37.967	278.729	89.391	115.500	-1.416
2900	38.044	280.062	93.191	115.225	-1.318
3000	38.117	281.353	97.000	114.973	-1.224
3100	38.188	282.604	100.815	114.743	-1.134
3200	38.256	283.818	104.637	114.532	-1.047
3300	38.322	284.996	108.466	114.339	-0.963
3400	38.386	286.141	112.301	114.163	-0.882
3500	38.448	287.255	116.143	114.000	-0.803
3600	38.509	288.339	119.991	113.849	-0.727
3700	38.569	289.394	123.845	113.709	-0.654
3800	38.628	290.424	127.700	113.579	-0.583
3900	38.686	291.428	131.570	113.458	-0.514
4000	38.744	292.408	135.442	113.344	-0.447
4100	38.801	293.365	139.319	113.236	-0.383
4200	38.858	294.301	143.202	113.133	-0.321
4300	38.915	295.216	147.099	113.035	-0.261
4400	38.972	296.111	151.009	112.941	-0.202
4500	39.029	296.988	154.885	112.851	-0.145
4600	39.087	297.846	158.791	112.765	-0.090
4700	39.145	298.688	162.702	112.683	-0.037
4800	39.204	299.512	166.600	112.605	0.014
4900	39.264	300.321	170.483	112.531	0.061
5000	39.324	301.115	174.353	112.461	0.109
5100	39.385	301.895	178.209	112.395	0.157
5200	39.448	302.660	182.050	112.333	0.205
5300	39.511	303.412	185.878	112.275	0.253
5400	39.576	304.151	189.693	112.221	0.301
5500	39.642	304.878	193.495	112.170	0.349
5600	39.709	305.593	197.283	112.121	0.397
5700	39.778	306.296	201.055	112.075	0.445
5800	39.848	306.989	204.812	112.032	0.493
5900	39.920	307.670	208.555	111.991	0.541
6000	39.993	308.342	212.283	111.952	0.589

PREVIOUS: June 1977 (1 atm)

CURRENT: June 1977 (1 bar)

Mercapto-D<sub>1</sub> (SD)

D<sub>1</sub>S<sub>1</sub>(g)

Deuterium (D<sub>2</sub>)

$M_r = 4.028204$

REFERENCE STATE—IDEAL GAS

0 to 6000 K Ideal Gas

$D_0 = 439.615 \pm 0.005 \text{ kJ}\cdot\text{mol}^{-1}$   
 $S^\circ(298.15 \text{ K}) = 144.960 \pm 0.04 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

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

Vibrational and Rotational Levels (cm<sup>-1</sup>)  
 Direct Summation of Electronic Ground State

$E = G - G_0 + F + G - G_0 + BZ - DZ^2 + HZ^3 - LZ^4 + \dots - G - G_0 + BZ - DZ^2 + HZ^3 + (H+LZ),$   
 where  $Z = J(J+1)$ ,  $Y = v+1/2$ , and we omit subscript  $v$  on  $G, F, B, D, H$ , and  $L$   
 $G = 3116.334Y - 62.50516Y^2 + 0.7797565Y^3 - 5.48262 \times 10^{-3}Y^4 + 2.25748 \times 10^{-3}Y^5 - 6.30154 \times 10^{-3}Y^6$   
 $B = 30.45273 - 1.102045Y + 0.0295505Y^2 - 5.99912 \times 10^{-3}Y^3 + 8.37740 \times 10^{-4}Y^4$   
 $D = 6.87040 \times 10^{-3}Y^3 + 2.80134 \times 10^{-6}Y^6 - 4.68952 \times 10^{-4}Y^7$   
 $H = 0.011525 - 3.6876 \times 10^{-4}Y + 4.1199 \times 10^{-3}Y^2 - 4.4723 \times 10^{-4}Y^3 + 1.7858 \times 10^{-3}Y^4$   
 $L = 6.55 \times 10^{-6} - 6.42 \times 10^{-4}Y + 6.03 \times 10^{-3}Y^2 - 2.15 \times 10^{-3}Y^3$   
 $L = 4.20 \times 10^{-9} - 6.32 \times 10^{-10}Y + 4.35 \times 10^{-11}Y^2$

$v_{\text{max}} = 21, J_{\text{max}} = 54 - 47v/v_{\text{max}}$   
 Normalized statistical weights = 2/3 (even  $J$ ) and 1/3 (odd  $J$ )

Ground State Configuration:  $1\Sigma_g^+$   $r_e = 0.7415 \text{ \AA}$

Enthalpy of Formation

Zero by definition. Refer to the monatomic deuterium gas table for a discussion of the dissociation energy.

Heat Capacity and Entropy

These are calculated by direct summation<sup>1</sup> over vibration-rotation energy levels of the electronic ground state. We performed the direct summation with an extended version of a program written by W. H. Evans and provided through cooperation of D. D. Wagman, both of the U. S. National Bureau of Standards. Contributions of excited states ( $T_0 > 90000 \text{ cm}^{-1}$ ) are negligible at 6000 K. Polynomials  $G, B$  and  $D$  are our fits of data from Stoicheff<sup>2</sup> and Bredohl and Herzberg.<sup>3</sup> Polynomials  $H$  and  $L$  are estimated by isotopic relations from those of H<sub>2</sub>, in order to provide a similar extrapolation to high  $J$  values. The adopted  $H$  polynomial is not more accurate than the relatively scattered data,<sup>2-4</sup> but it should be more consistent with our adopted approximation for the infinite-series ( $F$ ) equation for rotational levels. We assume that  $F$  has the form proposed by Khachkuruzov<sup>5</sup> and Woolley *et al.*<sup>6</sup> We use a linear approximation for the limiting values ( $J_{\text{max}}$ ) of rotational quantum number. The  $J_{\text{max}}$  equation is estimated; its second value has been revised from 52 (in the 1977 table) to 47 in order to yield  $C_p^\circ$  and  $S^\circ$  values that agree more closely with theory<sup>7</sup> near 6000 K. We omit the nuclear-spin contribution (R in 9) to entropy and Gibbs energy function. We adopt ortho-para "equilibrium"<sup>8</sup> D<sub>2</sub> as the reference state at all temperatures. Values differ from "normal" D<sub>2</sub> only at 100 K.<sup>6,7</sup> Our values can be compared with the theoretical results of Kosloff *et al.*<sup>9</sup> and Gurvich *et al.*<sup>9</sup> and with the earlier table of NBS.<sup>1</sup> Our  $S^\circ$  values deviate by 0.001<sup>8</sup> or -0.005<sup>9</sup> cal·K<sup>-1</sup>·mol<sup>-1</sup> at 6000 K. Our  $C_p^\circ$  values deviate by 0.01<sup>8</sup>, -0.002<sup>9</sup> or 0.002<sup>7</sup> at 5000 K and by 0.001<sup>8</sup> or -0.005<sup>9</sup> cal·K<sup>-1</sup>·mol<sup>-1</sup> at 6000 K.

References

- <sup>1</sup>JANAF Thermochemical Tables: H<sub>2</sub>(g), 3-31-77.
- <sup>2</sup>B. P. Stoicheff, *Can. J. Phys.* **35**, 730 (1957).
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- <sup>4</sup>P. J. Brannon, C. H. Church, and C. W. Peters, *J. Mol. Spectrosc.* **27**, 44 (1968).
- <sup>5</sup>G. A. Khachkuruzov, *Opt. Spectrosc.* **30**, 455 (1971).
- <sup>6</sup>H. W. Woolley, R. B. Scott, and F. G. Brickwedde, *J. Res. Natl. Bur. Stand.* **41**, 379 (1948).
- <sup>7</sup>S. Abramowitz *et al.*, *U. S. Natl. Bur. Stand., Rept. 10904*, 239, (July 1974).
- <sup>8</sup>R. Rosloff, R. D. Levine and R. B. Bernstein, *Mol. Phys.* **27**, 981 (1974).
- <sup>9</sup>L. V. Gurvich, I. V. Veits *et al.*, "Thermodynamic Properties of Individual Substances," 3rd ed., Vol. I, Nauka, Moscow, (1978).

Deuterium (D<sub>2</sub>)

Deuterium (D<sub>2</sub>)

D<sub>2</sub>(ref)

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S° - (G° - H°(T <sub>r</sub> ))/T	H° - H°(T <sub>r</sub> )	Δ <sub>f</sub> G°	
0	0	INFINITE	-8.569	0	0
100	30.317	112.789	-5.818	0	0
200	29.204	133.306	-2.865	0	0
250	29.185	139.819	-1.405	0	0
298.15	29.194	144.960	0	0	0
300	29.195	145.141	0.054	0	0
350	29.213	149.647	1.514	0	0
400	29.242	153.545	2.975	0	0
450	29.290	156.992	4.439	0	0
500	29.366	160.081	5.905	0	0
600	29.619	165.456	8.853	0	0
700	30.008	170.049	11.833	0	0
800	30.502	174.087	14.858	0	0
900	31.057	177.712	17.936	0	0
1000	31.636	181.014	21.070	0	0
1100	32.210	184.056	24.263	0	0
1200	32.762	186.882	27.512	0	0
1300	33.282	189.526	30.814	0	0
1400	33.766	192.010	34.167	0	0
1500	34.213	194.355	37.566	0	0
1600	34.625	196.576	41.008	0	0
1700	35.004	198.687	44.490	0	0
1800	35.353	200.698	48.008	0	0
1900	35.676	202.618	51.560	0	0
2000	35.975	204.456	55.142	0	0
2100	36.252	206.218	58.754	0	0
2200	36.512	207.910	62.392	0	0
2300	36.755	209.539	66.056	0	0
2400	36.984	211.108	69.743	0	0
2500	37.201	212.622	73.452	0	0
2600	37.407	214.085	77.182	0	0
2700	37.605	215.501	80.933	0	0
2800	37.795	216.872	84.703	0	0
2900	37.978	218.201	88.492	0	0
3000	38.156	219.492	92.298	0	0
3100	38.329	220.746	96.123	0	0
3200	38.498	221.965	99.964	0	0
3300	38.665	223.152	103.822	0	0
3400	38.829	224.309	107.697	0	0
3500	38.991	225.437	111.588	0	0
3600	39.152	226.533	115.495	0	0
3700	39.312	227.613	119.419	0	0
3800	39.470	228.663	123.358	0	0
3900	39.628	229.690	127.313	0	0
4000	39.785	230.696	131.283	0	0
4100	39.941	231.680	135.270	0	0
4200	40.096	232.644	139.271	0	0
4300	40.250	233.590	143.289	0	0
4400	40.402	234.517	147.321	0	0
4500	40.553	235.426	151.369	0	0
4600	40.701	236.319	155.432	0	0
4700	40.847	237.196	159.509	0	0
4800	40.989	238.058	163.601	0	0
4900	41.127	238.904	167.707	0	0
5000	41.262	239.736	171.826	0	0
5100	41.391	240.555	175.959	0	0
5200	41.515	241.360	180.105	0	0
5300	41.633	242.152	184.263	0	0
5400	41.745	242.931	188.431	0	0
5500	41.850	243.698	192.611	0	0
5600	41.947	244.453	196.801	0	0
5700	42.036	245.196	201.000	0	0
5800	42.117	245.928	205.208	0	0
5900	42.190	246.648	209.423	0	0
6000	42.253	247.358	213.645	0	0

