

Cs<sub>1</sub>(cr)

Cesium (Cs)

$$A_1 = 132.9054$$

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

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

$$\Delta_{\text{sub}}H^\circ(923 \text{ K}) = 2.087 \pm 0.004 \text{ kJ}\cdot\text{mol}^{-1}$$

$$S^\circ(298.15 \text{ K}) = 85.147 \pm 0.21 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_{\text{fus}} = 301.55 \pm 0.01 \text{ K}$$

**Enthalpy of Formation**

Zero by definition.

**Heat Capacity and Entropy**

The low temperature heat capacities, 0.19–301.55 K, have been measured by Dauphinee,<sup>1</sup> McCollum,<sup>2</sup> Martin,<sup>3</sup> Lien,<sup>4</sup> Filby,<sup>5</sup> and Morgan.<sup>6</sup> The adopted values are derived based on the  $C_p$  data reported by Filby<sup>5</sup> and Lien.<sup>4</sup> Lien measured the heat capacities in the temperature range 0.1874 to 1.20 K in the adiabatic demagnetization cryostat and at higher temperatures, 1.2 to 4.09 K, in the liquid-helium temperature cryostat. The Cs sample was obtained from a commercial source of 99.8 per cent purity. Filby determined the  $C_p$  values in the temperature ranges 0.4–1.5 K, 3–26 K and 20–320 K, using commercial samples of 99.9 per cent purity. These two sets of measurements are joined smoothly at 4 K.  $S^\circ(298.15 \text{ K})$  is derived from the adopted heat capacities, based on  $S^\circ(0.20 \text{ K}) = 0.0002 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ . Dauphinee<sup>1</sup> determined the heat capacities of Cs(cr) employing a sample badly contaminated with oxygen. In the temperature range of approximately 100 to 200 K, an anomaly of  $C_p$  curve somewhat similar to those found for sodium and potassium was reported. This anomaly was not observed by Filby who used the higher purity cesium sample. The  $C_p$  values reported by Dauphinee are lower than the adopted ones by about 0.5 to 1.5 per cent in the temperatures 55 to 220 K; above 270 K his reported heat capacities are unreasonably high. Therefore the data are not adopted for evaluation. McCollum<sup>2</sup> calculated the Debye  $\theta$  values from the measured low temperature heat capacities and plotted them, since no numerical data were reported these were not used. The low temperature  $C_p$  values determined by Martin<sup>3</sup> and Morgan<sup>6</sup> are in good agreement with the adopted ones.

**Fusion Data**

Refer to the liquid table for details.

**Sublimation Data**

$$\Delta_{\text{sub}}H^\circ(298.15 \text{ K})$$
 is calculated as the difference between  $\Delta H_f^\circ(298.15 \text{ K})$  for Cs(g) and Cs(cr).
**References**

- <sup>1</sup>T. M. Dauphinee, D. L. Martin and H. Preston-Thomas, Proc. Roy. Soc. (London) A233, 214 (1955);  $C_p$  (20–320 K).
- <sup>2</sup>D. C. McCollum, Jr. and H. B. Silsbee, Phys. Rev. 127, 119 (1962);  $C_p$  (1.3–12 K).
- <sup>3</sup>B. D. Martin, D. A. Zych and C. V. Heer, Phys. Rev. 135, A671 (1964);  $C_p$  (0.36–1.63 K).
- <sup>4</sup>W. H. Lien and N. E. Phillips, Phys. Rev. 133, A1370 (1964);  $C_p$  (0.19–4.09 K).
- <sup>5</sup>J. D. Filby and D. L. Martin, Proc. Roy. Soc. (London) A284, 83 (1965);  $C_p$  (0.7–320 K).
- <sup>6</sup>J. A. Morgan and J. C. Thompson, J. Chem. Phys. 47, 4607 (1967);  $C_p$  (2.1–4.2 K).

T/K	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$		log $K_f$
	$C_p^\circ$	$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	
0	0	0	0	0	0
100	25.812	54.952	-7.717	0	0
200	27.804	71.453	-5.568	0	0
250	29.201	79.784	-2.888	0	0
298.15	32.195	85.147	-1.468	0	0
301.550	32.501	85.149	0.060	0	0
350	34.840	90.550	1.749	-2.005	0.331
400	36.066	95.290	3.574	-1.815	0.653
450	36.777	99.582	5.347	-1.563	0.946
500	37.196	103.480	7.197	-1.274	1.210
600	37.530	110.295	10.935	-0.643	1.648
700	37.614	116.087	14.693	0.018	1.978
800	37.635	121.111	18.455	0.687	2.212
900	37.656	125.545	22.270	1.358	2.363
1000	37.656	129.513	25.986	-65.103	6.138

PREVIOUS:

CURRENT: June 1968

Cesium (Cs)

Cs<sub>1</sub>(cr)

Cesium (Cs)

$S^\circ(298.15\text{ K}) = [92.069] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}} = 301.55 \pm 0.01 \text{ K}$

Enthalpy of Formation

$\Delta_f H^\circ(\text{Cs, l}, 298.15 \text{ K})$  is calculated from that of the crystal by adding the enthalpy of fusion and the difference in enthalpy,  $H^\circ(301.55 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and liquid.

Heat Capacity and Entropy

The enthalpies of Cs(l) have been measured by Tepper *et al.*,<sup>1</sup> Achener,<sup>2</sup> and Lemmon *et al.*,<sup>3</sup> using drop calorimetry. Lemmon *et al.* used a cesium sample of 99.994 per cent purity and encapsulated in Nb-12r alloy. They found that Cs(l) does not behave as a normal liquid from about 100–300°C. The thermal conductivity measurements of Cs(l) show a change of slope at about 200°C and its electrical resistivity also shows scatter in this region. The heat capacities, 301.55–1435.2 K, derived from the reported enthalpies (corrected for vapor condensation), are consistent with the low temperature heat capacity data on Cs(cr) at 298.15 K, and are adopted.

Tepper *et al.* measured the enthalpies in the temperature range 351.1–1238 K. The reported enthalpy values are considerably higher, over 20 per cent, at the lower end of the measured temperature range than the adopted ones. However, the agreement becomes better at the higher temperature end. Achener determined the enthalpies of Cs(l) at the temperatures 340.1–1175.7 K. Using the reported enthalpies, the average heat capacity is derived to be 9.75 kcal·mol<sup>-1</sup>, which is unreasonably high by comparison with those for the other alkali metals. The above two sets of data are not used for evaluation. The enthalpies of Cs(l), 773–1423 K, were also measured by Shapiro,<sup>4</sup> and quoted by<sup>5</sup> The derived constant heat capacity, 7.60 cal·mol<sup>-1</sup>, is in reasonable agreement with the adopted ones.

Heat capacities of Cs(l), 301.55–373.2 K, were reported by Filby,<sup>5</sup> 301.55–320 K, Dauphinee,<sup>6</sup> 310–320 K, and Rengade,<sup>7</sup> 301.7–373.2 K.

The values obtained are consistent with the adopted ones.

$S^\circ(298.15 \text{ K})$  is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

The melting point and enthalpy of melting have been determined by many investigators. The results reported are presented in the table below. The adopted  $T_{\text{fus}}$  and  $\Delta_{\text{fus}} H^\circ$  are obtained from.<sup>5</sup> The two determinations of fraction melted against temperature are in very good agreement with one another and lead to a linear plot of reciprocal fraction melted against temperature thus indicating that the major impurity is solid insoluble. This is confirmed by a graph of excess heat capacity against the reciprocal of  $(T_0 - T)^2$ , where  $T_0$  is the melting point, which indicates an impurity (mainly oxygen) concentration of 0.06 atomic per cent.

$T_{\text{fus}}/\text{K}$	$\Delta_{\text{fus}} H^\circ/\text{kcal}\cdot\text{mol}^{-1}$	References
299.52	0.496	M. Eckardt and E. Graefe, <i>Z. Anorg. Chem.</i> <b>23</b> , 378 (1900)
301.35	—	A. Guntz and W. Broniewski, <i>J. Chim. Phys.</i> <b>7</b> , 474 (1909).
301.60 ± 0.05	0.500	E. Rengade <sup>7</sup>
301.75	—	J. H. Boer, J. Broos and H. Emmens, <i>Z. Anorg. Chem.</i> <b>191</b> , 118 (1930).
301.45	—	E. Rinck, <i>Compt. Rend.</i> <b>199</b> , 1217 (1934).
301.95 ± 0.1	—	L. Losana, <i>Gazz. Chim. Ital.</i> <b>65</b> , 855 (1935).
301.75	—	J. B. Taylor and J. Langmuir, <i>Phys. Rev.</i> <b>51</b> , 759 (1937).
301.79 ± 0.17	—	K. Clusius and H. Stern, <i>Z. Angew. Physik</i> <b>6</b> , 194 (1954).
—	0.510	W. D. Weatherford, Jr., <i>et al.</i> , WADD Tech. Rept. 61–96, November 1961.
301.67	0.470	A. W. Lemmon <i>et al.</i> <sup>3</sup>
301.55 ± 0.01	0.499 ± 0.01	J. D. Filby and D. L. Martin. <sup>5</sup>

Vaporization Data

$T_{\text{vap}}$  is the temperature at which the Gibbs energy change for the reaction Cs(l) = Cs(g) is zero. The differences between  $\Delta_f H^\circ(\text{Cs, g})$  and  $\Delta_f H^\circ(\text{Cs, l})$  at  $T_{\text{vap}}$  is  $\Delta_{\text{vap}} H^\circ$ . Due to the presence of dimer (Cs<sub>2</sub>) in the vapor, the boiling point (1 atm) of Cs(l) is calculated to be 941.3 K at which the vapor mixture contains 0.835 mol of monomer/mol of Cs(l) vaporized, or 9.0 per cent of dimer. The corresponding enthalpy of vaporization is evaluated as 15.26 kcal·mol<sup>-1</sup> of vapor mixture.

References

1. F. Tepper, A. Murchison, J. Zeleznak, and F. Roehlich, Thermophysical Properties of Rubidium and Cesium, RTD-TDR-63-4018, Part I, MSA Research Corporation, Callery, Pennsylvania, (November 1963).
2. Y. Achener, The Determination of the Latent Heat of Vaporization, Vapor Pressure, Enthalpy, Specific Heat, and Density of Liquid Rubidium and Cesium up to 1800 F, AGRN-8090, Aerojet-General Nuclronics, (January 1964).
3. A. W. Lemmon, Jr., H. W. Deem, E. A. Eldridge, E. H. Hall, J. Matolich, Jr., and J. F. Walling, The Specific Heat, Thermal Conductivity, and Viscosity of Liquid Cesium, BATT-4673-T7, Battelle Memorial Institute, (February 1964).
4. A. Shapiro and C. J. Meisl, General electric Company, Flight Propulsion Laboratory Department Report No. R60FFD358-A, (November 9, 1960).
5. J. D. Filby and D. L. Martin, Proc. Roy. Soc. (London) **A284**, 83 (1965).
6. T. M. Dauphinee, D. L. Martin, and H. Preston-Thomas, Proc. Roy. Soc. (London) **A233**, 214 (1955).
7. E. Rengade, Compt. Rend. **156**, 1897 (1913); Bull. Soc. Chim. France **15**, 130 (1914).

Cesium (Cs)

Cs(l)

$T/\text{K}$	$C_p^\circ$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$			Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$		
		$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	—	—	—	—	—	—	—
100	—	—	—	—	—	—	—
200	—	—	—	—	—	—	—
250	—	—	—	—	—	—	—
298.15	32.439	92.069	0.060	2.087	0.024	-0.004	
300	32.413	92.269	0.060	2.087	0.011	-0.002	
301.550	32.393	92.071	0.110	—	—	—	LIQUID
350	31.898	97.225	1.667	0.	0.	0.	
400	31.518	101.458	3.252	0.	0.	0.	
450	31.310	105.158	4.822	0.	0.	0.	
500	31.154	108.448	6.384	0.	0.	0.	
600	30.999	114.113	9.491	0.	0.	0.	
700	30.941	118.887	12.587	0.	0.	0.	
800	30.932	123.017	15.681	0.	0.	0.	
900	30.957	126.662	18.775	0.	0.	0.	
947.967	30.976	128.270	20.260	—	—	—	FUGACITY = 1 bar
1000	30.999	129.926	21.873	-67.129	3.699	-0.193	
1100	31.054	132.883	24.975	-66.105	10.733	-0.510	
1200	31.116	135.587	28.084	-65.075	17.673	-0.769	
1300	31.188	138.081	31.199	-64.040	24.526	-0.985	
1400	31.263	140.395	34.321	-62.998	31.300	-1.168	
1500	31.342	142.554	37.452	-61.950	37.999	-1.323	

PREVIOUS

CURRENT June 1968

Cesium (Cs)

Cs(l)

CRYSTAL-LIQUID

0 to 301.55 K crystal  
above 301.55 K liquid

Refer to the individual tables for details.

Cesium (Cs)

Cs<sub>1</sub>(cr,l)

T/K	C <sub>p</sub> <sup>o</sup>	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>
		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> )	Δ <sub>r</sub> H <sup>o</sup>	Δ <sub>r</sub> G <sup>o</sup>	
0	0	0	INFINITE	-7.717	0	0
100	25.812	54.952	10.635	-5.588	0	0
200	77.804	75.453	87.892	-2.888	0	0
250	29.201	79.784	85.856	-1.468	0	0
298.15	32.195	85.147	85.147	0	0	0
300	32.355	85.347	85.148	0.060	0	0
301.550	32.501	85.514	85.149	0.110	0	0
301.550	32.593	92.856	85.149	2.197	0	0
350	31.898	97.225	86.498	3.754	0	0
400	31.518	101.458	88.110	5.339	0	0
450	31.310	105.158	89.803	6.910	0	0
500	31.154	108.448	91.506	8.471	0	0
600	30.999	114.113	94.817	11.578	0	0
700	30.941	118.887	97.923	14.674	0	0
800	30.932	123.017	100.808	17.768	0	0
900	30.957	126.662	103.482	20.862	0	0
947.967	30.976	128.270	104.696	22.348	0	0
1000	30.999	129.926	105.966	23.960	-67.129	-0.193
1100	31.054	132.883	108.280	27.062	-66.105	-0.510
1200	31.116	135.587	110.445	30.171	-65.075	-0.769
1300	31.188	138.081	112.476	33.286	-64.040	-0.985
1400	31.263	140.395	114.389	36.409	-62.998	-1.168
1500	31.342	142.554	116.195	39.539	-61.950	-1.323

PREVIOUS

CURRENT June 1968

Cesium (Cs)

Cs<sub>1</sub>(cr,l)

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

A<sub>r</sub> = 132.9054 Cesium (Cs)

IDEAL GAS

Cesium (Cs)

IP(Cs, g) = 31406.432 ± 0.010 cm<sup>-1</sup>  
 S°(298.15 K) = 175.599 ± 0.025 J·K<sup>-1</sup>·mol<sup>-1</sup>

ΔH°(298.15 K) = 78.0 ± 1.0 kJ·mol<sup>-1</sup>  
 ΔH<sub>f</sub>°(298.15 K) = 76.5 ± 1.0 kJ·mol<sup>-1</sup>

Electronic Levels and Quantum Weights	g <sub>i</sub>
State	
5s <sub>1/2</sub>	2
5p <sub>1/2</sub>	2
5p <sub>3/2</sub>	4
5s <sub>1/2</sub>	2
5p <sub>3/2</sub>	4
IP	31406.432

Enthalpy of Formation

The enthalpy of formation of cesium gas is chosen to be the value recommended by CODATA.<sup>1</sup> This value was obtained from 2nd and 3rd law treatments of vapor pressure data. The reported vapor pressure were corrected for the effects of Cs(g), using D<sub>0</sub><sup>0</sup> = 38.02 kJ·mol<sup>-1</sup>. At higher pressures an alternate virial treatment was employed. As stated by CODATA,<sup>1</sup> the selected value is the weighted average of the 3rd law values of Δ<sub>sub</sub>H<sup>0</sup>(298.15 K) from the following:

Source	Δ <sub>sub</sub> H <sup>0</sup> (298.15 K), kJ·mol <sup>-1</sup>
Taylor and Langmuir <sup>2</sup>	76.71 ± 0.64
Bonilla <i>et al.</i> <sup>3</sup>	76.20 ± 1.28
Achener <sup>4</sup>	76.66 ± 1.05
Tepper <i>et al.</i> <sup>5</sup>	78.08 ± 1.08
Bohdansky and Schins <sup>6</sup>	76.10 ± 0.95
Stone <i>et al.</i> <sup>7</sup>	76.52 ± 1.08
Buck and Pauly <sup>8</sup>	76.77 ± 0.75
Shipil'rain and Belova <sup>9</sup>	76.62 ± 1.06
Volyak <i>et al.</i> <sup>10</sup>	76.48 ± 0.77
Novikov and Rosupkin <sup>11</sup>	76.57 ± 1.19
Ewing <i>et al.</i> <sup>12</sup>	76.44 ± 1.48
Shipil'rain <i>et al.</i> <sup>13</sup>	76.50 ± 1.12
Schins <i>et al.</i> <sup>14</sup>	76.34 ± 0.90
Shipil'rain and Nikanorov <sup>15</sup>	76.46 ± 1.21
Behrens <i>et al.</i> <sup>16</sup>	77.22 ± 1.15

The 2nd law calculations from the above sources led to values somewhat more positive<sup>1</sup>

Heat Capacity and Entropy

The thermal functions for the five alkali metal monatomic gases are calculated by the same procedure. Observed and estimated atomic energy levels are included in the partition function calculation, using an ionization potential lowering (IP-KT) technique as the cutoff procedure in the energy level summation.<sup>19</sup>

The lowest lying levels for these metals [14904 cm<sup>-1</sup> (Li), 16956 cm<sup>-1</sup> (Na), 12578 cm<sup>-1</sup> (K), 12578 cm<sup>-1</sup> (Cs)] do not contribute to the thermal functions below ~1000 K; there is only a translational contribution below this temperature. Above this approximate temperature, the thermal functions become increasingly sensitive to the partition function cutoff procedure used, due to the combined effect of the observation of atomic energy levels of high principal quantum number and a low ionization potential. Energy levels have been observed up to n = 42 (Li), 59 (Na), 79 (K), 77 (Rb), and 73 (Cs). However, not all predicted levels have been observed for each of these principal quantum numbers. The ionization potentials vary from 43487.29 cm<sup>-1</sup> for Li to 31406.1 cm<sup>-1</sup> for Cs. In calculating the thermal functions with the inclusion of missing levels up to the high principal quantum numbers just mentioned, the Gibbs energy functions show significant differences (depending on the cutoff procedure) above 3000 K.<sup>17</sup>

The atomic energy levels have been taken from the compilation of Moore.<sup>18,19</sup> Our calculated values for the thermal functions are similar to those recommended by CODATA.<sup>1</sup> They do differ for two reasons, however. First, the entropy differs by 0.1094 J·K<sup>-1</sup>·mol<sup>-1</sup> because this table uses a reference pressure of 1 bar, whereas the CODATA recommendations are based on 1 atm. Second, the entropies at 298.15 K for all alkali metal gases differs by ~0.004 J·K<sup>-1</sup>·mol<sup>-1</sup>, presumably due to the use of slightly different values for auxiliary data.

References

<sup>1</sup>J. D. Cox, Chairman, CODATA Task Group on Key Values for Thermodynamics, CODATA Special Report No. 8, (1980).

