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Enthalpy Reference Temperature = T. = 298.15 K

Mo₁(ref)

Standard State Pressure = $p^* = 0.1$ MPa

LJ·mol⁻ A.H.•

H*-H*(T;)

S -[G-H'(T,)]/T

7,

ideal monatomic gas

to 2896 to 4951.969 4951.969

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Refer to the individual tables for details.

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Molybdenum (Mo)

Mo₁(cr)

CURRENT March 1978

CRYSTAL

A, = 95.94 Molybdenum (Mo)

 $S^{\circ}(298.15 \text{ K}) = 28.605 \pm 0.050 \text{ J·K}^{-1} \cdot \text{mol}^{-1}$ Firs = 2896 ± 8 K

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

The low temperature heat capacities of Mo(cr) have been measured by Clusius and Franzosim1 between 16 and 256 K (63 measured C, points). The reported C, values are smoothed by fitting the data with orthogonal polynomials over selected overlapping temperature intervals. This fitting procedure also includes the smoothed C° values (275-335 K) reported in the critical evaluation by Dimars et al. so as to provide smoothly varying heat capacity values in the range 256-275 K. The data of Simon and Zeidler, 15-238 K, are as much as 2.5% high below 78 K and as much as 1% low above 78 K.

Below 20 K several investigators ⁴⁻⁷ have determined the heat capacity. Heiniger et all ² have summarized and critically reviewed this work as well as other studies. These sources give S'(20 K) values in the range 0.021-0.025 cal·K⁻¹-mol⁻¹. Adopting S'(20 K) = 0.024 cal·K⁻¹·mol⁻¹ and combining this with our analysis of the Clusius and Franzosoni work, we calculate S'(298,15 K) = 6.836 ± 0.012 cal·K⁻¹·mol⁻¹. This result agrees with the review of the heat capacity data (T <298.15 K) by Reilly and Furukawa' for Brewer.

capacity/enthalpy studies covering the 270-2800 K on NBS Standard Reference Material No. 781. In addition, the report contains a NBS results with those of all the principal investigators and critical evaluation is also given in the publication. These results are linearly extrapolated from 2800 K to 3300 K. The high temperature heat capacity values adopted by Brewer, 10 based on IPTS-48, are within 0.1% The high temperature heat capacity values, 273-2800 K, are those selected by Ditmars et al 2 This study reports three recent NBS hear bibliography of publications on the high temperature enthalpy and heat capacity of crystalline molybdenum. A graphical comparison of the of the NBS results between 298 and 900 K and are 0.2 to 0.3% higher between 1000 and 1400 K. Between 1500 and 1900 K, the difference at 2800 K is 0.5% lower than our adopted value. At 2800 K, the entropy difference is 0.004 cal·K-1·mol-1 with the JANAF value being rs less than 0.1%. From 2000 to 2300 K, the values are 0.2 to 0.3% lower and are 0.1% low to 0.2% high between 2400 to 2700 K. The value

Fusion Data

Refer to the liquid table for details.

Sublimation Data

Eight sublimation studies are discussed on the ideal gas table.

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Standard State Pressure = p = 0.1 MPa odod o ododdddddd odddd ddddd ddddd dd 0.050 1.258 3.460 4.436 ರರದಂದ ರ ದರದರದದದದದದ ದರದದದ ದದದದದ -31.771 -29.189 -26.268 ರೆದಿರರ ರ ರೆರರೆರರದೆರೆದರು ರೆರರೆರರ ರೆದರೆರರ ಕೆರೆರೆರರ ಕರ್ $H^{\bullet}-H^{\bullet}(T_{r})$ 0.0044 1.258 1.258 1.265 Enthalpy Reference Temperature = T, = 298.15 K $-[G^{\bullet}-H^{\bullet}(T_{i})]T$ 51.384 52.796 54.160 55.481 56.763 59.226 60.414 61.577 63.837 64.939 66.027 67.060 J·K-'mol-' 28.605 28.753 32.494 35.810 38.789 41.494 46.263 50.382 54.015 60.235 62.963 65.502 67.588 70.148 70.148 74.373 76.373 76.373 76.373 76.373 76.373 76.373 76.373 76.373 76.373 76.373 76.373 76.373 80.198 80.198 81.645 81 92.713 94.490 96.304 98.098 98.173 100.094 23.938 24.580 25.080 25.500 25.850 25.850 26.980 27.890 27.890 28.900 29.490 30.140 30.860 31.650 32.500 33.420 34.420 35.490 36.650 37.900 39.240 42.210 45.880 48.370 51.570 23.933 54.835 298.15 $\Delta_t H^{\circ}(0 \text{ K}) = 0 \text{ kJ} \cdot \text{mol}^{-1}$ Δ_tH°(298.15 K) = 0 kJ·mol⁻¹ $\Delta_{lu}H^{\circ} = 36.0 \pm 5.4 \text{ kJ} \cdot \text{mol}^{-1}$

Molybdenum (Mo)

PREVIOUS: December 1966

CURRENT: March 1978

A_r = 95.94 Molybdenum (Mo)

Molybdenum (Mo)

PREVIOUS: December 1966

$\Delta_1 H^{\circ}(298.15 \text{ K}) = [41.568] \text{ kJ·mol}^{-1}$ Enthalpy R $\Delta_{\text{lut}} H^{\circ} = 36.0 \pm 5.4 \text{ kJ·mol}^{-1}$	15 K) = [43.146] J·K ⁻¹ ·mol ⁻¹ 396 + 8 K
$\Delta_t H^{\circ}(298.15 \text{ K}) = [41.568] \text{ kJ} \cdot \text{mol}^{-1}$ Enthalpy R	$ 5K\rangle = [43 46 1.K^{-1} \cdot mo]^{-1}$

LIQUID

Molybdenum (Mo)

 $T_{\rm fus} = 2896 \pm 8 \, \rm K$

Enthalpy of Formation

The enthalpy of formation is calculated from that of the crystal by addition of $\Delta_{ho}H^{\circ}$ and the difference in enthalpy, $H^{\circ}(2896)$ H°(298.15 K), between the crystal and liquid.

Heat Capacity and Entropy

Enthalpy measurements via levitation calorimetry by Treverton and Margrave3 were over a sufficient range of temperature, 2692-3112 insufficient to define a liquid phase heat capacity value. Shaner et al. 3 and Dikther and Lebedev⁶ have reported $C_p^0(1)$ values of 1. to establish C₂(I) = 8.19 cal·K⁻¹·mol⁻¹. The enthalpy measurements of Berezin et al.² in the liquid region (14 pts., 2890-2925 K)

cal K^{-1} -mol⁻¹ and 14.0 cal K^{-1} -mol⁻¹, respectively, using pulse heating techniques. We adopt $C_p^o(1) = 9.0$ cal K^{-1} -mol⁻¹ as did Brewer. This value implies a heavier weighting of the drop calorimetric studies rather than pulse heating techniques. The magnitude of the difference of the $C_p^o(1)$ values derived from the various studies^{3,3,6} suggests further study this area. A glass transition is assumed at 2150 K below which the heat capacity is assumed to be that of the crystal The entropy is calcula in a manner analogous to the enthalpy of formation.

The adopted melting point, T_{tat} = 2896 \pm 8 K, is derived from the recent experimental study and critical evaluation of earlier data

2890–2925 K, respectively. They reported $\Delta_{nn}H^2 = 8.741 \pm 0.314$ kcal mol⁻¹ at an assumed melting temperature of 2890 K. Correcting th results to $T_{nn} = 2896$ K yields 8 693 \pm 0.314 kcal mol⁻¹. Shaner *et al.*, using a pulse–heating technique, reported enthalpy measureme Bererzin et al.² have measured the enthalpy of crystal and liquid molybdenum by levitation calorimetry in the range 1962-2869 K. (1978–4450 K) which gave $\Delta_{lu}H^{\circ} = 8.553$ kcal·mol⁻¹ at a melting point of 2883 K.

Freverton and Margrave 3 also used levitation calorimetry to measure the liquid phase enthalpy of molybdenum in the range 2693-3115 Using the enthalpy value for the liquid at the melting point as determined by Treverton and Margrave and the enthalpy value of the cry-

at the melting point as determined by our adopted functions, we calculate $b_{n}H^{-} = 1.24$ kcal-mol⁻¹. Lebedov et al.¹ reported $\Delta_{lan}H^{0} = 9.8$ kcal-mol⁻¹ (exploding wire technique) while Kostikov et al.¹ found $\Delta_{lan}H^{0} = 6.095$ kcal-mol⁻¹ (drop technique). We adopt $\Delta_{lan}H^{0} = 8.6 \pm 1.3$ kcal-mol⁻¹, which corresponds to $\Delta_{lan}S^{0} = 2.97$ cal-K⁻¹·mol⁻¹. This $\Delta_{lan}S^{0}$ appears high for a metal will bec (A2) structure; however, this value is supported by the studies of Berezin et al.² and Shaner et al.³ Brewer² selected a value $\Delta_{tor}H^{\circ} = 8.54 \pm 0.3 \text{ kcal-mol}^{-1} \text{ (IPTS-48)}.$

Vaporization Data

The boiling point and enthalpy of vaporization are calculated from the adopted functions and enthalpy of sublimation in order to main

proper themodynamic consistency.

Koch and Anable* have measured the vapor pressure of liquid molybdenum by a Langmuir free-evaporation method. They measured data points in the range 2895–2995 K. A 2nd and 3th law analysis gives $\Delta_{rup}H^{o}(298.15 \text{ K})$ values of 136.8 \pm 18.4 and 147.7 \pm 1.7 kcal·mol respectively. This corresponds to our adopted value of $\Delta_{uu}H^{o}(298.15 \text{ K}) = 147.565 \text{ kcal·mol}^{-1}$. Note, however, that there is a signific difference between the 2nd and 3rd law results.

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²B. Ya Berezin, V. Ya. Chekhovskoi, and A. E. Sheindlin, High Temperatures-High Pressures 3, 287 (1971).

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	Enthalpy Reference	ř	Temperature =	T, = 298.15 1	×	Standard State Pressure	Pressure = p	- 0.1 MPa
ol-1	7/K] :	J·K ⁻ 'mol'. S -[G'.	-[G*-H'(T,)]/T	H*H*(T,)	KJ-mod -	$\Delta_i G^{\bullet}$	log Kr
Ϋ́	986							
	298.15	23.932	43.146	43.146	ď	41.568	37.233	-6.523
	85	23.958	43.294	43.146 43.440	0.044	41.568	37.206 36.479	-6.478
2 K,	\$\$	25.080	50.351	101.44	2500	41.568	35.752	-4.669
16.7	7 <u>8</u>	25.850	56.035	45.938	5.049	41.568	34.298	-3.583
	88	26.980	64.922	48.028	7.665	41.568 41.568	32.844 31.390	-2859
ı the	888	27.440	68.555	52 232	13.059	41.568	29.935	-1.955
E 7	88	28.370	74.776	56.138	18.638	41.568	17.027	-1 412
1	1700	28.900	77.504 80.043	57.958 59.694	24.419	41.568 41.568	25.573	-1.214
	865	30.14 30.860 30.860	82.479 84.689	61.352 62.939 64.461	30.450	4 4 4 80 80 80 80 80 80	21.211	0.791
a by	000	32.500	88.914	65.925	36.782	41.568	18.303	-0.598
7	0021	33.420	90.912	67.337	43.469	41.568	15.395	-0.518 -0.447
hese	888	35.490	94.739	70.021	46.964 50.570	41.568	13.940	-0.383
ents	2100	37.900	98.407	12.551	54.297	41.568	11.032	-0.274
5 K.	2150.000	38.550 37.656	99.306 99.306	73.163 73.163	\$6.208 \$6.208	CLASS	RANSTHON	 e
ystal	2200	37.656	100.172	73.767	58.091	41.506	9.579 9.579	-0.227
864	540 540 540 540 540 540 540 540 540 540	37.656	103.448	76.106	65.622	40.900	6.699	91.0
ith a	2600	37.656	106.462	78.327	73.153	39.642	3.894	-0.078
e of	2800	37.656	107.884	79.395	76.919 80.684	38.700 37.475	2537 1219	-0.049 -0.023
	2896.000	37.656	110.522	81.414	84.299	CRYSTA	T <> LIQUID	B
	3000	37.656 37.656	110.574	81.454 82.446	84.450 88.215	ರ ರ	ೆ ೆ	ರ ರ
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icant	3800	37.656	118.716	87.936	110.809	ံ ဝံ	o o	io
	3200	37.656	119.748	88.782 89.610	114.575	ರರ	ರರ	o o
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nergy	2300	37.656 37.656	132.564	99.668 100.295	171.059	- 594.890	29.683	-0.298 -0.411
	2400	37.656	133.985	100.912	06581	-598.972	78 040	-0.320
	888	37.656	136.676	103.287	193.652	-608.795	102.474	-0.923
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Molybdenum (Mo)

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3400	37.656	116.564	73.962	141.080	o c	o c	o' c
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4	37.656	126273	84.795	182.502	óó	ó	o c
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800	37.656	129.549	88.390	197.564	jo	ဝံဝံ	ತ ರ
4900	37.656	130,326	89.238	201,330		ö	o
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2000	37.656	131.087	90.068	205.096	-591,385	5.731	-0.060
200	37.656	131,832	90.879	208.861	- 593.064	17.690	-0.181
2300	37.656	133.281	92.452	216.392	-596.860	41 713	-0.411
\$500	37.656	133.985	93.215	220.158	-598.972	53.781	-0.520
2000	37.66	256.364	70.56	476.577	-001.224	65.889	-0.62
888	37.656	136.676	96.120	235.220	-608.795	102.475	-0.728
3	000.	137.32	4.47	242.752	-614 401	32	2
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IL-LIQUID

CRYSTAL-LIQUID

Refer to the individual tables for details.

0 to 2896 K crystal above 2896 K liquid

Molybdenum (Mo)

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

Mo₁(g)

Molybdenum (Mo)

Molybdenum (Mo)

 $\Delta_t H^{\circ}(0 \text{ K}) = 657.37 \pm 3.8 \text{ kJ} \cdot \text{mol}^{-1}$ $I^{\circ}(298 \text{ 15 K}) = 658.98 \pm 3.8 \text{ kJ} \cdot \text{mol}^{-1}$

Δ_{p}				
	Veights 8,	2 -	 	
	ronic Levels and Quantum Weights €, cm ⁻¹ 8,	10768.33 10965.97		

State State 5.53 🖴 IP(Mo, g) = $57260 \pm 50 \text{ cm}^{-1}$ S°(298.15 K) = $181.951 \pm 0.04 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$

Enthalpy of Formation

The entitalpy of formation at 298 15 K for Mo(g) is simply the entitalpy of sublimation at 298.15 K, i.e. $Mo(cr) \rightarrow Mo(g)$. The following table summarizes the analysis of the numerous sublimation studies by a 2nd and 3rd law calculation. All temperatures have been corrected to IPTS-68. All studies are based on the Langmuir effusion method.