PREVIOUS: March 1977 (1 atm)

CURRENT: March 1982 (1 bar)

Deuterium (D<sub>2</sub>)

D<sub>2</sub>(ref)

Deuterium, Ion (D<sub>2</sub><sup>+</sup>)

IDEAL GAS

D<sub>2</sub>(g)

$S^\circ(298.15\text{ K}) = 156.735 \pm 0.04 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(0\text{ K}) = 1492.287 \pm 0.013 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = [1498.567] \text{ kJ}\cdot\text{mol}^{-1}$

Vibrational and Rotational Levels (cm<sup>-1</sup>)

Direct Summation using Energy-Level Equations for the <sup>2</sup>S<sub>g</sub><sup>+</sup> Electronic Ground State:

$$E = G - G_v + F - G - G_v + BZ - DZ^2 + HZ^3 - LZ^4 + \dots \quad G - G_v + BZ - DZ^2 + HZ^3 - LZ^4$$

where  $Z = N(N+1)$ ,  $Y = v+1/2$ , and we omit subscript  $v$  on  $G$ ,  $F$ ,  $B$ ,  $D$ ,  $H$ , and  $L$

$$G = 1643.29 Y - 33.7163 Y^2 + 0.329116 Y^3 - 0.00725916 Y^4$$

$$B = 14.9825 - 0.564098 Y + 0.00801011 Y^2 - 0.000230173 Y^3 \quad r_3 = 1.057 \text{ \AA}$$

$$D = 4.98379 \times 10^{-3} - 1.54039 \times 10^{-4} Y + 3.75711 \times 10^{-6} Y^2$$

$$H = 2.15408 \times 10^{-6} - 5.31503 \times 10^{-8} Y \text{ and } L = 1.00253 \times 10^{-9}$$

$$v_{\text{max}} = 26 \text{ and } N_{\text{max}} = 57 - 46v/v_{\text{max}}$$

electronic statistical weight = 2 and normalized rotational statistical weights = 2/3 (even  $N$ ) or 1/3 (odd  $N$ )

Enthalpy of Formation

$\Delta_f H^\circ(0\text{ K}) = 356.666 \pm 0.003 \text{ kcal}\cdot\text{mol}^{-1}$  is the ionization potential  $IP(D_2) = 124745.6 \pm 1.2 \text{ cm}^{-1}$ . Takezawa and Tanaka<sup>1</sup> determined  $IP = 124746.6 \pm 0.6 \text{ cm}^{-1}$  from Rydberg spectra of  $D_2^+$ . Similar studies on  $H_2$  by Herzberg and Jungen<sup>2</sup> revealed a bias of  $-1.0 \text{ cm}^{-1}$  attributed to a pressure shift in the spectra. We assume an equal shift for  $D_2^+$ , adjust  $IP$  by  $-1.0 \text{ cm}^{-1}$ , and increase the uncertainty due to this adjustment.  $\Delta_f H^\circ(0\text{ K})$  is converted to  $\Delta_f H^\circ(298.15\text{ K})$  by use of JANAF<sup>3</sup> enthalpies  $H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})$  for  $D_2$ ,  $D$ , and  $e$  (ref).  $\Delta_f H^\circ(298.15\text{ K})$  should not be interpreted as a room-temperature ionization threshold due to inclusion of these enthalpies and to threshold effects noted by Rosenstock *et al.*<sup>4</sup>

The adopted spectroscopic  $IP(D_2)$  receives strong support from a value calculated indirectly from experimental values<sup>5</sup> of  $D_2(D_2)$  and  $IP(D)$  combined with the theoretical value<sup>6</sup> of  $D_2(D_2)$ ; this indirect value differs by only  $0.4 \text{ cm}^{-1}$ . Rosenstock *et al.*<sup>4</sup> review several less accurate determinations of  $IP(D_2)$  and recommend a value calculated from  $IP(H_2)$  using differences in zero-point energies of the diatomic molecules and their ions. Repeating this calculation with JANAF values,<sup>3</sup> we predict an  $IP(D_2)$  which differs from the observed value by  $-32 \text{ cm}^{-1}$ . Inclusion of an empirical adjustment for  $IP(D) - IP(H)$  overcorrects the prediction, giving a deviation of  $+28 \text{ cm}^{-1}$ . These slight discrepancies are due<sup>3</sup> (refer to  $HD^+$ ,  $g$ ) to the approximate nature of the prediction. Villarejo's average photoionization result,<sup>6</sup>  $IP(D_2) = 124757 \pm 180 \text{ cm}^{-1}$ , deviates by  $+11 \text{ cm}^{-1}$  from the spectroscopic value.

Heat Capacity and Entropy

Thermodynamic functions for ortho-para "equilibrium"  $D_2$  are calculated by direct summation using the energy-level equations listed above. We use 1973 fundamental constants<sup>7</sup> in an extended version of a computer program written by W. H. Evans and provided by D. D. Wagman of the U. S. National Bureau of Standards. Excited electronic states are neglected because they do not contribute significantly. The electronic statistical weight is taken equal to the multiplicity since we neglect rotational splitting which should be very small (see  $HD^+$  and  $H_2^+$ ).<sup>3</sup>

Coefficients of the energy-level polynomials are calculated from the theoretical values of  $H_2^+$  using  $\rho = 0.707330$  in isotopic equations. Theoretical calculations<sup>8</sup> on  $D_2$  provide confirmation of  $B_v$ ,  $\omega_v$ , and  $\omega_{x,v}$ ; the latter two are confirmed by vibrational structure observed<sup>9</sup> in the photoionization threshold of  $D_2$ . We give the polynomial coefficients, especially higher order ones, to many more digits than are justified by their accuracy. The equations are very approximate near  $N_{\text{max}}$  but, judging by  $H_2^+$ , this should have little effect on the thermodynamic functions even at 6000 K. The approximate  $v_{\text{max}}$  is derived from the  $G$  polynomial.

The thermodynamic functions include contributions from quasi-bound levels lying above  $D_0^0 = 21712 \text{ cm}^{-1}$ . At 6000 K these levels contribute  $0.33 \text{ cal K}^{-1}\cdot\text{mol}^{-1}$  to  $C_p^\circ$  and  $0.041 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  to the Gibbs-energy function. Their contribution is negligible below 3000 K. Limiting rotational quantum numbers  $N_{\text{max}}$  are estimated from  $H_2$ ,  $H$ , and  $D_2^+$  by comparing energy increments and rotational quanta found above the respective values of  $D_0^0$ . The crudity of these estimates makes  $C_p^\circ$  at 6000 K somewhat more uncertain than in the case of  $H_2^+$ .