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T/K	C <sub>p</sub> <sup>o</sup>	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>
		S <sup>o</sup> - (G <sup>o</sup> - HF(T)) / T	H <sup>o</sup> - H(T <sub>r</sub> )	ΔG <sup>o</sup>	Δ <sub>sub</sub> H <sup>o</sup>	
0	0	INFINITE	0	78.019	INFINITE	
100	20.786	152.892	-6.197	78.019	78.019	
200	20.786	167.300	-4.119	77.950	68.156	
250	20.786	171.938	-2.040	77.348	58.578	
298.15	20.786	175.599	0	76.500	53.979	
300	20.786	175.599	0.038	76.479	49.532	
350	20.786	178.932	1.078	73.823	45.216	
400	20.786	181.708	2.117	72.178	41.178	
450	20.786	184.156	3.156	72.747	37.316	
500	20.786	186.346	4.196	72.225	33.276	
600	20.786	190.136	6.274	71.196	25.583	
700	20.786	193.340	8.353	70.178	18.061	
800	20.786	196.115	10.431	69.164	10.685	
900	20.786	198.564	12.510	68.148	3.436	
947.967	20.786	199.643	13.507	67.132	0	
1000	20.786	200.754	14.589	66.116	0	
1100	20.788	202.735	16.667	65.100	0	
1200	20.791	204.544	18.746	64.083	0	
1300	20.799	206.208	20.826	63.066	0	
1400	20.814	207.750	22.906	62.049	0	
1500	20.841	209.187	24.989	61.032	0	
1600	20.886	210.533	27.075	60.015	0	
1700	20.952	211.802	29.167	59.000	0	
1800	21.048	213.002	31.267	58.000	0	
1900	21.178	214.143	33.378	57.000	0	
2000	21.349	215.233	35.504	56.000	0	
2100	21.564	216.280	37.649	55.000	0	
2200	21.830	217.289	39.818	54.000	0	
2300	22.150	218.256	42.017	53.000	0	
2400	22.527	219.217	44.250	52.000	0	
2500	22.960	220.145	46.523	51.000	0	
2600	23.456	221.055	48.844	50.000	0	
2700	24.016	221.950	51.217	49.000	0	
2800	24.639	222.835	53.649	48.000	0	
2900	25.326	223.711	56.146	47.000	0	
3000	26.082	224.582	58.716	46.000	0	
3100	26.905	225.451	61.365	45.000	0	
3200	27.796	226.319	64.099	44.000	0	
3300	28.599	227.175	66.885	43.000	0	
3400	29.572	228.043	69.793	42.000	0	
3500	30.600	228.915	72.801	41.000	0	
3600	31.680	229.792	75.914	40.000	0	
3700	32.770	230.671	79.125	39.000	0	
3800	33.902	231.557	82.447	38.000	0	
3900	35.096	232.447	85.875	37.000	0	
4000	36.250	233.349	89.439	36.000	0	
4100	37.488	234.259	93.126	35.000	0	
4200	38.744	235.178	96.938	34.000	0	
4300	40.010	236.104	100.875	33.000	0	
4400	40.717	236.985	104.847	32.000	0	
4500	40.901	237.756	108.229	31.000	0	
4600	41.940	238.667	112.371	30.000	0	
4700	42.950	239.580	116.616	29.000	0	
4800	44.024	240.494	120.960	28.000	0	
4900	44.859	241.409	125.399	27.000	0	
5000	45.748	242.325	129.930	26.000	0	
5100	46.588	243.239	134.547	25.000	0	
5200	46.722	244.034	138.714	24.000	0	
5300	47.407	244.931	143.421	23.000	0	
5400	47.729	245.763	147.915	22.000	0	
5500	48.117	246.611	152.560	21.000	0	
5600	48.599	247.483	157.396	20.000	0	
5700	49.022	248.347	162.278	19.000	0	
5800	49.385	249.203	167.199	18.000	0	
5900	49.689	250.049	172.153	17.000	0	
6000	49.935	250.887	177.133	16.000	0	

PREVIOUS: June 1968 (1 atm)

CURRENT: December 1983 (1 bar)

Cesium (Cs)

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

## IDEAL GAS

Cesium, Ion (Cs<sup>+</sup>)Cesium, Ion (Cs<sup>+</sup>)Cs<sup>+</sup>(g)

IP(Cs<sup>+</sup>, g) = 202263 ± 2 cm<sup>-1</sup>  
 $S^{\circ}(298.15 \text{ K}) = 169.836 \pm 0.005 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$

$\Delta H^{\circ}(0 \text{ K}) = 453.72 \pm 2.1 \text{ kJ} \cdot \text{mol}^{-1}$   
 $\Delta H^{\circ}(298.15 \text{ K}) = [458.402] \text{ kJ} \cdot \text{mol}^{-1}$

Electronic Level and Quantum State	Weight
$S_0$	1

## Enthalpy of Formation

$\Delta H^{\circ}(\text{Cs}^+, \text{g}, 0 \text{ K})$  is calculated from  $\Delta H^{\circ}(\text{Cs}, \text{g}, 0 \text{ K})$  using the spectroscopic value of IP(Cs) = 31406.432 ± 0.010 cm<sup>-1</sup> (375.704 ± 0.001 kJ·mol<sup>-1</sup>) from Moore.<sup>2</sup> The ionization limit is converted from cm<sup>-1</sup> to kJ·mol<sup>-1</sup> using the factor, 1 cm<sup>-1</sup> = 0.01196266 kJ·mol<sup>-1</sup>, 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.

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

## Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Moore,<sup>6</sup> is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels and cutting off the summation in the partition function<sup>7</sup> has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of all levels other than the ground state; the first excited state is approximately 107392 cm<sup>-1</sup> above the ground state. Since inclusion of these excited states has no effect on the thermodynamic functions (to 6000 K), we list only the ground state. The reported uncertainty in  $S^{\circ}(298.15 \text{ K})$  is due to uncertainties in the relative ionic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the excited states and use of different fill and cutoff procedures.<sup>7</sup>

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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)	ΔH <sup>o</sup>	ΔG <sup>o</sup>	log K <sub>r</sub>
0	0	INFINITE	0	453.724		
100	20.786	1.47129	-188.317	-6.197	426.897	-74.791
200	20.786	1.61537	-171.738	-4.119	426.701	-74.295
250	20.786	1.66175	-170.178	-2.040	421.714	-62.937
298.15	20.786	1.69836	-169.836	0	416.667	-54.411
300	20.786	1.69965	-169.837	0.038	415.558	-47.772
350	20.786	1.73169	-170.090	1.078	406.392	-42.456
400	20.786	1.75945	-170.652	2.117	395.908	-34.467
450	20.786	1.78393	-171.379	3.156	385.247	-28.277
500	20.786	1.80583	-172.192	4.196	374.433	-24.448
600	20.786	1.84373	-173.915	6.274	363.486	-21.096
700	20.786	1.87577	-175.644	8.353	356.121	-18.602
800	20.786	1.90352	-177.313	10.431	351.983	-16.714
900	20.786	1.92801	-178.900	12.510	347.636	-15.133
1000	20.786	1.94991	-180.402	14.589	343.156	-13.788
1100	20.786	1.96972	-181.820	16.667	338.496	-12.629
1200	20.786	1.98780	-183.159	18.746	333.687	-11.620
1300	20.786	2.00444	-184.425	20.824	328.741	-10.732
1400	20.786	2.01985	-185.625	22.903	323.664	-9.945
1500	20.786	2.03419	-186.764	24.982	318.467	-9.242
1600	20.786	2.04760	-187.847	27.060	313.156	-8.609
1700	20.786	2.06020	-188.880	29.139	307.736	-8.037
1800	20.786	2.07208	-189.865	31.217	302.216	-7.517
1900	20.786	2.08332	-190.808	33.296	296.601	-7.042
2000	20.786	2.09398	-191.711	35.375	290.896	-6.606
2100	20.786	2.10413	-192.578	37.453	285.106	-6.205
2200	20.786	2.11379	-193.410	39.532	279.237	-5.834
2300	20.786	2.12300	-194.212	41.610	273.293	-5.491
2400	20.786	2.13188	-194.984	43.689	267.280	-5.171
2500	20.786	2.14037	-195.730	45.768	261.202	-4.873
2600	20.786	2.14852	-196.449	47.846	255.063	-4.594
2700	20.786	2.15636	-197.146	49.925	248.868	-4.333
2800	20.786	2.16392	-197.820	52.004	242.622	-4.088
2900	20.786	2.17122	-198.473	54.082	236.328	-3.858
3000	20.786	2.17826	-199.106	56.161	229.983	-3.640
3100	20.786	2.18508	-199.721	58.239	223.611	-3.435
3200	20.786	2.19168	-200.319	60.318	217.198	-3.242
3300	20.786	2.19807	-200.899	62.397	210.755	-3.058
3400	20.786	2.20428	-201.465	64.475	204.282	-2.884
3500	20.786	2.21031	-202.015	66.554	197.785	-2.719
3600	20.786	2.21616	-202.552	68.632	191.267	-2.562
3700	20.786	2.22186	-203.075	70.711	184.734	-2.412
3800	20.786	2.22740	-203.585	72.790	178.187	-2.270
3900	20.786	2.23280	-204.083	74.868	171.631	-2.134
4000	20.786	2.23806	-204.569	76.947	165.067	-2.005
4100	20.786	2.24319	-205.045	79.025	158.467	-1.881
4200	20.786	2.24820	-205.510	81.104	151.826	-1.762
4300	20.786	2.25309	-205.965	83.183	145.236	-1.649
4400	20.786	2.25787	-206.410	85.261	138.647	-1.541
4500	20.786	2.26254	-206.846	87.340	132.061	-1.437
4600	20.786	2.26711	-207.272	89.418	125.480	-1.338
4700	20.786	2.27158	-207.691	91.497	118.905	-1.242
4800	20.786	2.27596	-208.101	93.576	112.339	-1.151
4900	20.786	2.28024	-208.503	95.654	105.765	-1.062
5000	20.786	2.28444	-208.898	97.733	99.147	-0.977
5100	20.786	2.28856	-209.283	99.811	92.558	-0.895
5200	20.786	2.29260	-209.665	101.890	85.992	-0.817
5300	20.786	2.29656	-210.039	103.969	79.460	-0.741
5400	20.786	2.30044	-210.406	106.047	72.940	-0.668
5500	20.786	2.30426	-210.766	108.126	66.433	-0.598
5600	20.786	2.30800	-211.121	110.204	59.940	-0.531
5700	20.786	2.31168	-211.469	112.283	53.461	-0.465
5800	20.786	2.31529	-211.812	114.362		
5900	20.786	2.31885	-212.149	116.440		
6000	20.786	2.32234	-212.481	118.519		

PREVIOUS December 1970 (1 atm)

CURRENT, December 1983 (1 bar)

Cesium, Ion (Cs<sup>+</sup>)Cs<sup>+</sup>(g)

Cs<sup>-</sup>(g)

M<sub>r</sub> = 132.90595 Cesium, Ion (Cs<sup>-</sup>)

IDEAL GAS

Cesium, Ion (Cs<sup>-</sup>)

EA(Cs, g) = 0.471630 ± 0.000025 eV  
 S<sup>o</sup>(298.15 K) = 169.836 ± 0.005 J·K<sup>-1</sup>·mol<sup>-1</sup>

Δ<sub>f</sub>H<sup>o</sup>(0 K) = 32.51 ± 0.5 kJ·mol<sup>-1</sup>  
 Δ<sub>f</sub>H<sup>o</sup>(298.15 K) = [24.798] kJ·mol<sup>-1</sup>

Electronic Level and Quantum State	Weight
<sup>1</sup> S <sub>0</sub>	1

**Enthalpy of Formation**

The enthalpy of formation, at 0 K, for Cs<sup>-</sup>(g) is calculated from the adopted electron affinity, EA(Cs, g) = 0.471630 ± 0.000025 eV, (45.505 ± 0.002 kJ·mol<sup>-1</sup>). This value, recommended by Hotoop and Lineberger,<sup>1</sup> was measured by a tunable laser photodetachment threshold technique.<sup>4,5</sup> Additional discussion on Cs<sup>-</sup>(g) may be obtained in the critical discussions of Hotoop and Lineberger,<sup>1,7</sup> Rosenstock *et al.*,<sup>2</sup> and Massey.<sup>3</sup>

Δ<sub>f</sub>H<sup>o</sup>(Cs<sup>-</sup>, g, 298.15 K) is obtained from Δ<sub>f</sub>H<sup>o</sup>(Cs, g, 0 K) by using EA(Cs, g) with JANAF<sup>6</sup> enthalpies, H<sup>o</sup>(0 K) - H<sup>o</sup>(298.15 K), for Cs<sup>-</sup>(g), Cs(g), and e<sup>-</sup>(ref). Δ<sub>f</sub>H<sup>o</sup>(Cs<sup>-</sup>, g) → Cs + 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>2</sup> Δ<sub>f</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 ion convention which excludes the enthalpy of the electron.

**Heat Capacity and Entropy**

The ground state configuration for Cs<sup>-</sup>(g) is given by Hotoop and Lineberger,<sup>1,7</sup> and Rosenstock *et al.*<sup>2</sup> Lacking any experimental evidence as to the stability of any excited states, we assume that no stable excited states exist.

**References**

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T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [G <sup>o</sup> - HF(T)]/T	H <sup>o</sup> - H <sup>o</sup> (T)	Δ <sub>f</sub> H <sup>o</sup>	Standard State Pressure = P <sup>o</sup> = 0.1 MPa	log K <sub>f</sub>
0	0	INFINITE	-6.197	32.514		-1.017
100	20.786	147.129	-4.119		5.802	-0.990
200	20.786	161.537	-2.040		5.685	-0.444
250	20.786	166.175	-1.001		2.972	-0.065
298.15	20.786	169.836	0		1.777	0.206
300	20.786	169.965	0.038	24.798	-3.878	0.405
350	20.786	173.169	1.078	24.738		
400	20.786	175.945	2.117	21.043		
450	20.786	178.393	3.156	19.438		
500	20.786	180.583	4.196	17.888		
600	20.786	184.373	6.274	13.220		
700	20.786	187.577	8.353	10.123		
800	20.786	190.352	10.431	7.030		
900	20.786	192.801	12.510	3.935		
1000	20.786	194.991	14.589	-66.291		
1100	20.786	196.972	16.672	-68.370		
1200	20.786	198.780	18.746	-70.449		
1300	20.786	200.444	20.824	-72.528		
1400	20.786	201.985	22.903	-74.609		
1500	20.786	203.419	24.982	-76.691		
1600	20.786	204.760	27.060	-78.777		
1700	20.786	206.020	29.139	-80.869		
1800	20.786	207.208	31.217	-82.969		
1900	20.786	208.332	33.296	-85.080		
2000	20.786	209.399	35.375	-87.206		
2100	20.786	210.413	37.453	-89.351		
2200	20.786	211.380	39.532	-91.520		
2300	20.786	212.304	41.610	-93.719		
2400	20.786	213.188	43.689	-95.952		
2500	20.786	214.037	45.768	-98.226		
2600	20.786	214.852	47.846	-100.546		
2700	20.786	215.636	49.925	-102.919		
2800	20.786	216.392	52.004	-105.351		
2900	20.786	217.122	54.082	-107.848		
3000	20.786	217.826	56.161	-110.418		
3100	20.786	218.508	58.239	-113.067		
3200	20.786	219.168	60.318	-115.801		
3300	20.786	219.808	62.397	-118.587		
3400	20.786	220.428	64.475	-121.495		
3500	20.786	221.031	66.554	-124.503		
3600	20.786	221.616	68.632	-127.617		
3700	20.786	222.186	70.711	-130.828		
3800	20.786	222.740	72.790	-134.151		
3900	20.786	223.280	74.868	-137.578		
4000	20.786	223.806	76.947	-141.142		
4100	20.786	224.319	79.025	-144.828		
4200	20.786	224.820	81.104	-148.640		
4300	20.786	225.309	83.183	-152.578		
4400	20.786	225.787	85.261	-156.649		
4500	20.786	226.254	87.340	-160.846		
4600	20.786	226.711	89.418	-165.163		
4700	20.786	227.158	91.497	-169.607		
4800	20.786	227.596	93.576	-174.178		
4900	20.786	228.025	95.654	-178.876		
5000	20.786	228.445	97.733	-183.693		
5100	20.786	228.856	99.811	-188.629		
5200	20.786	229.260	101.890	-193.686		
5300	20.786	229.656	103.969	-198.864		
5400	20.786	230.044	106.047	-204.164		
5500	20.786	230.426	108.126	-209.596		
5600	20.786	230.800	110.204	-215.163		
5700	20.786	231.168	112.283	-220.867		
5800	20.786	231.530	114.362	-226.709		
5900	20.786	231.885	116.440	-232.689		
6000	20.786	232.234	118.519	-238.807		

PREVIOUS:

CURRENT: December 1983 (1 bar)

Cesium, Ion (Cs<sup>-</sup>)

Cs<sup>-</sup>(g)

## CRYSTAL

## Cesium Fluoride (CsF)

 $M_r = 151.903803$ 

## Cesium Fluoride (CsF)

Cs<sub>2</sub>F<sub>2</sub>(cr)

$S^\circ(298.15 \text{ K}) = [88.3 \pm 8] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$   
 $T_{\text{fus}} = 976 \text{ K}$   
 $\Delta H_f^\circ(0 \text{ K}) = \text{Unknown}$   
 $\Delta H_f^\circ(298.15 \text{ K}) = -554.7 \pm 2 \text{ kJ} \cdot \text{mol}^{-1}$   
 $\Delta_{\text{sub}}H_f^\circ = 21.7 \text{ kJ} \cdot \text{mol}^{-1}$

## Enthalpy of Formation

The enthalpy of solution ( $\Delta_{\text{sol}}H_f^\circ$ ) of CsF(cr) in water at 298.15 K has been carefully determined with an adiabatic calorimeter by Somsen.<sup>1</sup> Based on the reported value,  $\Delta_{\text{sol}}H_f^\circ(298.15 \text{ K}) = -8.62 \pm 0.04 \text{ kcal} \cdot \text{mol}^{-1}$  and  $\Delta H_f^\circ(298.15 \text{ K}) = -61.69^\circ$  and  $-79.5 \text{ kcal} \cdot \text{mol}^{-1}$  for Cs<sup>+</sup>(aq) and F<sup>-</sup>(aq,  $\infty$ ), respectively, the enthalpy of formation for CsF(cr) is calculated to be  $-132.57 \text{ kcal} \cdot \text{mol}^{-1}$  which is adopted. The value,  $\Delta_{\text{sub}}H_f^\circ(298.15 \text{ K}) = -8.81 \pm 0.2 \text{ kcal} \cdot \text{mol}^{-1}$  for CsF(cr), was reported by Parker<sup>2</sup> which is in agreement with the value measured by Somsen.<sup>1</sup>

## Heat Capacity and Entropy

The heat capacities of CsF(cr) are estimated according to the method of Kristov,<sup>3</sup> based on  $H^\circ(976 \text{ K}) - H^\circ(298.15 \text{ K}) = 9.4 \text{ kcal} \cdot \text{mol}^{-1}$  reported by Dworkin.<sup>4</sup> The entropy,  $S^\circ(298.15 \text{ K})$ , is estimated such that the calculated and observed vapor pressures are in good agreement (refer to CsF(g) and Cs<sub>2</sub>F<sub>2</sub>(g) tables for details).

## Fusion Data

$T_{\text{fus}}$  and  $\Delta_{\text{sub}}H_f^\circ$  are obtained from Bredig<sup>5</sup> and Dworkin.<sup>6</sup> Buhalova<sup>7</sup> reported  $T_{\text{fus}} = 958 \text{ K}$ , which is not adopted.