98.15 K), I	2nd law 3rd law cal·K-'-mol-'	158.5	156.2 ± 1.4	158.4 ± 2.6 157.8 ± 0.8 -0.3 ± 1.1	158.4 ± 1.2	148.8	156.9 ± 0.6	158.2 ± 1.4
	7/K	1201–2396	2068-2500	2144-2537	2154-2466	1601-2297	2089-2493	2293–2673
Data	Points	edu	. 6	12	6	Eda	12	01
	Source	_	2	'n	4	5	•	7

to 298.15 K, we calculate $\Delta_{ab}H^0(298.15 \text{ K}) = 149.8 \text{ kcal·mol}^{-1}$.

We adopt $\Delta_{ab}H^0(298.15 \text{ K}) = 157.5 \pm 0.9 \text{ kcal·mol}^{-1}$ from a consideration of five studies. ¹⁻³6.7 Brewer ¹² has adopted a value 0.2 kcal·mol ⁻¹ less positive, however his vapor pressure analysis is based on the 1948 temperature scale. A mass spectrometric study of the enthalpy of sublimation of molybdenum^{*} yielded, $\Delta_{ab}H^o(2500 \text{ K}) = 144.1 \pm 2.2 \text{ kcal-mol}^{-1}$; correcting

Heat Capacity and Entropy

and cut-off procedures.¹¹ In fact, the inclusion of some higher states (n = 5, 6, 7) and consideration of various cut-off procedures leads to calculational differences in the Gibbs energy function of roughly 0.1 cal·K⁻¹ mol⁻¹ or greater at temperatures in excess of 7600 K. The thermal functions adopted here are the same as those of Brewer.¹² unaffected up to 4000 K. The reported uncertainty in S'(298.15 K) is due to uncertainties in the relative atomic gas and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states and utilization of proper fill The efectronic energy levels are given in the compilations by Moore, 10 Although we have only listed the ground state, first excited state, and the ionization limit for Mo(g), all levels listed by Moore, 10 as well as estimated levels, are used in our highest observed excited state, and the ionization limit for Mo(g), all levels listed by Moore, 10 as well as estimated levels, are used in our calculations. The observed levels are too numerous to list completely. An examination of the estimates for missing levels suggests that they levels (for n = 5, 6, 7), the cut-off procedure, and the inclusion of n = 6, 7 levels up to 3000 K. The Gibbs energy function is essentially all he above 20000 cm-1. Our calculations indicate that for Mo(g) the thermochemical functions are independent of the estimated missing

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CURRENT March 1978 (1 bar) Standard State Pressure = $p^* = 0.1$ MPa -106.729 -90340 -68.497 -68.497 -61.256 -40.401 -30.342 -20.843 -20.843 -20.843 -20.843 -11.567 -11.573 -11.57 -3.685 -3.376 -3.086 -2.814 -2.557 -5.676 -5.206 -4.771 -4.369 -2315 -1.800 -1.865 -1.469 -1.284 -1.107 -0.938 -0.475 NFINITE -336.252 -164.110 -129.679 -107.441 -- FUGACTTY - 1 bar 282.518 255.541 222.541 222.541 222.541 220.600 200.832 11.360 11 350.919 337.079 323.318 309.636 296.036 41.807 29.962 18.092 6.195 657.367 658.373 650.655 611.266 611.276 605.373 882.525 882.525 882.525 882.525 882.525 882.526 882.526 882.526 882.748 882.748 872.74 654.147 653.307 652.406 651.437 650.396 632.892 630.596 628.082 589.392 588.258 587.212 586.261 585.412 584.672 584.048 583.033 583.358 583.832 584.456 585.233 658.974 658.800 658.372 658.372 658.127 657.589 656.995 656.352 656.353 656.353 658.980 -6.197
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-1 134.938 142.946 148.537 160.150 166.168 172.323 178.613 185.035 191.585 Enthalpy Reference Temperature = T. = 298.15 K 215.113 215.703 216.287 216.865 217.438 218.006 218.571 219.133 219.692 220.248 $S^{\bullet} - [G^{\bullet} - H^{\bullet}(T_{r})]T$ 199.963 200.396 200.298 200.298 201.835 201.835 206.544 206.544 207.137 200.346 200.346 200.346 200.346 200.346 210.041 210.04 220.803 221.356 221.908 222.459 222.746 223.010 J·K⁻¹mol⁻¹ 227.473 228.332 229.233 231.070 231.070 231.505 231.80 251.588 252.674 253.766 254.865 255.969 249.995 250.510 182.079 185.283 188.059 190.507 192.697 196.487 199.691 202.467 204.915 209.086 210.895 212.560 214.102 215.540 216.888 218.158 219.360 220.505 221.600 222.652 223.667 224.652 225.611 0. 159.243 173.651 178.290 181.951 PREVIOUS March 1978 (1 atm) 0 20786 2078 53,001 55 185 56 640 58.072 1951.969 5000 5100 5300 5300 5300 5500 5500 5700 5800 5800 5800 5900

Mo;(g)

M, = 95.93945 Molybdenum, lon (Mo*)

IDEAL GAS

Molybdenum, lon (Mo⁺)

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CURRENT March 1984 (1 bar)

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PREVIOUS March 1978 (1 atm)

$P(Mo^+, g) = 130300 \pm 500 \text{ cm}^{-1}$ S°(298.15 K) = 180 669 ± 0.05 J·K·mol ⁻¹				$\Delta_t H^{\circ}(0 \text{ K}) = 1342.35 \pm 4.0 \text{ kJ} \cdot \text{mol}^{-1}$ $\Delta_t H^{\circ}(298.15 \text{ K}) = [1350 159] \text{ kJ} \cdot \text{mol}^{-1}$	L	eference Ter	emperature =	Enthalpy Reference Temperature = T, = 298.15 K J·K-'mol-'		Standard State Pressure = p° = 0.1 MPa kJ·mol ⁻¹	Pressure = p	- 0.1 MPa
					7.K	ប	$S^{\bullet} - [G^{\bullet} - H^{\bullet}(T_{\bullet})]H$	-H'(T,)]/T	$H^{\bullet}-H^{\bullet}(T_t)$	$\Delta_i H^{\bullet}$	₽'0	log Kr
	Electronic State	Electronic Levels and Quantum Weights State	antum Weights		0000	0. 20.786 20.786	0. 1 157.962 172.369	INFINITE 199.149 182.570	-6.197 -4.119 -2.040	1342,349		
	\$ ₅₂₂	0.00			28.15 S1.85	20.786	180.669	180.669	0.038	1350.159	1298.567	-227.503
	ؠڴڴ	12034.06	400		85 63 85 63 85 85 85 85 85 85 85 85 85 85 85 85 85	20.786 20.786 20.786	184,002 186,777 189,226	180.922 181.485 182.211	1.078 2.117 3.156	1351.057 1351.893 1352.707	1289.520 1280.672 1271.720	-192.450 -167.239 -147.617
	్డ్ క్ల క	13460.70			8 888	20.786 20.786 20.786	191.416 198.409 201.185	183.024 184.748 186.477 188.146	4.196 6.274 8.353 10.431	1353.502 1355.043 1356.527 1357.963	1262.679 1244.368 1225.804 1207.031	-131.911 -108.332 -91.471 -78.811
Enthalpy of Formation		•		070 - 800 - 07 - 03 - 07 00 07 07 07 07 07 07 07 07 07 07 07		20.786	203.633	189.733	12.510	1359.354	1188.081	-68.954 -61.061
Δρf*(Mo*, g, 0 K) is calculated from Δρf*(Mo, g, 0 K) using the spectrosco kJ-mol ⁻¹) from Moore. The ionization limit is converted from cm ⁻¹ to kJ-mol ⁻¹ derived from the 1973 CODATA fundamental constants ³ Rosenstock et al. * and I appearance potential data.	o, g, 0 K) using nverted from cn istants ³ Rosenste	the spectrosco n ⁻¹ to kJ·mol ⁻¹ ock et al. ⁴ and l	pic value of IP using the facto Levin and Lias	Δμ ² (Mo ² , g, 0 K) is calculated from Δμ ² (Mo, g, 0 K) using the spectroscopic value of IP(Mo) = 57260 ± 50 cm · (684,982 ± 0.60 · mol ⁻¹) from Moore. The ionization limit is converted from cm ⁻¹ to kJ·mol ⁻¹ using the factor, I cm ⁻¹ = 0.01196266 kJ·mol ⁻¹ , which is rived from the 1973 CODATA fundamental constants ³ Rosenstock <i>et al.</i> ⁴ and Levin and Lias ⁵ have summarized additional ionization and pecarance potential data.		20.787 20.789 20.794 20.804	207.804 209.613 211.277 212.819 214.255	192.652 193.992 195.258 196.458 197.597	16.667 18.746 20.825 22.905 24.986	1361,993 1363,232 1364,409 1365,517 1366,552	1149.742 1130.392 1110.940 1091.401 1071.784	-54.597 -49.205 -44.638 -40.721
$A_{\mu}H^{\circ}(Mo^{\bullet}, g, 298 15 K)$ is calculated from $\Delta_{\mu}H^{\circ}(Mo)$ $Mo^{\bullet}(g)$, and e (ref), $\Delta_{\mu}H^{\circ}(Mo \rightarrow Mo^{\bullet} + e^{-}, 298.15 K)$ and to threshold effects discussed by Rosenstock et al. convention that excludes the enthalpy of the electron.	(Mo, g, 0 K) by 5 K) differs fron 11 al. ⁴ ∆ _r H°(298 ron.	using IP(Mo) w n a room tempe .15 K) should b	rith JANAF¹ en rature threshold e changed by -	$\Delta_H^{*}(Mo^{\bullet}, g. 298 15 \text{ K})$ is calculated from $\Delta_H^{*}(Mo, g. 0 \text{ K})$ by using IP(Mo) with JANAF¹ entralpies, $H^{*}(0 \text{ K})$ – $H^{*}(298 15 \text{ K})$, for Mo(g), $Mo^{\bullet}(g)$, and e (ref). $\Delta_H^{*}(Mo \to Mo^{\bullet} + e^{-}, 298.15 \text{ K})$ differs from a room temperature threshold energy due to inclusion of these entralpies and to threshold effects discussed by Rosenstock et al. $^{4}\Delta_H^{*}(298.15 \text{ K})$ should be changed by $-6.197 \text{ kJ} \cdot mol^{-1}$ if it is to be used in the ion convention that excludes the enthalpy of the electron.	280 280 280 280 280 280 280 280 280 280	20.860 20.917 21.004 21.128 21.300	215.600 216.866 218.064 219.202 220.290	198.681 199.714 200.700 201.644 202.549	27.070 29.159 31.255 33.361 35.482	1367.507 1368.379 1369.162 1369.853	1052.102 1032.362 1012.573 992.743 972.879	-34.348 -31.721 -29.384 -77.292 -25.409
Heat Capacity and Entropy The information on electronic energy levels and	f quantum weig	thts, given by N	foore, ⁶ is incon	eat Capacity and Entropy The information on electronic energy levels and quantum weights, given by Moore, is incomplete because many theoretically predicted	2100 2200 2300 2400	21.526 21.816 22.176 22.176	221.335 222.343 223.320 224.273	203.419 204.257 205.064 205.845	37.623 39.789 41.988 44.227	1370.939 1371.328 1371.611	952.988 933.076 913.149 893.212	-23.704 -22.154 -20.738
levels have not been observed. Although we have listed only the ground, the fit nonzation cotential for Mo*(s), all levels listed by Moore, as well as estimated	listed only the	ground, the fir	st excited state, levels, are used	levels have not been observed. Although we have listed only the ground, the first excited state, the highest observed excited state, and the nonzation notential for MoYo, all levels listed by Moore, as well as estimated levels, are used in the calculation. The observed levels are		23.131	225.206	206.601	46.514	1371.847	873.270	-18.246
too numerous to list completely. The calculations indicate that for Mo'(g), the transition gives (for $n = 4$, 5), the cut-off procedure, and the inclusion of $n = 5$	indicate that for	or Mo ⁺ (g), the tlusion of $n = 5$	hermodynamic levels up to 40	too numerous to list completely. The calculations indicate that for Mo'(g), the thermodynamic functions are independent of the estimated missing levels (for n = 4, 5), the cut-off procedure, and the inclusion of n = 5 levels up to 4000 K, the Gibbs energy function showing massing levels (for n = 4, 5), the cut-off procedure, and the inclusion of n = 5 levels up to 4000 K, the Gibbs energy function showing massing levels (for n = 4, 5), the cut-off procedure, and the inclusion of n = 5 levels up to 4000 K, the Gibbs energy function showing		74.423 76.060 26.060	227.033 227.935 228.834	208.047 208.741 209.418	51.263 53.744 56.306	1371.561 1371.129 1334.529	833.390 813.465 793.610	-16.123 -15.175 -14.294
and the fundamental constants. Extension of these and use of different fill and cut-off procedures.	calculations at	bove 6000 K m	ay require cons	and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states (n>5), and use of different fill and cut-off procedures.	33.00	28.028	230.635	210.729	64.566	1336.559	756.239	-12.743
References					3,400	31.528	233.79	212.606 213.213	70.628	1340.416 1341.946	699.906 681.046	-10.753
¹ JANAF Thermochemical Tables: Mo(g), 3-31-78; e (ref), 3-31-82. ² C. E. Moore, U. S. Nat. Bur. Stand., NSRDS-NBS-34, 8 pp.(1970). ³ E. R. Cohen and B. N. Taylor, J. Phys. Chem. Ref. Data 2, 663 (1973).	78; e ⁻ (ref), 3-3 BS-34, 8 pp.(15 tef. Data 2, 663	11–82. 970). (1973).	Í		3600 3700 3800 3900	34.156 35.541 36.963 38.419	235.254 236.209 237.176 238.155	213.812 214.404 214.991 215.572	77.193 80.677 84.302 88.071	1343.607 1345.405 1347.343 1349.425	662.140 643.186 624.181 605.124	-9.607 -9.080 -8.580 -8.105
⁷ H. M. Kosenstock, K. Draxl et al., J. Phys. Chem. Ref. Data 6, Supp. 1, 783 pp. (1971). ⁷ R. D Levin and S. G. Lias, U. S. Natl. Bur. Stand. NSRDS-NBS-71, 634 pp. (1982).	n. Ket. Data 6, nd. NSRDS-NE	Supp. 1, 783 pl 3S-71, 634 pp.	(1982).		4100	39.904	240.150	216.149	91.987	1351.653	586 011 566.841	2227-
°C E. Moore, U.S. Nat. Bur. Stand., NSRDS-NBS-35, Volume III, (1970) [Reprint of NBS Circular 467, Volume III, 1958] ⁷ J R. Downey, Jr., The Dow Chemical Company, AFOSR-TR-78-0960, Contract No. F44620-75-1-0048, (1978).	SS-35, Volume , AFOSR-TR-	III, (1970) [Re 78-0960, Contr	print of NBS C act No. F44620	ircular 467, Volume III, 1938]. -75-1-0048, (1978).	984 984 986 986 986 986	42.942 44.491 46.057	241.166 242.195 243.235 244.288	217.292 217.859 218.424 218.987	100.270 104.642 109.169	1359.247 1359.247 1362.087	528.319 508.962 489.540	-6.042 -6.042
					4400 4400	49.235 50.847	245.352	219.549	118.697	1368.242	470.049	-5.338
					2008 2008 2008 2009	52.473 54.112 55.765	241.516 248.615 249.725	220.869 221.228 221.787	138.86/ 134.196 139.690	1378.680 1378.680 791.101	430.833 411.146 397.093	-4.383 -4.148
					\$200 \$300	57.429 59.102 60.781	250.845 251.977 253.118	222.346 222.904 223.464	145.349 151.176 157.170	793.394 795.708 798.046	389.190 381.242 373.249	-3.986 -3.830 -3.679
					\$400 \$500	64.142	255.432	224.024	163.332	802.800	365.212	-3.533
					\$200 \$200 \$200	67.470 69.103	258.772	225.708 226.271	182.825	807.674 810.159	340.837	-3.12
					\$200 \$200 \$200	70.706 72.268	260.165 261.366	226.835 227.401	196.644 203.793	812.679 815.229	324.370 316.072	-2872 -2.752