References

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T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T)]/T	H <sup>o</sup> - H <sup>o</sup> (T)	Δ <sub>f</sub> H <sup>o</sup>	Δ <sub>f</sub> G <sup>o</sup>	log K <sub>f</sub>
0	0	0	0	1492.287	1488.801	-260.832
100	29.192	124.796	-8.651	1498.567	1488.741	-259.213
200	29.221	182.774	-5.798	1498.566	1488.741	-259.213
298.15	29.510	145.027	-2.879	1498.567	1488.741	-259.213
300	29.519	156.735	0	1498.566	1488.741	-259.213
400	30.282	156.917	0.055	1500.749	1483.131	-193.938
500	31.332	157.901	3.041	1502.978	1480.971	-154.716
600	32.420	162.666	9.309	1505.297	1476.353	-128.528
700	33.417	169.255	12.002	1507.688	1471.580	-99.719
800	34.285	173.785	13.988	1510.128	1465.982	-70.799
900	35.028	177.241	15.484	1512.595	1460.316	-48.755
1000	35.664	179.582	17.259	1515.075	1454.574	-25.990
1100	36.214	199.007	26.584	1517.556	1448.184	-68.769
1200	36.695	202.179	30.230	1520.031	1441.768	-112.759
1300	37.123	205.133	33.922	1522.499	1435.146	-157.665
1400	37.510	207.899	37.653	1524.956	1428.334	-202.592
1500	37.867	210.499	41.427	1527.405	1421.347	-247.549
1600	38.201	212.954	45.226	1529.845	1414.197	-292.506
1700	38.518	215.279	49.062	1532.278	1406.894	-337.463
1800	38.825	217.490	52.929	1534.705	1399.449	-382.420
1900	39.125	219.597	56.827	1537.130	1391.869	-427.377
2000	39.422	221.611	60.754	1539.553	1384.160	-472.334
2100	39.719	223.540	64.711	1541.977	1376.331	-517.291
2200	40.017	225.396	68.698	1544.404	1368.386	-562.248
2300	40.317	227.182	72.715	1546.836	1360.331	-607.205
2400	40.620	228.904	76.761	1549.275	1352.170	-652.162
2500	40.923	230.568	80.829	1551.721	1343.907	-697.119
2600	41.225	232.179	84.946	1554.176	1335.546	-742.076
2700	41.523	233.741	89.083	1556.642	1327.091	-787.033
2800	41.814	235.256	93.250	1559.117	1318.543	-831.990
2900	42.094	236.728	97.446	1561.607	1309.908	-876.947
3000	42.360	238.153	101.669	1564.097	1301.186	-921.904
3100	42.607	239.553	105.917	1566.600	1292.381	-966.861
3200	42.832	240.909	110.189	1569.110	1283.495	-1011.818
3300	43.032	242.231	114.483	1571.624	1274.531	-1056.775
3400	43.204	243.524	118.795	1574.140	1265.490	-1101.732
3500	43.345	244.772	123.123	1576.655	1256.376	-1146.689
3600	43.453	245.995	127.465	1579.166	1247.190	-1191.646
3700	43.526	247.187	131.812	1581.671	1237.933	-1236.603
3800	43.565	248.346	136.167	1584.165	1228.610	-1281.560
3900	43.577	249.480	140.524	1586.646	1219.221	-1326.517
4000	43.534	250.582	144.879	1589.109	1209.768	-1371.474
4100	43.467	251.657	149.230	1591.552	1200.254	-1416.431
4200	43.365	252.703	153.571	1593.970	1190.681	-1461.388
4300	43.232	253.722	157.902	1596.362	1181.051	-1506.345
4400	43.068	254.714	162.217	1598.723	1171.365	-1551.302
4500	42.875	255.680	166.514	1601.051	1161.626	-1596.259
4600	42.655	256.620	170.791	1603.344	1151.836	-1641.216
4700	42.411	257.534	175.044	1605.598	1141.996	-1686.173
4800	42.145	258.424	179.272	1607.813	1132.108	-1731.130
4900	41.859	259.291	183.473	1609.986	1122.175	-1776.087
5000	41.556	260.133	187.643	1612.106	1112.199	-1821.044
5100	41.237	260.953	191.783	1614.202	1102.179	-1865.999
5200	40.905	261.751	195.890	1616.242	1092.120	-1910.954
5300	40.562	262.526	199.964	1618.227	1082.021	-1955.909
5400	40.210	263.281	204.006	1620.185	1071.886	-2000.864
5500	39.850	264.016	208.006	1622.197	1061.714	-2045.819
5600	39.485	264.731	212.079	1624.234	1051.509	-2090.774
5700	39.116	265.426	216.126	1626.279	1041.271	-2135.729
5800	38.744	266.103	220.148	1628.308	1031.001	-2180.684
5900	38.371	266.763	224.136	1630.316	1020.701	-2225.639
6000	37.998	267.404	228.093	1632.347	1010.373	-2270.594

D<sub>2</sub>(g)

Deuterium, Ion (D<sub>2</sub><sup>+</sup>)

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

Deuterium, Ion (D<sub>2</sub><sup>+</sup>)

IDEAL GAS

Deuterium, Ion (D<sub>2</sub><sup>+</sup>)

D<sub>2</sub>(g)

$S^\circ(298.15\text{ K}) = 158.26 \pm 0.4\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(0\text{ K}) = [241.4 \pm 42]\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = [235.365]\text{ kJ}\cdot\text{mol}^{-1}$

Electronic Level and Quantum Weight State	$\epsilon$ , cm <sup>-1</sup>	g
$X^2\Sigma_g^+$	0	2
$\omega_e$	[1202] cm <sup>-1</sup>	
$B_e$	[12.7] cm <sup>-1</sup>	
$\omega_e x_e$	[17.5] cm <sup>-1</sup>	
$\alpha_e$	[0.141] cm <sup>-1</sup>	
$\sigma = 2$		
$r_e = [1.15]\text{ \AA}$		

Enthalpy of Formation

The enthalpy of formation at 0 K for D<sub>2</sub><sup>+</sup>(g) is based on the electron affinity (EA) value derived from a Rydberg-Klein-Rees configuration interaction calculation for H<sub>2</sub><sup>+</sup>. This study by Sharpe<sup>1</sup> led to EA(H<sub>2</sub>) = -2.5 eV. Assuming the same value for D<sub>2</sub> and using auxiliary data,<sup>2</sup> we calculate  $\Delta_f H^\circ(0\text{ K}) = 57.7 \pm 10\text{ kcal}\cdot\text{mol}^{-1}$  and  $D_0^0(D_2^+) = 30.0 \pm 10\text{ kcal}\cdot\text{mol}^{-1}$ , the latter value assumes dissociation into ground state D<sub>2</sub>(g) and D<sup>+</sup>(g). The adopted EA(H<sub>2</sub>) value is suggested to be the more reliable value of eight studies considered by Rosenstock *et al.*<sup>3</sup> In terms of molecular orbitals, the ground state for D<sub>2</sub><sup>+</sup>(g) is the (1σ<sub>g</sub>)<sup>2</sup>(2pσ<sub>g</sub>)<sup>2</sup>Σ<sub>g</sub><sup>+</sup> state involving two bonding electrons and one antibonding electron. As stated by Massey,<sup>4</sup> we should expect only a weakly-bound molecule as compared with D<sub>2</sub>(g) for which the ground state has no electrons in an antibonding orbital. We would expect, however, the ground state to be (1σ<sub>g</sub>)<sup>2</sup>(1σ<sub>u</sub>)<sup>0</sup>. Our calculated EA(D<sub>2</sub>) value is consistent with this viewpoint. Further discussion of the D<sub>2</sub><sup>+</sup>(g) ion may be found in Massey.<sup>4</sup>

$\Delta_f H^\circ(0\text{ K})$  is converted to  $\Delta_f H^\circ(298.15\text{ K})$  by use of JANAF<sup>5</sup> enthalpies,  $H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})$ , for D<sub>2</sub>(g), D<sub>2</sub><sup>+</sup>(g), and e<sup>-</sup>(ref).  $\Delta_f H^\circ(298.15\text{ K})$  should not be interpreted as a room temperature electron affinity due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*<sup>3</sup>

Heat Capacity and Entropy

The vibrational constants for H<sub>2</sub><sup>+</sup>(g) are estimated to be the same as in the isoelectronic species He<sub>2</sub><sup>+</sup>. The vibrational constants for D<sub>2</sub><sup>+</sup>(g) are calculated from those of H<sub>2</sub><sup>+</sup>(g) using isotopic relations.<sup>6</sup> The internuclear distance is estimated to be ~8% larger than that for He<sub>2</sub><sup>+</sup>(g). The same relationship appeared to exist for the (N<sub>2</sub><sup>+</sup>, NO, O<sub>2</sub><sup>+</sup>) isoelectronic series.  $B_e$  is calculated from  $r_e$ , whereas  $\alpha_e$  is calculated assuming a Morse function for the ground state.

The ground and excited electronic states are discussed in detail by Massey.<sup>4</sup> No excited state contributions are included in this calculation.

References

- <sup>1</sup>T. E. Sharpe, Lockheed Report LMSC 5-10-69-9 (1969).
- <sup>2</sup>JANAF Thermochemical Tables: D(g), D<sub>2</sub>(g), D<sub>2</sub><sup>+</sup>(g), and e<sup>-</sup>(ref), H<sub>2</sub><sup>+</sup>(g), H<sub>2</sub><sup>+</sup>(g), 9-30-77.
- <sup>3</sup>H. M. Rosenstock, K. Draxl, B. W. Steiner, and J. T. Herron, *J. Phys. Chem. Ref. Data* 6, Supp. 1, 783 pp. (1977).
- <sup>4</sup>H. S. W. Massey, "Negative Ions", 3rd ed., Cambridge University Press, Cambridge, 741 pp. (1976).
- <sup>5</sup>B. Rosen, Ed., "Spectroscopic Data Relative to Diatomic Molecules", Pergamon Press, New York, (1970).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (C <sub>p</sub> <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> ))/T <sub>r</sub>	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	Δ <sub>f</sub> H <sup>o</sup>	
0	0	0	INFINITE	241.418	
100	29.190	126.100	184.605	-8.714	-41.636
200	29.403	146.375	160.977	-8.850	-41.382
250	29.771	152.971	158.755	-2.924	-35.540
298.15	30.315	158.259	158.259	-1.446	-31.176
300	30.338	158.447	158.260	0	-27.795
350	31.023	163.174	158.632	1.590	-25.101
400	31.745	167.364	159.466	3.159	-18.230
450	32.447	171.144	160.557	4.764	-14.466
500	33.101	174.597	161.791	6.403	-12.103
600	34.226	180.735	164.449	9.771	-10.401
700	35.121	186.081	167.166	13.240	-9.865
800	35.832	190.819	169.832	16.789	-9.865
900	36.404	195.073	172.404	20.467	-9.865
1000	36.875	198.934	174.867	24.067	-9.865
1100	37.270	202.468	177.218	27.103	-9.865
1200	37.610	205.725	179.459	31.510	-9.865
1300	37.907	208.748	181.598	35.295	-9.865
1400	38.173	211.567	183.659	39.000	-9.865
1500	38.413	214.239	185.590	42.929	-9.865
1600	38.634	216.695	187.457	46.782	-9.865
1700	38.840	218.944	189.246	50.655	-9.865
1800	39.033	221.069	190.964	54.549	-9.865
1900	39.216	223.084	192.615	58.462	-9.865
2000	39.390	225.000	194.204	62.392	-9.865
2100	39.558	227.326	195.736	66.339	-9.865
2200	39.721	229.170	197.214	70.303	-9.865
2300	39.878	230.540	198.642	74.283	-9.865
2400	40.032	232.440	200.024	78.279	-9.865
2500	40.182	234.277	201.361	82.290	-9.865
2600	40.329	235.956	202.658	86.315	-9.865
2700	40.474	237.481	203.916	90.345	-9.865
2800	40.617	238.851	205.138	94.410	-9.865
2900	40.757	240.083	206.325	98.479	-9.865
3000	40.896	241.667	207.480	102.561	-9.865
3100	41.034	243.010	208.605	106.658	-9.865
3200	41.170	244.315	209.700	110.768	-9.865
3300	41.305	245.584	210.769	114.892	-9.865
3400	41.439	246.819	211.811	119.029	-9.865
3500	41.573	248.022	212.828	123.180	-9.865
3600	41.705	249.195	213.822	127.344	-9.865
3700	41.837	250.340	214.794	131.521	-9.865
3800	41.968	251.457	215.744	135.711	-9.865
3900	42.099	252.549	216.674	139.914	-9.865
4000	42.229	253.617	217.584	144.131	-9.865
4100	42.359	254.661	218.476	148.360	-9.865
4200	42.488	255.683	219.349	152.602	-9.865
4300	42.617	256.685	220.206	156.858	-9.865
4400	42.745	257.666	221.046	161.126	-9.865
4500	42.873	258.628	221.871	165.407	-9.865
4600	43.001	259.572	222.680	169.700	-9.865
4700	43.129	260.498	223.475	174.007	-9.865
4800	43.256	261.407	224.256	178.326	-9.865
4900	43.383	262.300	225.023	182.658	-9.865
5000	43.510	263.178	225.778	187.003	-9.865
5100	43.637	264.041	226.519	191.360	-9.865
5200	43.763	264.889	227.249	195.730	-9.865
5300	43.890	265.724	227.967	200.113	-9.865
5400	44.016	266.546	228.674	204.508	-9.865
5500	44.142	267.355	229.370	208.916	-9.865
5600	44.268	268.151	230.055	213.336	-9.865
5700	44.394	268.936	230.731	217.769	-9.865
5800	44.519	269.709	231.396	222.215	-9.865
5900	44.645	270.471	232.052	226.673	-9.865
6000	44.770	271.222	232.698	231.144	-9.865