## Sublimation Data

$\Delta_{\text{sub}}H_f^\circ(298.15 \text{ K})$  is calculated as the difference between  $\Delta H_f^\circ(298.15 \text{ K})$  for CsF(g) and CsF(cr).

## References

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T/K	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$		log $K_r$
	$C_p^\circ$	$S^\circ - (G^\circ - H^\circ(T_r))/T_r$	$H^\circ - H^\circ(T_r)$	$\Delta_r H_f^\circ$	
0					
100					
200					
298.15	51.965	88.282	0.	-554.673	92.044
300	52.007	88.604	0.096	-554.665	91.445
400	53.764	103.805	5.384	-556.266	67.221
500	55.564	115.996	10.851	-555.615	52.700
600	57.363	126.286	16.497	-554.811	43.032
700	59.120	135.260	22.322	-553.860	36.138
800	60.877	143.269	28.321	-552.758	30.976
900	62.634	150.541	34.497	-551.504	26.970
976.000	63.952	155.672	39.308	-- CRYSTAL --> LIQUID	--
1000	64.350	157.231	40.848	-617.224	23.580
1100	65.856	163.438	47.362	-614.649	20.655
1200	66.944	169.217	54.004	-611.958	18.228
1300	67.697	174.607	60.739	-609.188	16.183
1400	68.157	179.642	67.533	-606.370	14.439
1500	68.492	184.356	74.366	-603.525	12.934
1600	68.743	188.785	81.228	-600.663	11.623
1700	68.910	192.958	88.112	-597.794	10.473
1800	68.994	196.899	95.007	-594.928	9.455
1900	69.036	200.631	101.909	-592.073	8.548
2000	69.036	204.172	108.813	-589.236	7.736

PREVIOUS:

CURRENT: June 1968

## Cesium Fluoride (CsF)

Cs<sub>2</sub>F<sub>2</sub>(cr)

Cs<sub>3</sub>F<sub>3</sub>(l)

M<sub>r</sub> = 151.903803 Cesium Fluoride (CsF)

LIQUID

Cesium Fluoride (CsF)

S°(298.15 K) = [90.099] J·K<sup>-1</sup>·mol<sup>-1</sup>  
 T<sub>m</sub> = 976 K  
 $\Delta_f H^\circ(298.15 \text{ K}) = [-543.849] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{vap}} H^\circ = 21.7 \text{ kJ}\cdot\text{mol}^{-1}$

**Enthalpy of Formation**  
 $\Delta_f H^\circ(\text{CsF}, l, 298.15 \text{ K})$  is calculated from  $\Delta_f H^\circ(\text{CsF}, \text{cr}, 298.15 \text{ K})$  by adding  $\Delta_{\text{melt}} H^\circ$  and the difference enthalpy,  $H^\circ(976 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and liquid.

**Heat Capacity and Entropy**  
 Dworkin<sup>1</sup> measured the heat capacity of CsF(l) at the melting point to be 17.7 cal·K<sup>-1</sup>·mol<sup>-1</sup>, which is adopted and assumed to be constant in the temperature range 298–3000 K.  
 The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

**Fusion Data**  
 Refer to the crystal table for details.

**Vaporization Data**  
 T<sub>vap</sub> = 1504 K is the temperature at which the calculated vapor pressures of CsF(g) and Cs<sub>3</sub>F<sub>3</sub>(g) equal one atmosphere. The vapor composition at T<sub>vap</sub> is calculated as CsF 80.3% and Cs<sub>3</sub>F<sub>3</sub> 19.7%. The enthalpy required to vaporize one mole of liquid to the above vapor mixture at T<sub>m</sub> is  $\Delta_{\text{vap}} H^\circ$ .  
 T<sub>vap</sub> has been observed as 1524 and 1526 K by Wartenberg<sup>1</sup> and Ruff,<sup>2</sup> respectively, which are in fair agreement with the calculated one, 1504 K.

**References**  
<sup>1</sup>H. von Wartenberg and H. Schulz, Z. Elektrochem. 22, 568 F(1921).  
<sup>2</sup>O. Ruff, G. Schmidt and S. Muggdan, Z. anorg. allgem. Chem. 123, 83 (1922).

T/K	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> H°	Δ <sub>f</sub> G°	log K <sub>r</sub>
0							
100	74.057	90.099	90.099	0.	-543.849	-515.094	90.242
200	74.057	90.557	90.101	0.137	-543.801	-514.916	89.655
298.15	74.057	111.862	93.005	7.543	-543.284	-504.999	65.946
300	74.057	128.387	98.491	14.948	-540.693	-495.728	51.788
600	74.057	141.890	104.633	22.354	-538.131	-486.976	42.395
700	74.057	153.305	110.792	29.760	-535.598	-478.651	35.717
800	74.057	163.194	116.738	37.165	-533.090	-470.687	30.733
900	74.057	171.917	122.394	44.571	-530.606	-463.036	26.874
976.000	74.057	177.921	126.487	50.199	---	---	---
1000	74.057	179.720	127.743	51.977	---	---	---
1100	74.057	186.778	132.794	59.382	-595.271	-451.961	23.608
1200	74.057	193.222	137.565	66.788	-591.804	-437.798	20.789
1300	74.057	199.150	142.077	74.194	-588.351	-423.950	18.454
1400	74.057	204.638	146.352	81.599	-584.909	-410.390	16.490
1500	74.057	209.747	150.410	89.005	-581.479	-397.094	14.816
1600	74.057	214.577	154.270	96.411	-578.062	-384.043	13.374
1700	74.057	219.016	157.948	103.817	-574.656	-371.230	12.119
1800	74.057	223.243	161.459	111.222	-571.265	-358.699	11.019
1900	74.057	227.253	164.818	118.628	-567.897	-346.497	10.046
2000	74.057	231.052	168.035	126.034	-564.530	-334.573	9.182
2100	74.057	234.665	171.123	133.439	-561.191	-322.924	8.408
2200	74.057	238.110	174.090	140.845	-557.874	-310.043	7.712
2300	74.057	241.402	176.945	148.251	-554.583	-298.319	7.083
2400	74.057	244.554	179.697	155.656	-551.320	-286.743	6.512
2500	74.057	247.577	182.352	163.062	-548.089	-275.310	5.992
2600	74.057	250.482	184.917	170.468	-544.894	-264.010	5.516
2700	74.057	253.277	187.398	177.873	-541.740	-252.837	5.080
2800	74.057	255.970	189.799	185.279	-538.630	-241.784	4.678
2900	74.057	258.569	192.126	192.685	-535.570	-230.846	4.306
3000	74.057	261.079	194.383	200.090	-532.565	-220.016	3.963
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PREVIOUS: Cs<sub>3</sub>F<sub>3</sub>(l)

CURRENT: June 1968

Cs<sub>3</sub>F<sub>3</sub>(l)

Cesium Fluoride (CsF)



Cesium Fluoride (CsF)

Cesium Fluoride (CsF)

Cs<sub>3</sub>F<sub>4</sub>(cr,l)

0 to 976 K crystal  
above 976 K liquid

Refer to the individual tables for details.

T/K	C <sub>p</sub> <sup>o</sup>	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>
		J·K <sup>-1</sup> ·mol <sup>-1</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> )	Δ <sub>r</sub> H <sup>o</sup>	
0				0		
100				0.096	-554.673	92.044
200				5.384	-554.665	91.445
298.15	51.965	88.282	88.282	10.831	-514.238	67.211
300	52.007	88.604	88.283	10.831	-556.266	52.700
400	53.764	103.805	90.344		-504.434	
500	55.564	115.996	94.294			
600	57.363	126.286	98.790			
700	59.120	135.260	103.372			
800	60.877	143.269	107.867			
900	62.634	150.541	112.211			
976.000	63.952	155.672	115.397			
976.000	74.057	171.921	115.397	61.023		
1000	74.057	179.720	116.920	62.800	-595.272	23.608
1100	74.057	186.778	122.955	70.206	-591.805	20.789
1200	74.057	193.222	128.546	77.611	-588.351	18.454
1300	74.057	199.150	133.752	85.017	-584.910	16.490
1400	74.057	204.638	138.622	92.423	-581.480	14.816
1500	74.057	209.747	143.195	99.828	-578.062	13.374
1600	74.057	214.577	147.505	107.234	-574.657	12.119
1700	74.057	219.016	151.581	114.640	-571.266	11.019
1800	74.057	223.249	155.446	122.045	-567.890	10.046
1900	74.057	227.253	159.121	129.451	-564.531	9.182
2000	74.057	231.052	162.624	136.857	-561.192	8.408
2100	74.057	234.665	165.969	144.262	-557.875	7.712
2200	74.057	238.110	169.170	151.668	-554.583	7.083
2300	74.057	241.402	172.240	159.074	-551.320	6.512
2400	74.057	244.554	175.188	166.479	-548.090	5.992
2500	74.057	247.577	178.023	173.885	-544.895	5.516
2600	74.057	250.482	180.755	181.291	-541.740	5.080
2700	74.057	253.277	183.389	188.697	-538.631	4.678
2800	74.057	255.970	185.933	196.102	-535.571	4.306
2900	74.057	258.569	188.394	203.508	-532.566	3.963
3000	74.057	261.079	190.775	210.914	-529.620	3.644

PREVIOUS.

CURRENT June 1968

Cesium Fluoride (CsF)

Cs<sub>3</sub>F<sub>4</sub>(cr,l)

Cesium Fluoride (CsF)

Cesium Fluoride (CsF)

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

S°(298.15 K) = 243.21 ± 0.04 J·K<sup>-1</sup>·mol<sup>-1</sup> ΔH<sub>f</sub>°(0 K) = -354.0 ± 2 kJ·mol<sup>-1</sup> ΔH<sub>f</sub>°(298.15 K) = -356.5 ± 2 kJ·mol<sup>-1</sup>

Electronic Level and Quantum State	Weight g <sub>i</sub>
1Σ <sup>+</sup>	0
ω <sub>e</sub> = 353 ± 4 cm <sup>-1</sup>	
B <sub>e</sub> = 0.18437 cm <sup>-1</sup>	
ω <sub>e</sub> x <sub>e</sub> = 1.23 cm <sup>-1</sup>	
α <sub>e</sub> = 0.001105 cm <sup>-1</sup>	
σ = 1	
r <sub>e</sub> = 2.345 Å	

Enthalpy of Formation

The vapor pressures of CsF(cr) and CsF(l) were measured by the manometric method by Wartenberg,<sup>1</sup> Russ,<sup>2</sup> and Cantor,<sup>3</sup> the torsion-fiber effusion method by Pugh<sup>4</sup> and the Knudsen effusion method by Scheer.<sup>5</sup> Based on the reported total pressures, the corresponding partial pressures of CsF(g) and CsF<sub>2</sub>(g) were evaluated using the adjusted enthalpies of vaporization and Gibbs energy functions such that the calculated and observed total pressures are in reasonable agreement, and the derived enthalpy changes by the 2nd and 3rd law methods are consistent. The results obtained are presented in the table below. The value of ΔH<sub>f</sub>°(CsF, g, 298.15 K) is adopted as -82.5 ± 0.5 kcal·mol<sup>-1</sup>.

The dissociation energy (D<sub>0</sub>) of CsF(g) has been reported using the spectroscopic convergence limit as 5.65 eV (130.3 kcal·mol<sup>-1</sup>) and 5.5 eV (126.8 kcal·mol<sup>-1</sup>) by Herzberg<sup>6</sup> and Gaydon,<sup>9</sup> respectively. Based on the above two D<sub>0</sub> and ΔH<sub>f</sub>°(0 K) = 18.68 and 18.36 for Cs(g) and F(g), we obtain the corresponding value for ΔH<sub>f</sub>°(CsF, g, 298.15 K) as -93.86 and -90.39 kcal·mol<sup>-1</sup>, which are not adopted.

Source	Reaction*	Method	ΔH°(298.15 K), kcal·mol <sup>-1</sup>	Drift	ΔH°(298.15 K), kcal·mol <sup>-1</sup>
1	B	Manometric	45.39 ± 0.15	-0.28 ± 0.10	-85.00
2	B	Manometric	44.78 ± 1.70	0.11 ± 1.18	-85.04
3	B	Manometric	44.83	0.05 ± 0.04	-85.09
4	A	Torsion fibre	48.52 ± 0.03	-1.18 ± 0.04	-85.00
5	A	Knudsen	48.43 ± 0.27	-2.35 ± 0.35	-85.96

Reactions: (A) CsF(cr) = CsF(g) (B) CsF(l) = CsF(g)

Heat Capacity and Entropy

The ground state configuration was reported by Herzberg.<sup>6</sup> The molecular constants are obtained from Honig *et al.*,<sup>7</sup> who observed the microwave spectra of CsF(g) at temperatures of about 700°C. Based on the J = 1 → 2 transition, the molecular constants are derived. The vibrational frequency (ω<sub>e</sub>) has been reported, from different kinds of spectra, in the range 270–385 cm<sup>-1</sup> by many investigators, e.g. radiofrequency, infrared, ultraviolet, microwave, etc. The value of ω<sub>e</sub> adopted was reported by Baikov and Vasilievskii,<sup>8</sup> who also reviewed the ω<sub>e</sub> values obtained by the earlier investigators.

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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° - (C <sub>p</sub> <sup>o</sup> - RT)/T	H° - H°(T <sub>r</sub> )	ΔH <sub>f</sub> <sup>o</sup>	
0	0	0	INFINITE	-353.988	INFINITE
100	30.506	206.799	273.829	-361.319	188.734
200	34.207	229.206	246.449	-355.543	96.015
250	35.207	236.954	243.800	-355.977	71.433
298.15	35.838	243.213	243.213	0	65.413
300	35.857	243.435	243.214	0.066	65.028
350	36.298	248.998	244.632	1.871	56.104
400	36.611	253.866	244.631	3.694	39.174
450	36.842	258.192	245.902	5.531	24.574
500	37.019	262.083	247.529	7.377	9.988
600	37.276	268.857	250.639	11.093	33.695
700	37.456	274.617	253.432	14.830	29.186
800	37.598	279.628	256.400	18.583	25.794
900	37.707	284.063	259.232	22.348	23.147
1000	37.805	288.041	261.917	26.124	20.829
1100	37.891	291.648	264.459	29.909	18.757
1200	37.971	294.949	266.864	33.702	17.052
1300	38.046	297.991	269.143	37.502	15.598
1400	38.117	300.813	271.305	41.311	14.352
1500	38.185	303.445	273.361	45.126	13.271
1600	38.251	305.912	275.319	48.948	12.325
1700	38.316	308.233	277.188	52.776	11.507
1800	38.379	310.424	278.974	56.611	10.777
1900	38.441	312.501	280.684	60.452	10.133
2000	38.502	314.474	282.325	64.299	9.484
2100	38.555	316.355	283.901	68.152	8.942
2200	38.623	318.150	285.417	72.012	8.449
2300	38.683	319.868	286.878	75.877	7.999
2400	38.742	321.516	288.287	79.748	7.586
2500	38.801	323.098	289.648	83.625	7.206
2600	38.860	324.621	290.964	87.508	6.855
2700	38.919	326.089	292.238	91.397	6.529
2800	38.977	327.505	293.473	95.292	6.226
2900	39.035	328.874	294.670	99.193	5.944
3000	39.093	330.199	295.832	103.099	5.681
3100	39.151	331.481	296.962	107.011	5.434
3200	39.209	332.723	298.060	110.929	5.202
3300	39.267	333.933	299.129	114.853	4.978
3400	39.324	335.106	300.170	118.783	4.774
3500	39.381	336.246	301.184	122.718	4.584
3600	39.439	337.357	302.174	126.659	4.400
3700	39.496	338.438	303.139	130.606	4.226
3800	39.553	339.492	304.082	134.558	4.061
3900	39.611	340.520	305.003	138.516	3.903
4000	39.668	341.524	305.904	142.480	3.753
4100	39.725	342.504	306.785	146.450	3.610
4200	39.782	343.462	307.646	150.425	3.473
4300	39.839	344.399	308.490	154.406	3.343
4400	39.896	345.313	309.317	158.393	3.218
4500	39.953	346.213	310.127	162.385	3.098
4600	40.010	347.091	310.921	166.384	2.983
4700	40.067	347.952	311.700	170.388	2.872
4800	40.124	348.796	312.464	174.397	2.765
4900	40.181	349.624	313.214	178.412	2.663
5000	40.238	350.437	313.950	182.433	2.564
5100	40.295	351.234	314.673	186.460	2.468
5200	40.352	352.017	315.384	190.492	2.377
5300	40.408	352.786	316.082	194.530	2.287
5400	40.465	353.542	316.769	198.574	2.201
5500	40.522	354.285	317.445	202.623	2.118
5600	40.579	355.016	318.109	206.678	2.037
5700	40.636	355.733	318.763	210.739	1.959
5800	40.692	356.442	319.406	214.805	1.883
5900	40.749	357.138	320.040	218.878	1.809
6000	40.806	357.823	320.664	222.955	1.737

PREVIOUS: June 1968 (1 atm)

CURRENT: June 1968 (1 bar)

Cesium Fluoride (CsF)

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

Cs<sub>2</sub>H<sub>3</sub>O<sub>4</sub>(cr)

Cesium Hydroxide (CsOH)

M<sub>r</sub> = 149.91274

CRYSTAL(α-β-γ)

Cesium Hydroxide (CsOH)

$S^{\circ}(298.15\text{ K}) = 98.7 \pm 4.2\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{m}}(\alpha\text{-}\beta) = 410 \pm 1\text{ K}$   
 $T_{\text{m}}(\beta\text{-}\gamma) = 493 \pm 1\text{ K}$   
 $T_{\text{m}} = 588 \pm 1\text{ K}$

#### Enthalpy of Formation

The enthalpy of formation of CsOH(cr) is obtained from the enthalpy of hydrolysis of metallic cesium, the enthalpy of solution of the hydroxide in water, and appropriate auxiliary data.

Beketov<sup>1</sup> and de Forcrand<sup>2</sup> determined the enthalpy of solution of crystalline CsOH in water. Parker<sup>3</sup> analyzed these data and selected  $\Delta_{\text{sol}}H^{\circ}(\text{CsOH, cr}) = -17.1 \pm 0.2\text{ kcal}\cdot\text{mol}^{-1}$ . This value is adopted here.

Discordant values for the enthalpy of hydrolysis of metallic cesium have been reported by Vorob'yev *et al.*<sup>4</sup> and Gunn.<sup>5</sup> For the reaction  $\text{Cs}(\text{cr}) + (n+1)\text{H}_2\text{O}(\text{l}) = \text{CsOH}\cdot n\text{H}_2\text{O} + 0.5\text{H}_2(\text{g})$ , they reported enthalpies of hydrolysis of  $-46.5 \pm 0.20$  ( $n = 1030$ ) and  $-48.346 \pm 0.20$  ( $n = 3000$ ) kcal·mol<sup>-1</sup>, respectively. From these values  $\Delta_{\text{f}}H^{\circ}(\text{CsOH}\cdot n\text{H}_2\text{O, 298.15 K}) = -114.82 \pm 0.20$  and  $-116.661 \pm 0.020\text{ kcal}\cdot\text{mol}^{-1}$  are calculated based on  $\Delta_{\text{f}}H^{\circ}(\text{H}_2\text{O, l, 298.15 K}) = -68.315\text{ kcal}\cdot\text{mol}^{-1}$ .