Heat Capacity and Entropy

Molybdenum, Ion (Mo⁻)

CURRENT March 1984 (1 bar)

PREVIOUS March 1978 (1 atm)

. GAS
IDEAL

M, = 95.94055 Molybdenum, Ion (Mo-)

Mo₁(g)

EA(Mo, g) = 0.746 ± 0.010 eV S°(298.15 K) = 180.669 ± 0.003 J·K⁻¹·mol⁻¹

Molybdenum, Ion (Mo⁻)

0.0

 $\Delta_t H^{\circ}(0 \text{ K}) = 585.390 \pm 1.5 \text{ kJ} \cdot \Delta_t H^{\circ}(298.15 \text{ K}) = [580.805] \text{ kJ} \cdot$ State 6S₅₂2 $\Delta_H^{H'}(Mo^-, g, 0K)$ is calculated from $\Delta_H^{H'}(Mo, g, 0K)^1$ using the adopted electron affinity of EA(Mo) = 0.746 ± 0.01 (71 978 ± 0.965 kJ-mol⁻¹). This value, recommended by Hotop and Lineberger,² is based on a laser photodetachment electron spectro study. Additional information on Mo-(g) may be obtained in the critical discussions of Hotop and Lineberger, 4 Rosenstock et al

Enthalpy of Formation

 Δ_H^{μ} (Mo⁻, g, 298.15 K) is obtained from Δ_H^{μ} (Mo, g, 0 K) by using EA(Mo) with JANAF¹ enthalpies, H° (0 K) – H° (298.15 K) Mo⁻(g), Mo₂(g), and e⁻(ref) Δ_H^{μ} (Mo⁻ \rightarrow Mo + e⁻, 298.15 K) differs from a room-temperature threshold energy due to inclusion of enthalpies and to threshold effects discussed by Rosenstock *et al.*³ Δ_H^{μ} (298.15 K) should be changed by +6.197 kJ·mol⁻1f it is to be in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The ground state electronic configuration for Mo (g) is given by Hotop and Lineberger and Rosenstock et al ³ Lacking any experii evidence as to the stability of any excited states, we assume that no stable excited states exist.

JANAF Thermochemical Tables: Mo(g), 3-31-78; e (ref), 3-31-82.
 Hotop and W. C. Lineberger, J. Phys. Chem. Ref. Data, 14, 731 (1985).
 C. S. Feigerle, R. R. Cordermann, S. V. Bobashev and W. C. Lineberger, J. Chem. Phys. 74, 1580 (1981).
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 H. M. Rosenstock, K. Dratl et al., J. Phys. Chem. Ref. Data 6, Supp. 1, 783 pp. (1977).
 H. S. W. Massey, "Negative Ions," 3rd ed., Cambridge University Press, Cambridge, 741 pp. (1976).

-lom-l	Enthalpy R	eference Te	mperature	Enthalpy Reference Temperature = T, = 298.15 K		Standard State Pressure = $p^* = 0.1$ MPa	Pressure = f	. = 0.1 MPa
l-mol_	7/K	ູ່	J.K-'mot'' S -[G	-H(T,)]T	$H^{\circ}-H^{\circ}(T_{*})$	Ld.mol ⁻¹	₽ .G•	log Kr
	280 0 280 0 280 0	0. 20.786 20.786 20.786	0. 157.962 172.370	INFINITE 199.149 182.570 181.011	-6.197 -4.119 -2.040 -1.001	585.390		
	298.15	20.786		180.669	ó	580,805	541.722	-94.907
	300	20.786 20.786	180.798 184.002	180.669 180.923	0.038	580.761 579.547	541.480 535.028	-94.280 -79.849
ometry	8 2 5	20.786 20.786	186.777	181.485	3.156 3.156 4.196	578,305 577,040 57,757	528.753 522.635 516.658	-69.048 -60.666
ıl.5 and	88	20.786	195.205	184.748	6.274	573.140	505.083	-43.971
K). or	888	20.786	201.185	188.146	8.353 10.431	570.467 567.746	483.205	-36.859
of these	88	20.786	205.823	189.733	14589	562.167	472.804	-24.170
pe nsed	1200	20.786 20.786	207.805 209.613	192.653 193.992	16.667 18.746	559.304 556.386	452.905 443.360	-21.507 -19.299
	0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	20.786 20.786 20.786	211 <i>277</i> 212,817 214,251	195.258 196.458 197.597	20.824 22.903 24.982	553.405 550.355 547.230	434.062 424.996 416.150	-17.441 -15.857 -14.492
imental	1600	20.786	215.593	198.680	29.139	544.023	399,084	-13.304
	0081	20.786	218.041	200.698	33.296	537,336	390.850	-11.342
	2000	20.786	220231	202.544	37.453	526 509	367.777	-9.136
	220	20.786	222.212	204.243	39.532	522.653	359.784	-8.542 -8.005
	2400 2500	20.786	224.021	205.817	43.689	514515 510212	345,333	-7.516 -7.070
	2600 2700	20.786 20.786	225.685 226.469	207.282 207.979	47.846	505.726 501.019	331,585 324,976	-6.662
	2888	20.786 20.786 20.786	22,722 22,725 28,659	208.652 209.306 209.939	52.004 54.082 56.161	496.028 454.787 451.022	318.547 312.351 307.503	-5.943 -5.626 -5.354
	3200	20.786	229.341	210.554	58.239 60.318	447.256	302.781	-5.102
	3400	20.786	230.640	211.732	62.397	435.959	289.330	-4.649 -4.445
	3600	20.786	232.449	213,384	68.632	428.428	280.922	-4.076
	3800 3800 3900	20.786 20.786 20.786	233.018 233.573 234.113	213.907 214.418 214.916	72.790 72.790 74.868	424.662 420.897 417.131	276.876 272.932 269.088	-3.752 -3.604
	4000	20.786	234.639	215.402	76.947	413.366	265.340	-3.465
	4200	20.786	235.653	216.343	81.104 83.183	405.834	258.123	-3.210 -3.093
	4500 4500	20.786 20.786	236.620 237.087	217.243 217.678	85.261 87.340	398.303 394.538	251.266 247.967	-2.983 -2.878
	4400	20.786	237.54	218.105	89.418 91.497	390.772 387.006	244.751 241.617	-2.685
	2000	20.786	238.857	219.336	95.654 97.733	379.475	235.589	-251 -2491
	5200	20.786	239.689	220.118	99.811	-221.120	247.557	-2.536
	2400 2400 2500 2500	20.786 20.786 20.786	240.877 240.877 241.258	220.872 221.239 221.599	103.969 106.047 108.126	-232.447 -238.325 -244.342	266.154 275.617 285.189	-2623 -2666 -2709
	\$600 \$700	20.786	241.633 242.001	221.954	110.204	-250.498 -256.788	294.873 304.667	-2.750 -2.792
	2800	20.786 20.786 20.786	242.362 242.718 243.067	222.982 223.314	114,362 116,440 118,519	-269.760 -269.760 -276.437	324.590 334.720	-2834 -2874 -2914
			1			ţ	The second	

Mo₁O₁(g)

	=	
п		

$\Delta_i H^0(0 \text{ K}) = 310.25 \pm 33.5 \text{ kJ}$	14 5 C + 310 06 + 33 5 L1
h	86C) ₀ HV
	-'-mol-'
	.15 K) = 241.764 ± 8.4 J·K ⁻¹ ·mol ⁻¹

Molybdenum Oxide (MoO)

$\Delta_i H^0(0 \text{ K}) = 310.25 \pm 33.5 \text{ kJ·mol}^{-1}$ $\Delta_i H^0(298.15 \text{ K}) = 310.96 \pm 33.5 \text{ kJ mol}^{-1}$
$S^{\circ}(298.15 \text{ K}) = 241.764 \pm 8.4 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$

Epr (276:12 N) = 310 90 :			ķ
			σ=1 r _c =[1.74] Å
	Electronic Levels and Quantum Weights	0 [3] [450] [5]	$\omega_c x_c = [3.99] \text{ cm}^{-1}$ $\alpha_c = [0.00309] \text{ cm}^{-1}$
•	Electronic	[4]	$\omega_e = [1000 \pm 20] \text{ cm}^{-1}$ $B_e = [0.40604] \text{ cm}^{-1}$

Enthalpy of Formation

The enthalpy of formation of MoO(g) is taken from the critical analysis of the Mo-O system by Brewer. The adopted value i $\Delta_t H^0(298.15 \, \text{K}) = 74.32 \pm 8 \, \text{kral·mol}^{-1}$. All the current JANAF Thermochemical Tables for molybdenum-oxygen species are based on th internally consistent values of Brewer.

Choudary et al. have reviewed earlier data and evaluations of $\Delta_i H^\circ$ for MoO(g). They have also presented new data between 1462 an 1908 K. For the treaction 2 MoO₂(g) = MoO(g) + MoO₃(g), the 3rd law values are mostly in the range -2.4 to -4.6 kcal mol⁻¹ compared 2nd law values of -7.8 kcal·mol⁻¹ or more negative. Δμ⁰/R = -2200 ± 2000 K was selected by Brewer¹ for the reaction as written.

Heat Capacity and Entropy

The ground state configuration is assumed to be similar to that for gaseous WO₂. Swaminathan and Krisnamurthy* observed ten ban systems which they attributed to molybdenum oxide with lower state values of $\omega_s = 950 \pm 10$ cm⁻¹ forms and Stafford' also observed a ban with a peak at 969 cm⁻¹ in the vapor above MoO₃(ct). It is surprising that the observed vibrational frequency of MoO(g) is lower than 105. cm 1 observed for WO(g). The latter comes not only from electronic spectra of the gas but also from infrared observation in matrix isolation the former comes only from tentative assignments of electronic spectra presumably arising from MoO(g). It is possible that the observed states could be low lying excited states. We tentatively assume the fundamental vibrational frequency to be $1000 \pm 20 \text{ cm}^{-1}$. The anharmonicity correction x_k is estimated from the relation x_k = 0.014 given by Barrow and Caunt. The constant (0.014) is assumed to be the same at that for WO(g). The value of α_e is calculated from the Morse potential function. Schroder? gave a relationship between bond order and Mointernuclear distance which yields values of 1.74 Å for a bond order of two and 1.62 Å for a bond order of three. A value 1.74 ± 0.05 Å wa

The suggestion of Hewett et al., that the electronic structure of MoO should be closer to that of CrO than WO, was followed in using the same treatment as for MoF₂ where g = 3 was taken for the ground state and g = 5 for a low-lying excited state at 450 cm⁻¹.

¹L. Brewer, Materials and Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, personal communication September 29, 1978, preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy Agency, Vienna, Austria.

²U. V. Choudary, K. A. Gingerich and J. E. Kingcade, J. Less-Common Metals 42, 111 (1975).

JANAF Thermochemical Tables: WO(g) and WO₃(g), 9-30-66.

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 W. D. Hewett, Jr., J. H. Newton, and W. Weltner, Jr., J. Phys. Chem. 79, 2640 (1975).