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1977 (1 bar)

Deuterium, Ion (D<sub>2</sub><sup>+</sup>)

D<sub>2</sub>(g)

D<sub>2</sub>N<sub>1</sub>(g)

M<sub>r</sub> = 18.034904 Amidogen-D<sub>2</sub>(ND<sub>2</sub>)

IDEAL GAS

Amidogen-d<sub>2</sub> (ND<sub>2</sub>)

S<sup>0</sup>(298.15 K) = 204.291 J·K<sup>-1</sup>·mol<sup>-1</sup> Δ<sub>f</sub>H<sup>0</sup>(0 K) = 188.276 ± 8.4 kJ·mol<sup>-1</sup> Δ<sub>f</sub>H<sup>0</sup>(298.15 K) = 185.351 ± 8.4 kJ·mol<sup>-1</sup>

State	Electronic Levels (Quantum Weights) and Vibrational Frequencies (Degeneracies)	ν <sub>i</sub> , cm <sup>-1</sup>	ν <sub>j</sub> , cm <sup>-1</sup>
X <sup>2</sup> B <sub>1</sub>	0	[2305](1)	[2367](1)
X <sup>2</sup> A <sub>1</sub> (σ)	10393	[2305](1)	[2367](1)

Point Group: C<sub>2v</sub>  
 Bond Distance: N-D = 1.024 Å  
 Bond Angle: D-N-D = 103.4°  
 Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = 5.7948 × 10<sup>-119</sup> g<sup>3</sup>·cm<sup>6</sup>

Enthalpy of Formation

Δ<sub>f</sub>H<sup>0</sup>(298.15 K) of ND<sub>2</sub>(g) was calculated from the JANAF selection<sup>1</sup> for Δ<sub>f</sub>H<sup>0</sup>(298.15 K) of NH<sub>3</sub>(g), the JANAF thermal functions,<sup>1</sup> and the zero point energies of H<sub>2</sub>(g), D<sub>2</sub>(g), NH<sub>2</sub>(g), and ND<sub>2</sub>(g). The zero point energies of H<sub>2</sub>(g) and D<sub>2</sub>(g) were those given by Herzberg and Monfils.<sup>2</sup> The zero point energies of NH<sub>2</sub>(g) and ND<sub>2</sub>(g) were estimated from vibrational frequencies given by Milligan and Jacox<sup>3</sup> who observed the infrared and visible spectrum of matrix-isolated NH<sub>2</sub> and ND<sub>2</sub>.

Heat Capacity and Entropy

The bond distance and angle are from the electronic absorption spectrum of NH<sub>2</sub>, as summarized by Herzberg<sup>4</sup> The vibrational frequencies for the ground state are from Milligan and Jacox,<sup>3</sup> those for the excited state are estimated by comparison with NH<sub>2</sub>.<sup>4</sup> The National Bureau of Standards prepared this table<sup>5</sup> by critical analysis of data existing in 1972. Using S<sup>0</sup>, C<sub>p</sub><sup>0</sup> and Δ<sub>f</sub>H<sup>0</sup> selected by NBS,<sup>5</sup> we recalculate the table in terms of current JANAF reference states for the elements.

References

- <sup>1</sup>JANAF Thermochemical Tables. NH<sub>3</sub>(g), 7-31-72 (NBS)(6-30-77).
- <sup>2</sup>G Herzberg and A. Monfils, *J. Mol. Spectrosc.* **5**, 482 (1960).
- <sup>3</sup>D. E. Milligan and M. E. Jacox, *J. Chem. Phys.* **43**, 4487 (1965).
- <sup>4</sup>G. Herzberg, "Electronic Spectra of Polyatomic Molecules," D Van Nostrand Co., Inc., New York, (1966).
- <sup>5</sup>S. Abramowitz *et al.*, U. S. Nat. Bur. Stand. Report 10904, 239, (July 1972).

T/K	Enthalpy Reference Temperature = T, = 298.15 K		Standard State Pressure = P <sup>0</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>0</sup>	S <sup>0</sup> - [C <sub>p</sub> <sup>0</sup> - H <sup>0</sup> (T)]/T	H <sup>0</sup> - H <sup>0</sup> (T)	Δ <sub>f</sub> H <sup>0</sup>	
0	0	INFINITE	INFINITE	188.276	INFINITE
100	33.259	167.708	234.234	187.401	-99.193
200	33.439	190.787	207.397	186.323	-50.361
298.15	34.422	204.291	204.291	185.351	196.226
300	34.427	204.504	204.292	185.334	196.293
400	36.062	214.625	205.661	184.476	200.085
500	37.949	222.871	208.302	183.775	204.065
600	39.953	229.967	211.334	183.231	208.177
700	41.945	236.277	214.455	182.825	215.847
800	43.815	242.002	217.546	182.535	216.610
900	45.509	247.262	220.559	182.337	220.882
1000	47.007	252.136	223.476	182.210	225.173
1100	48.308	256.679	226.290	182.136	229.473
1200	49.442	260.932	229.020	182.101	233.778
1300	50.421	264.929	231.613	182.096	238.085
1400	51.279	268.697	234.129	182.112	242.391
1500	52.036	272.262	236.533	182.145	246.696
1600	52.714	275.642	238.892	182.192	250.997
1700	53.329	278.856	241.149	182.250	255.296
1800	53.898	281.921	243.329	182.319	259.591
1900	54.430	284.849	245.438	182.399	263.882
2000	54.936	287.654	247.479	182.490	268.168
2100	55.424	290.346	249.457	182.595	272.449
2200	55.902	292.936	251.375	182.713	276.725
2300	56.368	295.431	253.236	182.846	280.996
2400	56.827	297.840	255.045	182.996	285.260
2500	57.278	300.169	256.804	183.164	289.518
2600	57.722	302.424	258.515	183.351	293.768
2700	58.160	304.611	260.182	183.556	298.011
2800	58.589	306.734	261.807	183.782	302.246
2900	59.009	308.797	263.392	184.027	306.473
3000	59.417	310.804	264.939	184.292	310.690
3100	59.813	312.759	266.450	184.576	314.899
3200	60.195	314.664	267.927	184.879	319.098
3300	60.565	316.522	269.372	185.199	323.288
3400	60.919	318.335	270.785	185.537	327.467
3500	61.259	320.106	272.169	185.890	331.637
3600	61.580	321.837	273.525	186.257	335.796
3700	61.883	323.528	274.854	186.638	339.944
3800	62.169	325.182	276.156	187.029	344.082
3900	62.436	326.801	277.434	187.430	348.210
4000	62.683	328.384	278.688	187.839	352.328
4100	62.915	329.935	279.919	188.255	356.435
4200	63.128	331.454	281.128	188.675	360.531
4300	63.322	332.942	282.316	189.098	364.618
4400	63.499	334.399	283.483	189.522	368.695
4500	63.660	335.828	284.631	189.946	372.762
4600	63.803	337.229	285.759	190.369	376.821
4700	63.932	338.603	286.869	190.789	380.869
4800	64.045	339.950	287.961	191.205	384.909
4900	64.146	341.271	289.035	191.615	388.940
5000	64.233	342.568	290.093	192.020	392.964
5100	64.303	343.841	291.134	192.418	396.978
5200	64.363	345.090	292.160	192.808	400.985
5300	64.413	346.317	293.170	193.189	404.985
5400	64.451	347.521	294.166	193.562	408.978
5500	64.480	348.704	295.146	193.926	412.963
5600	64.499	349.866	296.113	194.280	416.943
5700	64.509	351.008	297.066	194.625	420.916
5800	64.509	352.130	298.006	194.959	424.883
5900	64.503	353.232	298.933	195.284	428.844
6000	64.492	354.316	299.847	195.598	432.801

PREVIOUS: June 1977 (1 atm)

CURRENT: June 1977 (1 bar)

Amidogen-D<sub>2</sub>(ND<sub>2</sub>)

D<sub>2</sub>N<sub>1</sub>(g)

Diazene-D<sub>2</sub>, Cis (N<sub>2</sub>D<sub>2</sub>)

## IDEAL GAS

M<sub>r</sub> = 32.041604

Diazene-D<sub>2</sub>, Cis (DNND)D<sub>2</sub>N<sub>2</sub>(g)

$$\Delta H_f^\circ(0 \text{ K}) = 214.039 \pm 2.1 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H_f^\circ(298.15 \text{ K}) = 224.092 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