In both investigations the possibility of hydroxide and oxide contamination of the metal samples was reduced by repeated distillation of the metal under vacuum, and spectroscopic analysis of each sample indicated low concentrations of the lighter alkali metals. Vorob'yev *et al.*<sup>4</sup> determined the amount of reaction by both weighing the metal sample and titrating the final hydroxide solution. Gunn<sup>5</sup> determined the amount of reaction by both weighing the sample and recovering the hydrogen formed in the hydrolysis. The systematically high hydrogen yields (0.05–0.16%) obtained by Gunn<sup>5</sup> suggest the presence of lighter alkali metals in higher concentrations than indicated by the spectroscopic analysis of the cesium, and the flame–photometric analyses of the final hydroxide solutions. However, the presence of lighter alkali metals at these concentrations should not introduce any serious error in the enthalpy of hydrolysis, since their heats<sup>6</sup> are quite similar to cesium.

The major difference between the two measurements lies in the instrumentation used to investigate the reaction. Vorob'yev *et al.*<sup>4</sup> used a hermetically sealed static calorimeter which was not stirred. In the absence of proper agitation, temperature gradients and chemical inhomogeneities are likely to arise in the final state. Without any indication of the performance of this calorimeter, the results of Vorob'yev *et al.*<sup>4</sup> are questionable. On the other hand, Gunn [5] carried out the hydrolysis reaction in a closed bomb calorimeter, agitation being effected by rocking the assembly through an angle of approximately 150°.<sup>7</sup> Where comparisons are possible, all indications are that the results are quite reliable. Therefore, we adopt  $\Delta_{\text{f}}H^{\circ}(\text{CsOH}\cdot n\text{H}_2\text{O, 298.15 K}) = -116.661 \pm 0.020\text{ kcal}\cdot\text{mol}^{-1}$  from the work of Gunn.<sup>5</sup> Combining this result with the enthalpy of solution of CsOH(cr) given above, we derive  $\Delta_{\text{f}}H^{\circ}(\text{CsOH, cr, 298.15 K}) = -99.6 \pm 0.2\text{ kcal}\cdot\text{mol}^{-1}$  ( $-416.73 \pm 0.8\text{ kJ}\cdot\text{mol}^{-1}$ ).

#### Heat Capacity and Entropy

Heat capacities for CsOH(cr) over the entire temperature range 298–1000 K are estimated by comparison with similar data for the other alkali metal hydroxides and halides.<sup>8</sup> Likewise,  $S^{\circ}(298.15\text{ K})$  is estimated to be  $23.6\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  ( $98.7\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ ) for CsOH(cr) by comparison with similar data for the alkali metal halides and lighter hydroxides.<sup>9</sup>

#### Transition and Fusion Data

The temperatures and enthalpies of the polymorphic transitions and melting of CsOH(cr) are from the work of Reshetnikov and Baranskaya.<sup>10</sup> These data were determined thermographically with  $\Delta_{\text{m}}H = 1.575\text{ kcal}\cdot\text{mol}^{-1}$  for NaOH(cr) as a standard.

#### Sublimation Data

$\Delta_{\text{sub}}H^{\circ}(298.15\text{ K})$  for the monomer and dimer are calculated from the adopted enthalpies of formation of the crystal and the respective gaseous species.

#### References

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T/K	Enthalpy Reference		Temperature = T, = 298.15 K		Standard State Pressure = P° = 0.1 MPa	
	C <sub>p</sub> <sup>o</sup>	S°	-(G°-H°(T))/T	H°-H°(T)	Δ <sub>f</sub> H°	log K <sub>r</sub>
0						
200						
298.15	67.872	98.742	98.742	0	-416.726	64.948
300	67.990	99.163	98.744	0.126	-416.714	64.498
400	74.392	119.617	101.489	7.251	-417.807	46.287
410.000	74.990	121.461	101.954	7.998	ALPHA <--> BETA	
410.000	75.278	124.625	101.954	9.295	TRANSITION	
493.000	82.174	139.114	107.010	15.827	BETA <--> GAMMA	
493.000	83.680	151.420	107.010	21.894	TRANSITION	
500	83.680	152.600	107.640	22.480	-408.701	35.433
588.000	83.680	166.166	115.411	29.844	-- GAMMA <--> LIQUID	
600	83.680	167.856	116.443	30.848	-406.484	28.335
700	83.680	180.729	124.733	39.216	-404.309	23.292
800	83.680	191.929	132.450	47.584	-402.179	19.531
900	83.680	201.786	139.617	55.952	-400.095	16.620
1000	83.680	210.602	146.282	64.320	-465.187	14.111

PREVIOUS.

CURRENT: June 1971

Cesium Hydroxide (CsOH)

Cs<sub>2</sub>H<sub>3</sub>O<sub>4</sub>(cr)

Cs<sub>2</sub>H<sub>3</sub>O<sub>4</sub>(l)

M<sub>r</sub> = 149.91274 Cesium Hydroxide (CsOH)

LIQUID

Cesium Hydroxide (CsOH)

S°(298.15 K) = [118.513] J·K<sup>-1</sup>·mol<sup>-1</sup>  
T<sub>ref</sub> = 588 ± 1 K

Δ<sub>liq</sub>H°(298.15 K) = [-405.970] kJ·mol<sup>-1</sup>  
Δ<sub>liq</sub>H° = 4.56 ± 0.4 kJ·mol<sup>-1</sup>

**Enthalpy of Formation**

Δ<sub>f</sub>H°(CsOH, l, 298.15 K) is calculated from that of the crystal by adding Δ<sub>liq</sub>H° and the difference enthalpy, H°(588 K) - H°(298.15 K), between the crystal and liquid.

**Heat Capacity and Entropy**

C<sub>p</sub>° for liquid CsOH is estimated to be 19.5 cal·K<sup>-1</sup>·mol<sup>-1</sup> by comparison with similar data for the other liquid alkali metal hydroxides [1]. It is assumed constant in the temperature range 298–2000 K.

S°(298.15 K) is calculated in a manner analogous to that used for the enthalpy of formation.

**Fusion Data**

Refer to the crystal table for details.

**Vaporization Data**

T<sub>ref</sub> is calculated as the temperature at which Δ<sub>v</sub>G° for the vaporization process is zero. The difference in the enthalpy of formation of CsOH(l) and CsOH(g) at the boiling point is the heat of vaporization.

**Reference**

<sup>1</sup>JANAF Thermochemical Tables: refer to all alkali metal hydroxide liquid tables.

Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa			
T/K	C <sub>p</sub> ° J·K <sup>-1</sup> ·mol <sup>-1</sup>	S° - [G° - H°(T <sub>r</sub> )]/T J·K <sup>-1</sup> ·mol <sup>-1</sup>	H° - H°(T <sub>r</sub> ) kJ·mol <sup>-1</sup>	Δ <sub>f</sub> H° kJ·mol <sup>-1</sup>	log K <sub>r</sub>
0					
100	81.588	118.513	0.000	-405.970	64.096
200	81.588	119.017	0.151	-405.933	63.658
298.15	81.588	121.715	8.510	-405.992	63.658
300	81.588	122.758	16.469	-398.472	45.929
400	81.588	133.704	23.648	---	35.560
500	81.588	141.309	24.627	---	---
588.000	81.588	147.860	32.786	---	---
600	81.588	148.660	40.945	---	---
700	81.588	154.091	49.104	---	---
800	81.588	159.985	57.263	---	---
900	81.588	165.549	65.421	---	---
1000	81.588	170.806	73.580	---	---
1100	81.588	175.777	81.739	---	---
1200	81.588	180.487	89.898	---	---
1300	81.588	184.957	98.057	---	---
1400	81.588	189.209	106.215	---	---
1500	81.588	193.261	114.374	---	---
1600	81.588	197.130	122.533	---	---
1700	81.588	200.830	130.692	---	---
1800	81.588	204.374	138.851	---	---
1900	81.588	207.851	147.010	---	---
2000	81.588	211.247	155.169	---	---

PREVIOUS:

CURRENT: June 1971

Cesium Hydroxide (CsOH)

Cs<sub>2</sub>H<sub>3</sub>O<sub>4</sub>(l)

Cesium Hydroxide (CsOH)

CRYSTAL ( $\alpha$ - $\beta$ - $\gamma$ )-LIQUID

$M_r = 149.91274$

Cesium Hydroxide (CsOH)

$Cs_2H_3O_4(cr,l)$

0 to 410 K crystal, alpha  
 410 to 493 K crystal, beta  
 493 to 588 K crystal, gamma  
 above 588 K liquid

Refer to the individual tables for details.

T/K	C <sub>p</sub> <sup>a</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
		S° - [C <sub>p</sub> - H(T <sub>r</sub> )]/T	H° - H(T <sub>r</sub> )	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0						
100						
200						
298.15	67.872	98.742	98.742	0	-416.726	-370.716
300	67.990	99.163	98.744	0.126	-416.714	-370.431
400	74.392	119.617	101.489	7.251	-417.807	-354.453
410.000	74.990	121.461	101.954	7.998	ALPHA $\leftrightarrow$ BETA	
410.000	75.228	124.625	101.954	9.295	TRANSITION	
493.000	82.174	139.114	107.010	15.827	BETA $\leftrightarrow$ GAMMA	
493.000	83.680	151.420	107.010	21.894	TRANSITION	
500	83.680	152.600	107.640	22.480	-408.701	-339.169
588.000	83.680	166.166	115.411	29.844	GAMMA $\leftrightarrow$ LIQUID	
588.000	81.588	173.922	115.411	34.404	TRANSITION	
600	81.588	175.570	116.598	35.383	-401.949	-325.564
700	81.588	188.147	125.944	43.542	-399.983	-312.989
800	81.588	199.041	134.415	51.701	-398.062	-300.694
900	81.588	208.651	142.140	59.860	-396.187	-288.636
1000	81.588	217.247	149.229	68.018	-461.488	-273.084
1100	81.588	225.023	155.771	76.177	-458.682	-254.380
1200	81.588	232.122	161.842	84.336	-455.916	-235.930
1300	81.588	238.653	167.503	92.495	-453.188	-217.708
1400	81.588	244.699	172.804	100.654	-450.499	-199.696
1500	81.588	250.328	177.787	108.812	-447.847	-181.874
1600	81.588	255.594	182.487	116.971	-445.234	-164.228
1700	81.588	260.540	186.934	125.130	-442.659	-146.744
1800	81.588	265.204	191.154	133.289	-440.125	-129.411
1900	81.588	269.615	195.169	141.448	-437.633	-112.217
2000	81.588	273.800	198.996	149.606	-435.187	-95.153

PREVIOUS

CURRENT June 1971

Cesium Hydroxide (CsOH)

$Cs_2H_3O_4(cr,l)$

Cesium Hydroxide (CsOH)

IDEAL GAS

Cs<sub>2</sub>H<sub>3</sub>O<sub>2</sub>(g)

S°(298.15 K) = 254.78 ± 0.42 J·K<sup>-1</sup>·mol<sup>-1</sup>

ΔH°(0 K) = -254.9 ± 12.6 kJ·mol<sup>-1</sup>  
 ΔH°(298.15 K) = -259.4 ± 12.6 kJ·mol<sup>-1</sup>

M<sub>r</sub> = 149.91274 Cesium Hydroxide (CsOH)

Vibrational Frequencies and Degeneracies  
 ν, cm<sup>-1</sup>

- 335.6 (1)
- 306 (2)
- [3610](1)

Ground State Quantum Weight: 1 σ=1

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

Bond Distances: Cs-O = 2.391 ± 0.002 Å; O-H = [0.96 ± 0.01] Å

Bond Angle: Cs-O-H = 180°

Rotational Constant: B<sub>0</sub> = 0.184795 cm<sup>-1</sup>

Enthalpy of Formation

Jensen and Padley<sup>1</sup> determined an equilibrium constant for the reaction Cs(g) + H<sub>2</sub>O(g) = CsOH(g) + H(g) at 2475 K by atomic absorption spectroscopy in a hydrogen-oxygen-nitrogen flame. These workers pointed out that interference from ionization of the metal had introduced some uncertainty in their equilibrium data. Using all JANAF functions,<sup>2</sup> 3rd law analysis of the equilibrium constant gives ΔH°(298.15 K) = 27.4 kcal·mol<sup>-1</sup>. This leads to an enthalpy of formation, ΔH°(CsOH, g, 298.15 K) = -64.2 ± 3.0 kcal·mol<sup>-1</sup>, and a corresponding bond dissociation energy of 91 kcal·mol<sup>-1</sup>. Cotton and Jenkins<sup>3</sup> investigated the same equilibrium in a fuel-rich hydrogen-oxygen-nitrogen flame and eliminated the ionization problem by working at a lower temperature (1570 K). 3rd law analysis of their equilibrium data gives ΔH°(298.15 K) = 28.9 kcal·mol<sup>-1</sup>, which results in ΔH°(CsOH, g, 298.15 K) = -62.7 ± 2.0 kcal·mol<sup>-1</sup> corresponding to D<sub>0</sub>(Cs-OH) = 89.6 kcal·mol<sup>-1</sup>. Smith and Sugden<sup>4</sup> had earlier reported a D<sub>0</sub> = 91 ± 1 kcal·mol<sup>-1</sup> from flame studies. Electron impact studies<sup>5,6</sup> have also led to values for the bond dissociation energy of CsOH(g). This method resulted in values of 82 ± 3<sup>5</sup> and 86 ± 3 kcal·mol<sup>-1</sup>.<sup>6</sup>

Cotton and Jenkins<sup>3</sup> also reported bond dissociation energies for LiOH(g), KOH(g), and NaOH(g) which are in good agreement with JANAF enthalpy of formation data<sup>7</sup> for these hydroxides. Furthermore, the position of the hydroxides in the order of increasing bond dissociation energy established from their data, i.e. NaOH < KOH < CsOH < LiOH, is that predicted by comparison with similar data on the stabilities of the alkali metal halides.<sup>8</sup> However, trends within the bond dissociation energies for the halides suggest that the value D<sub>0</sub> = 89.6 kcal·mol<sup>-1</sup> for CsOH may be slightly high. The difference in D<sup>0</sup> for potassium and sodium compounds is from 0.1 kcal·mol<sup>-1</sup> for the fluorides to 0.4 kcal·mol<sup>-1</sup> for the chlorides more than the difference in D<sub>0</sub> for the cesium and potassium compounds. Assuming this same trend in D<sub>0</sub> is prevalent in the hydroxides as well, then D<sub>0</sub>(Cs-OH) - D<sub>0</sub>(K-OH) must be less than 3.9 kcal·mol<sup>-1</sup> (see NaOH(g) table). We adopt D<sub>0</sub>(CsOH) = 89.0 ± 3.0 kcal·mol<sup>-1</sup>, which results in the difference D<sub>0</sub>(Cs-OH) - D<sub>0</sub>(K-OH) = 3.6 kcal·mol<sup>-1</sup>. This adopted bond dissociation energy corresponds to ΔH°(CsOH, g, 298.15 K) = -62.0 ± 3.0 kcal·mol<sup>-1</sup>.

Heat Capacity and Entropy

The microwave spectra of gaseous CsOH have been studied in a high temperature spectrometer by Kuczowski *et al.*<sup>9</sup> and Lide *et al.*<sup>10</sup> completely eliminated Acquista *et al.*<sup>11</sup> observed the infrared spectra of CsOH and CsOD in an argon matrix at liquid hydrogen temperatures. The isotope shift of the bending mode, ν<sub>2</sub>, was quite large (80 cm<sup>-1</sup>), and the ratio of ν<sub>2</sub> for CsOH and CsOD was in excellent agreement with the value calculated for a linear molecule and a harmonic oscillator. The infrared results when used in combination with the microwave data indicate a linear equilibrium configuration for CsOH. We adopt this configuration along with the bond distances and angles determined by Lide *et al.*<sup>10</sup> from their microwave data.

The Cs-O stretching mode, ν<sub>1</sub>, and the bending frequency, ν<sub>2</sub>, are from the matrix isolation studies of Acquista *et al.*<sup>11</sup> The OH stretching frequency, ν<sub>3</sub>, is an estimate from the recent work of Jensen.<sup>12</sup>

References

- <sup>1</sup>D. E. Jensen and P. J. Padley, *Trans. Faraday Soc.*, **62**, 2132 (1966).
- <sup>2</sup>JANAF Thermochemical Tables: Cs(g), 6-30-68; H<sub>2</sub>O(g), 3-31-61; H(g), 9-30-65.
- <sup>3</sup>D. H. Cotton and D. R. Jenkins, *Trans. Faraday Soc.*, **65**, 1537 (1969).
- <sup>4</sup>H. Smith and T. M. Sugden, *Proc. Roy. Soc. A*, **219**, 204 (1953).
- <sup>5</sup>A. M. Emel'yanov, A. V. Gusarov, L. N. Gorokhov, and N. A. Sadovnikova, *Teor. Eksp. Khim.*, **3**, 226 (1967).
- <sup>6</sup>L. N. Gorokhov, A. V. Gusarov, and I. G. Panchenkov, *Russ. J. Phys. Chem. (English Transl.)*, **44**, 150 (1970).
- <sup>7</sup>Ref. 2; LiOH(g), 3-31-66; NaOH(g) and KOH(g), 12-31-70.
- <sup>8</sup>Ref. 2; See recent review of the fluorides by J. Chao, *Thermochimica Acta*, **1**, 71 (1970).
- <sup>9</sup>R. L. Kuczowski, D. R. Lide, Jr., and L. C. Krisher, *J. Chem. Phys.*, **44**, 3131 (1966).
- <sup>10</sup>D. R. Lide, Jr., and R. L. Kuczowski, *J. Chem. Phys.*, **46**, 4768 (1967).
- <sup>11</sup>N. Acquista, S. Abramowitz, and D. R. Lide, *J. Chem. Phys.*, **49**, 780 (1968).
- <sup>12</sup>D. E. Jensen, *J. Phys. Chem.*, **74**, 207 (1970).