-	Enthalpy Reference	eference Te	Temperature	= T, = 298.15 K	İ	Standard State Pressure	l K	$p^{\circ} = 0.1 \text{ MPa}$
,	τÆ	೮	S - [G	-[G*-H*(T,)]/T	$H^{\bullet}-H^{\bullet}(T_{r})$	A.II.	4.G•	log K,
	0	0.	Ö	INFINITE	-9.636	310.249	310.249	INFINITE
	38€	34.472	227.640	245.025	-6.714	311.228	300.056	-156.733 -75.449
	SZ 5	35.531	235.461	242.355	-1.724	311.073	283.322	-59.197
	208.15	30.02	241.704	241.764	Ö.	310.959	277.988	-48.702
	38	36.242	247.558	242.705	1.874	310.954	272.268	-48.366
	\$ \$	36.478	252.407	243.183 244.451	3.689 5.511	310,635	261.300	-34.837
	00 50 50 50 50 50 50 50 50 50 50 50 50 5	36.567	260.545	245.871	7337	310,205	255.852	-26.729
	88	36.732 36.879	267.227 272.901	248.890 251.925	11.002	309.674 309.054	245.030	-21.332
	88	37.006	277.834	254.862	18.377	308.359	223.672	-14.604
ر 2.	88	37.207	286.114	260.314	25.799	306.769	202.679	-12370 -10587
<u>2</u>	200 1700 1700	37.287	289.664	262.824	33.256	305.876	192.313	-9.132
ğ	1300	37 418	295.904	267.446	36.995	303.882	171.832	-6.904
2	88	31.413	298.679 301.266	269.579 271.606	40.740 44.490	302.770 301.574	161.715 151.681	-6.034 -5.282
	8 2 2 2 2 2 3 2 3	37.568	303.689	273.537	48.244	300.288	141.730	-4.627
	0081	37.649	308.119	277.138	55.766	297.419	122.078	-3.543
덛	200 200 200 200 200 200 200 200 200 200	37.721	310.155	278.822 280.438	59.533 63.303	295.821 294.104	112.380	-3.090
5 %	2100	37.754	313.931	281.989	7,07,07	292.259	93.247	-2319
}	2300	37.817	317.368	284.918	74.634	288.146	74.479	066.1- 169.1-
S	7500 2500	37.846 37.875	318.978 320.524	286.304 287.642	78.417	285.859 283.405	56.094	-1.420
<u>ک</u> و	2600	37.903	322.010	288.936	85.992	280.760	47.054	-0.945
4 Q	2800	37.958	324821	291.400	89.784 93.578	274.720	38.119 29.295	-0.737
æ	888	38.011	326.153 327.441	292.575 293.716	97.376 101.175	235.298 233.344	20.640 13.272	-0.372 -0.231
<u>9</u>	3200	38.036	328.688	294.824	104.978	231.383	5.969	-0.101
:	3300	38.087	331,068	296.949	112.590	27.4	-8.450	0.134
	3200	38.136	333.310	298.964	120.212	223.462 223.471	-15.568 -22.629	0738
Ę	3600 3700	38.161 38.185	334,385 335,431	299.933 300.878	124.027	221.486	-29.632	0.430
25	3800	38.209 38.233	336.449 337.442	301.801 302.702	131.664	215.486	-43.474	0.598
	9	38.257	338.410	303.583	139,311	213.477	-57.106	0.746
	200	38.304	340278	305.286	143.138	209.447	-63.845	0.813
	964	38.327 38.350	341.180 342.061	306.110 306.917	150.798	207.426 205.402	-71.178 -83.773	0.938 0.995
	4500	38.374	342.923	307.708	158.468	203.373	-90.323	1.048
	902	38.420	344.593	309.242	166.148	199.305	-96.827	 1.188
	4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	38.443 38.466	345.402 346.195	309.987 310.718	169.991 173.836	197.265	-109.704 -116.077	1.194
-	2000	38 489	346.972	311.435	177.684	-398.212	-116.678	1.219
	2200	38.512	347.735	312.140	181.534	-401.945 -405.828	-111.011 -105.269	1.137
	2400	38,557	349.217	313.511	189.241 193.098	-409.860 -414.040	-93.450 -93.555	0.980 0.905
	2500	38.602	350.646	314.836	196.957	-418.366	-87.581	0.832
	888 888 888	38.623	351.342	315.481	200.818 204.682	-422.836 -427.446	-81.526 -75.391	0.760 0.691
	2800	38.670 38.693	352.698 353.359	316.741 317.356	208.548 212.416	-432.196 -437.081	-69.173 -62.873	0.623 7250
	0009	38.715	354,010	317.962	216.286	-442.103	~56.488	0.492
	PREVIOUS.	September 1	September 1978 (1 atm)			CURRENT		September 1978 (1 bar)

NENTIE 28631 143.443 143.443 143.443 143.443 143.443 144.66 145.441 145.443 144.66 145.443 145

354.141 337.411 320.858

570.389

577.049

84.947

58.515 67.038 75.820 84.870

304.482

565.090

03.810

107.046

165.725 171.927 177.933 183.770 189.461 195.028

94.680 97.588

4.197

422.843 422.843 405.397 -388.132 -272.260 -256.416 -240.749

-555.770

134.459 145.313

114.919 118.694 122.372

106.893

13.608 03,688

-225.262 -209.954 -194.828 -179.882 -165.118

\$44.736 \$40.669

156.502 168.038 179.930 192.190 204.827

125.962 129.472 132.908 136.276 139.583

200.487 205.852 211.138 216.355 221.514

124,470

548.608

536.405

-150,536

-527.301 -522.500 -517.593 -548.535

142.832 146.030 149.179 152.284 155.348

226.622 231.689 236.720 241.722 246.701

-531.664 -513.011 -494.558

476.324 458 300

583.757 582.293 580.692 578.946

6.125 12.713 19.674 26.932 34.454 27.227

91.441 102.623 112.664 121.816 130.264

73.935 76.488 78.965 81.437 83.948

46.460 48.764 53.333

56.095 63.551 67.936

532.011

587.852

46.459

46.459 46.806 64.076 78.758

55.898

log K

 $\Delta_t H$

 $S^{\bullet} - [G^{\bullet} - H^{\bullet}(T_{\epsilon})]T$

ن:

Mo₁O₂(cr)

Standard State Pressure = p = 0.1 MPa

Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$

J-K-1mol-1

CURRENT September 1978

CRYSTAL

Molybdenum Oxide (MoO₂)

 $\Delta_t H^{\circ}(0 \text{ K}) = -582.90 \pm 2.1 \text{ kJ·mol}^{-1}$ $\Delta_t H^{\circ}(298.15 \text{ K}) = -587.85 \pm 2.9 \text{ kJ} \cdot \text{mol}^{-1}$ $S^{\circ}(298.15 \text{ K}) = 46.459 \pm 0.42 \text{ J·K}^{-1} \cdot \text{mol}^{-1}$

Enthalpy of Formation

Pearson Notation: mP12

cal-K⁻¹-mol⁻¹ in this tabulation, the entitlapy of formation should also have been revised. With the exeption of the data from tollowing equilibrium studies suggest $\Delta_H^0(298.15 \, \text{K}) = -141.20$ kcal-mol⁻¹ in comparison with the calorimetric mean of $\Delta_H^0(298.15 \, \text{K}) = -140.8 \, \text{kcal-mol}^{-1}$ for MoO₂(cr). In addition, eight recent emf studies (published since the analysis by Brewer) also yield a value of $\Delta_H^0(298.15 \, \text{K}) = -141.2 \, \text{kcal-mol}^{-1}$. Although there is some overlap in the values for Δ_H^0 derived from equilibrium and calorimetric studies, the equilibrium studies appear to be more negative by 0.4 kcal·mol-1. Brewerl noted (in reference to MoO₂(cr) were made more regative by 0.5 kcal mol-1 with a corresponding decrease of 0.5 kcal mol-1 for MoO₂(g) and MoO(g) and 0.8 The adopted enthalpy of formation of MoO₂(cr) at 298.15 K is -140.5 ± 0.2 kcal·mol⁻¹. This value is chosen so as to be in agreement with Brewer' who has performed a critical analysis of all data pertaining to the molybdenum-oxygen system. However, Brewer' chose to adopt the value previously used by JANAF; ¹⁴ a value which was derived as a weighted average of two calorimetric determinations and seven equilibrium studies, the latter results based on 5°(298.15 K) = 11.954 cal·K⁻¹·mol⁻¹. In revising the 5°(298.15 K) value to 11.04 $\Delta_H^2(298.15 \, \text{K}) = -140.5 \, \text{kcal·mol}^{-1}$, however, that a better overall fit of all Mo-O data would be obtained if the enthalpy of formation of ccal-mol" for MoO, (g). Such a change could be accommodated in the MoO, tables.

complete. The authors also digested the products with NH₄OH to remove the trioxide. The residue was the dioxide, as indicated by both gnition of the bomb products from the calorimetric studies of Staskiewicz et. al 2 indicated that oxidation was only about 70 percent oxidation and reduction. This evidence does not necessarily eliminate the possibility of known intermediate oxides in the combustion products. Mah³ found 72-75 percent conversion to trioxide by weighing the total combustion products; no additional analysis was performed.

				Data	∆H°(298.15	H°(298.15 K). kcal·mol ⁻¹	-1 Drift	Δ47°(298.15 K)
Source	Method	Reaction	<i>1/</i> K	Points	2nd law	3rd law	Ä	kcal·mol-1
Staskiewicz et. al.2	Calorimetric	4	1		-37.12		ı	-140.86 ± 0.13**
Mah³	Calorimetric	<	ì	1	-37.52		ı	$-140.64 \pm 0.13**$
Rapp*	emf	8	1023-1323	32	-13.26	-1418	-0.8 ± 0.1	-141 46
•		ပ	1023-1273	23	-25.64	-26.65	-0.9 ± 0.1	-141.25
Barbi ⁵	emţ	i.	873-1073	Edn.	-140.4	-139.45	6:0	-139.45
Gleiser and Chipman	Equilibrium	۵	1296-1341	. 6	+ 3.02	-6.57	-3.6 ± 1.5	-141.84
Gokcen,	Equilibrium	ш	949-1344	Eqn.	- 19.88	-25.50	-3.4	-141.11
Collins*	Equilibrium	ш	973-1173	Edn.	-22.18	-25.46	-1.5	-141.07
Tonosaki ⁹	Equilibrium	ш	981-1096	Edii.	-18.86	-25.86	-3.0	-140.47

**Auxiliary data for MoO₃(cr) are taken from corresponding measurements of the same authors. See also JANAF. 13

 $Mo(cr) + O_2(g) = MoO_2(cr)$ derived by the author from the cell reaction 2 Fe_xO(cr) + Mo(cr) = MoO_x(cr) + 2 xFe(cr) E. $Mo(cr) + 2 H_2O(g) = MoO_2(cr) + 2 H_2(g)$ using A.G. data for Fe,O(cr) B. 2 Fe_xO(α) + Mo(cr) = MoO₂(cr) + 2 xFe(cr) C. 2 NiO(cr) + Mo(cr) = MoO₂(cr) + 2 Ni(cr) A. MoO₂(cr) + 1/2 O₂(g) = MoO₃(cr)

D. $Mo(cr) + 2 CO_2(g) = MoO_2(cr) + 2 CO(g)$

measured low temperature heat capacities from 53.3 to 296 K. King et al. 11 measured the high temperature enthalpy changes from Heat Capacity and Entropy

The entropy \$'(298.15 K) = 11.104 cal·K⁻¹·mol⁻¹ is obtained from the low temperature heat capacity data, based on \$'(51 K) = 0.36 cal·K⁻¹·mol⁻¹. As discussed by Brewer, Ghose et. al.¹² used neutron diffraction measurements to demonstrate the absence of a permanent 399 to 1801 K by drop calorimetry. The adopted heat capacities are derived from these two sets of data, subject to the constraint that they oin smoothly at 298.15 K. Deviations of the enthalpy data from the adopted values are -1.3 to +0.7%, excluding the point at 1801 K. This soint at the highest temperature deviates by +2.3%, which suggests that the apparent heat capacity is rising very rapidly. No explanation for ragnetic moment. Thus no additional heat capacity or entropy contribution below 50 K due to a possible antiferromagnetic effect is necessary. this rapid rise is available.

L. Brewer, Materials and Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, personal communication, September 29, 1978, preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy References

Molybdenum Oxide (MoO₂)

PREVIOUS: June 1967

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

²H. A. Staskiewicz, J. R. Tucker and P. E. Snyder, J. Amer. Chem. Soc. 77, 2987 (1955) Agency, Vienna, Austria.

A. D. Mah, J. Phys Chem. 61, 1572 (1957). A. Rapp, Trans. AIME 227, 371 (1963).

Continued on page 1598

3.713 3.3706 3.3

-37.208 -39.978 -43.035 -82.343 -84.176

116.745 122.569 128.409 134.264 140.136 146.026 151.935

343.944 345.815 347.629 349.391 351.103 352.768 354.389 355.968 357.508

395.542 397.677 399.744 401.748

58.634 58.809 58.994 59.188

393,332

58.471

-100.980 -101.435 -101.832 -102.173

-86.009 -87.838 -89.664 -91.484

403.692 405.581 407.418 409.207 410.951 412.652 414.313 415.937 417.524 419.077

59.603 59.822 60.046 60.276

157.864 163.814 169.785 175.778 181.794 187.833 193.896 193.896 199.983 206.093

-102.697 -102.884 -103.021 -103.111

-95.103 -96.900 -98.687 100.464

360.476 361.909 363.310 364.679 366.020

60.510

-103.158 -103.117 -103.034 -102.911 -102.750

103.987 105.731 107.465 109.187 110.898

218.386 224.568 230.774 237.004 243.256

420.598 422.087 423.548 424.980 426.385

61.941 62.177 62.409 62.638 62.863

-102.550 102.041 101.733 -95.660

249.531 255.828 262.148 268.488 274.849

112.599 -114.290 -115.971 -117.644 -710.695

427.764 429.118 430.449 431.756 433.041

-83.326 -70.926 -58.457 -45.919

-728.787

-714.033 -717.513

281.230 287.630 294.050

435.548 436.770 437.974 439.158

434,305

63.909 64.100 64.285

-67.336 -70.545 -70.543 -76.331 -76.331 -81.792 -84.394 -85.903 -93.890 -93.890 -93.890 -93.890 -93.890

-26222 -28.100 -30.127 -32.313 -34.666

333.613 335.825 337.959 340.021 342.014

380.922 383.614 386.191 388.664 391.042

57.805 57.920

58.176

-18.778 -20.035 -21.400 -22.880 -24.485

321.166 323.864 326.450 328.932 331.317

57.243 57.365 57.479 57.587 57.694

375.148 378.105

53.480 59.165 64.867 70.585 76.315 82.057 87.811

365.281

\$6.942 \$7.104

Mo₁O₂(g)

Standard State Pressure = p* = 0.1 MPa

Enthalpy Reference Temperature = T, = 29&15 K

W_r = 127.9388 Molybdenum Oxide (MoO₂)

log K,

 $H^{\bullet}-H^{\bullet}(T_{i})$

 $S^{\bullet} - [G^{\bullet} - H^{\bullet}(T_{*})]T$

-21.286 -23.410 -25.477 -27.498 -29.481

-8.331 -8.759 -9.141 -9.490

-21.206

-8.314

276.990

0. 234,266 260,251 269,395 276,990

-51.380 -54.756 -58.060 -61.292 -64.451

-13.847 -14.678 -15.579 -16.557 -17.621

-33,355 -37,127 -40,809 -44,409 -47,932

-10.435 -11.051 -11.688 -12.360 -13.077

326.336 332.813 338.668 344,008 353.444 357.657 361.591

310.914

CURRENT September 1978 (1 bar)