## Vibrational Frequencies and Degeneracies

$\nu$ , cm <sup>-1</sup>	$\nu$ , cm <sup>-1</sup>
[2300](1)	[2400](1)
[1490](1)	[1150](1)
[1058](1)	[750](1)

Ground State Quantum Weight: 1

Point Group: C<sub>2v</sub>

Bond Distances: N-N = [1.230] Å; N-D = [1.014] Å

Bond Angle: D-N-N = [100]°

Product of Moments of Inertia: I<sub>AB</sub>I<sub>C</sub> = 3.8165 × 10<sup>-117</sup> g<sup>3</sup>·cm<sup>6</sup>

σ = 2

## Enthalpy of Formation

$\Delta H_f^\circ(\text{N}_2\text{D}_2, \text{g}, 298.15 \text{ K})$  was estimated from  $\Delta H_f^\circ(\text{N}_2\text{H}_2, \text{g}, 298.15 \text{ K}) = 50.9 \pm 5 \text{ kcal}\cdot\text{mol}^{-1}$ , given in the JANAF Thermochemical Tables,<sup>1</sup> the appropriate thermal functions (see tables for N<sub>2</sub>D<sub>2</sub>, H<sub>2</sub>, D<sub>2</sub>, and N<sub>2</sub>H<sub>2</sub>)<sup>1</sup> and the estimated zero point energies. The zero point energies for H<sub>2</sub>(g), D<sub>2</sub>(g) are those given by Herzberg and Monfils.<sup>2</sup> The zero point energies for N<sub>2</sub>D<sub>2</sub>(g) and N<sub>2</sub>H<sub>2</sub>(g) are taken to be one half the sum of the vibrational frequencies given above and for N<sub>2</sub>H<sub>2</sub>(g).<sup>1</sup>

## Heat Capacity and Entropy

The bond distances and angle are assumed the same as were obtained from a quantum mechanical calculation for N<sub>2</sub>H<sub>2</sub> by Wheland and Chen.<sup>3</sup> The principal moments of inertia are: I<sub>a</sub> = 0.5832, I<sub>b</sub> = 2.1780, I<sub>c</sub> = 2.7612 × 10<sup>-39</sup> g·cm<sup>2</sup>. The infrared spectrum of N<sub>2</sub>H<sub>2</sub>(g) has been observed using matrix isolation techniques by Rosengren and Pimentel;<sup>4</sup> they also observed absorptions at 1481 and 1058 cm<sup>-1</sup> attributed to trans-HNND and at 946 cm<sup>-1</sup> attributed to trans-DNND. For cis-HNND, they assigned  $\nu_1$  or  $\nu_2 = 3074 \text{ cm}^{-1}$  and  $\nu_3 = 1279 \text{ cm}^{-1}$ . Based on these observations and the vibrational frequencies adopted for N<sub>2</sub>H<sub>2</sub>(g),<sup>1</sup> the vibrational frequencies for N<sub>2</sub>D<sub>2</sub> are estimated.

The National Bureau of Standards prepared this table<sup>5</sup> by critical analysis of data existing in 1972. Using molecular constants and  $\Delta H_f^\circ$  selected by NBS,<sup>5</sup> we recalculate the table in terms of 1973 fundamental constants,<sup>6</sup> 1975 atomic weights,<sup>7</sup> and current JANAF reference states for the elements.

## References

- <sup>1</sup>JANAF Thermochemical Tables: N<sub>2</sub>H<sub>2</sub>(g), 12-31-65; H<sub>2</sub>(ref. st.), 3-31-77; N<sub>2</sub>D<sub>2</sub>(g), 6-30-77.
- <sup>2</sup>G. Herzberg and A. Monfils, *J. Mol. Spectrosc.* **5**, 482 (1960).
- <sup>3</sup>G. W. Wheland and P. S. K. Chen, *J. Chem. Phys.* **24**, 482 (1956).
- <sup>4</sup>G. Rosengren and G. Pimentel, *J. Chem. Phys.* **24**, 67 (1956).
- <sup>5</sup>S. Abramowitz *et al.*, *U. S. Nat. Bur. Stand., Report 10904*, p. 239, (July 1972).
- <sup>6</sup>CODATA Task Group on Fundamental Constants, CODATA Bulletin **11**, (December 1973).
- <sup>7</sup>IUPAC Commission on Atomic Weights, *Pure Appl. Chem.* **47**, 75 (1975), **37**, 589 (1974).

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (G <sup>o</sup> - H(T))/T	H <sup>o</sup> - H(T)	ΔH <sup>o</sup>	Standard State Pressure = P <sup>o</sup> = 0.1 MPa	log K <sub>r</sub>
0	0	INFINITE	0	INFINITE	214.039	INFINITE
100	33.278	186.132	-6.982	-10.308	220.359	-115.104
200	34.771	209.482	-3.605	-3.605	229.987	-60.066
250	36.691	217.435	-2.242	-1.821	235.310	-49.165
298.15	39.024	224.092	0	0	240.643	-42.160
300	39.119	224.333	0.072	0.072	240.851	-41.936
350	41.779	230.562	2.094	2.094	246.554	-36.796
400	44.483	236.317	4.251	4.251	252.376	-32.957
450	47.125	241.710	6.541	6.541	258.286	-29.981
500	49.652	246.807	8.961	8.961	264.260	-27.607
600	54.274	256.278	14.163	14.163	276.337	-24.057
700	58.283	264.953	19.796	19.796	288.507	-21.529
800	61.703	272.965	25.800	25.800	300.715	-19.635
900	64.591	280.404	32.119	32.119	312.977	-18.162
1000	67.018	287.339	38.703	38.703	325.323	-16.983
1100	69.056	293.825	45.509	45.509	337.793	-16.017
1200	70.750	299.900	52.513	52.513	349.430	-15.210
1300	72.140	305.633	59.654	59.654	361.537	-14.527
1400	73.240	311.030	66.939	66.939	373.597	-13.939
1500	74.483	316.134	74.336	74.336	385.626	-13.429
1600	75.375	320.970	81.830	81.830	397.618	-12.981
1700	76.143	325.563	89.407	89.407	409.575	-12.585
1800	76.808	329.935	97.056	97.056	421.498	-12.232
1900	77.386	334.103	104.766	104.766	433.389	-11.915
2000	77.891	338.086	112.530	112.530	445.248	-11.629
2100	78.335	341.897	120.342	120.342	457.078	-11.369
2200	78.726	345.550	128.195	128.195	468.879	-11.133
2300	79.073	349.058	136.086	136.086	480.654	-10.916
2400	79.381	352.430	144.009	144.009	492.402	-10.717
2500	79.656	355.676	151.961	151.961	504.127	-10.533
2600	79.903	358.805	159.939	159.939	515.877	-10.363
2700	80.125	361.825	167.941	167.941	527.506	-10.205
2800	80.326	364.742	175.963	175.963	539.165	-10.058
2900	80.507	367.564	184.005	184.005	550.800	-9.921
3000	80.672	370.296	192.064	192.064	562.418	-9.793
3100	80.822	372.944	200.139	200.139	574.018	-9.672
3200	80.959	375.512	208.228	208.228	585.600	-9.559
3300	81.084	378.006	216.331	216.331	597.166	-9.452
3400	81.199	380.428	224.445	224.445	608.716	-9.352
3500	81.305	382.783	232.570	232.570	620.250	-9.257
3600	81.402	385.075	240.706	240.706	631.771	-9.167
3700	81.492	387.307	248.850	248.850	643.278	-9.081
3800	81.576	389.481	257.004	257.004	654.772	-9.000
3900	81.653	391.601	265.165	265.165	666.254	-8.923
4000	81.724	393.669	273.334	273.334	677.725	-8.850
4100	81.791	395.688	281.510	281.510	689.184	-8.780
4200	81.853	397.660	289.692	289.692	700.633	-8.714
4300	81.911	399.586	297.880	297.880	712.072	-8.650
4400	81.965	401.470	306.074	306.074	723.502	-8.589
4500	82.016	403.313	314.273	314.273	734.923	-8.531
4600	82.064	405.116	322.477	322.477	746.336	-8.475
4700	82.108	406.881	330.686	330.686	757.742	-8.421
4800	82.150	408.610	338.899	338.899	769.139	-8.370
4900	82.189	410.305	347.116	347.116	780.530	-8.321
5000	82.227	411.965	355.336	355.336	791.914	-8.273
5100	82.262	413.594	363.561	363.561	803.292	-8.227
5200	82.295	415.192	371.789	371.789	814.665	-8.183
5300	82.326	416.760	380.020	380.020	826.032	-8.141
5400	82.356	418.299	388.254	388.254	837.394	-8.100
5500	82.384	419.810	396.491	396.491	848.751	-8.061
5600	82.410	421.295	404.731	404.731	860.104	-8.023
5700	82.435	422.755	412.973	412.973	871.457	-7.986
5800	82.459	424.186	421.218	421.218	882.810	-7.950
5900	82.482	425.597	429.463	429.463	894.166	-7.916
6000	82.504	426.984	437.714	437.714	905.438	-7.883

PREVIOUS: June 1977 (1 atm)

CURRENT: June 1977 (1 bar)

Diazene-D<sub>2</sub>, Cis (DNND)D<sub>2</sub>N<sub>2</sub>(g)



Water-d<sub>2</sub> (D<sub>2</sub>O) D<sub>2</sub>O(g)

$M_r = 20.020004$  Water-D<sub>2</sub>(D<sub>2</sub>O)

$\Delta H_f^\circ(0\text{ K}) = -246.251 \pm 0.067$  kJ·mol<sup>-1</sup>  
 $\Delta H_f^\circ(298.15\text{ K}) = -249.203 \pm 0.067$  kJ·mol<sup>-1</sup>