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)]/T	H° - H°(T)	ΔH°	
0	0	0	-11.834	-254.950	INFINITE
100	34.721	207.752	-8.801	-257.018	135.077
200	45.601	235.675	-4.709	-258.508	67.791
250	48.173	246.150	-2.360	-258.906	54.281
298.15	49.723	254.778	0	-259.408	45.537
300	49.771	255.085	0.092	-259.430	45.257
350	50.815	262.841	2.608	-262.071	38.747
400	51.525	269.676	5.168	-267.572	30.833
450	52.035	275.775	7.758	-273.797	20.040
500	52.420	281.279	10.369	-280.500	26.984
600	52.991	290.889	15.641	-294.372	22.389
700	53.459	299.093	20.964	-295.912	19.096
800	53.915	306.261	26.333	-266.112	16.618
900	54.388	312.639	31.748	-266.981	14.685
1000	54.877	318.394	37.211	-247.971	12.940
1100	55.371	323.648	42.723	-239.003	11.349
1200	55.857	328.487	48.285	-230.300	10.025
1300	56.325	332.976	53.894	-221.611	8.904
1400	56.769	337.167	59.549	-212.916	7.945
1500	57.184	341.098	65.247	-204.275	7.114
1600	57.568	344.801	70.985	-195.627	6.387
1700	57.922	348.302	76.759	-186.991	5.746
1800	58.246	351.622	82.568	-178.366	5.176
1900	58.543	354.779	88.408	-169.750	4.667
2000	58.813	357.789	94.276	-161.143	4.209
2100	59.060	360.664	100.170	-152.544	3.794
2200	59.285	363.417	106.087	-143.950	3.418
2300	59.490	366.057	112.026	-135.362	3.074
2400	59.677	368.593	117.985	-126.773	2.759
2500	59.848	371.033	123.961	-118.186	2.469
2600	60.005	373.383	129.954	-109.597	2.202
2700	60.148	375.650	135.961	-101.003	1.954
2800	60.279	377.840	141.983	-92.404	1.724
2900	60.400	379.958	148.017	-83.796	1.509
3000	60.511	382.007	154.063	-75.177	1.309
3100	60.614	383.993	160.119	-66.544	1.121
3200	60.708	385.919	166.185	-57.896	0.945
3300	60.796	387.788	172.260	-49.232	0.779
3400	60.876	389.604	178.344	-40.545	0.623
3500	60.951	391.370	184.435	-31.853	0.475
3600	61.021	393.088	190.534	-23.099	0.335
3700	61.086	394.761	196.639	-14.335	0.202
3800	61.146	396.391	202.751	-5.541	0.076
3900	61.203	397.980	208.869	3.286	-0.044
4000	61.255	399.530	214.992	12.149	-0.158
4100	61.304	401.043	221.120	21.051	-0.268
4200	61.350	402.521	227.252	29.994	-0.373
4300	61.394	403.965	233.390	38.979	-0.473
4400	61.434	405.377	239.531	47.975	-0.570
4500	61.472	406.758	245.676	56.979	-0.661
4600	61.508	408.110	251.825	66.081	-0.750
4700	61.542	409.433	257.978	75.220	-0.836
4800	61.573	410.729	264.134	84.428	-0.919
4900	61.604	411.999	270.292	93.675	-0.999
5000	61.632	413.244	276.454	102.973	-1.076
5100	61.659	414.464	282.619	112.322	-1.150
5200	61.684	415.662	288.786	121.646	-1.222
5300	61.708	416.837	294.956	131.089	-1.292
5400	61.731	417.991	301.128	140.549	-1.359
5500	61.753	419.124	307.302	150.058	-1.425
5600	61.773	420.237	313.478	159.650	-1.489
5700	61.793	421.330	319.656	169.294	-1.551
5800	61.811	422.405	325.836	178.991	-1.612
5900	61.829	423.462	332.018	188.740	-1.671
6000	61.846	424.501	338.134	198.542	-1.728

PREVIOUS: June 1971 (1 atm)

CURRENT: June 1971 (1 bar)

Cesium Hydroxide (CsOH)

Cs<sub>2</sub>H<sub>3</sub>O<sub>2</sub>(g)

Cesium Hydroxide, Ion (CsOH<sup>+</sup>)

$S^\circ(298.15\text{ K}) = [268.7 \pm 8.4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

Electronic Levels and Quantum Weights	
State	$g_i$
$^2\Pi$	0
$^2\Sigma^+$	[32000]
Vibrational Frequencies and Degeneracies	
$\nu_i$ , $\text{cm}^{-1}$	

$\sigma = 1$

Point Group:  $[C_{\infty v}]$   
 Bond Distances: Cs-O =  $[2.40] \text{ \AA}$ ; O-H =  $[1.03] \text{ \AA}$   
 Bond Angle: Cs-O-H =  $[180]^\circ$   
 Rotational Constant:  $B_0 = [0.182583] \text{ cm}^{-1}$

Enthalpy of Formation

The appearance potential of CsOH<sup>+</sup> has been determined by Emel'yanov *et al.*<sup>1</sup> as  $7.21 \pm 0.14 \text{ eV}$  and by Gorokhov *et al.*<sup>2</sup> as  $7.40 \pm 0.15 \text{ eV}$ . These values correspond to  $\Delta_f H^\circ(0 \text{ K}) = 166.3 \pm 3.0 \text{ kcal}\cdot\text{mol}^{-1}$  and  $170.7 \pm 5 \text{ kcal}\cdot\text{mol}^{-1}$ , respectively, for the process  $e^- + \text{CsOH}(\text{g}) \rightarrow \text{CsOH}^+(\text{g}) + 2e^-$ . Since there may be excess energy involved, we prefer the lower value. Combining this result with JANAF auxiliary data,<sup>3</sup> we derive  $\Delta_f H^\circ(\text{CsOH}^+, \text{g}, 0 \text{ K}) = 105 \pm 10 \text{ kcal}\cdot\text{mol}^{-1}$  ( $439.32 \pm 41.8 \text{ kJ}\cdot\text{mol}^{-1}$ ).

Heat Capacity and Entropy

The correlation diagram of Walsh<sup>4</sup> for HAB molecules predicts that CsOH<sup>+</sup> (7 valence electrons) should be linear with the unpaired electron in a pi orbital. Therefore, we estimate the ground state of CsOH<sup>+</sup> to be  $^2\Pi$ . CsOH<sup>+</sup> is isoelectronic with OH<sup>+</sup> and SH<sup>+</sup>. A first excited state is estimated at  $32000 \text{ cm}^{-1}$  to be  $^2\Sigma^+$  by analogy with these isoelectronic molecules. The bonding in CsOH<sup>+</sup> is assumed to be weakened relative to that in CsOH by the loss of the bonding electron from the neutral species. The vibrational frequencies are estimated from those for CsOH with somewhat lower values due to the weaker bonding. The Cs-O and O-H bond distances are increased slightly over those for CsOH.

References

- <sup>1</sup>A. M. Emel'yanov, A. V. Gusarov, L. N. Gorokhov, and N. A. Sadovnikova, *Teor. Eksp. Khim.* **3**, 226 (1967).
- <sup>2</sup>L. N. Gorokhov, A. V. Gusarov, and I. G. Panchenkov, *Russ. J. Phys. Chem.* **44**, 150 (1970).
- <sup>3</sup>JANAF Thermochemical Tables: CsOH(g), 6-30-71; OH(g), 12-31-70; SH(g), 6-30-67.
- <sup>4</sup>A. D. Walsh, *J. Chem. Soc.* **1953**, 2288.

Cesium Hydroxide, Ion (CsOH<sup>+</sup>)

Cs<sub>2</sub>H<sub>3</sub>O<sub>2</sub>(g)

T/K	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		$S^\circ - [G^\circ - H^\circ(T_r)]/T$	Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$		$\log K_r$
	$C_p^\circ$	$S^\circ - [G^\circ - H^\circ(T_r)]/T$		$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	
0	0	INFINITE	-12.154	439.320		
100	36.400	220.076	-9.068			
200	46.942	249.166	-4.810			
250	49.177	259.903	-2.402			
298.15	50.492	268.686	0	441.379	430.466	-75.416
300	50.532	268.998	0.093	441.398	430.398	-74.939
350	51.403	276.858	2.643	459.830	428.860	-64.004
400	51.993	283.762	5.229	440.394	427.255	-55.794
450	52.414	289.912	7.840	440.985	425.577	-49.400
500	52.753	295.451	10.469	441.590	424.278	-44.278
600	53.215	305.110	15.767	442.816	420.167	-36.579
700	53.628	313.345	21.110	444.044	416.295	-31.064
800	54.049	320.533	26.493	445.268	412.247	-26.917
900	54.498	326.925	31.920	446.489	408.046	-23.682
1000	54.971	332.691	37.394	380.582	407.409	-21.281
1100	55.452	337.953	42.915	382.829	409.983	-19.468
1200	55.929	342.798	48.484	385.084	412.332	-17.949
1300	56.390	347.293	54.100	387.348	414.232	-16.656
1400	56.827	351.488	59.761	389.618	415.731	-15.541
1500	57.236	355.423	65.465	391.892	416.882	-14.569
1600	57.616	359.150	71.207	394.169	420.073	-13.714
1700	57.966	362.633	76.987	396.442	421.623	-12.955
1800	58.287	365.956	82.800	398.709	423.039	-12.276
1900	58.580	369.115	88.643	400.964	424.329	-11.666
2000	58.848	372.127	94.515	403.202	425.500	-11.113
2100	59.092	375.004	100.412	405.417	426.561	-10.610
2200	59.315	377.758	106.325	407.604	427.516	-10.159
2300	59.518	380.399	112.274	409.755	428.373	-9.751
2400	59.703	382.936	118.236	411.864	429.137	-9.340
2500	59.873	385.377	124.215	413.926	429.814	-8.980
2600	60.027	387.728	130.210	415.932	430.410	-8.647
2700	60.169	389.996	136.220	417.877	430.930	-8.337
2800	60.300	392.187	142.243	419.754	431.379	-8.047
2900	60.419	394.305	148.278	421.555	431.757	-7.777
3000	60.529	396.355	154.327	423.274	432.084	-7.523
3100	60.631	398.342	160.385	424.904	432.351	-7.285
3200	60.725	400.268	166.453	426.439	432.566	-7.061
3300	60.811	402.138	172.529	427.911	432.732	-6.850
3400	60.892	403.955	178.615	429.251	432.858	-6.650
3500	60.967	405.721	184.708	430.480	432.945	-6.461
3600	61.036	407.439	190.808	431.593	433.000	-6.283
3700	61.101	409.113	196.915	432.598	433.024	-6.113
3800	61.161	410.743	203.028	433.480	433.023	-5.952
3900	61.218	412.332	209.147	434.249	432.998	-5.799
4000	61.271	413.883	215.271	434.869	432.958	-5.654
4100	61.322	415.397	221.401	435.356	432.904	-5.515
4200	61.369	416.875	227.536	435.707	432.839	-5.383
4300	61.414	418.319	233.675	435.972	432.769	-5.257
4400	61.456	419.732	239.818	436.291	432.690	-5.136
4500	61.496	421.113	245.966	436.540	432.513	-5.020
4600	61.535	422.465	252.118	436.732	432.332	-4.910
4700	61.572	423.789	258.273	436.882	432.148	-4.805
4800	61.607	425.086	264.432	436.994	431.957	-4.704
4900	61.641	426.356	270.594	437.068	431.762	-4.607
5000	61.674	427.602	276.760	437.102	431.566	-4.514
5100	61.706	428.824	282.929	437.098	431.362	-4.425
5200	61.737	430.022	289.101	437.055	431.157	-4.338
5300	61.767	431.199	295.276	436.974	430.942	-4.256
5400	61.797	432.353	301.455	436.855	430.718	-4.176
5500	61.826	433.488	307.636	436.698	430.481	-4.100
5600	61.854	434.602	313.820	436.504	430.232	-4.026
5700	61.882	435.697	320.007	436.273	430.000	-3.956
5800	61.910	436.773	326.196	436.007	429.788	-3.888
5900	61.937	437.832	332.389	435.701	429.591	-3.822
6000	61.965	438.873	338.442	435.354	429.337	-3.759

PREVIOUS: December 1971 (1 atm)

CURRENT: December 1971 (1 bar)

Cesium Hydroxide, Ion (CsOH<sup>+</sup>)

Cs<sub>2</sub>H<sub>3</sub>O<sub>2</sub>(g)

Cesium Oxide (CsO)

IDEAL GAS

$M_r = 148.9048$  Cesium Oxide (CsO)

$Cs_2O_1(g)$

$S^\circ(298.15\text{ K}) = [225.5 \pm 4.2] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $\Delta H_f^\circ(0\text{ K}) = [64.9 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta H_f^\circ(298.15\text{ K}) = [62.8 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$

Electronic Levels and Quantum Weights State	$\epsilon_e$ , $\text{cm}^{-1}$	$g_e$
[ <sup>2</sup> I]	0	[4]

$\omega_e x_e = [1.0] \text{ cm}^{-1}$   $\sigma = 1$   
 $B_e = [0.198] \text{ cm}^{-1}$   $\alpha_e = [0.001] \text{ cm}^{-1}$   $r_e = [2.40] \text{ \AA}$

Enthalpy of Formation

The enthalpy of formation is estimated from three calculated values. The methods of estimation are described as follows. Brewer and Margrave<sup>1</sup> suggested that the  $\Delta H_f^\circ$  value for MO(g) from the gaseous ions can be taken as the mean of the corresponding  $\Delta H_f^\circ$  values for the alkali fluoride and chloride with a maximum uncertainty of 10 kcal·mol<sup>-1</sup>. Adopting  $\Delta H_f^\circ(298.15\text{ K}) = -131.1$  and  $-109.6$  kcal·mol<sup>-1</sup> for the reaction  $Cs^+(g) + F^-(g) = CsF(g)$  and  $Cs^+(g) + Cl^-(g) = CsCl(g)$ , respectively, we obtain  $\Delta H_f^\circ(298.15\text{ K}) = -120.4$  kcal·mol<sup>-1</sup> for  $Cs^+(g) + O^-(g) = CsO(g)$  which leads to  $\Delta H_f^\circ(298.15\text{ K}) = 12.0$  kcal·mol<sup>-1</sup>. The  $\Delta H_f^\circ(298.15\text{ K})$  values of the above species are taken from the respective JANAF Thermochemical Tables.

Based on the assumption that  $D_0(Cs-O) = 1/2 [D_0(Cs_2O) + D_0(O_2)]$ , we derive  $D_0(Cs-O, g, 298.15\text{ K}) = 65.2$  kcal·mol<sup>-1</sup> and  $\Delta H_f^\circ(298.15\text{ K}) = 12.7$  kcal·mol<sup>-1</sup> for CsO(g).

Adopting the Cs-O bond energy as half of the atomization energy of Cs<sub>2</sub>O, we calculate  $D_0(Cs-O) = 60 \pm 10$  kcal·mol<sup>-1</sup> and  $\Delta H_f^\circ(CsO, g, 298.15\text{ K}) = 17 \pm 10$  kcal·mol<sup>-1</sup>.

The enthalpy of formation for CsO(g) is tentatively selected as  $15 \pm 10$  kcal·mol<sup>-1</sup>.

Heat Capacity and Entropy

The ground state configuration is assumed to be the same as that of the isoelectronic molecule OH(g).  $\omega_e$  is estimated from those of LiO(g), CsF(g), and CsCl(g). The bond distance is taken from that in CsOH(g) reported by Lide and Kuczkowski.<sup>2</sup>  $\omega_e x_e$  is estimated by comparison with those of the other alkali oxides. The values of  $B_e$  and  $\alpha_e$  are calculated from  $r_e$ ,  $\omega_e$  and  $\omega_e x_e$  by the method suggested by Herzberg.<sup>3</sup>

References

- L. Brewer and J. L. Margrave, *J. Phys. Chem.* **59**, 421 (1955).
- D. R. Lide, Jr. and R. L. Kuczkowski, *J. Chem. Phys.* **46**, 4768 (1967).
- G. Herzberg, "Spectra of Diatomic Molecules," D. Van Nostrand Co., Inc., New York, (1950).

T/K	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^\circ = 0.1\text{ MPa}$		log $K_r$
	$C_p^\circ$	$S^\circ - [C_p^\circ - H_f^\circ(T_r)]/T$	$H^\circ - H_f^\circ(T_r)$	$\Delta G^\circ$	
0	0.	0.	INFINITE	INFINITE	INFINITE
100	31.670	217.938	287.000	64.939	-29.606
200	35.247	241.201	258.847	64.311	-12.889
250	36.016	249.156	256.140	63.552	-9.578
298.15	36.481	255.542	255.542	63.187	-7.453
300	36.495	255.768	255.543	62.741	-7.385
350	36.816	261.419	255.988	60.141	-5.880
400	37.044	266.351	256.982	57.483	-4.763
450	37.216	270.724	258.270	54.913	-3.901
500	37.351	274.653	259.715	52.489	-3.216
600	37.555	281.482	262.791	47.775	-2.202
700	37.709	287.283	265.886	42.889	-1.489
800	37.833	292.326	268.882	37.830	-0.963
900	37.945	296.789	271.740	32.644	-0.562
1000	38.046	300.793	274.448	27.336	-0.440
1100	38.139	304.423	277.011	21.920	-0.503
1200	38.228	307.746	279.456	16.414	-0.536
1300	38.313	310.809	281.733	10.827	-0.601
1400	38.397	313.651	283.912	5.269	-0.659
1500	38.478	316.303	285.984	0.748	-0.673
1600	38.558	318.789	287.958	-4.730	-0.703
1700	38.638	321.129	289.841	-10.190	-0.729
1800	38.716	323.340	291.641	-15.726	-0.752
1900	38.794	325.435	293.365	-21.331	-0.773
2000	38.871	327.427	295.019	-27.006	-0.793
2100	38.948	329.325	296.607	-32.752	-0.810
2200	39.024	331.139	298.136	-38.569	-0.826
2300	39.100	332.875	299.609	-44.357	-0.841
2400	39.176	334.541	301.030	-50.117	-0.855
2500	39.252	336.142	302.403	-55.849	-0.868
2600	39.328	337.683	303.730	-61.554	-0.880
2700	39.403	339.168	305.015	-67.234	-0.892
2800	39.478	340.603	306.261	-72.889	-0.903
2900	39.554	341.989	307.469	-78.520	-0.914
3000	39.629	343.331	308.642	-84.128	-0.924
3100	39.704	344.632	309.782	-89.714	-0.934
3200	39.779	345.894	310.891	-95.279	-0.943
3300	39.854	347.119	311.971	-100.823	-0.953
3400	39.928	348.310	313.022	-106.346	-0.962
3500	40.003	349.468	314.047	-111.848	-0.972
3600	40.078	350.596	315.046	-117.329	-0.981
3700	40.152	351.695	316.022	-122.791	-0.990
3800	40.227	352.767	316.975	-128.234	-0.999
3900	40.302	353.813	317.906	-133.659	-1.008
4000	40.376	354.834	318.817	-139.066	-1.018
4100	40.451	355.832	319.707	-144.455	-1.027
4200	40.525	356.808	320.579	-149.826	-1.036
4300	40.600	357.762	321.433	-155.179	-1.045
4400	40.674	358.697	322.269	-160.514	-1.053
4500	40.749	359.612	323.089	-165.832	-1.064
4600	40.823	360.508	323.893	-171.134	-1.074
4700	40.898	361.387	324.681	-176.419	-1.084
4800	40.972	362.249	325.455	-181.689	-1.094
4900	41.047	363.094	326.214	-186.944	-1.104
5000	41.121	363.924	326.960	-192.184	-1.114
5100	41.195	364.739	327.693	-197.409	-1.124
5200	41.270	365.540	328.413	-202.619	-1.134
5300	41.344	366.327	329.121	-207.814	-1.144
5400	41.418	367.100	329.817	-213.004	-1.155
5500	41.493	367.861	330.502	-218.189	-1.165
5600	41.567	368.609	331.176	-223.369	-1.176
5700	41.641	369.346	331.839	-228.544	-1.187
5800	41.716	370.070	332.492	-233.714	-1.198
5900	41.790	370.784	333.135	-238.879	-1.209
6000	41.864	371.487	333.768	-244.039	-1.220

PREVIOUS: December 1968 (1 atm)

CURRENT: December 1968 (1 bar)

Cesium Oxide (CsO)

$Cs_2O_1(g)$



Cesium (Cs<sub>2</sub>)

$$M_r = 265.8108$$

$$D_0^0 = 43.389 \pm 0.096 \text{ kJ mol}^{-1} \quad \Delta H_f^0(0 \text{ K}) = 111.77 \pm 0.26 \text{ kJ mol}^{-1} \quad r_e, \text{ \AA}$$

$$S^0(298.15 \text{ K}) = 284.675 \pm 0.084 \text{ J K}^{-1} \text{ mol}^{-1} \quad \Delta H_f^0(298.15 \text{ K}) = 107.37 \pm 0.30 \text{ kJ mol}^{-1}$$

State	$T_e$	$\omega_e$	$10^3 \omega_e x_e$	$10^5 \omega_e^2 x_e$	$10^7 \omega_e^3 x_e$	$10^9 \omega_e^4 x_e$	$10^8 D_e$	$10^{10} B_e$	$10^8 D_e$	$10^8 \gamma_e$	$10^8 \gamma_e$	$r_e, \text{ \AA}$
X <sup>1</sup> $\Sigma_g^+$	0	42.0194	8.191	-9.0404	-3.2912 <sup>b</sup>	2.215	1.1743	1.2608 <sup>c</sup>	3.73	[8.5833]	—	4.646 <sup>c</sup>
C <sup>1</sup> $\Pi_u$	15949 <sup>a</sup>	29.664	4.202	—	—	6.6503	—	—	—	—	—	4.34 <sup>c</sup>

(a) The dissociation energy,  $D_0^0$ , for the C<sup>1</sup> $\Pi_u$  state is 18228 cm<sup>-1</sup>.  
 (b)  $-5.8173 \times 10^{-9}(v+1/2)^4 - 4.5832 \times 10^{-12}(v+1/2)^2$  for  $\Sigma_g^+$ .  
 (c)  $+5.8751 \times 10^{-10}(v+1/2)^3 - 3.0391 \times 10^{-12}(v+1/2)^4 + 1.8161 \times 10^{-14}(v+1/2)^5$  for  $\Sigma_g^+$ .  
 (d)  $+9.2704 \times 10^{-13}(v+1/2)^2 - 9.7917 \times 10^{-15}(v+1/2)^3$  for  $\Sigma_g^+$ .  
 (e) As determined from  $B_e$ .