745.740

Molybdenum Oxide (MoO₂)

IDEAL GAS

 $S^{*}(298.15 \text{ K}) = [276.990 \pm 8.4] \text{ J. K}^{-1} \cdot \text{mol}^{-1}$ $\Delta_{*}H^{\circ}(0 \text{ K}) = 1157.294 \pm 20.9 \text{ kJ} \cdot \text{mol}^{-1}$

 $\Delta_t H^{\circ}(0 \text{ K}) = -6.32 \pm 12.6 \text{ kJ} \cdot \text{mol}^{-1}$ $\Delta_t H^{\circ}(298.15 \text{ K}) = -8.31 \pm 12.6 \text{ kJ} \cdot \text{mol}^{-1}$

Vibrational Frequencies and Degeneracies Electronic Levels and Quantum Weights (1) 000 (2) (3) (3) 950 (1) e, cm

522 [13000]

Product of the Moments of Inertia: $I_A I_B I_C = 5.663388 \times 10^{-115} \text{ g}^3 \cdot \text{cm}^6$ Bond Distance: Mo-O = 1.73 A Bond Angle: O-Mo-O = 116 Point Group: C₂,

 $\sigma = 2$

Enthalpy of Formation

slightly exceed those of Burns et al.² and are 50% lower than those of Chizhikov et al.⁶ The adopted AG values for the formation of MoO_A(g) from Mo(cr) and O_A(g) average 1 kcal-mol⁻¹ more negative than those determined by Franklin and Stickney.⁷ The only recent determination that deviates senously is that of Belton and Jordan⁴ who determined the volatility of molybdenum in steam-hydrogen mixtures at 1200 and The adopted enthalpy of formation for MoO₂(g) at 298.15 K is -1.99 ± 3 kcal·mol⁻¹. This value was adopted by Brewer¹ who has R = 69700 ± 1500 K for the sublimation process MoO₂(cr) = MoO₂(g). The vapor pressures of MoO₂ calculated from the adopted tabulation 1500°C. The variation of their results with water partial pressure at 1383 to 1500°C indicate an intercept corresponding to non-hydrated species which they attribute to MoO₃ and MoO₂. They assumed the ratio of MoO₂ to MoO₃ to be that observed by Burns et al. 2 and obtained partial pressures of MoO₂ about six times higher than calculated from the adopted values. Their values would require that $\Delta_t H^*$ (298 15 K/)R adopted Δ_{sub}H°(298.15 K)/ of Mo(cr) + O_{xg}) = MoO_x(g) be made more negative by 3200 K. If both $\Delta_{xx}H^{\circ}$ and Δ_{yH}^{*} (cr) were shifted by their assigned uncertainties performed a critical analysis of all data pertaining to the molybdenum-oxygen system. Brewer indicated, a change of 2000 K could be accomodated.

Burns et al.? have investigated mass-spectrometrically the vapor in equilibrium with powdered MoO_A(cr) and also reported the partial (cr) by the Knudsen effusion method. More recently there have been mass spectroscopic Knudsen cell studies of Chizhikov et al. of the vapor over MoO₂(cr) between 1500 and 1730 K and the Langmuir type studies of Franklin and Stickney⁷ on the vapor resulting from oxygen on pressures of MoO₂(g), MoO₃(g), (MoO₃)₃(g) and (MoO₃)₃(g). DeMaria et al. ³ have measured the partial pressures of gaseous oxides MoO₃ MoO2, and O(g) in the Mo-Al₂O3 system by mass spectrometry. Blackbum et al. * and Plante* have studied the vapor pressures above MoO3, a molybdenum surface.

			Data	∆.H°(298.15 K)	kcal·mol		AH*(298.15 K)
Source	Reaction	T/K	Points	2nd law 3rd law cal·K ⁻¹ ·n	3rd law	loc	kcal-mol-1
Burns et al.2	MoO ₂ (cr) → MoO ₂ (g)	1598-1777	*=	137.6 ± 3.0	137.38	-07 ± 1.8	-1.67
DeMaria et al.3	$Mo(cr)+2O(g) \rightarrow MoO_2(g)$	2262-2466	6	-61.3 ± 320	138.83	-20.0 ± 13.6	
Blackburn et al.4	$MoO_2(cr) \rightarrow MoO_2(g)$	1818-2028	7	107.6 ± 6.8	126.55	-99 ± 3.5	•
Plante ⁵	$MoO_2(cr) \rightarrow MoO_2(g)$	1611-1802	9	151.1 ± 13.4	142.89	-50 ± 7.7	
Chizhikov et al.6	$MoO_2(cr) = MoO_2(g)$	1500-1750	Edn	131.3 ± 0.2	136.88	3.4 ± 0.1	
Franklin and Stickney7	$Mo(cr)+O_2(g) = MoO_2(g)$	1900-2500	Egn	-0.2 ± 1.3	-0.80	-0.3 ± 0.6	-0.80
Beltonand Jordan*	Mo(cr)+2H ₂ O(g) =	1473-1773	Egn	-1181 ± 0.1	16601	-6.5 ± 0.0	
	MoO ₂ (g)+2H ₂ (g)						
	** Animal minute of the failure of abstract and	incidents for ment.	and the				

*2 points rejected due to failure of statistical test

Heat Capacity and Entropy

Continued on page 1598

natrices at 4 K. The adopted bond distance and angle and two stretching frequencies are derived from this study. Brewer' adopted the same Hewett et al. 9 have reviewed the spectroscopic studies on MoO₂(g). In addition they have studied spectroscopically MoO₂in neon and argon values. The bending frequency (300 cm⁻¹) is estimated by comparison with other transition metal dioxides.

Molybdenum Oxide (MoO₂)

PREVIOUS September 1978 (1 atm)

Molybdenum Oxide (MoO₂₇₅₀)

PREVIOUS:

CURRENT September 1978

 $\Delta_c H^{\circ}(0 \text{ K}) = \text{Unkno}$ $\Delta_t H^{\circ}(298.15 \text{ K}) = -708.41 \pm 3.3 \text{ kJ} \cdot \text{mc}$ $S^{\circ}(298.15 \text{ K}) = [69.936 \pm 1.7] \text{ J K}^{-1} \cdot \text{mol}^{-1}$ Pearson Notation: mP60 $T_{\rm tr} = 875 \pm 50 \, \rm K$

CRYSTAL

Molybdenum Oxide (MoO₂₇₅₉)

For this oxide, the atomic ratio of oxygen to molybdenum is 2.750 or 11/4. The formula MoO2750 (upon which this tabulation is ba is more indicative of the oxygen content relative to MoO₂ and MoO₃, as opposed to Mo₂O₁₁. The thermochemical values describing MoC are numerically 1/4 those of Mo₂O₁₁. Enthalpy of Formation

The high temperature emf measurements^{1,23} on compositions between MoO₂ and MoO₃ gave widely divergent results, some of which contradicted by the Mo-O phase diagram recommended by Brewer 4 Brewer 4 found that it was more practical to determine a $\Delta_d H^o(298.15)$ 1091 ± 7 K. For Mo₂O₁(cr) = MoO₂(cr) + 3 MoO₂(l), Brewer⁴ obtained Δ₂G*RT = 0.863 ± 0.05 at 1091 K. This yielded, using auxil data, $\Delta H'R = 1280 \pm 400$ K for the disproportionation of Mo₄O₁₁ to crystalline MoO₂ and MoO₃ at 298.15 K. This heat of reaction yi $\Delta_4 H'(298.15 \text{ K})R = -85203 \pm 200$ K for Mo₄O₁₁, from which we calculate $\Delta_4 H'(MoO_2r_3$, cr, 298.15 K) = -169.315 \pm 0.4 kcal·mol⁻¹. increase the uncertainty in Δ_H to \pm 0.8 kcal·mol⁻¹ which better represents the effect of errors in reducing a Δ_G ° value at 1091 K to a Δ_G value for Mo,O₁₁(cr) by fixing the thermodynamic properties from the peritectic equilibrium together with the thermodynamic data for liquid. From the phase diagram, 4 MoO₂ and Mo₂O₁₁ solids are in equilibrium with the peritectic liquid of 74.2 \pm 0.1 atomic % oxyge value at 298.15 K.

Heat Capacity and Entropy

temperature enthalpy data of MoO, fom 379 to 971 K. Their values agree with the adopted JANAF values for MoO, within 2% below 500 but the deviations increase rapidly at higher temperatures becoming 10% high at 950 K. Thus, the adopted heat capacity values for Mo₄O₁₁(were higher by 3% at 400 K, decreasing to 1.5% at 700 K. As these differences were within the scatter of the experimental measureme Brewer' assumed $\Delta C_o^* = 0$ and $\Delta S^* = 0$ for the formation of $Mo_0 I_{11}$ from 3 $MoO_1(cr)$ and $MoO_2(cr)$. Bousquet et. al. also measured the Mo_sO_{se}(cr). Brewer¹ compared their values of MoO₂(cr) and MoO₃(cr) mixtures with the same composition. For Mo₂O₁₁(cr), the entha Bousquet et. al. weed differential enthalpy analysis to obtain enthalpies between 379 and 971 K for Mo₄O₁₁(cr), Mo₈O₂₁(cr) based on the assumption $\Delta C_p^{\bullet} = 0$ as discussed in the preceding paragraph, may be less reliable at higher temperatures

Phase Data

875 K. However, a graphical examination of their data suggests two comments. First, the data point at 670 K may be a typographical ern perhaps 62.58 cal g⁻¹ should be 52.58 cal g⁻¹. Second, a transition at approximately 850 K with a corresponding heat of 0.7 kcal-mol⁻¹ co be easily derived. To be consistent with Brewer, we assume a transition at 875 ± 50 K with a corresponding zero heat of transition. $Mo_{O,I}(oP60)$ disproportionates to MoO_2 and liquid at 1091 \pm 7 K, according to the phase diagram of Phillips and Chang. ⁷³ $Mo_{O,I}(oF)$ transforms on cooling below 875 \pm 50 K to Mo, O_{11} (mP60). Bousquet et al. 6 did not interpret their enthalpy data to include a transition

In addition to the discussion of the molybdenum oxygen system by Brewer, Cmelin Handbuch der Anorganischen Chemie, has rece presented a thorough summary of the literature dealing with the phase diagram and properties of the oxide phases Ekstrom and Tilley¹⁰ hereviewed the work of Ekstrom as well as the earlier work of Kihlborg¹¹ on the phases in the Mo-O system.

LeBresq, J. J. Ochlig, and F. Marion, C. R. Acad. Sci. (Paris), Ser. C. 268, 1047 (1969).
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¹⁰T. Ekstrom and R. J. D. Tilley, J. Solid State Chem. 19, 125 (1976).
¹¹L. Kihlborg, Acta Chem. Scand. 13, 954 (1959).

II-loc	Enthalpy R	eference Te	mperature	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ $1 \cdot \text{K}^{-1} \text{mol}^{-1}$		Standard Sta	Standard State Pressure = $p^* = 0.1 \text{ MPa}$ k1-mol ⁻¹	p* = 0.1 MPa
- <u>-</u> <u>-</u>	τÆ	ಟ		-[G*-H*(T,)]/T	$H^{\bullet}-H^{\circ}(T_t)$	 V H.	δ _G •	log Kr
sed)	200°							
J _{2.750}	298.15	70.135	69.936	69.936	o'	-708.412	-636.633	111.535
	9 9 9	70.354	20.370	69.937 7.807	0.130	-708.401	-636.188	110.770
5 K	8	82.797	109.722	78.438	15.642	-706 185	-588.572	61.488
1	88	86.626	125.158	84.968	24.114	-704.674	-565.189	49.204
en at	88	94.145	151.100	98.369	42.185	-701.059	-542.073	33.901
liary	88	98.072	162.414	104.864	51.795	688899	-496612	28.823
ields	8	607701	0067/1	751.111	90.00	-090.402	-4/4.203	24.113
. We	82	110.638	192.323	123.094	83.074	-690.678	-430,346	18.732
Δ _r H°	000	115.050	201.352	128.769	94.358	-687.302	-408.786	16.425
	1200	124.139	218.447	139.599	118.271	-679.539	-366.489	12.762
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Mo₁O₂₈₇₅(cr)

M_r = 141.9383 Molybdenum Oxide (MoO₂₈₇₅)

CURRENT: September 1978

Molybdenum Oxide (MoO₂₈₇₅)

 $S^{\circ}(298 \ 15 \ \text{K}) = [73.849 \pm 1.71 \ \text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}]$

Enthalpy of Formation

 $\Delta_d H^{\circ}(298.15 \text{ K}) = -727.13 \pm 2.5 \text{ kJ·mol}$

is more indicative of the oxygen content relative to MoO₂ and MoO₃, as opposed to Mo₂O₂. The thermochemical values describing MoO₂1. The high temperature emf measurements 123 on compositions between MoO₂ and MoO₃ gave widely divergent results, some of which ar For this oxide, the atomic ratio of oxygen to molybdenum is 2.875 or 23/8 The formula MoO21315 (upon which this tabulation is based are numerically 1/8 those of Mo₈O₂₃.

1058 ± 5 K. For the equilibrium Mo₃O₂₃(cr) = Mo₄O₁₁(cr) + 4 MoO₃(1), Brewer* calculated a A₂G*RT value at 1058 K. This yielded, usin auxiliary data, $\Delta H''(298.15 \text{ K}) = 200 \text{ K}$ for the disproportionation of Mo₄O₂ to crystalline Mo₄O₁₁ and MoO₃ at 298.15 K. This enthalpy o reaction yields $\Delta H''(298.15 \text{ K}) = -173.788 \pm 0.3 \text{ kcal-mol}^{-1}$ contradicted by the Mo-O phase diagram recommended by Brewer 4 Brewer 4 found that it was more practical to determine a Δ_H ?(298, 15 K value for MoO2x13 by fixing the thermodynamic properties from the peritectic equilibria together with the thermodynamic data for the liquic From the Mo-O phase diagram, 4 Mo₂O₃ and Mo₂O₁₁ solids are in equilibrium with the perifectic liquid of 74.45 \pm 0.1 atomic % oxygen is We increase the uncertainty in ΔH^o to \pm 0.6 kcal-mol⁻¹, a value which better represents the effect of uncertainties in reducing a ΔG^o valu at 1058 K to a A_tH° value at 298.15 K.