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>a</sup>	S° - [G° - H°(T)]/T	H° - H°(T)	Δ <sub>r</sub> H°	
0	0	INFINITE	-9.958	-246.251	INFINITE
100	33.299	161.256	-728.287	-743.148	171.128
200	33.449	184.861	-201.451	-248.222	62.649
298.15	34.255	198.339	0	-249.203	41.090
300	34.278	198.551	0.063	-249.221	40.820
400	35.635	208.591	3.577	-250.135	29.954
500	37.184	216.707	7.197	-250.954	23.411
600	38.835	223.631	10.997	-251.681	18.005
700	40.545	229.745	14.966	-252.320	13.901
800	42.251	235.271	19.106	-252.872	10.742
900	43.892	240.343	23.414	-253.346	8.170
1000	45.424	245.048	27.881	-253.744	6.127
1100	46.826	249.444	32.494	-254.078	4.632
1200	48.091	253.574	37.241	-254.354	3.026
1300	49.225	257.469	42.108	-254.581	1.714
1400	50.236	261.155	47.082	-254.767	0.643
1500	51.136	264.652	52.151	-254.917	0.000
1600	51.938	267.978	57.306	-255.038	-0.6034
1700	52.653	271.149	62.536	-255.136	-1.2549
1800	53.292	274.177	67.834	-255.214	-1.9159
1900	53.866	277.074	73.192	-255.277	-2.5866
2000	54.382	279.850	78.605	-255.328	-3.2698
2100	54.848	282.515	84.067	-255.371	-3.9170
2200	55.270	285.076	89.573	-255.407	-4.5281
2300	55.654	287.541	95.119	-255.439	-5.1038
2400	56.004	289.918	100.702	-255.470	-5.6456
2500	56.326	292.210	106.319	-255.500	-6.1548
2600	56.621	294.425	111.967	-255.531	-6.6321
2700	56.894	296.566	117.643	-255.564	-7.0781
2800	57.146	298.641	123.345	-255.601	-7.4935
2900	57.380	300.651	129.071	-255.642	-7.8797
3000	57.598	302.600	134.820	-255.688	-8.2373
3100	57.802	304.492	140.590	-255.740	-8.5678
3200	57.993	306.330	146.380	-255.799	-8.8725
3300	58.172	308.117	152.189	-255.864	-9.1541
3400	58.342	309.856	158.014	-255.937	-9.4148
3500	58.501	311.550	163.856	-256.018	-9.6577
3600	58.652	313.200	169.714	-256.107	-9.8851
3700	58.795	314.809	175.587	-256.205	-10.0991
3800	58.931	316.379	181.473	-256.312	-10.2935
3900	59.060	317.911	187.373	-256.428	-10.4705
4000	59.184	319.408	193.285	-256.554	-10.6320
4100	59.301	320.871	199.209	-256.690	-10.7798
4200	59.414	322.301	205.145	-256.837	-10.9160
4300	59.522	323.700	211.092	-256.994	-11.0435
4400	59.626	325.070	217.049	-257.165	-11.1645
4500	59.726	326.414	223.017	-257.342	-11.2800
4600	59.822	327.725	228.994	-257.522	-11.3918
4700	59.914	329.012	234.976	-257.734	-11.4999
4800	60.003	330.270	240.971	-257.947	-11.6053
4900	60.089	331.513	246.982	-258.173	-11.7088
5000	60.172	332.728	252.995	-258.409	-11.8108
5100	60.254	333.920	259.016	-258.658	-11.9113
5200	60.333	335.091	265.045	-258.918	-12.0105
5300	60.410	336.241	271.083	-259.190	-12.1085
5400	60.484	337.371	277.127	-259.473	-12.2053
5500	60.556	338.481	283.179	-259.768	-12.3010
5600	60.626	339.573	289.238	-260.075	-12.3956
5700	60.694	340.647	295.304	-260.392	-12.4893
5800	60.764	341.703	301.377	-260.721	-12.5821
5900	60.832	342.742	307.457	-261.060	-12.6741
6000	60.898	343.765	313.544	-261.410	-12.7653

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

**Water-d<sub>2</sub> (D<sub>2</sub>O)** D<sub>2</sub>O(g)

$M_r = 20.020004$  Water-D<sub>2</sub>(D<sub>2</sub>O)

$\Delta H_f^\circ(0\text{ K}) = -246.251 \pm 0.067$  kJ·mol<sup>-1</sup>  
 $\Delta H_f^\circ(298.15\text{ K}) = -249.203 \pm 0.067$  kJ·mol<sup>-1</sup>

$\sigma = 2$

Vibrational Frequencies and Degeneracies  
 $\nu$ , cm<sup>-1</sup>       $\nu$ , cm<sup>-1</sup>       $\nu$ , cm<sup>-1</sup>  
 2671.69(1)    1178.33(1)    2788.02(1)

Ground State Quantum Weight: 1  
 Point Group: C<sub>2v</sub>  
 Bond Distances: O-D = 0.958 Å  
 Bond Angle: D-O-D = 104.45°  
 Product of the Moments of Inertia:  $I_A I_B I_C = 3.9948 \times 10^{-119}$  g<sup>3</sup>·cm<sup>6</sup>

**Enthalpy of Formation**  
 Rossini *et al.*<sup>1</sup> measured the ratio of the heats of formation of D<sub>2</sub>O(l)/H<sub>2</sub>O(l). Recalculation of their results using  $\Delta H_f^\circ(298.15\text{ K})$  of H<sub>2</sub>O(l) = -68.315 ± 0.010 kcal·mol<sup>-1</sup> (refer to H<sub>2</sub>O(g) table,<sup>15</sup> yields  $\Delta H_f^\circ(298.15\text{ K})$  of D<sub>2</sub>O(l) = -2.1098 ± 0.01492 ×  $\Delta H_f^\circ(\text{HDO}(l) - \text{H}_2\text{O}(l))$ , 298.15 K] ± 0.16 kcal·mol<sup>-1</sup>. Using a value of 32 ± 30 kcal·mol<sup>-1</sup> for the reaction H<sub>2</sub>O(l) = 2 HDO(l) from<sup>1</sup> (some justification that the uncertainty may be smaller is given by Van Hook,<sup>3</sup> refer also to HDO table,<sup>15</sup> one obtains  $\Delta H_f^\circ(\text{D}_2\text{O}(l) - \text{H}_2\text{O}(l))$ , 298.15 K] = -2.094 ± 0.016 kcal·mol<sup>-1</sup>.

The difference between the heats of vaporization of D<sub>2</sub>O(l) and H<sub>2</sub>O(l) at 298.15 K were evaluated as follows. A) By direct calorimetry, Rossini *et al.*<sup>1</sup> determined the ratio of the heats of vaporization of H<sub>2</sub>O(l)/D<sub>2</sub>O(l) at 298.15 K, and zero pressure to be 0.969503 ± 0.000070. B) Bartholome and Clusius<sup>4</sup> determined the heat of vaporization of D<sub>2</sub>O(l) by direct calorimetry at 0°C. Recalculation of their results, using the energy equivalent of a Bunsen ice calorimeter given by<sup>5</sup> (compression correction assumed zero) and neglecting gas imperfection corrections, yields 12.637 ± 0.026 kcal·mol<sup>-1</sup>. The heat of vaporization of D<sub>2</sub>O(l) at 25°C was calculated using a heat of fusion of D<sub>2</sub>O(l) selected by<sup>6</sup> and,<sup>7</sup> the condensed phase data of D<sub>2</sub>O(l) given by Long and Kemp<sup>8</sup> and the gas phase thermal functions of Friedman and Haar (refer to the next section) C) The difference in heats of vaporization of D<sub>2</sub>O(l) and H<sub>2</sub>O(l) was derived by differentiating the formula given by Jones<sup>9</sup> (refer to Liu and Lindsay<sup>10</sup> for a comparison with other measurements) for the ratio of the vapor pressures of H<sub>2</sub>O(l)/D<sub>2</sub>O(l) as a function of temperature, and assuming negligible corrections for gas imperfection (refer to Kell, Laurin and Whalley,<sup>11</sup> however).

Source	Method	$\Delta_{\text{vap}}H^\circ(\text{D}_2\text{O}(l) - \text{H}_2\text{O}(l))$ , 298.15 K], kcal·mol <sup>-1</sup>
Knowlton, Johnston, Rossini	Calorimetry	0.331 ± 0.008*
Bartholome and Clusius	Calorimetry	0.340 ± 0.028*
Jones	Vapor Pressure	0.307 ± 0.020

\*Calculated from  $\Delta_{\text{vap}}H^\circ(298.15\text{ K})$  of H<sub>2</sub>O(l) = 10.520 ± 0.002 kcal·mol<sup>-1</sup>.<sup>12</sup>

Selecting 0.331 ± 0.008 kcal·mol<sup>-1</sup> for the difference in the heats of vaporization, one obtains -1.763 ± 0.018 kcal·mol<sup>-1</sup> for  $\Delta_{\text{vap}}H^\circ(298.15\text{ K})$  of D<sub>2</sub>O(g) - H<sub>2</sub>O(g). The "spectroscopic" value for this difference was calculated to be -1.768 ± 0.015 kcal·mol<sup>-1</sup> based on the zero point energies given by Hultson<sup>13</sup> for H<sub>2</sub>O(g) and D<sub>2</sub>O(g), and by Herzberg and Monfils<sup>14</sup> for H<sub>2</sub>O(g) and D<sub>2</sub>O(g), and the appropriate thermal functions (H<sub>2</sub>O(g), H<sub>2</sub>(ref. st.), D<sub>2</sub>O(g)),<sup>15</sup> To close the consistency check, the "spectroscopic" value of  $\Delta_{\text{vap}}H^\circ(298.15\text{ K})$  of D<sub>2</sub>O(g) minus HDO(g) is -0.916 ± 0.0015 kcal·mol<sup>-1</sup> and the "nonspectroscopic" value for this difference (refer to HDO table, reaction A)<sup>15</sup> is (-1.763 ± 0.0018) + (0.846 ± 0.006) = -0.917 ± 0.019 kcal·mol<sup>-1</sup>. The average value of -1.766 ± 0.016 kcal·mol<sup>-1</sup> for  $\Delta_{\text{vap}}H^\circ(298.15\text{ K})$  of D<sub>2</sub>O(g) - H<sub>2</sub>O(g) and  $\Delta_{\text{vap}}H^\circ(298.15\text{ K})$  of H<sub>2</sub>O(g) = -57.795 ± 0.010 kcal·mol<sup>-1</sup> are used to obtain  $\Delta_{\text{vap}}H^\circ(298.15\text{ K})$  for D<sub>2</sub>O(g) = -59.561 ± 0.016 kcal·mol<sup>-1</sup>.