**Enthalpy of Formation**  
 Using the adopted value of the ground state dissociation energy for Cs<sub>2</sub>(g),  $D_0^0 = 43.389 \text{ kJ mol}^{-1}$ , and the recommended  $\Delta H_f^0(\text{Cs, g, 0 K}) = 155.160 \text{ kJ mol}^{-1}$  from NBS,<sup>6</sup> we calculate the adopted value of  $\Delta H_f^0(\text{Cs}_2, \text{g, 0 K}) = 111.77 \text{ kJ mol}^{-1}$ . This value is in essential agreement with the NBS recommended value of 111.7 kJ mol<sup>-1</sup>. Correcting the adopted  $\Delta H_f^0(0 \text{ K})$  to 298.15 K using the current value of  $H^0(298.15 \text{ K}) - H^0(0 \text{ K}) = 11.029 \text{ kJ mol}^{-1}$  for Cs<sub>2</sub>(g) and the NBS value of  $H^0(298.15 \text{ K}) - H^0(0 \text{ K}) = 7.711 \text{ kJ mol}^{-1}$  for Cs(cr) 6, we obtain  $\Delta H_f^0(\text{Cs}_2, \text{g, 298.15 K}) = 107.38 \text{ kJ mol}^{-1}$ .

**Heat Capacity and Entropy**  
 The heat capacity and entropy were calculated using a direct summation technique similar to the Li<sub>2</sub>(g) calculation<sup>7</sup> using ground state data from Raab *et al.*,<sup>4</sup> as recommended by Swalley.<sup>8</sup> Spectroscopic data for the C<sup>1</sup> $\Pi_u$  state of Cs<sub>2</sub>(g) at  $T_e = 15949 \text{ cm}^{-1}$  come from the work of Raab *et al.*<sup>4</sup> The other low lying states of Cs<sub>2</sub>(g) at  $T_e = 7850 \text{ cm}^{-1}$ ,<sup>13</sup> the B<sup>1</sup> $\Pi_u$  state at  $13044 \text{ cm}^{-1}$ ,<sup>15</sup> and the  $\Sigma_g^+$  state at  $T_e = 16720 \text{ cm}^{-1}$ .<sup>14</sup> These states have not been characterized satisfactorily to date. To include the excited states in the thermodynamic calculation in an approximate manner, we proceeded as with the Na<sub>2</sub>(g) species as follows.<sup>7</sup> The C<sup>1</sup> $\Pi_u$  state was included using the spectroscopic data reported by Raab.<sup>4</sup> To account for the  $\Pi_u$ , B<sup>1</sup> $\Pi_u$ , and  $\Sigma_g^+$  states, the rotational levels of the C<sup>1</sup> $\Pi_u$  state were weighted  $\times 1/3$  to account for the sixfold degeneracy of the  $\Pi_u$  state, the threefold degeneracy of each of the  $\Pi_u$  states and the singly degenerate  $\Sigma_g^+$  state. Note that the  $\Sigma_g^+$  state is weakly bound and was neglected. Due to the minimal number of vibrational and rotational levels used by<sup>7</sup> to generate Dunham coefficients for the C<sup>1</sup> $\Pi_u$  state, we artificially truncated the  $G(v)$  expression after the  $\omega_e x_e$  term and the  $B(v)$  expression after the  $\alpha_e$  term. For the same reason, we used Herzberg's method (see Li<sub>2</sub> table) to estimate  $D_e = 8.5833 \times 10^{-9} \text{ cm}^{-1}$  rather than use the value of 1. As with the Na<sub>2</sub>(g) calculation, the above method certainly underestimates the  $\Pi_u$  and B<sup>1</sup> $\Pi_u$  contributions but at the same time overestimates the  $\Sigma_g^+$  contribution to the thermodynamic functions. The contribution of the excited states to the free energy function is negligible at temperatures below 2000 K and only contribute ca.  $0.25 \text{ J K}^{-1} \text{ mol}^{-1}$  at 6000 K. This method of treating the excited states does result, however, in a more realistic high temperature heat capacity. The rotational levels of the ground state were weighted in accordance with the nuclear spin of the atom ( $I = 7/2$ ); even  $J$  weight = 5833, odd  $J$  weight = 4167. The adopted value of  $S^0(298.15 \text{ K})$  is larger than the NBS adopted value 6 by  $0.74 \text{ J K}^{-1} \text{ mol}^{-1}$  but is in exact agreement with that adopted by Gurvich, *et al.*<sup>9</sup>

**References**  
<sup>1</sup>M. Raab, H. Weickenmeier, and W. Demtroder, *Chem. Phys. Lett.* **88**, 377 (1982).  
<sup>2</sup>W. C. Swalley, Director, Iowa Laser Facility and Professor of Chemistry and Physics, University of Iowa, personal communication, (1982).  
<sup>3</sup>R. P. Benedict, D. L. Drummond and L. A. Schlie, *J. Chem. Phys.* **66**, 4600 (1977).  
<sup>4</sup>M. Raab, G. Honing, W. Demtroder, and C. R. Vidal, *J. Chem. Phys.* **76**, 4370 (1982).  
<sup>5</sup>K. P. Huber and G. Herzberg, "Constants of Diatomic Molecules," Van Nostrand Reinhold Co., New York, (1981).  
<sup>6</sup>D. D. Wagman, *et al.*, *J. Phys. Chem. Ref. Data* **11**, Supp. 2 (1982).  
<sup>7</sup>JANAF Thermochemical Tables: Li<sub>2</sub>(g), 12-31-82; Na<sub>2</sub>(g), 12-31-82.  
<sup>8</sup>L. V. Gurvich, *et al.*, *Thermodynamic Properties of Individual Substances*, Vol. IV, 3rd ed., Nauka, Moscow, (1982).

Cesium (Cs<sub>2</sub>)

## IDEAL GAS

Cesium (Cs<sub>2</sub>)

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>e</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
		S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>e</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>e</sub> )/T	ΔH <sup>o</sup>	ΔG <sup>o</sup>	
0	0	INFINITE	-11.029	111.770	111.770	INFINITE
100	37.404	243.396	-7.502	118.414	87.900	-51.008
200	37.872	269.484	-7.335	288.161	84.860	-22.171
298.15	38.250	284.675	0	284.675	73.263	-12.835
300	38.258	284.912	0.071	107.317	73.052	-12.719
400	38.686	295.977	3.918	100.605	63.581	-8.277
500	38.962	304.645	7.803	98.227	54.553	-5.678
600	38.757	311.739	11.694	95.904	45.796	-3.987
700	37.949	317.660	15.534	91.551	37.630	-2.808
800	36.671	322.648	19.268	85.098	29.807	-1.946
900	35.150	326.881	23.001	78.502	22.300	-1.294
1000	33.582	330.503	26.297	72.400	16.175	-0.851
1100	32.089	333.633	29.779	66.743	10.631	-0.407
1200	30.734	336.366	33.719	61.408	5.639	-0.1604
1300	29.537	338.777	37.192	56.354	1.177	-0.1725
1400	28.497	340.927	40.215	51.587	-3.129	-0.208
1500	27.602	342.862	42.797	47.146	-5.609	-0.258
1600	26.836	344.618	44.156	43.000	-7.660	-0.317
1700	26.183	346.225	45.328	39.134	-9.285	-0.384
1800	25.631	347.706	46.807	35.544	-11.587	-0.454
1900	25.166	349.079	48.536	32.200	-14.644	-0.525
2000	24.781	350.359	50.432	29.100	-18.450	-0.600
2100	24.468	351.561	52.468	26.230	-23.000	-0.680
2200	24.221	352.693	54.693	23.576	-28.330	-0.760
2300	24.037	353.765	57.131	21.200	-34.500	-0.840
2400	23.912	354.786	60.000	19.076	-41.500	-0.920
2500	23.842	355.760	63.230	17.156	-49.300	-1.000
2600	23.826	356.693	66.808	15.414	-57.900	-1.080
2700	23.861	357.594	70.776	13.820	-67.300	-1.160
2800	23.944	358.464	75.082	12.350	-77.500	-1.240
2900	24.073	359.306	79.768	11.000	-88.500	-1.320
3000	24.245	360.123	84.858	9.750	-100.300	-1.400
3100	24.456	360.923	90.392	8.600	-113.000	-1.480
3200	24.704	361.703	96.344	7.540	-126.500	-1.560
3300	24.986	362.468	102.764	6.560	-140.800	-1.640
3400	25.297	363.218	109.688	5.650	-155.900	-1.720
3500	25.634	363.956	117.132	4.800	-171.800	-1.800
3600	25.994	364.683	125.100	4.000	-188.500	-1.880
3700	26.371	365.401	133.600	3.250	-206.000	-1.960
3800	26.764	366.109	142.640	2.550	-224.300	-2.040
3900	27.168	366.810	152.220	1.900	-243.400	-2.120
4000	27.579	367.503	162.350	1.300	-263.300	-2.200
4100	27.994	368.189	173.040	0.750	-284.000	-2.280
4200	28.410	368.868	184.290	0.250	-305.500	-2.360
4300	28.824	369.542	196.100	-0.200	-328.000	-2.440
4400	29.232	370.209	208.480	-0.650	-351.500	-2.520
4500	29.632	370.870	221.440	-1.100	-376.000	-2.600
4600	30.022	371.526	234.980	-1.550	-401.500	-2.680
4700	30.400	372.176	249.110	-2.000	-428.000	-2.760
4800	30.763	372.820	263.830	-2.450	-455.500	-2.840
4900	31.110	373.458	279.150	-2.900	-484.000	-2.920
5000	31.440	374.089	295.080	-3.350	-513.500	-3.000
5100	31.752	374.715	311.620	-3.800	-544.000	-3.080
5200	32.043	375.335	328.770	-4.250	-575.500	-3.160
5300	32.315	375.948	346.540	-4.700	-608.000	-3.240
5400	32.566	376.554	364.940	-5.150	-641.500	-3.320
5500	32.795	377.154	383.980	-5.600	-676.000	-3.400
5600	33.004	377.746	403.680	-6.050	-711.500	-3.480
5700	33.197	378.332	424.040	-6.500	-748.000	-3.560
5800	33.358	378.911	445.070	-6.950	-785.500	-3.640
5900	33.505	379.483	466.790	-7.400	-824.000	-3.720
6000	33.650	380.047	489.220	-7.850	-863.500	-3.800

PREVIOUS June 1968 (1 atm)

CURRENT December 1983 (1 bar)

Cesium (Cs<sub>2</sub>)Cs<sub>2</sub>(g)

Cs<sub>2</sub>F<sub>2</sub>(g)

M<sub>r</sub> = 303.807606 Cesium Fluoride ((CsF)<sub>2</sub>)

IDEAL GAS

Cesium Fluoride ((CsF)<sub>2</sub>)

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)	ΔH <sup>o</sup>	log K <sub>r</sub>
0	0	INFINITE	-19.273	-885.119	INFINITE
100	62.412	272.336	-420.380	-887.854	463.353
200	76.312	321.055	-359.539	-889.036	231.330
300	78.605	338.355	-313.628	-889.500	184.881
298.15	79.888	352.319	0	-890.104	154.858
300	79.926	352.813	0.148	-890.134	153.896
350	80.750	365.200	0.168	-895.093	131.646
400	81.296	376.021	0.218	-895.881	114.941
450	81.675	385.619	0.253	-896.575	101.938
500	81.950	394.239	0.276	-897.305	91.526
600	82.310	409.218	0.288	-898.778	75.891
700	82.529	421.921	0.291	-900.280	64.704
800	82.672	432.952	0.284	-901.815	56.300
900	82.741	442.695	0.274	-903.386	49.752
1000	82.842	451.420	0.264	-904.998	44.118
1100	82.984	459.318	0.253	-906.654	39.184
1200	83.164	466.532	0.242	-908.350	35.074
1300	83.368	473.172	0.232	-910.084	31.597
1400	83.598	479.251	0.223	-911.856	28.618
1500	83.809	484.868	0.216	-913.663	26.037
1600	83.926	490.405	0.210	-915.502	23.789
1700	83.959	495.439	0.205	-917.369	21.817
1800	83.980	500.186	0.201	-919.261	20.019
1900	83.988	504.676	0.198	-921.175	18.436
2000	83.983	508.937	0.196	-923.108	17.011
2100	83.975	512.990	0.195	-925.058	15.723
2200	83.964	516.855	0.194	-927.021	14.551
2300	83.951	520.548	0.194	-929.000	13.482
2400	83.936	524.084	0.194	-931.000	12.500
2500	83.919	527.477	0.194	-933.029	11.602
2600	83.899	530.736	0.194	-935.082	10.767
2700	83.876	533.872	0.194	-937.156	9.996
2800	83.850	536.894	0.194	-939.248	9.279
2900	83.821	539.811	0.194	-941.356	8.612
3000	83.790	542.628	0.194	-943.478	7.989
3100	83.757	545.353	0.194	-945.612	7.406
3200	83.722	547.992	0.194	-947.756	6.858
3300	83.686	550.550	0.194	-949.918	6.344
3400	83.649	553.031	0.194	-952.097	5.859
3500	83.611	555.440	0.194	-954.292	5.402
3600	83.572	557.782	0.194	-956.502	4.969
3700	83.532	560.059	0.194	-958.726	4.559
3800	83.491	562.276	0.194	-960.963	4.170
3900	83.449	564.435	0.194	-963.212	3.800
4000	83.406	566.540	0.194	-965.472	3.448
4100	83.362	568.592	0.194	-967.742	3.113
4200	83.317	570.595	0.194	-969.999	2.792
4300	83.271	572.551	0.194	-972.232	2.486
4400	83.224	574.463	0.194	-974.441	2.193
4500	83.179	576.331	0.194	-976.616	1.914
4600	83.133	578.158	0.194	-978.757	1.645
4700	83.130	579.946	0.194	-980.863	1.386
4800	83.131	581.696	0.194	-982.934	1.137
4900	83.131	583.410	0.194	-984.970	0.898
5000	83.132	585.089	0.194	-986.972	0.668
5100	83.132	586.736	0.194	-988.940	0.445
5200	83.133	588.350	0.194	-990.875	0.232
5300	83.133	589.933	0.194	-992.778	0.025
5400	83.134	591.487	0.194	-994.649	-0.174
5500	83.134	593.013	0.194	-996.486	-0.367
5600	83.134	594.511	0.194	-998.290	-0.554
5700	83.135	595.982	0.194	-1000.053	-0.736
5800	83.135	597.428	0.194	-1001.777	-0.912
5900	83.135	598.849	0.194	-1003.462	-1.082
6000	83.136	600.246	0.194	-1005.108	-1.248

CURRENT: June 1968 (1 bar)

PREVIOUS: June 1968 (1 atm)

Cs<sub>2</sub>F<sub>2</sub>(g)

Cesium Fluoride ((CsF)<sub>2</sub>)

ΔH<sup>o</sup>(0 K) = -885.12 ± 8.4 kJ·mol<sup>-1</sup>  
 ΔH<sup>o</sup>(298.15 K) = -890.10 ± 8.4 kJ·mol<sup>-1</sup>

Vibrational Frequencies and Degeneracies	
ν, cm <sup>-1</sup>	ν, cm <sup>-1</sup>
[200](1)	[120](1)
[110](1)	[220](1)
[210](1)	[230](1)

Ground State Quantum Weight: (1)

Bond Distance: Cs-F = [2.55] Å

Bond Angles: F-Cs-F = [85]°, Cs-F-Cs = [95]°

Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [3.127422 × 10<sup>-112</sup>] g<sup>3</sup>·cm<sup>6</sup>

**Enthalpy of Formation**

Evidence from the velocity distribution in molecular beams<sup>1</sup> has shown that alkali halide vapors contain significant amounts of polymeric species. Using the same method Eisenstadt<sup>2</sup> determined the molecular composition of CsF vapor in the temperature range 838-919 K. Based on the reported equilibrium constants for the reaction (CsF)<sub>2</sub>(g) = 2CsF(g), we evaluate the enthalpy change, ΔH<sup>o</sup>(298.15 K), by the 2nd and 3rd law methods to be 40.53 ± 1.75 and 42.34 ± 0.26 kcal·mol<sup>-1</sup>, respectively. Employing ΔH<sup>o</sup>(298.15 K) = 42.34 and ΔH<sup>o</sup>(CsF, g, 298.15 K) = -85.2 kcal·mol<sup>-1</sup>, we obtained ΔH<sup>o</sup>(298.15 K) = -212.74 kcal·mol<sup>-1</sup> for Cs<sub>2</sub>F<sub>2</sub>(g), which is adopted.

**Heat Capacity and Entropy**

The Cs<sub>2</sub>F<sub>2</sub> molecule is assumed to have a rhombic configuration of symmetry D<sub>2h</sub> as Cs<sub>2</sub>Cl<sub>2</sub>.<sup>3</sup> The Cs-F bond distance is taken as the same as that in CsF(g). The bond angles and vibrational frequencies are estimated by comparison with those of the other dimeric alkali halides.<sup>3,4</sup> The principal moments of inertia are: I<sub>A</sub> = 15.9040 × 10<sup>-39</sup>, I<sub>B</sub> = 132.5032 × 10<sup>-39</sup>, and I<sub>C</sub> = 148.4071 × 10<sup>-39</sup> g·cm<sup>2</sup>.

**References**

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- M. Eisenstadt, G. M. Rothberg and P. Kusch, J. Chem. Phys. 29, 797 (1958).
- J. Berkowitz, J. Chem. Phys. 29, 1386 (1958).
- J. Berkowitz, J. Chem. Phys. 32, 1519 (1960).