Heat Capacity and Entropy

Mo₂O₂₆(cr). Brewer* compared their values with values of MoO₂(cr) and MoO₃(cr) mixtures with the same composition. For Mo₂O₂₃(cr), th enthalpies were lower by 15% at 400 K, lower by 3% at 500 K, and higher at higher temperatures, becoming 6% high at 700 K. As thes Bousquet et al. 6 used differential enthalpy analysis to obtain enthalpies between 379 and 971 K for Mo₄O₁₁(cr), Mo₄O₂₂(cr), an differences were within the scalter of the experimental measurements, Brewer' assumed ΔG^* = 0 and ΔS^* = 0 for the formation of Mo₄O(cr from 3MoO₂(cr) and MoO₂(cr).

Bousquet et al. ⁶ also measured high temperature enthalpy data of MoO₃ from 379 to 971 K. Their values agree with the adopted JANA! values² for MoO₃(cr) within 2% below 500 K, but the deviations increase rapidly at higher temperatures becoming 10% high at 950 K. Thu the adopted heat capacity values for Mo₂O₂(cr), based on the assumption ΔC_0^* = 0 as discussed in the preceding paragraph, may be less reliable at higher temperatures.

Phase Data

The phase Mo₈O₂₁(mP62) was found by Kihlborg, and Bousquet and Guillon, at temperatures up to 1058-1063 K. Bousquet and Guillor observed Mo₂O₂₁ to disproportionate to Mo₂O₁₁(cr) and MoO₃(g) at 1053 K by differential thermal analysis Brewer* adopted Mo₂O₂₂ as stable phase which disproportionates to Mo₄O₁₁ and liquid at a temperature, $T_{em} = 1058 \pm 5$ K, which is slightly above the disproportionation temperature of Mo₂O₂

In addition to the discussion of the molybdenum-oxygen system by Brewer, Gmeli Handbuch der Anorganischen Chemie has recently presented a thorough summary of the literature dealing with the phase diagram and properties of the oxide phases. Ekstrom and Tilley have reviewed the work of Ekstrom as well as the earlier work of Kihlborg!! on the phases in the Mo-O system.

¹H. Le Bresq, J. J. Ochlig, and F. Marion, C. R. Acad. Sci. (Paris), Ser. C, 268, 1047 (1969).

²S. Zador and C. B. Alcock, J. Chem. Thermodyn. 2, 9 (1970).

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⁴L. Brewer, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of Caliromia, Berkeley, persona communication, September 29, 1978, preliminary draft of review to be submitted for publication to Atomic Energy Review, International Atomic Energy Agency, Vienna, Austria.

JANAF Thermochemical Tables: MoO₂(cr), MoO₃(cr), and MoO_{2,250}(cr), 9-30-78.

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^oT. Ekstrom and R. J. D. Tilley, J. Solid State Chem. 19, 125 (1976).

$\Delta_t H^o(0 \text{ K}) = \text{Unknown}$	Enthalpy F	leference Te	mperature	Enthalpy Reference Temperature = T, = 29&15 K	_	Standard Sta	Standard State Pressure = p° = 0.1 MPa	, = 0.1 MPa
-727.13 ± 2.5 кЈ·то ''	r.ĸ	ប	راميا . چ – (3	nol-' -[G*-H*(T,)]/T	$H^{\circ}-H^{\circ}(T_t)$	K-mol ⁻¹	$\Delta_i G^{\bullet}$	log Kr
this tabulation is based) lues describing MoO ₂₁₇₅	880							
:	298.15	72.508	73.849	73.849	0	-727.128	-652.662	114.344
sults, some of which are mine a $\Delta_t H^{\circ}(298.15 \text{ K})$	888	80.651 120.08	74298 96.385	73.850	7.831	-727.116	-652.200 -627.358	113.558 81.925
amic data for the liquid.	8 8	89.201	130.786	85.62	16.133	- 723.229	-602.813	50.368
0 I atomic % oxygen at 8 K. This vielded using	92	93.079	144.826	96.297	33.970	-721.468	-554.586	41.384
15 K. This enthalpy of	88	101.256	169.189	109.864	53.393	-717.229	-507.435	29.451
3.788 ± 0.3 kcal·mol ⁻¹ .	3 2	110.062	190,353	172 617	03.734	-711806	-484.259	25.295
n reducing a A _t G value	025	114.658	200.126	128.667	85 751	-708.592	-438.723	19.097
	84.5 86.8	124.166	218.510	140.205	109.627	-701.096 -696.197	-394.318 -372.553	14 712 14 712 12 973
in For Mo,O ₂₃ (cr), and								
high at 700 K. As these formation of Mo-Ofer)								
vith the adopted JANAF								
aph, may be less reliable								
. Bousquet and Guillon ⁸								
r adopted Mo _s O ₂₃ as a gette disproportionation								
on Chemie ⁹ has recently strom and Tilley ¹⁰ have								
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PREVIOUS.

CURRENT: September 1978

Mo₁O₂₈₈₉(cr)

 $\Delta_t H^{\circ}(298.15 \text{ K}) = -729.16 \pm 2.5 \text{ kJ·mc}$ $S^{\circ}(298.15 \text{ K}) = [74.281 \pm 1.71 \text{ J·K}^{-1} \cdot \text{mol}^{-1}$ Pearson Notation: mP70

 $\Delta_t H^{\circ}(0 \text{ K}) = \text{Unknc}$

Enthalpy of Formation

Molybdenum Oxide (MoO₂₈₈₉)

MoO2 gry are numerically 1/9 those of Most

For this oxide, the atomic ratio of oxygen to molybdenum is 2.889 or, more exactly, 269. The formula MoO2289 (upon which this tabular is based) is more indicative of the oxygen content relative to MoO, and MoO,, as opposed to Mo_OO_s. The thermochemical values describ

contradicted by the Mo-O phase diagram recommended by Brewer. Brewer found that it was more practical to determine a AH (298.15 1053 \pm 5 K. For the equilibrium Mo₂O₂₆(cr) = Mo₂O₂₆(cr) + MoO₂(l), Brewer' calculated a Δ_1G^2RT value at 1053 K. This yielded us auxiliary data'. $\Delta_1H^3R = 50 \pm 50$ K for the disproportionation of Mo₂O₂₆ to crystalline Mo₂O₂₅ and MoO₃ at 298.15 K. This enthalpy reaction yields AH"(298.15 K)R = -87699 ± 150 K from which we calculate AH"(MOO_1183, CT, 298 15 K) = -174.275 ± 0.3 kcal mol We increase the uncertainty in ΔH^0 to \pm 0.6 kcal·mol⁻¹, a value which better represents the effects of uncertainties in reducing a ΔG^0 va value for MoO2119 by fixing the thermodynamic properties from the peritectic equilibria together with the thermodynamic data for the liqu From the Mo-O phase diagram, * Mo,O₃, and Mo,O₂₃ solids are in equilibrium with the peritectic liquid of 74.6 ± 0.1 atomic % oxygen The high temperature emf measurements 123 on compositions between MoO2 and MoO3 gave widely divergent results, some of which of 1053 K to a $\Delta_t H^{\circ}$ value at 298.15 K.

Heat Capacity and Entropy

within the scatter of the experimental measurements, Brewer* assumed $\Delta C_p^* = 0$ and $\Delta S^* = 0$ for the formation of $Mo_0O_{2d}(x)$ from $MoO_2(x)$ Mo₂O₂₆(σ). Brewer* compared their values with values of MoO₂(σ) and MoO₃(σ) mixtures with the same composition. For Mo₃O₂₆(σ), enthalpies were lower by 10% at 400 K but crossed over between 500 and 600 K and were 3% higher at 700 K. As these differences w Bousquet et al.⁶ used differential enthalpy analysis to obtain enthalpies between 379 and 971 K for Mo₄O₁₁(cr), Mo₄O₂₁(cr),

Bousquet et al. also measured high temperature enthalpy data of MoO, from 379 to 971 K. Their values agree with the adopted JANAF values for MoO₃(cr) within 2% below 500 K, but the deviations increase rapidly at higher temperatures becoming 10% high at 950 K. Thus, the adopted heat capacity values for Mo₂O₂(cr), based on the assumption $\Delta C_p^o = 0$ as discussed in the preceding paragraph, may be less reliable at hgher temperatures.

Mo₂O_{2ss} (mP70) disproportionates at 1053 ± 5 K to Mo₄O₁₁ and liquid according to the phase diagram of Phillips and Chang, ^{7,8} Brewer⁴ adopted a phase diagram which included Mo₃O₂₃ which Phillips and Chang^{1,3} did not have.

In addition to the discussion of the molybdenum-oxygen system by Brewer, Gmelin Handbuch der Anorganischen Chemie has recently presented a thorough summary of the literature dealing with the phase diagram and properties of the oxide phases. Ekstrom and Tilley to have reviewed the work of Ekstrom as well as the earlier work of Kihlborg" on the phases in the Mo-O system.

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¹ANAF Thermochemical Tables: MoO₁(cr), MoO₁(cr), and Mo₂O₂₁(cr), 9-30-78.
¹ Bousquet, J. C. David, M. Diot, and A. Guillon, Bull. Soc. Chim. Fr. (6), 2390 (1968)

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¹⁰T. Ekstrom and R. J. D. Tilley, J. Solid State Chem. 19, 125 (1976).

¹¹L. Kihiborg, Acta Chem. Scand. 13, 954 (1959).

7. C, S - (G*-H*(T,))/T 0 100	own ol ⁻¹	Enthalpy R	Reference To	emperature	Enthalpy Reference Temperature = T, = 298.15 K		Standard Stat	Standard State Pressure = p° = 0.1 MPa k1·mol ⁻¹	° = 0.1 MPa
100 208 228.15 72.772 74.281 74.281 300 72.995 74.732 74.282 400 80.973 86.896 500 89.487 131.409 89.843 700 93.343 145.494 89.843 700 93.343 145.494 89.843 100 101.611 188.225 103.700 110.0713 180.870 116.922 1100 110.476 191.181 123.208 1200 115.105 200.991 135.164 1400 129.595 228.218 146.396 1	······································	TÆ	ប	S - [G	$-H^{\prime}(T_{i})]T$	$H^{\bullet}-H^{\bullet}(T_{i})$	$\Delta_t H^{\bullet}$	Δ_{G}	log Kr
298.15 72.772 74.281 74.281 300 72.955 74.732 74.282 400 80.9723 96.895 77.235 500 80.5559 113.465 80.083 600 80.487 131.449 80.843 700 91.343 145.494 96.806 800 97.415 188.225 103.700 100.01.611 180.870 116.477 1100 110.476 191.181 122.284 1300 115.105 20.991 133.164 1400 129.595 228.218 146.396 1	rion	088							
300 72.995 74.732 74.282 400 83.973 96.896 77.250 500 85.550 115.463 83.088 600 89.487 131.409 89.843 700 93.383 145.494 96.806 800 97.415 188.225 103.700 900 101.611 169.940 110.417 1000 105.773 180.870 116.922 1100 110.476 191.181 123.284 1200 115.105 200.991 133.164 1400 124.679 219.449 140.863 1		298.15	277.77	74.281	74.281	o	-729.165	-654.461	114.659
400 80,923 96,896 77,250 500 85,550 111,463 83,088 600 83,487 131,499 83,843 800 97,415 154,549 66,806 900 101,611 169,940 110,470 1000 110,573 180,870 110,470 1200 110,576 191,181 122,208 1200 115,605 200,991 129,244 1400 124,679 219,449 140,863 11 1500 129,595 228,218 146,396	ä	300	72,995	74.732	74.282	0.135	-729.153	-653.998	113.871
500 85.559 115.463 83.088 600 89.487 131.409 89.843 700 93.383 145.494 96.806 800 97.415 158.225 103.700 900 101.611 168.940 116.417 100 105.973 180.870 116.922 1100 110.476 191.181 122.284 120 115.105 20.991 135.184 130 19.846 210.391 133.164 1400 124.679 219.449 140.863 150 129.595 228.218 146.396 1	8	9	80.923	96.896	77.250	7.858	-728.175	-629.078	82.149
600 89.487 131.449 89.843 700 93.343 145.494 96.806 800 97.415 138.225 103.700 100.611 169.940 110.417 1000 110.573 180.870 116.922 1100 110.476 191.181 123.284 1300 115.105 20.991 139.184 1400 129.595 228.218 146.396 1		200	85.550	115.463	83.088	16.188	-726.812	-604.456	63.147
700 93.33 145.494 86.806 800 97.415 158.225 103.700 900 101.611 169.940 110.417 1000 110.573 100.870 110.422 1100 110.476 191.181 122.208 1200 115.165 200.991 129.284 1400 124.679 219.449 140.863 1	1 1	8	89.487	131.409	89.843	24.940	-725.239	- 580 129	50.505
800 97415 182225 103.700 900 101.611 169.940 110.417 1000 105.973 180.870 116.922 1100 110.476 191.181 123.203 1200 115.105 200.991 123.204 1300 19.846 210.391 135.164 1400 124.679 219.449 140.863 1500 129.595 228.218 146.396	a l	90	93.383	145.494	96.806	34.082	-723.469	-556.082	41 495
900 101.611 169.940 110.417 1000 105.973 180.870 116.922 11000 115.05 105.973 180.870 116.922 1100 115.105 205.991 135.164 1300 119.465 210.391 135.164 140.0 129.595 228.218 146.396 1	Sills	8	97.415	158,225	103.700	43.621	-721 470	-532.303	34.756
1000 105.973 180.870 116.922 1100 110.476 191.181 123.208 1200 115.105 200.991 129.284 1300 119.846 210.391 135.164 1400 124.679 219.449 140.853 1500 129.595 228.218 146.396	Jo.	8	101.611	0+6.691	110.417	53.571	-719204	-508.790	29.529
1100 110,476 191,181 123,208 1200 120,181 123,284 1300 19,846 210,391 135,164 1400 124,679 219,449 140,863 1500 129,595 228,218 146,396 1	ī	0001	105.973	180.870	116.922	63.949	-716.637	-485.545	25.362
1200 115,105 200.991 132.284 1300 119,846 2103.91 135,164 1400 124,679 219,449 140,863 1500 129,595 228,218 146,396 1		1100	110.476	191.181	123.208	74.770	-713.746	-462.573	21 966
1300 119,846 210,391 133,164 1400 124,679 219,449 140,863 1 1500 129,595 228,218 146,396 1	2	1200	115.105	200.991	129.284	86.048	-710.511	-439.879	19.147
1400 129.595 228.218 146.396 1	_	1300	119.846	210.391	135.164	97.795	-706 919	-417.470	16.774
1500 129.595 228.218 146.396 1		1400	124.679	219 449	140.863	110.021	-702.961	-395,351	14.751
and the		1200	129.595	228.218	146.396	122.734	-698.631	-373,528	13 007
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Molybdenum Oxide (MoO₂₈₈₉)