**Heat Capacity and Entropy**  
 The thermodynamic functions of this table are analogous to those in the JANAF table for H<sub>2</sub>O(g);<sup>15</sup> both tables are taken from Friedman and Haar.<sup>16</sup> Friedman and Haar applied their non-rigid-rotor, anharmonic-oscillator treatment (with vibrational-rotational coupling terms and low-temperature rotational corrections) to the infrared-spectra analyses of Benedict *et al.*,<sup>17</sup> and of Benedict *et al.*<sup>18</sup> In the present table for D<sub>2</sub>O, the values of C<sub>p</sub> of Friedman and Haar between 4000 and 5000 K were extrapolated linearly (except with a term in T<sup>-2</sup>) from 5000 to 6000 K.

The National Bureau of Standards prepared this table<sup>19</sup> by critical analysis of data existing in 1972. Using S°(298.15 K) and C<sub>p</sub> values selected by NBS,<sup>19</sup> we recalculate the table in terms of the current JANAF reference states for the elements.<sup>15</sup>

**References**  
<sup>1</sup>F. D. Rossini, J. W. Knowlton, and H. L. Johnston, J. Res. Nat. Bur. Stand. 24, 369 (1940).  
<sup>2</sup>W. C. Duer and G. L. Bertrand, J. Chem. Phys. 53, 3020 (1970).  
 Continued on page 1048

D<sub>2</sub>S<sub>1</sub>(g)Hydrogen Sulfide-D<sub>2</sub>(D<sub>2</sub>S)

IDEAL GAS

Hydrogen Sulfide-d<sub>2</sub> (D<sub>2</sub>S)

J. Phys. Chem. Ref. Data, Monograph 9

$$\Delta_f H^\circ(298.15 \text{ K}) = 215.284 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1} \quad \Delta_f H^\circ(0 \text{ K}) = -20.997 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = -23.891 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$$

Vibrational Frequencies and Degeneracies	
$\nu$ , cm <sup>-1</sup>	$\sigma$ , cm <sup>-1</sup>
1896.38(1)	
855.45(1)	
1999 (1)	

Ground State Quantum Weight: 1  
 Point Group: C<sub>2v</sub>  
 Bond Distance: S-D = 1.328 Å  
 Bond Angle: D-S-D = 92.2°  
 Product of the Moments of Inertia:  $I_A I_B I_C = 0.3445 \times 10^{-117} \text{ g}^3 \cdot \text{cm}^6$

### Enthalpy of Formation

$\Delta_f H^\circ(\text{D}_2\text{S}, g, 298.15 \text{ K})$  was determined by Kapustinskii and Kankovskii<sup>1</sup> to be  $-5.692 \pm 0.06 \text{ kcal}\cdot\text{mol}^{-1}$  (recalculated) from the reaction: (a+b)D<sub>2</sub>S(g) + (1.5a+0.5b)O<sub>2</sub>(g) = aSO<sub>2</sub>(g) + (a+b)D<sub>2</sub>O(g) + bS(rhombic). The difference of  $\Delta_f H^\circ(\text{D}_2\text{S}, g, 298.15 \text{ K})$  minus H<sub>2</sub>S(g) for their work was calculated using their results for  $\Delta_f H^\circ(\text{H}_2\text{S}, g, 298.15 \text{ K})$ ,  $-4.92 \pm 0.08 \text{ kcal}\cdot\text{mol}^{-1}$  (recalculated), in the hope of eliminating possible systematic error due to uncertainty in the product formed.

The "spectroscopic" value of  $\Delta_f H^\circ(\text{D}_2\text{S}, g, 298.15 \text{ K})$ -H<sub>2</sub>S(g) was calculated from the appropriate thermal functions (see H<sub>2</sub>, D<sub>2</sub>, H<sub>2</sub>S)<sup>5</sup> and the zero point energies of H<sub>2</sub>S(g), D<sub>2</sub>S(g),<sup>2,3</sup> D<sub>2</sub>(g),<sup>4</sup> and H<sub>2</sub>(g).<sup>4</sup>

The equilibrium data of Grafé *et al.*<sup>5</sup> for the exchange reaction H<sub>2</sub>(g) + D<sub>2</sub>S(g) = D<sub>2</sub>(g) + H<sub>2</sub>S(g) were analyzed by third and second law methods.

Source	$\Delta_f H^\circ(298.15 \text{ K})$ of D <sub>2</sub> S(g)-H <sub>2</sub> S(g), kcal·mol <sup>-1</sup>
Kapustinskii and Kankovskii <sup>1</sup>	-0.771 ± 0.10
Spectroscopic <sup>4</sup>	-0.810 ± 0.01
Grafé, Clusius, and Kruis <sup>5</sup> Third Law	-0.826 ± 0.05
Second Law	-0.887 ± 0.02

A weighted average of  $-0.81 \pm 0.02 \text{ kcal}\cdot\text{mol}^{-1}$  was selected for  $\Delta_f H^\circ(298.15 \text{ K})$  of D<sub>2</sub>S(g) minus H<sub>2</sub>S(g) and was added to the selected value of  $\Delta_f H^\circ(298.15 \text{ K})$  of H<sub>2</sub>S(g)<sup>6</sup> to determine  $\Delta_f H^\circ(298.15 \text{ K})$  of D<sub>2</sub>.

### Heat Capacity and Entropy

The thermodynamic functions were estimated from those in the present table for H<sub>2</sub>S(g)<sup>6</sup> by adding those for D<sub>2</sub>S(g) and subtracting those for H<sub>2</sub>(g), where both the added and subtracted functions were generated using the rigid-rotor harmonic oscillator approximation. In this calculation the molecular constants for D<sub>2</sub>S were taken from Miller, Leroy and Meggers.<sup>2</sup>

The National Bureau of Standards prepared this table<sup>7</sup> by critical analysis of data existing in 1972. Using S<sup>0</sup>(298.15 K) and C<sub>p</sub> values selected by NBS,<sup>7</sup> we recalculate the table in terms of the current JANAF reference states for the elements.

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T/K	Enthalpy References		Temperature = T <sub>2</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (C <sub>p</sub> <sup>o</sup> - H(T <sub>2</sub> ))/T	H <sup>o</sup> - H(T <sub>2</sub> )	Δ <sub>f</sub> H <sup>o</sup>	Δ <sub>f</sub> G <sup>o</sup>		
0	0	INFINITE	INFINITE	-20.997	INFINITE		
100	33.263	177.971	245.585	-6.761	-26.377	15.778	
200	33.932	201.151	218.221	-3.414	-31.201	8.149	
298.15	35.761	215.284	215.284	0	-35.500	6.184	
300	35.794	215.506	215.285	0.066	-35.371	6.159	
400	37.999	226.102	216.715	3.755	-38.856	5.074	
500	40.342	234.833	219.489	7.672	-41.300	4.315	
600	42.673	242.396	222.600	11.824	-43.189	3.760	
700	44.936	249.140	225.995	16.202	-44.177	3.337	
800	46.748	255.284	229.216	20.782	-45.086	3.003	
900	48.488	260.664	232.479	25.547	-45.980	2.669	
1000	49.827	266.044	235.579	30.464	-46.946	2.139	
1100	51.028	270.850	238.570	35.508	-47.939	1.705	
1200	52.049	275.335	241.449	40.664	-48.969	1.344	
1300	52.923	279.537	244.219	45.913	-49.978	1.038	
1400	53.672	283.487	246.884	51.244	-50.801	0.776	
1500	54.321	287.212	249.451	56.644	-51.447	0.549	
1600	54.886	290.737	251.920	62.105	-51.977	0.351	
1700	55.379	294.079	254.303	67.619	-52.433	0.176	
1800	55.823	297.257	256.602	73.179	-52.821	0.021	
1900	56.208	300.286	258.822	78.781	-53.148	-0.118	
2000	56.568	303.178	260.968	84.420	-53.420	-0.243	
2100	56.881	305.946	263.045	90.093	-53.650	-0.356	
2200	57.166	308.599	265.053	95.796	-53.848	-0.458	
2300	57.430	311.146	267.004	101.525	-54.016	-0.552	
2400	57.676	313.592	268.905	107.281	-54.159	-0.638	
2500	57.902	315.953	270.750	113.060	-54.282	-0.717	
2600	58.107	318.230	272.514	118.830	-54.390	-0.790	
2700	58.300	320.426	274.248	124.681	-54.484	-0.850	
2800	58.480	322.550	275.935	130.520	-54.565	-0.920	
2900	58.647	324.605	277.578	136.377	-54.635	-0.978	
3000	58.810	326.596	279.179	142.250	-54.694	-1.032	
3100	58.965	328.527	280.740	148.138	-54.746	-1.083	
3200	59.112	330.401	282.263	154.042	-54.794	-1.131	
3300	59.245	332.222	283.749	159.960	-54.834	-1.176	
3400	59.379	333.993	285.201	165.891	-54.868	-1.218	
3500	59.509	335.716	286.620	171.836	-54.898	-1.258	
3600	59.630	337.394	288.007	177.793	-54.926	-1.296	
3700	59.748	339.029	289.264	183.762	-54.952	-1.331	
3800	59.860	340.624	290.512	189.744	-54.976	-1.364	
3900	59.975	342.181	291.922	195.714	-54.999	-1.397	
4000	60.082	343.700	293.266	201.737	-55.020	-1.428	
4100	60.187	345.185	294.515	207.750	-55.039	-1.457	
4200	60.291	346.637	295.738	213.774	-55.056	-1.485	
4300	60.392	348.057	296.939	219.808	-55.072	-1.511	
4400	60.488	349.446	298.116	225.852	-55.087	-1.536	
4500	60.588	350.807	299.272	231.906	-55.101	-1.560	
4600	60.676	352.139	300.407	237.970	-55.114	-1.584	
4700	60.768	353.445	301.522	244.042	-55.126	-1.606	
4800	60.865	354.726	302.617	250.123	-55.137	-1.627	
4900	60.953	355.982	303.693	256.214	-55.148	-1.648	
5000	61.045	357.214	304.751	262.314	-55.158	-1.667	
5100	61.124	358.424	305.792	268.423	-55.168	-1.686	
5200	61.216	359.611	306.815	274.540	-55.178	-1.705	
5300	61.300	360.778	307.822	280.665	-55.187	-1.722	
5400	61.383	361.923	308.814	286.800	-55.196	-1.739	
5500	61.467	363.052	309.790	292.942	-55.205	-1.756	
5600	61.551	364.160	310.751	299.093	-55.214	-1.772	
5700	61.634	365.250	311.697	305.252	-55.223	-1.787	
5800	61.710	366.323	312.630	311.419	-55.231	-1.802	
5900	61.798	367.379	313.549	317.595	-55.239	-1.817	
6000	61.873	368.418	314.455	323.779	-55.247	-1.831	