Cesium Hydroxide ((CsOH)<sub>2</sub>)

IDEAL GAS

M<sub>r</sub> = 299.82548

Δ<sub>r</sub>H<sup>0</sup>(0 K) = -674.7 ± 41.8 kJ·mol<sup>-1</sup>  
 Δ<sub>r</sub>H<sup>0</sup>(298.15 K) = -687.8 ± 41.8 kJ·mol<sup>-1</sup>

S<sup>0</sup>(298.15 K) = 360.7 ± 12.6 J·K<sup>-1</sup>·mol<sup>-1</sup>

Vibrational Frequencies and Degeneracies  
 ν, cm<sup>-1</sup>

[200](1)	[1250](1)
[110](1)	[1250](1)
[210](1)	[1250](1)
[120](1)	[1250](1)
[220](1)	[3700](1)
[230](1)	[3700](1)

Ground State Quantum Weight: 1

Point Group: C<sub>2h</sub> σ = 2  
 Bond Distances: Cs-O = [2.63] Å; O-H = [0.96] Å  
 Bond Angles: Cs-O-Cs = [90]°; Cs-O-H = [110]°  
 Product of Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [5.396347 × 10<sup>-112</sup>] g<sup>3</sup>·cm<sup>6</sup>

Enthalpy of Formation

Schoonmaker and Porter<sup>1</sup> analyzed the vapors in equilibrium with liquid CsOH and mixed KOH-CsOH condensed phases with a mass spectrometer and reported the presence of appreciable concentrations of dimer in the temperature range 650-700 K. By applying the method of relative equilibrium constants, these workers calculated the difference in the free energies of dimerization for KOH-CsOH. A 3rd law analysis of their free energy data for this pair leads to a difference in the enthalpies of dimerization of 4.9 kcal·mol<sup>-1</sup> at 298.15 K for CsOH and KOH. Based upon the adopted value for KOH(g), Δ<sub>r</sub>H<sup>0</sup>(dimerization, 298.15 K) = -45.3 ± 3.0 kcal·mol<sup>-1</sup>; we derive Δ<sub>r</sub>H<sup>0</sup>(dimerization, 298.15 K) = -40.4 ± 4.0 kcal·mol<sup>-1</sup> for 2 CsOH(g) = Cs<sub>2</sub>(OH)<sub>2</sub>(g). Combining this result with the enthalpy of formation for the gaseous monomer<sup>2</sup>, that for the dimer is Δ<sub>r</sub>H<sup>0</sup>(Cs<sub>2</sub>(OH)<sub>2</sub>, g, 298.15 K) = -164.4 ± 10.0 kcal·mol<sup>-1</sup> (-687.8 ± 41.8 kJ·mol<sup>-1</sup>).

Heat Capacity and Entropy

Buchler *et al.*<sup>3</sup> investigated the geometries of several molecules containing cesium by the deflection of molecular beams in an inhomogeneous electric field. Their results for Cs<sub>2</sub>(OH)<sub>2</sub>(g) indicated that the molecule was nonpolar which implies a planar configuration for at least the Cs<sub>2</sub>O part of the molecule. Several structural models proposed for the dimers of the alkali metal hydroxides each incorporate this planar configuration for the alkali and oxygen atoms. Bauer *et al.*<sup>4</sup> calculated entropies of dimerization for NaOH(g) and KOH(g) with a dimer model consisting of a square planar configuration for the alkali and oxygen atoms with two hydrogen bonded bridges between the oxygens and hydrogens. Schoonmaker and Porter<sup>1</sup> adopted the same alkali-oxygen configuration but did not allow for hydrogen bonding between the oxygens and hydrogens. Berkowitz *et al.*<sup>5</sup> relied on the apparent similarity of the alkali halides and hydroxides in forming dimeric species to propose a structural model for Li<sub>2</sub>(OH)<sub>2</sub>(g). This model consisted of a trans-configuration with hydrogens above and below the plane of a rhombus formed by the lithium and oxygen atoms, the Li-O-Li bond angle being 100°. We adopt a structure for Cs<sub>2</sub>(OH)<sub>2</sub>(g) which is similar to the model of Berkowitz *et al.*<sup>5</sup> for Li<sub>2</sub>(OH)<sub>2</sub>(g) but with the Cs-O-Cs bond angle equal to 90°. The cesium and oxygen atoms form a square planar configuration. The Cs-O-H bond angle is assumed equal to 110°. The Cs-O bond distance is estimated as being 10% longer than that in CsOH(g). The O-H bond distance is estimated to be the same as in H<sub>2</sub>O(g). The principal moments of inertia are: I<sub>A</sub> = [20.4212] × 10<sup>-39</sup>, I<sub>B</sub> = [152.8696] × 10<sup>-39</sup>, and I<sub>C</sub> = [172.8610] × 10<sup>-39</sup> g·cm<sup>2</sup>.

Acquista *et al.*<sup>7</sup> observed the infrared spectra of matrix isolated CsOH and reported bands in the region 300-200 cm<sup>-1</sup> whose relative intensities decreased with increasing temperature. Since the dimer to monomer ratio decreases with increasing temperature, these bands appeared to arise from polymeric species of CsOH, but no definite assignments could be made. Similar results have been reported for R<sub>2</sub>OH and NaOH from infrared studies<sup>8</sup> of these molecules trapped in inert matrices. Berkowitz *et al.*<sup>6</sup> estimated vibrational frequencies for Li<sub>2</sub>(OH)<sub>2</sub>(g) by comparison with those for dimeric Li<sub>2</sub>F<sub>2</sub>(g). The frequencies for Li<sub>2</sub>F<sub>2</sub>(g) had been estimated earlier by Berkowitz<sup>9</sup> using an ionic model and normal coordinate analysis. It has now been established experimentally that these estimated frequencies for Li<sub>2</sub>F<sub>2</sub>(g) are too low (Refer to Li<sub>2</sub>F<sub>2</sub>(g) table for details). Until definite assignments for the dimer hydroxides can be made from infrared studies, we tentatively adopt the six estimated frequencies for Cs<sub>2</sub>F<sub>2</sub>(g) (Refer to CsF<sub>2</sub>(g) table for details) and apply them directly to Cs<sub>2</sub>(OH)<sub>2</sub>(g). The remaining O-H stretching and bending frequencies are estimates from the work of Berkowitz *et al.*<sup>6</sup>.

References

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Cesium Hydroxide ((CsOH)<sub>2</sub>)

T/K	C <sub>p</sub> <sup>0</sup>	S <sup>0</sup> - (G <sup>0</sup> - H <sup>0</sup> (T))/T	H <sup>0</sup> - H <sup>0</sup> (T)	Δ <sub>r</sub> H <sup>0</sup>	Standard State Pressure = p <sup>0</sup> = 0.1 MPa	log K <sub>r</sub>
0	0	INFINITE	0	0	-674.683	INFINITE
100	62.412	280.202	-19.417	-674.683	-680.415	349.994
200	76.646	328.962	-7.833	-684.265	-687.977	171.877
250	79.900	346.426	-3.917	-686.043	-691.350	136.092
298.15	82.807	360.748	0	-687.850	-694.507	112.915
300	82.919	361.260	0.153	-687.923	-694.237	112.172
350	85.963	374.271	4.375	-694.016	-696.132	94.937
400	88.968	385.947	8.749	-695.764	-697.741	81.768
450	91.824	396.592	13.270	-697.362	-699.141	71.868
500	94.461	406.406	17.928	-698.830	-700.370	63.765
600	99.017	424.045	27.609	-701.451	-702.425	51.575
700	102.729	439.597	37.703	-703.743	-704.069	42.838
800	105.812	453.521	48.134	-705.788	-705.402	36.264
900	108.443	466.140	58.850	-707.641	-706.491	31.137
1000	110.738	477.687	69.812	-709.383	-707.369	26.639
1100	112.767	488.338	80.989	-710.966	-708.043	22.634
1200	114.576	498.229	92.358	-712.342	-708.542	19.299
1300	116.193	507.463	103.898	-713.565	-708.913	16.479
1400	117.640	516.130	115.591	-714.654	-709.173	14.063
1500	118.938	524.291	127.421	-715.629	-709.361	11.972
1600	120.101	532.005	139.374	-716.498	-709.481	10.144
1700	121.148	539.318	151.437	-717.263	-709.533	8.533
1800	122.081	546.270	163.599	-717.937	-709.524	7.102
1900	122.923	552.891	175.850	-718.529	-709.467	5.824
2000	123.680	559.128	188.181	-719.043	-709.363	4.674
2100	124.364	565.069	200.583	-719.487	-709.216	3.635
2200	124.980	570.727	213.051	-719.863	-709.033	2.692
2300	125.539	576.137	225.578	-720.172	-708.818	1.831
2400	126.045	581.349	238.157	-720.425	-708.574	1.043
2500	126.504	586.416	250.785	-720.633	-708.307	0.318
2600	126.923	591.346	263.457	-720.800	-708.013	-0.350
2700	127.304	596.143	276.168	-720.936	-707.696	-1.068
2800	127.653	600.809	288.916	-721.043	-707.357	-1.742
2900	127.977	605.344	301.698	-721.123	-706.995	-2.077
3000	128.285	610.378	314.510	-721.180	-706.610	-2.575
3100	128.578	614.588	327.350	-721.216	-706.204	-3.042
3200	128.873	618.673	340.216	-721.235	-705.778	-3.479
3300	129.010	622.639	353.106	-721.238	-705.336	-3.890
3400	129.221	626.493	366.017	-721.226	-704.878	-4.278
3500	129.417	630.242	378.949	-721.199	-704.403	-4.643
3600	129.598	633.891	391.900	-721.157	-703.907	-4.989
3700	129.767	637.444	404.869	-721.101	-703.393	-5.316
3800	129.923	640.905	417.853	-721.032	-702.863	-5.627
3900	130.069	644.283	430.853	-720.951	-702.319	-5.923
4000	130.205	647.578	443.867	-720.858	-701.763	-6.204
4100	130.333	650.795	456.894	-720.754	-701.197	-6.472
4200	130.452	653.937	469.933	-720.639	-700.622	-6.729
4300	130.563	657.001	482.986	-720.514	-700.037	-6.974
4400	130.667	660.011	496.045	-720.380	-699.442	-7.208
4500	130.766	662.948	509.117	-720.237	-698.837	-7.432
4600	130.858	665.833	522.202	-720.085	-698.222	-7.648
4700	130.943	668.638	535.288	-720.028	-697.597	-7.856
4800	131.026	671.396	548.387	-719.966	-696.963	-8.055
4900	131.104	674.099	561.494	-719.899	-696.313	-8.248
5000	131.176	676.748	574.608	-719.827	-695.649	-8.434
5100	131.245	679.346	587.729	-719.750	-694.972	-8.613
5200	131.310	681.891	600.857	-719.660	-694.285	-8.785
5300	131.372	684.397	613.991	-719.558	-693.589	-8.953
5400	131.431	686.853	627.138	-719.445	-692.884	-9.114
5500	131.486	689.266	640.271	-719.322	-692.171	-9.271
5600	131.539	691.635	653.428	-719.189	-691.453	-9.423
5700	131.589	693.964	666.584	-719.046	-690.729	-9.571
5800	131.636	696.253	679.746	-718.893	-690.000	-9.714
5900	131.682	698.503	692.912	-718.730	-689.267	-9.854
6000	131.725	700.717	706.082	-718.557	-688.531	-9.989

PREVIOUS June 1971 (1 atm)

CURRENT: June 1971 (1 bar)

Cesium Hydroxide ((CsOH)<sub>2</sub>)

Cs<sub>2</sub>H<sub>2</sub>O<sub>2</sub>(g)

Cs<sub>2</sub>O(g)

M<sub>r</sub> = 281.8102 Cesium Oxide (Cs<sub>2</sub>O)

IDEAL GAS

Cesium Oxide (Cs<sub>2</sub>O)

S<sup>o</sup>(298.15 K) = [-318.1 ± 8.4] J·K<sup>-1</sup>·mol<sup>-1</sup> ΔH<sup>o</sup>(0 K) = -86.2 ± 41.8 kJ·mol<sup>-1</sup> ΔH<sup>o</sup>(298.15 K) = -92.0 ± 41.8 kJ·mol<sup>-1</sup>

Vibrational Frequencies and Degeneracies  
ν, cm<sup>-1</sup>

- (290)(1)
- [130](1)
- [300](1)

Ground State Quantum Weight: [1]

Bond Distance: Cs-O = [2.4] Å

Bond Angle: Cs-O-Cs = [105]°

Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [1.415602 × 10<sup>-11</sup>] g<sup>3</sup>·cm<sup>6</sup>

σ = 2

Enthalpy of Formation

The appearance potentials of CsOH and Cs<sub>2</sub>O ions were investigated by Ermel'yanov *et al.*,<sup>1</sup> using the electron-impact method with a mass spectrometer fitted with a heated ion source and a Pt effusion chamber. The enthalpy of atomization of Cs<sub>2</sub>O was derived as 117 ± 10 kcal·mol<sup>-1</sup>. Based on this value we calculate the enthalpy of formation ΔH<sup>o</sup>(298.15 K) of Cs<sub>2</sub>O to be -22 ± 10 kcal·mol<sup>-1</sup> (-92.0 ± 41.8 kJ·mol<sup>-1</sup>), employing ΔH<sup>o</sup>(0 K) = 18.68 and 58.99 kcal·mol<sup>-1</sup> for Cs(g) and O(g), respectively. Brewer and Mastick<sup>2</sup> calculated theoretically the stability of gaseous alkali oxides according to ionic models and gave the enthalpies of formation from gaseous atoms for Cs<sub>2</sub>O(g) as -24 kcal·mol<sup>-1</sup>. The ΔH<sup>o</sup>(298.15 K) value is evaluated to be 72.2 kcal·mol<sup>-1</sup>, which is not adopted.

Heat Capacity and Entropy

The molecular structure of Cs<sub>2</sub>O(g) has been determined to be nonlinear by Buchler *et al.*,<sup>3</sup> using electric-deflection method. The Cs-O bond distance is assumed to be the same as that in CsOH(g) reported by Lide and Kuczukowski.<sup>4</sup> The bond angle is estimated by comparison with that in the H<sub>2</sub>O molecule. Three vibrational frequencies are estimated from those for H<sub>2</sub>O(g). The principal moments of inertia are: I<sub>A</sub> = 5.3492 × 10<sup>-39</sup>, I<sub>B</sub> = 160.0237 × 10<sup>-39</sup>, and I<sub>C</sub> = 165.3730 × 10<sup>-39</sup> g·cm<sup>2</sup>.

References

- <sup>1</sup>A. M. Ermel'yanov, A. V. Gusarov, L. N. Gorokhov, and N. A. Sadownikova, *Teor. Eksp. Khim.* **3**, 226 (1967).
- <sup>2</sup>L. Brewer and D. F. Mastick, *J. Amer. Chem. Soc.* **73**, 2045 (1951).
- <sup>3</sup>A. Buchler and J. L. Stauffer and W. Klenperer, *J. Chem. Phys.* **46**, 605 (1967).
- <sup>4</sup>D. R. Lide, Jr. and R. L. Kuczukowski, *J. Chem. Phys.* **46**, 4768 (1967).

T/K	C <sub>p</sub> <sup>o</sup> J·K <sup>-1</sup> ·mol <sup>-1</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - R ln(T <sub>2</sub> /T <sub>1</sub> )]/T J·K <sup>-1</sup> ·mol <sup>-1</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )/T kJ·mol <sup>-1</sup>	Standard State Pressure = P <sup>o</sup> = 0.1 MPa ΔG <sup>o</sup> kJ·mol <sup>-1</sup>	log K <sub>r</sub>
0	0	0	INFINITE	-86.211	INFINITE
100	43.945	262.828	363.083	-94.875	49.537
200	52.588	296.481	323.084	-100.376	26.307
250	54.345	308.420	318.595	-103.265	21.576
298.15	55.388	318.088	318.088	-105.530	18.488
300	55.420	318.431	318.089	-105.614	18.389
350	56.109	327.079	318.767	-107.104	15.984
400	56.574	334.554	320.280	-108.410	14.157
450	56.902	341.237	322.244	-109.591	12.720
500	57.141	347.246	324.449	-110.634	11.558
600	57.457	357.694	329.145	-112.441	9.789
700	57.651	366.567	333.873	-114.760	8.500
800	57.778	374.274	338.452	-117.087	7.513
900	57.866	381.085	342.818	-119.953	6.731
1000	57.929	387.185	346.955	-123.346	6.106
1100	57.976	392.708	350.867	-127.263	5.618
1200	58.012	397.755	354.567	-131.709	5.246
1300	58.040	402.399	358.070	-136.683	4.969
1400	58.062	406.701	361.392	-142.190	4.741
1500	58.080	410.708	364.548	-148.233	4.558
1600	58.094	414.457	367.551	-154.918	4.418
1700	58.106	417.979	370.415	-162.250	4.318
1800	58.117	421.300	373.151	-170.233	4.241
1900	58.123	424.443	375.768	-178.862	4.181
2000	58.133	427.424	378.277	-188.141	4.138
2100	58.139	430.261	380.686	-198.068	4.108
2200	58.144	432.966	383.002	-208.644	4.088
2300	58.149	435.550	385.230	-219.869	4.073
2400	58.153	438.025	387.372	-231.744	4.062
2500	58.157	440.399	389.432	-244.269	4.054
2600	58.160	442.680	391.456	-257.444	4.048
2700	58.163	444.875	393.394	-271.269	4.043
2800	58.166	446.991	395.271	-285.744	4.038
2900	58.168	449.032	397.089	-300.869	4.033
3000	58.170	451.004	398.854	-316.644	4.028
3100	58.172	452.911	400.567	-333.069	4.023
3200	58.174	454.758	402.221	-350.144	4.018
3300	58.176	456.548	403.821	-367.869	4.013
3400	58.177	458.285	405.366	-386.244	4.008
3500	58.179	459.972	406.961	-405.269	4.003
3600	58.180	461.611	408.556	-424.944	3.998
3700	58.181	463.205	409.915	-445.269	3.993
3800	58.182	464.756	411.137	-466.244	3.988
3900	58.183	466.268	412.277	-487.869	3.983
4000	58.184	467.741	413.338	-510.144	3.978
4100	58.185	469.177	414.310	-533.069	3.973
4200	58.185	470.579	415.193	-556.644	3.968
4300	58.186	471.949	416.000	-580.869	3.963
4400	58.187	473.286	416.734	-605.744	3.958
4500	58.187	474.594	417.404	-631.269	3.953
4600	58.188	475.873	418.025	-657.444	3.948
4700	58.188	477.124	418.593	-684.269	3.943
4800	58.189	478.349	419.117	-711.744	3.938
4900	58.189	479.549	419.600	-740.869	3.933
5000	58.190	480.725	420.046	-771.644	3.928
5100	58.190	481.877	420.454	-803.069	3.923
5200	58.191	483.007	420.820	-835.144	3.918
5300	58.191	484.115	421.147	-867.869	3.913
5400	58.191	485.203	421.434	-901.244	3.908
5500	58.192	486.271	421.681	-935.269	3.903
5600	58.192	487.319	421.893	-970.944	3.898
5700	58.192	488.349	422.070	-1008.269	3.893
5800	58.193	489.361	422.214	-1047.244	3.888
5900	58.193	490.356	422.326	-1087.869	3.883
6000	58.193	491.334	422.406	-1130.144	3.878

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

Cesium Oxide (Cs<sub>2</sub>O)

Cs<sub>2</sub>O(g)

Cesium Sulfate, I (Cs<sub>2</sub>SO<sub>4</sub>)Cesium Sulfate, I (Cs<sub>2</sub>SO<sub>4</sub>)M<sub>r</sub> = 361.8684

## CRYSTAL(I)

Cesium Sulfate, I (Cs<sub>2</sub>SO<sub>4</sub>)

S°(298.15 K) = [264.834] J·K<sup>-1</sup>·mol<sup>-1</sup>  
 T<sub>m</sub>(I→II) = 940 ± 5 K  
 T<sub>fus</sub>(I→I) = 1278 ± 5 K

ΔH°(298.15 K) = [-1410.152] kJ·mol<sup>-1</sup>  
 Δ<sub>wp</sub>H°(II→I) = 4.310 ± 0.8 kJ·mol<sup>-1</sup>  
 Δ<sub>wp</sub>H°(I→I) = 35.690 ± 0.8 kJ·mol<sup>-1</sup>

## Enthalpy of Formation

Δ<sub>f</sub>H°(Cs<sub>2</sub>SO<sub>4</sub>, cr, I, 298.15 K) is calculated from Δ<sub>f</sub>H°(Cs<sub>2</sub>SO<sub>4</sub>, cr, II, 298.15 K) by adding the enthalpy of transition (II → I) and the difference in enthalpy, H°(940)-H°(298.15 K), between the II and I crystalline forms.