PREVIOUS:

CRYSTAL

Molvbdenum Oxide (MoO₂)

CURRENT September 1978

 $S^{\circ}(298.15 \text{ K}) = 77.760 \pm 1.3 \text{ J·K}^{-1} \cdot \text{mol}^{-1}$ Pearson Notation: oP16 Fins = 1074 ± 5 K

Enthalpy of Formation

tem The adopted enthalpy of formation, -178.1 kcal mol-1, is the weighted average of two calorimetric determinations. 12 The result of and other calorimetric determinations, all for the reaction $Mo(cr) + 3/2 O_{\lambda}(g) \rightarrow MoO_{\lambda}(cr)$, are given below Staskiewicz et al.! four oxidation was only about 80% complete and tentatively attributed this to formation of MoO₄cr) Using their analytical results and their of enthalpy of combustion for the dioxide, we obtain $\Delta_t H^{2}(MOO_s, cr, 298.15 \, K) = -177.98 \, kcal \cdot mol^{-1}$. Subsequent discovery of intermediate between MoO₂ and MoO₃ raises a possible uncertainty concerning the incomplete oxidation. Mah² also reported that comb of the Mo(cr) sample ranged from 84 to 93 percent complete, as determined only by weight gam of the total combustion products prolonged low temperature ignition. In contrast, the earlier workers reported almost complete combustion. Neumann et al. ³ found abou completion using a wet analysis involving aqua regia. Moose and Parr found that in several combustions, they obtained over 99% comp based on the weight of the oxide formed

Source	Year	Δ _r H°(298 15 K), kcal·mol ⁻¹
	1955	-177.98
7	1957	-178.16
ı	1934	-180.4
•	1924	-175.6

Heat Capacity and Entropy

399.3 to 1063.9 K by drop calorimetry. The adopted heat capacities are derived from these two sets of data, subject to the constraint tha join smoothly near 300 K. Deviations of the enthalpy data from the adopted values are -0.65% to +0.17%. Seltz et al.? have also mee low temperature heat capacities from 70 to 298.7 K which are not in agreement with the values adopted, the discrepancy has been disc Smith et al 5 measured low temperature heat capacities from 18.3 to 299.8 K. King et al. 6 measured high temperature enthalpy daz by Smith. Cosgrove and Snyder8 measured high temperture enthalpy data

from 273 to 1068 K by drop calorimetry. Their smooth values are about 2% higher than the values adopted in the tabulation. Bousquet also measured high temperature enthalpy data from 379 to 971 K. Their values agree with the adopted values within 2% below 500

cal-K -1 mol -1. The increasing scatter in the C, data below 40 K (indicative of a loss of calorimeter sensitivity) coupled with uncertain recognizing the need for new low temperature C, measurements. It is surprising that the entropy of MoO3(cr) is larger than that of Wi by about 0.4 cal·K-1mol-1. This may be due to the difference in the crystal structures, MoO3 being orthorhomibe (oP16) and WO3, mono the deviations increase rapidly at higher temperature becoming +10% at 950 K.

The entropy, S'(298.15 K) = 18.585 cal·K⁻¹·mol⁻¹, is obtained from the low temperature heat capacity data of Smith et al., ⁵ bas S°(20 K) = 0.197 cal·K-1 mol-1. This starting entropy was obtained by the authors from a T² extrapolation of the data. Recently, Mi and Westrum¹⁰ have shown that the T² limiting law is inappropriate for Mo5₂ and a T³ law is suggested for this and other compound below 100 K. If the same bias is present in the C_p^a data of Smith et al. for MoO), and a T^3 extrapolation is used, our analysis sugg to bias suggests an uncertainty of ±0.3 cal·K⁻¹ mol⁻¹ for S'(298.15 K). Therefore, we adopt the author's original interpretation tamellar lattices. They have also shown that the heat capacity data of Smith et al for MoS₂ was positively biased by ~0.07 cal·K⁻¹ reduction of ~0.12 cal·K⁻¹-mol⁻¹ in S°(298.15 K). Other treatments result in estimated decreases in S°(298.15 K) ranging from 0.08 and also to uncertainty in the entropy extrapolation below 50 K for WO₃(cr).

Fusion Data

the crystal and liquid based on the enthalpy data of King. Cosgrove and Snyder⁸ found the melting point 1068 K by the cooling curve in and derived $\Delta_{tu}H^{\circ} = 12.54$ kcal-mol⁻¹ from their smooth enthalpy values at the melting point. The adopted melting pount, 1074 ± 5 K, is obtained from King et al. The enthalpy of fusion is calculated from the adopted enthalp

References

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23. Bousquet, J. C. David, M. Diot and A. Guillon, Bull Soc. Chim. France, 2390 (1968).

, = 0.1 MPa	log Kr	INFINITE 375.563 181.125	117.045	64.405	42.280	30.054	QI	22,326 19,447 17,023 14,956 13,176				
Pressure = 1	δ.	-740.150 -718.992 -693.504	-668.079 -667.601	-616.494	- 591.403 - 566.599 - 542 072	-517.821 -493.847	T <>	-470.158 -446.759 -423.657 -400.860 -378.374				
Standard State Pressure = p° = 0.1 MPa	Δ'H°	-740.150 -743.735 -745.249	-745 170 -745.158 -744 111	-742.696	- 739.250 - 737.186	-734.839 -732.172	CRYSTAL	-729.156 -725.775 -722.014 -717.862 -713.312				
	H*-H*(T,)	-12.590 -11.326 -6.632	0. 0.139 8.098	16.650	35.027 35.006 176	55.018 65.691	73.889	76.833 88.455 100.573 113.195 126.331				
Enthalpy Reference Temperature = T, = 298.15 K	-[G*-H"(T,)]/T	INFINITE 132.814 84.136	77.760 17.761 15808	86.830	100.927	114.906	126.387	128.046 134.291 140.336 146.198 151.892				
emperature =	S - [G		78.224	120.130	150.936	176.037	195.186	197.894 208.004 217.700 227.052 236.113				
ference T	೮	0. 31.648 59.279	74 881 75.107	87.751	95.814	104.441	112.562	113.792 118.679 123.683 128.779 133.959				
Enthalpy Re	7.K	100 200 200	298.15 300 400	8 8	858	888	1074 000	1200 1200 1300 1500				
$\Delta_t H^{\circ}(0 \text{ K}) = -740.15 \pm 0.4 \text{ kJ} \cdot \text{mol}^{-1}$	Δ_{fr} (290.13 K) = -/45.17 ± 0.4 KJ·mol Δ_{hw} = -48.534 ± 4.2 kJ mol ⁻¹	rimetric determinations. 12 The result of these	e given below Staskiewicz et al. 1 found that Using their analytical results and their value	oxidation. Mah ² also reported that combustion	gain of the total combustion products upon ombustion. Neumann et al. 3 found about 97%	bustions, they obtained over 99% completion,		1 1	easured high temperature enthalpy data from sets of data, subject to the constraint that they 6 to +0.17% Seltz et al., have also measured adopted, the discrepancy has been discussed	ues adopted in the tabulation. Bousquet et al. ⁹ adopted values within 2% below 500 K, but	theat capacity data of Smith et al., 5 based on extrapolation of the data. Recenly, McBride suggested for this and other compounds with as positively biased by ~0.07 cal·K ⁻¹ ·mol ⁻¹ extrapolation is used, our analysis suggests a ses in S'(298 15 K) ranging from 0.08 to 0.17 eter sensitivity) coupled with uncertainty due put the author's original interpretation while by of MoO ₃ (cr) is larger than that of WO ₃ (cr) is orthorhomibe (oP16) and WO ₃ monoclinic, is calculated from the adopted enthalpies of ing point 1068 K by the cooling curve method	

Molybdenum Oxide (MoO₃)

PREVIOUS. June 1967

CURRENT. September 1978

Molybdenum Oxide (MoO₃)

Mo₁O₃(I)

M_r = 143.9382 Molybdenum Oxide (MoO₃)

LIQUID $S^{\circ}(298.15 \text{ K}) = [114.935] \text{ J·K}^{-1} \cdot \text{mol}^{-1}$ $T_{\rm fut} = 1074 \pm 5 \, \rm K$

Enthalpy of Formation

 $\Delta_t H''(MoO)$, 1, 298.15 K) is calculated from that of the crystal by adding the enthalpy of fusion, $\Delta_t \mu H'$, and the difference in enth H°(1074 K)-H°(298.15 K), between the crystal and liquid.

The heat capacity is derived from the enthalpy data (1074-1392 K) measured by King et al. The heat capacity is assumed constant and below the measured range. At 750 K, a glass transition is assumed, below which the heat capacity is taken to be the same as that crystal. S°(MoO), 1, 298.15 K) is calculated in a manner analogous to that used for the enthalpy of formation. Heat Capacity and Entropy

Cosgrove and Snyder² also measured enthalpy data for MoO₃(1) in the temperature range from 1068 to 1300 K. Their smooth value 2.5 to 4.0 percent higher than our tabulated values.

Fusion Data

Refer to the crystal table for details

Vaporization Data

Effusion3 and transpiration4 measurements indicate that MoO3(g) is not the major species found in the vapor above MoO3 condensed ph primarily on the transpiration measurements of Ackermann et al. Feiser, using indirect methods, reported a normal boiling point of 14: Both sets of measurements indicate the presence of polymeric species (MoO₃), where the predominant species near the normal boiling are those for x = 3 and 4. At higher temperatures the equilibrium shifts toward lower x but MoO₃(I) will reach 1 atm at 1380 \pm 30 K l We adopt Brewer's estimate and emphasize that this represents vaporization to a mixture of gases, (MoO3),

G. King, W. W. Weller and A. U. Christensen, U. S. Bur. Mines RI 5664, 29 pp. (1960).

²L. A. Cosgrove and P. E. Snyder, J Amer. Chem. Soc. 75, 1227 (1953).

³I. Berkowitz, M. G. Inghram and W. A. Chupka, J. Chem. Phys. 26, 842 (1957).

(September 29, 1978), of preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Es Brewer, Materials and Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, personal communic R. J. Ackermann, R. J. Thorn, C. Alexander and M. Tetenbaum, J. Phys Chem. 64, 350 (1960).

Agency, Vienna, Austria. ⁶J. Feiser, Metall Erz. 28, 297 (1931).

-	Enthalny D	forence T.	- dunament	N 51 805 = T = emisses Terrestation	 	Standard Sta	Standard State Pressure = " = 0.1 MPs	. = 0.1 MPa	_
Δ_{eff} (296.13 K) = [-105.127] KJ·III01 Δ_{eff} 48.534 ± 4.2 kJ·mol ⁻¹	M fd mine		L·K-'mol-'-	- 11		kJ·mol-!			
	T/K	ប	s -[G	$-[G^{\bullet}-H^{\bullet}(T_{*})]T$	$H^{\bullet}-H^{\bullet}(T_{\bullet})$	$\Delta_t H^{ullet}$	•9₹	log Kr	
n, $\Delta_{hw}H^{\circ}$, and the difference in enthalpy,	088								
e best canacity is assumed constant above	298.15 300 400	74.881 75.107 83.094	115.399 138.240	114.935 114.936 117.996	0. 0.139 8.098	-703.727 -703.714 -702.668	-637.719 -637.310 -615.317	111.726 110.966 80.352	
icity is taken to be the same as that of the of formation.	888	91.776	157.305	124.005	16.650 25.627	-701.252 -699.631	-593.638 -572.264 -551.178	62.017 49.820 41.129	
1068 to 1300 K. Their smooth values are	750.000	_	194.79	141.660	39.848 39.848	dLAS	GLASS <> LIQUID TRANSITION		
	888		202.985 217.937 231.313	145.240 152.503 159.727	46.196 58.891 71.586	-694,343 -689,523 -684,833	-530.415 -510.214 -490.544	34.633 29.612 25.623	,
	1074 000	126.951	240.376	164.975	80,980	CRYST	CRYSTAL <> LIQUID	Q D	
the vapor above MoO ₃ condensed phases.	1200 1200 1400 1400	126.951 126.951 126.951 126.951	243.413 254.459 264.620 274.028	166.794 173.645 180.258 186.624	84281 96.976 109.671 122.366	-680.265 -675.811 -671.472 -667.247	-471.337 -452.541 -434.112 -416.012	22.382 19.699 17.443	
1) will reach I atm at 1380 ± 30 K based	0091 1800	126.951	290.980	192.746	153,001	-659.152	-380.680	12.428	
reported a normal boiling point of 1438 K. es, (MoO ₃) _k .	0081 5 0080 5 0080 5	126.951 126.951 126.951	298.677 305.933 312.797	204.293 209.740 214.985	160.452 173.147 185.842 198.537	-655.290 -651.560 -647.968 -644.573	-363.395 -346.333 -329.475 -312.801	11.166 10.050 9.058	
onis Badelav nascoral communication									
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PREVIOUS: June 1967

3)	
(MoO	
n Oxide	
Molybdenun	

CRYSTAL-LIQUID

Refer to the individual tables for details. 0 to 1074 K crystal (oP16) above 1074 K liquid

Molybdenum Oxide (MoO₃)

No₁O₃(g)

Molybdenum Oxide (MoO3)

CURRENT September 1978 (1 bar)