PREVIOUS: June 1977 (1 atm)

CURRENT: June 1977 (1 bar)

Hydrogen Sulfide-D<sub>2</sub>(D<sub>2</sub>S)D<sub>2</sub>S<sub>1</sub>(g)

Ammonia-d<sub>3</sub> (ND<sub>3</sub>)

IDEAL GAS

M<sub>r</sub> = 20.049006 Ammonia - D<sub>3</sub>(ND<sub>3</sub>)

D<sub>3</sub>N<sub>1</sub>(g)

S°(298.15 K) = 203.931 J·K<sup>-1</sup>·mol<sup>-1</sup>      Δ<sub>f</sub>H°(0 K) = -51.622 ± 0.4 kJ·mol<sup>-1</sup>  
 Δ<sub>f</sub>H°(298.15 K) = -58.576 ± 0.4 kJ·mol<sup>-1</sup>

Vibrational Frequencies and Degeneracies

2495(1)
793(1)
2652(2)
1225(2)

Ground State Quantum Weight: 1      σ(external) = 3

Point Group: C<sub>3v</sub>      σ(internal) = 2

Bond Length: N-D = 1.0124 Å

Bond Angle: 106.67°

Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = 2.5775 × 10<sup>-118</sup> g<sup>3</sup>·cm<sup>6</sup>

Enthalpy of Formation

A "spectroscopic" value for the difference in Δ<sub>f</sub>H°(298.15 K) of ND<sub>3</sub>(g) minus NH<sub>3</sub>(g) of -3.029 ± 0.01 kcal·mol<sup>-1</sup> was calculated from the appropriate thermal functions (refer to H<sub>2</sub>, D<sub>2</sub>, NH<sub>3</sub>,<sup>67</sup> zero point energies of ND<sub>3</sub>(g) and NH<sub>3</sub>(g),<sup>1</sup> and the zero point energies of H<sub>2</sub>(g) and D<sub>2</sub>(g) given by Herzberg and Montfils.<sup>1</sup>

Analysis of the equilibrium data of Schulz and Schaefer<sup>6</sup> for K<sub>2</sub> (1 atm, 660-773 K) for 1/2ND<sub>2</sub>(g) + 3/2D<sub>2</sub>(g) = ND<sub>3</sub>(g) gave the following:

third law	second law <sup>a</sup>	Δ <sub>f</sub> H°(298.15 K), kcal·mol <sup>-1</sup>	Drift	ΔS°(obsv.-calc., 298.15 K)
-13.80	-13.0 ± 0.38	-13.80	-1.2	+1.3 ± 0.5 cal·K <sup>-1</sup> ·mol <sup>-1</sup>

<sup>a</sup> Assuming ΔC<sub>p</sub>° = 1.237-0.00608(T-700) cal·K<sup>-1</sup>·mol<sup>-1</sup>

Using the results from the same authors' data for NH(g),<sup>6</sup> one obtains a difference in Δ<sub>f</sub>H°(298.15K) for ND<sub>3</sub>(g) minus NH<sub>3</sub>(g) of -2.93 ± 0.14 kcal·mol<sup>-1</sup> (third law) and -2.22 ± 0.4 kcal·mol<sup>-1</sup> (second law). The third law value agrees with the "spectroscopic" value within combined uncertainty intervals.

A value of -3.03 ± 0.1 kcal·mol<sup>-1</sup> was added to the JANAF selection for Δ<sub>f</sub>H°(298.15 K) of NH<sub>3</sub>(g), -10.97 ± 0.10 kcal·mol<sup>-1</sup>,<sup>6</sup> to obtain Δ<sub>f</sub>H°(298.15 K) of ND<sub>3</sub>(g).

Heat Capacity and Entropy

The thermodynamic functions were estimated from those in the present table for NH<sub>3</sub>(g)<sup>6</sup> by adding those for ND<sub>3</sub>(g) and subtracting those for NH<sub>3</sub>(g), where both the added and subtracted functions were generated using the rigid-rotor harmonic oscillator approximation. In this calculation the molecular constants for ND<sub>3</sub> were taken from Duncan and Mills<sup>1</sup> and Benedict and Plyler.<sup>2</sup>

The National Bureau of Standards prepared this table<sup>7</sup> by critical analysis of data existing in 1972. Using S°, C<sub>p</sub>° and Δ<sub>f</sub>H° selected by NBS,<sup>7</sup> we recalculate the table in terms of current JANAF reference states for the elements.

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T/K	Enthalpy Reference Temperature = T, = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S° - [G° - F°(T <sub>r</sub> )]/T	H° - F°(T)	Δ <sub>f</sub> H°	
0	0	INFINITE	-10.234	-51.622	INFINITE
100	33.296	166.193	-6.929	-45.604	23.821
200	34.551	189.507	-3.637	-36.317	9.485
298.15	38.225	203.931	0	-25.984	4.552
300	38.305	204.168	0.071	-25.782	4.489
400	42.924	215.622	4.133	-14.558	1.901
500	47.375	225.883	8.650	-6.739	0.307
600	51.472	234.888	13.595	-6.207	8.923
700	55.208	243.108	18.932	-63.362	20.917
800	58.589	250.704	24.625	-63.987	-1.154
900	61.601	257.782	30.638	-63.953	-2.617
1000	64.258	264.413	36.933	-63.979	-3.289
1100	66.576	270.649	43.478	-63.873	-3.292
1200	68.592	276.530	50.238	-63.660	-3.544
1300	70.346	281.991	57.187	-63.361	-3.757
1400	71.869	287.361	64.269	-62.993	-3.939
1500	73.199	292.366	71.534	-62.573	-4.093
1600	74.362	297.128	78.933	-62.107	-4.230
1700	75.379	301.667	86.421	-61.604	-4.349
1800	76.278	306.002	94.005	-61.072	-4.454
1900	77.069	310.148	101.673	-60.516	-4.547
2000	77.768	314.119	109.416	-59.942	-4.630
2100	78.387	317.928	117.224	-59.353	-4.704
2200	78.940	321.588	125.091	-58.754	-4.771
2300	79.429	325.108	133.010	-58.147	-4.831
2400	79.868	328.498	140.975	-57.535	-4.886
2500	80.257	331.766	148.982	-56.920	-4.935
2600	80.601	334.921	157.025	-56.306	-4.981
2700	80.906	337.969	165.101	-55.694	-5.023
2800	81.182	340.916	173.203	-55.087	-5.061
2900	81.416	343.769	181.240	-54.486	-5.096
3000	81.634	346.533	189.288	-53.893	-5.129
3100	81.814	349.213	197.361	-53.310	-5.159
3200	81.973	351.813	205.450	-52.739	-5.187
3300	82.107	354.337	213.559	-52.181	-5.213
3400	82.224	356.790	221.771	-51.639	-5.237
3500	82.326	359.175	230.099	-51.112	-5.259
3600	82.408	361.496	238.536	-50.604	-5.280
3700	82.466	363.754	246.980	-50.115	-5.300
3800	82.508	365.954	255.428	-49.647	-5.319
3900	82.537	368.098	263.881	-49.201	-5.336
4000	82.550	370.188	272.344	-48.779	-5.353
4100	82.548	372.226	280.816	-48.382	-5.368
4200	82.534	374.215	289.294	-48.011	-5.383
4300	82.506	376.157	297.780	-47.667	-5.397
4400	82.467	378.053	306.175	-47.352	-5.410
4500	82.414	379.906	314.583	-47.065	-5.422
4600	82.349	381.716	322.990	-46.809	-5.434
4700	82.276	383.487	331.389	-46.583	-5.445
4800	82.186	385.218	339.782	-46.389	-5.456
4900	82.082	386.912	348.174	-46.227	-5.466
5000	81.965	388.569	356.569	-46.099	-5.476
5100	81.818	390.190	364.967	-46.006	-5.486
5200	81.780	391.779	373.366	-45.942	-5.495
5300	81.746	393.336	381.764	-45.902	-5.503
5400	81.712	394.864	390.162	-45.884	-5.512
5500	81.680	396.363	398.561	-45.887	-5.520
5600	81.649	397.834	406.960	-45.911	-5.528
5700	81.619	399.279	415.359	-45.953	-5.535
5800	81.591	400.698	423.758	-46.013	-5.542
5900	81.564	402.093	432.157	-46.089	-5.549
6000	81.538	403.464	440.556	-46.180	-5.556

PREVIOUS: June 1977 (1 atm)

CURRENT: June 1977 (1 bar)

Ammonia - D<sub>3</sub>(ND<sub>3</sub>)

D<sub>3</sub>N<sub>1</sub>(g)

## Continued from page 1036

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