## Heat Capacity and Enthalpy

High-temperature enthalpies of the I-phase of Cs<sub>2</sub>SO<sub>4</sub> have been determined by Denielou *et al.*, (960–1260 K)<sup>2</sup> and by Politschuk *et al.*, (950.7–1254.5 K).<sup>3</sup> We have adopted heat capacities based upon the enthalpies of Denielou *et al.*<sup>2</sup> We have extrapolated the heat capacities smoothly to 298.15 K below the II → I transition and extended C<sub>p</sub> above the melting point to 1500 K.

S°(298.15 K) is calculated in a manner similar to that used for the enthalpy of formation.

## Transition Data

The high-temperature hexagonal modification of cesium sulfate is denoted Cs<sub>2</sub>SO<sub>4</sub>, cr, I, in accordance with the usual nomenclature. This modification has been referred to as the α-phase in contrast to our use of α to refer to the low-temperature phase for the other members of the alkali metal sulfates.<sup>1</sup>

## Fusion Data

The adopted melting point, T<sub>fus</sub> = 1278 ± 5 K, was determined from the work of Denielou *et al.*, (1274 ± 3 K),<sup>2</sup> Politschuk *et al.*, (1281 K),<sup>3</sup> Rassonskaya and Semendyaeva, (1283 K),<sup>4</sup> and from the compilation of Stern and Weise (1277 K).<sup>5</sup> The enthalpy of fusion, Δ<sub>wp</sub>H° = 8.530 ± 0.2 kcal·mol<sup>-1</sup>, is calculated from the difference between the smoothed relative enthalpy of the liquid and the adopted enthalpy value for the I form at T<sub>fus</sub>.

## References

- <sup>1</sup>JANAF Thermochemical Tables: Cs<sub>2</sub>SO<sub>4</sub>(cr, II), 6–30–79; Na<sub>2</sub>SO<sub>4</sub>(cr, V), K<sub>2</sub>SO<sub>4</sub>(cr, ex), 6–30–78.
- <sup>2</sup>L. Denielou, Y. Fournier, J. P. Petitfret, and C. Tequi, C. R. Acad. Sci., Paris, 270, 1854 (1970).
- <sup>3</sup>A. F. Politschuk, T. A. Tishura, and A. N. Buderina, Ukr. Khim. Zh. 40, 120 (1974).
- <sup>4</sup>I. S. Rassonskaya and N. K. Semendyaeva, Russ. J. Inorg. Chem. 15, 27 (1970).
- <sup>5</sup>K. H. Stern and E. L. Weise, NSRDS - NBS 7, (1966).

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> J·K <sup>-1</sup> ·mol <sup>-1</sup>	S° J·K <sup>-1</sup> ·mol <sup>-1</sup>	H°-H°(T <sub>r</sub> )/T	Δ <sub>f</sub> H° kJ·mol <sup>-1</sup>	
0					
100					
200					
298.15	108.700	264.834	0.	-1410.152	228.885
300	108.784	265.506	0.201	-1410.221	227.361
400	112.131	297.150	11.209	-1420.312	165.713
500	120.081	322.947	22.784	-1423.046	128.561
600	132.256	345.866	35.373	-1428.574	103.718
700	147.737	367.416	49.373	-1430.624	85.937
800	163.218	388.154	64.921	-1431.748	72.590
900	178.699	408.272	82.016	-1433.308	62.147
940.000	184.891	416.177	89.288	---	---
1000	194.179	427.901	100.660	-1613.897	53.161
1100	209.660	447.135	120.852	-1606.752	45.513
1200	225.141	466.041	142.592	-1598.155	39.171
1278.000	237.233	480.596	160.625	---	---
1300	240.622	484.675	165.882	---	33.836
1400	256.103	503.073	190.718	---	29.393
1500	271.583	521.270	217.103	-1563.560	25.387

PREVIOUS

CURRENT: June 1979

Cesium Sulfate, I (Cs<sub>2</sub>SO<sub>4</sub>)Cs<sub>2</sub>O<sub>7</sub>S<sub>1</sub>(cr)

Cs<sub>2</sub>O<sub>4</sub>S<sub>1</sub>(cr)

Cesium Sulfate, II (Cs<sub>2</sub>SO<sub>4</sub>)

CRYSTAL(II)

Cesium Sulfate, II (Cs<sub>2</sub>SO<sub>4</sub>)

M<sub>r</sub> = 361.8684

S<sup>o</sup>(298.15 K) = 211.88 ± 0.21 J·K<sup>-1</sup>·mol<sup>-1</sup>  
 T<sub>m</sub>(α→β) = 940 ± 5 K  
 $\Delta_f H^\circ(0 \text{ K}) = -1433.16 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15 \text{ K}) = -1442.64 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{tr}} H^\circ(\alpha \rightarrow \beta) = 4.310 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$

**Enthalpy of Formation**

The enthalpy of solution at infinite dilution of Cs<sub>2</sub>SO<sub>4</sub> has been measured by Kuznetsova *et al.*,<sup>1</sup> (3.980 kcal·mol<sup>-1</sup>), and by Borob'ev *et al.*,<sup>2</sup> (4.11 ± 0.80 kcal·mol<sup>-1</sup>). We adopt the mean of these values 4.05 ± 0.1 kcal·mol<sup>-1</sup>. When this result is combined with enthalpies of formation of the infinitely dilute ions from CODATA,<sup>3</sup> we obtain  $\Delta_f H^\circ(\text{Cs}_2\text{SO}_4, \infty\text{H}_2\text{O}, 298.15 \text{ K}) = -340.746 \pm 0.12 \text{ kcal}\cdot\text{mol}^{-1}$  and  $\Delta_f H^\circ(\text{Cs}_2\text{SO}_4, \text{cr}, 298.15 \text{ K}) = -344.80 \pm 0.2 \text{ kcal}\cdot\text{mol}^{-1}$ .

**Heat Capacity and Entropy**

The low temperature heat capacities of Cs<sub>2</sub>SO<sub>4</sub> were measured by Paukov *et al.*<sup>4</sup> by adiabatic calorimetry over the region 12.82–308.72 K. The curve of C<sub>p</sub>-T was graphically extrapolated to 0 K. Our adopted value of S<sup>o</sup>(298.15 K) = 50.64 ± 0.05 cal·K<sup>-1</sup>·mol<sup>-1</sup> is based on S<sup>o</sup>(12 K) = 0.309 cal·K<sup>-1</sup>·mol<sup>-1</sup> as estimated by Paukov *et al.*<sup>4</sup> They also estimated H<sup>o</sup>(12 K)-H<sup>o</sup>(0 K) = 2.83 cal·K<sup>-1</sup>·mol<sup>-1</sup>, which leads to H<sup>o</sup>(298.15 K)-H<sup>o</sup>(0 K) = 6.628 ± 0.006 kcal·mol<sup>-1</sup>. These values of S<sup>o</sup>(12 K) and H<sup>o</sup>(12 K)-H<sup>o</sup>(0 K) are almost identical to estimates obtained using a Debye T<sup>-3</sup>-law extrapolation. We have smoothed the experimental data of Paukov *et al.*<sup>4</sup> by fitting to orthogonal polynomials.

High temperature heat capacities of Cs<sub>2</sub>SO<sub>4</sub> have been measured by Shmidt<sup>5</sup> by adiabatic calorimetry over the range 297.5–774.0 K. Enthalpy measurements by drop calorimetry were carried out by Denielou *et al.*,<sup>6</sup> (400–910 K) and by Politschuk *et al.*,<sup>7</sup> (803.3–933.4 K). We have joined the low temperature C<sub>p</sub> data of Paukov<sup>4</sup> to the high temperature C<sub>p</sub> data of Shmidt<sup>5</sup> and then merged this into C<sub>p</sub> values derived from the measurements of Denielou *et al.*<sup>6</sup> above 700 K. We have extrapolated the data smoothly to 1200 K.

**Transition Data**

Cs<sub>2</sub>SO<sub>4</sub>(cr, II) is the low-temperature form of cesium sulfate (often denoted as Cs<sub>2</sub>SO<sub>4</sub>, β). The crystals are orthorhombic, space group D<sub>2h</sub><sup>16</sup>-Pmcn.<sup>8</sup> The transformation to the high-temperature I-phase (hexagonal, Cs<sub>2</sub>SO<sub>4</sub>, I) occurs at 940 ± 5 K.<sup>2,7</sup> The enthalpy of transition is determined by taking the difference between the adopted enthalpy curves of II- and I-Cs<sub>2</sub>SO<sub>4</sub>, extended to 940 K.

**References**

- <sup>1</sup>G. P. Kuznetsova, G. A. Lovetskaya, V. M. Presnyakova, and B. O. Stepin, *Russ. J. Phys. Chem.* **48**, 2141 (1974).
- <sup>2</sup>A. F. Borob'ev, N. A. Ibragim, and S. M. Skuratov, *Russ. J. Inorg. Chem.* **11**, 13 (1966).
- <sup>3</sup>CSU-CODATA Task Group on Key Values for Thermodynamics, *J. Chem. Thermodyn.* **10**, 903 (1978).
- <sup>4</sup>I. E. Paukov, L. M. Khriplovich, and A. M. Korotkikh, *Russ. J. Phys. Chem.* **42**, 661 (1968).
- <sup>5</sup>N. E. Shmidt, *Russ. J. Phys. Chem.* **12**, 929 (1967).
- <sup>6</sup>L. Denielou, Y. Fournier, J. P. Pettiet and C. Tequi, *C. R. Acad. Sci., Paris*, **270**, 1854 (1970).
- <sup>7</sup>A. F. Politschuk, T. A. Tishura, and A. N. Buderina, *Ukr. Khim. Zh.*, **40**, 120 (1974).
- <sup>8</sup>C. N. R. Rao and B. Prakash, *NSRDS-NBS* **56**, (1975).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K			Standard State Pressure = p <sup>o</sup> = 0.1 MPa		
	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>	Δ <sub>f</sub> G <sup>o</sup>	log K <sub>f</sub>
0	0	0	0	-1433.163	-1433.163	INFINITE
100	89.287	91.922	INFINITE	-1438.791	-1401.080	731.849
200	114.767	162.172	317.566	-1441.328	-1362.260	355.786
298.15	135.143	211.878	223.551	0	-1323.155	231.811
300	135.478	212.715	211.878	0.250	-1322.413	230.253
400	151.223	253.916	217.391	14.610	-1280.787	167.254
500	164.337	289.120	228.298	30.411	-1238.562	129.392
600	176.816	320.158	241.069	47.453	-1196.356	104.152
700	192.255	348.512	254.416	65.867	-1154.417	86.144
800	212.464	375.547	267.877	86.136	-1112.937	72.667
900	228.697	401.504	281.293	108.190	-1071.010	62.160
940.000	235.337	411.592	286.624	117.470	-----	-----
1000	245.266	426.458	294.570	131.888	-1017.551	53.151
1100	261.835	450.612	307.663	157.244	-1602.852	45.509
1200	278.362	474.103	320.558	184.254	-1588.984	39.193

PREVIOUS:

CURRENT June 1979

Cs<sub>2</sub>O<sub>4</sub>S<sub>1</sub>(cr)

Cesium Sulfate, II (Cs<sub>2</sub>SO<sub>4</sub>)

Cs<sub>2</sub>O<sub>4</sub>S<sub>4</sub>(l)Cesium Sulfate (Cs<sub>2</sub>SO<sub>4</sub>)

LIQUID(l)

Cesium Sulfate (Cs<sub>2</sub>SO<sub>4</sub>)

$S^{\circ}(298.15\text{ K}) = [246.449] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}}(l \rightarrow \text{I}) = 1278 \pm 5 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $\Delta H^{\circ}(298.15\text{ K}) = [-1400.139] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{liq}}H^{\circ}(l \rightarrow \text{I}) = 35.690 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$

**Enthalpy of Formation**

$\Delta_{\text{f}}H^{\circ}(\text{Cs}_2\text{SO}_4, \text{I}, 298.15\text{ K})$  is calculated from  $\Delta_{\text{f}}H^{\circ}(\text{Cs}_2\text{SO}_4, \text{cr}, \text{I}, 298.15\text{ K})$  by adding  $\Delta_{\text{liq}}H^{\circ}$  and the difference in enthalpy,  $H^{\circ}(1278) - H^{\circ}(298.15\text{ K})$ , between the I crystal and liquid.<sup>1</sup>

**Heat Capacity and Entropy**

Enthalpies for Cs<sub>2</sub>SO<sub>4</sub>(l) have been measured by Denielou *et al.*<sup>2</sup> and by Polishchuk *et al.*<sup>3</sup> We adopt enthalpies based on the work of Denielou *et al.*<sup>2</sup> This leads to a constant heat capacity of  $49.4 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  at temperatures above an assumed glass transition at 780 K. Below the glass transition, the heat capacity is taken as that of the low temperature II phase.  $S^{\circ}(298.15\text{ K})$  is calculated in a manner analogous to that used for the enthalpy of formation.

**Fusion Data**

Refer to the I-crystal table for details.

**References**

- <sup>1</sup>JANAF Thermochemical Tables: Cs<sub>2</sub>SO<sub>4</sub>(cr, I), 6-30-79.
- <sup>2</sup>L. Denielou, Y. Fournier, J.-P. Petit, and C. Tequi, C. R. Acad. Sci. Paris **270**, 1854 (1970).
- <sup>3</sup>A. F. Polishchuk, T. A. Tishura, and A. N. Budarina, Ukr. Khim. Zh. **40**, 120 (1974).

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )/J	Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
		S <sup>o</sup> - (S <sup>o</sup> - IF(T <sub>r</sub> ))/T	J·K <sup>-1</sup> ·mol <sup>-1</sup>		ΔH <sup>o</sup>	ΔG <sup>o</sup>	
0							
100							
200							
298.15	135.143	246.449	246.449	0.	-1400.139	-1290.958	226.171
300	135.478	247.286	246.452	0.250	-1400.159	-1290.281	224.658
400	151.293	288.488	251.962	14.610	-1406.897	-1252.112	163.509
500	164.537	323.692	262.869	30.411	-1407.406	-1213.344	126.357
600	176.816	354.729	275.640	47.453	-1406.482	-1174.595	102.258
700	192.235	383.084	288.988	65.867	-1404.117	-1136.113	84.778
800	212.464	409.874	302.434	85.952	-1400.103	-1098.078	71.697
880.000	241.626	431.400	313.174	104.039			
880.000	206.690	431.400	313.174	104.039			
900	206.690	436.045	315.853	108.173	-1447.139	-1059.609	61.498
1000	206.690	457.822	328.980	128.842	-1575.703	-1009.458	32.729
1100	206.690	477.521	341.603	149.511	-1568.081	-953.203	45.264
1200	206.690	495.506	353.689	170.180	-1560.555	-897.638	39.073
1278.000	206.690	508.522	362.746	186.301			
1300	206.690	512.050	365.243	190.849	-1553.113	-842.697	33.860
1400	206.690	527.367	376.383	211.518	-1546.751	-788.526	29.413
1500	206.690	541.627	386.636	232.187	-1538.463	-734.480	23.577
1600	206.690	554.967	396.932	252.856	-1531.249	-681.116	22.236
1700	206.690	567.497	406.600	273.524	-1524.110	-628.202	19.302
1800	206.690	579.311	415.870	294.193	-1517.048	-575.706	16.707
1900	206.690	590.486	424.769	314.862	-1510.070	-523.600	14.395
2000	206.690	601.088	433.332	335.531	-1503.179	-471.859	12.324
2100	206.690	611.173	441.553	356.200	-1496.384	-420.460	10.438
2200	206.690	620.788	449.484	376.869	-1489.693	-369.382	8.770
2300	206.690	629.975	457.133	397.538	-1483.114	-318.607	7.236
2400	206.690	638.772	464.519	418.207	-1476.658	-268.116	5.835
2500	206.690	647.210	471.659	438.876	-1470.335	-217.891	4.553
2600	206.690	655.316	478.568	459.545	-1464.154	-167.915	3.373
2700	206.690	663.117	485.760	480.214	-1458.178	-118.174	2.286
2800	206.690	670.633	491.747	500.883	-1452.466	-68.654	1.281
2900	206.690	677.886	498.041	521.552	-1446.981	-19.341	0.348
3000	206.690	684.894	504.153	542.221	-1441.084	29.780	-0.519

PREVIOUS:

CURRENT: June 1979

Cesium Sulfate (Cs<sub>2</sub>SO<sub>4</sub>)Cs<sub>2</sub>O<sub>4</sub>S<sub>4</sub>(l)

Cs<sub>2</sub>O<sub>4</sub>(cr,l)

M<sub>r</sub> = 361.8684 Cesium Sulfate (Cs<sub>2</sub>SO<sub>4</sub>)

CRYSTAL(I-II)-LIQUID

Cesium Sulfate (Cs<sub>2</sub>SO<sub>4</sub>)

0 to 940 K crystal, II  
940 to 1278 K crystal, I  
above 127 K liquid

Refer to the individual tables for details.

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> H°	
		J·K <sup>-1</sup> ·mol <sup>-1</sup>	J·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	
0	0	INFINITE	INFINITE	-1433.163	INFINITE
100	89.287	91.922	317.566	-1401.080	731.849
200	114.767	162.172	223.531	-1441.328	335.786
298.15	135.143	211.878	211.878	0	231.811
300	135.478	212.715	211.880	0.250	230.253
400	151.293	253.916	217.391	14.610	167.254
500	164.537	289.120	228.298	30.411	129.392
600	176.816	320.158	241.069	47.453	104.152
700	192.235	348.512	254.416	63.667	86.144
800	212.468	375.547	267.877	86.136	72.667
900	228.697	401.504	281.293	108.190	62.160
940.000	235.337	411.592	286.624	117.470	62.160
940.000	184.891	416.177	286.624	121.780	53.161
1000	194.179	427.901	294.750	133.152	45.513
1100	209.660	447.135	307.731	153.344	39.171
1200	225.141	466.041	320.138	175.084	
1278.000	237.233	480.596	329.488	193.116	
1278.000	206.690	508.522	329.488	228.806	
1300	206.690	512.050	332.548	233.353	33.860
1400	206.690	577.367	345.923	254.022	29.413
1500	206.690	541.627	358.500	274.691	25.577
1600	206.690	554.967	370.367	295.560	22.236
1700	206.690	567.497	381.598	316.029	19.302
1800	206.690	579.311	392.257	336.698	16.707
1900	206.690	590.486	402.399	357.367	14.395
2000	206.690	601.088	412.070	378.035	12.324
2100	206.690	611.173	421.313	398.704	10.458
2200	206.690	620.788	430.163	419.373	8.770
2300	206.690	629.975	438.653	440.042	7.236
2400	206.690	638.772	446.809	460.711	5.835
2500	206.690	647.210	454.657	481.380	4.553
2600	206.690	655.316	462.220	502.049	3.373
2700	206.690	663.117	469.517	522.718	2.286
2800	206.690	670.633	476.567	543.387	1.281
2900	206.690	677.886	483.384	564.056	0.348
3000	206.690	684.894	489.985	584.725	-0.519

PREVIOUS:

CURRENT: June 1979

Cesium Sulfate (Cs<sub>2</sub>SO<sub>4</sub>)

Cs<sub>2</sub>O<sub>4</sub>(cr,l)





## Cesium

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## Continuation of discussions of selected Cs species

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<sup>11</sup>JANAF Thermochemical Tables:  $\text{Li}_2\text{SO}_4(\text{g})$ , 12-31-78;  $\text{K}_2\text{SO}_4(\text{g})$ , Na<sub>2</sub>SO<sub>4</sub>(g), 6-30-78.