127.292 148.485 169.761 191.116 212.559

-1061.885 -1066.587 -1071.446 -1076.463

22.485 43.295 64.181

1037.070

388.825

419.339 422.566 424.125 424.125 427.169 427.169 430.107 430.107 431.538

503.409 505.021 506.602 508.153 509.676

82.981

1033.511

434 798

347.344

494.849 498.379 500.090 501.766

82.943 82.952 82.967 82.967 82.967

1048.742

-1057.343

-198.463 -192.088 -185.621 -179.005

365.416 368.055 406.969 408.435

198.276 206.538 214.804 23.073 231,345 239,619 247,896 256,175

377.716 380.363 382.930 385.422 387.843

447.624 450.740 453.743 456.642 459.445

82.521 82.566 82.606 82.642 82.643

363.087

-163.183 -155.200 -147.169 -139.090

-409.925 -411.439 -412.977 -414.537

390.197 392.487 394.716 396.889 399.006

464.782 467.328 469.799 472.199

82.704 82.731 82.735 82.738 82.738

462.156

\$2,444,50 \$2

-416.120

426.037

905.884

314.174 322.465 330.757 339.050

410.702 412.502 414.264 415.990 417.682

485.308 487.305 489.256 491.162 493.026

52.892 82.904 82.915 82.925 82.934

-122.796 -114.582 -106.322 -98.019 -89.675

264.456 272.738 281.023 289.308 297.596

401.072 403.088 405.057 406.981 408.862

474.532 476.801 479.010 481.163 483.261

52.817 52.835 52.851 52.865

Mo₁O₃(q)

Standard State Pressure = $p^* = 0.1$ MPa

Enthalpy Reference Temperature = T. = 298.15 K

M_r = 143.9382 Molybdenum Oxide (MoO₃)

S -[G-H(T,)]T

IDEAL GAS Molybdenum Oxide (MoO₃)

 $S^{(298.15 \text{ K})} = [283.897 \pm 12.6] \text{ J·K}^{-1} \cdot \text{mol}^{-1}$ $\Delta_{\rm e}H^{\circ}(0 \text{ K}) = 1740.126 \pm 21.3 \text{ kJ·mol}^{-1}$

 $\Delta_i H^{\circ}(0 \text{ K}) = -342.22 \pm 20.9 \text{ kJ} \cdot \text{mol}^{-1}$ $\Delta_c H^{\circ}(298.15 \text{ K}) = -346.44 \pm 20.9 \text{ kJ·mol}^{-1}$

Product of the Moments of Inertia: $I_A I_B I_C = \{3.0307222 \times 10^{-114}\}$ g³-cm⁶ Vibrational Frequencies and Degeneracies v, cm_1 924 (2) [310](2) Ground State Quantum Weight; [1] Bond Distance Mo-O = [1.73] A ν, cm⁻¹ (1)(1) 978 (1) Bond Angle. O-Mo-O = 99° Point Group: C3.

Enthaloy of Formation

mass spectrometry Plante, Blackburn et al. 3 and Chizhikov et al. 4 also investigated the vapor pressures above molybdenum dioxide by a Knudsen effusion method. These studies — involve the disproportionation of MoO₂(cr) to Mo(cr) and MoO₃(g). DeMaria et al. 3 reported Burns et al. I determined the partial pressures of gaseous oxides MoO₂, MoO₃, MoO₃, and (MoO₃) in equilibrium with powdered MoO₂ partial pressures of MoO(g), MoO₂(g), MoO₃(g) and O(g) in the Mo-Al₂O₂system from mass spectrometry 윤

-303.302 -297.751 -292.189

347.756

-314,373

20,454

330,707

73.289 77.266 78.381 79.214

-286.612 -281.017 -275.400 -269.756 -264.083

348.051 348.282 348.582 348.962 349.430

377.493

79.851 80.348 80.742 81.059 31.318

330.707 328.052 325.353 322.627 319.885

347.249

-330,804

-346.435 346.451

283.897 284,265

59.378 59.518 53.017 55.979 58.449 70.494 -258.376 -252.629 -246.841 -241.005

407.763 412.711 417.386 421.816 426.024

81.532 81.711 81.862 81.990 82.100

349.995 -351.452 -352.363 -353.408

-223.174 -223.170 -217.102 -210.965 -204.754

148.799 157.030 165.269 173.513 181.763

363.092 366.222 369.243 372.161 374.983

430.032 433.858 437.517 441.023

22.1% 22.278 22.351 22.415

-354.598 355.942 357.451 359.136 361.007

40.575

Source	Source Reaction		T/K	Data Points	Δ _t H*(298.15 K), kcal·mol ⁻¹ 2nd law 3rd law), kcal·mol ⁻¹ 3rd law	Drift cal·K ⁻¹ ·mol ⁻¹	Δ _t H°(298.15 K) kcal·mol ⁻¹
-	1.5 MoO ₂ (cr)	5 MoO ₂ (cr) → MoO ₃ (g) + 0.5 Mo(cr) 1481-1777 34	1481-1777	22	131.7 ± 1.5	128.0 ± 0.8	28.0 ± 0.8 -2.2 ± 0.9	-82.8
~	1.5 MoO ₂ (cr)	→ MoO ₃ (g) + 0.5 Mo(cr) 1592-1918	1592-1918	119	133.5 ± 1.4	1240 ± 1.3	-6.3 ± 0.8	8.98-
	1.5 MoO ₂ (cr)	→ MoO ₃ (g) + 0.5 Mo(cr) 1818-2028	1818-2028	7	108.8 ± 6.4	121.2 ± 1.6	6.3 ± 3.4	-89.5
•	1.5 MoO ₂ (cr)	→ MoO ₃ (g) + 0.5 Mo(cr) 1500-1730	1500-1730	Ega	137.9	133.1 ± 0.5	-3.0	-77.6
n	Mo(cr) + 3 O(g	$fo(cr) + 3 O(g) \rightarrow MoO_3(g)$	2281–2416	9	-210.5 ± 28.0	-253.7 ± 4.0	-18.6 ± 11.8	-75.0

adopted value differs slightly from the value of -82.57 kcal·mol⁻¹ adopted by Brewer, ⁷ which is also based on Burns *et al.* ¹ The difference is a result of slight differences in Gibbs energy functions in the respective auxiliary data for Mo(cr). ^{6,4} The deat of atomization calculated from the JANAF tables 6 is $\Delta_{\rm a}H^9(0\,{\rm K}) = 415.9 \pm 5.1$ kcal·mol⁻¹. The selected enthalpy of formation is -82.8 kcal·mol⁻¹, based on the 3rd law value of $\Delta_t H^2$ (298.15 K) of Burns et al. The choice is made because there is serious doubt about the data of Blackburn³ as discussed by Burns et all. In addition, the assumption made by Plante² that they only vapor species of any importance is MoO₃ may be erroneous. The mass specrometric work of Burns et al 1 is thus preferred. Our

Heat Capacity and Entropy

In a recent IR matrix isolation study, Hewett et al. * observed peaks at 976 and 922 cm-1 which they assigned to stretching modes of an estimated bending force constant (f_a) of 0.296 mdyn/Å. Variations of 20% in f_a changed the calculated stretching frequencies by only a few cm⁻¹. The calculated stretching frequencies were more sensitive to the estimated pyramidal angle (β) which was adjusted to obtain the best fit to the observed stretching frequencies of oxide molecules containing ¹⁶O, ¹⁶O, and mixed ¹⁶O-¹⁶O. The final results yielded best fit to the observed stretching frequencies of oxide molecules containing 16 O, 16 O, and mixed 16 O- 16 O. The final results yielded $\beta = 61.5 \pm 2^{\circ}$ and values of 261, 275 and 275 cm⁻¹ for the bending frequencies of Mo 16 O. Due to the insensitivity of the normal coordinate The pyramidal angle of 61.3° corresponds to an O-Mo-O bond angle of 99° Based on the adopted structure, the principal moments of inertia analysis to fa these bending frequencies are useful only for comparing changes due to isotopic substitution. In contrast, we adopt bending frequencies of 310, 310 and 340 cm⁻¹ and a bond distance of 1.73 Å as selected by Brewer⁷ for consistency with other metal oxides. The pyramidal angle of 61.5° is adopted, the possible effect of using a shorter bond distance during the normal coordinate analysis is unknown. MoO₃(g). We add 2 cm⁻¹ to these frequencies to correct for the matrix effect. The observation of two stretching modes in the infrared spectrum suggests a pyramidal C₃, structure for MoO₃(g). Hewett *et al.* performed a normal coordinate analysis using a bond distance of 1.8 Å and are $I_A = I_B = [12.8372 \times 10^{-3}]$ and $I_C = [18.3999 \times 10^{-39}]$ g cm². The thermochemical functions are consistent with those of Brewer.

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DeMaria, R. P. Burns, J. Drowart and M. G. Inghram, J. Chem. Phys. 32, 1373 (1960)

L. Brewer, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, personal PREVIOUS: September 1978 (1 am) communication of preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy JANAF Thermochemical Tables: Mo(cr) and Mo(g), 3–31–78; MoO₂(cr), 9–30–78; O(g), 3–31–77; WO₁(g), 9–30–66. Agency, Vienna, Austria; (September 29, 1978).

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Mo₁S₂(cr)

Standard State Pressure = p^* = 0.1 MPa

Enthalpy Reference Temperature = T. = 298.15 K

M_r = 160.06 Molybdenum Sulfide (MoS₂)

Y.

 $H^{\bullet}-H^{\bullet}(T_{\bullet})$

 $S^{*} - [G^{*} - H^{*}(T_{*})]T$

267.156 -267.100 -263.822 -259.125

276.144

110.098 68.080 62.572 62.573 62.573 65.146

0. 24.050 51.840 63.555 63.680 68.910 71.756

298.15

°28

62.965 82.099 97.805

0. 12.991 39.359 62.572

-276.155 -281.141 -284.502

CURRENT: June 1978

(23)	
de (Mo	
Sulfie	
mnu	

Molybde

CRYSTAL

 $\Delta_t H^{\circ}(0 \text{ K}) = -273.31 \pm 2.5 \text{ kJ·mol}^{-1}$ $\Delta_t H^{\circ}(298.15 \text{ K}) = -276.14 \pm 2.5 \text{ kJ·mol}^{-1}$ A...H" - Unknown $S^{(298.15 \text{ K})} = 62.572 \pm 0.08 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ $f_{ta} = 2023 \pm 50 \text{ K [p = 1 atm S}_{2}(g)]$ Pearson Notation: hP6

Enthalpy of Formation

The adopted enthalpy of formation is from Brewer' and is a weighted average of calorimetric² and equilibrium³ values. O'Hare et al.² obtained $\Delta_t H^0(298.15 \, K) = 6.58 \pm 1.2 \, kcal·mol⁻¹ using a fluorine bomb calorimeter. Larson and Elliout³ studied the equilibrium MoO₂(cr) + 2 SO₂(g) = MoS₂(cr) + 3 O₂(g) via emf technique (1051–1372 K); using auxiliary data¹⁴ Brewer calculated <math>\Delta_t H^0(MoS_3, 298.15 \, K) = -66.64 \pm 0.6 \, kcal·mol⁻¹ from their results. Thermodynamic analysis of other calorimetric and equilibrium measurements²⁻³ are summarized by O'Hare et. al.² and Mills.⁴$

Heat Capacity and Entropy

The adopted values of C, are from Brewer! and are based on experimental C, data (6-346 K) of McBride and Westrum? and high temperature enthalpy data (523-1204 K) of Fredrickson and Chasanov. ¹⁰ C, values above 1200 K are extrapolated. The recent enthalpy data (500-1700 K) of Volovik et. al. ¹¹ agrees with enthalpies in this table to within ±2% to 2000 K. Older C, data of Smith et. al. ¹² and Anderson ¹³ contain considerable scatter and are given no weight.

46.2292 46.596 46.59

-197.623 -179.680 -161.841 -144.098 -126.444 -108,869

-395.620 -394.356 -393.101 -391.861 -390.646

103.329 108.122 112.691 117.052

157.341 164.263 170.699 176.721 182.383

59.413 75.411 83.537 91.744 00.030

389.463

-56.555 -39.233 -21.958 -4.726 12.469 29.633

133.959 133.959 142.632 151.383 160.211 169.115

210.876 214.947 218.871 222.660

125.211 129.039 132.717 136.255 139.665 142.956 146.137 146.137

187.730 192.802 197.628 202.235 206.645

79.119 79.998 80.835 81.677 82.467 83.262 84.057 84.810 84.810 86.358 86.358 87.906 88.639 88.639

-386.171 -385.182

-253.800 -248.105 -242.159 -233.867 -215.682

288.951 290.530 398.134 396.882

75.897 81.756 87.494 93.018 98.297

111.057 122.511 132.610 141.650 149.842

73.597 75.019 76.232 77.278 78.241

0.118 6.781 13.825 21.096 28.528 36.092 43.769 51.545

\$'(298.15 K) is obtained from the appropriate integration of the adopted C; data based on \$'(10 K) = 0.012 cal·K⁻¹·mol⁻¹

The crystal structure of MoS2 is (AP6). Mering and Levialdi " have shown that nonstoichiometric sulfur-rich modifications (which have essentially the hP6 structure with expansion and distortion of the lattice) can be prepared as metastable compositions up to MoS_{2.95} amorphous metastable phases are obtained with higher sulfur contents. For information on other metastable phases, refer to and. ¹⁵ According to Brewer's lead to the contents of the phase diagram the compositional range of stability decreases as the temperature increases.

Incongruent melting points up to 350 K lower may be obtained depending upon the pressure of S₂(g). The adopted melting point is that selected by Brewer¹ for an S₂(g) pressure of 1 atm. Mills² adopted a 1 atm value of 1458 K which appears much too low. Based on Cannon's evidence¹⁶ of a melting point in excess of 2073 K, Brewer¹ adopted a congruent melting point of 2173 K. However, congruent melting is observed only at high sulfur pressures; the melting point of 2173 K corresponds to a Szg) pressure of ~4 arm.

References

L. Brewer, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, personal communication of preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy

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Cannon, Nature 183, 1612 (1959) supplement, (1969)

Molybdenum Sulfide (MoS₂)

PREVIOUS:

CURRENT: June 1978

Mo2S3(cr)

Standard State Pressure = p° = 0.1 MPa

log Kr

ΔĦ

 $H^{\bullet}-H^{\bullet}(T_t)$

 $S^{\bullet} - [G^{\bullet} - H^{\bullet}(T_{\bullet})]T$

ڻ

Enthalpy Reference Temperature - T, - 298.15 K

J-K-'mol-'

M, = 288.06 Molybdenum Sulfide (Mo₂S₃)

CRYSTAL

Molybdenum Sulfide (Mo₂S₃)

Δ_tH°(0 K) = Unknown $\Delta_t H^{\circ}(298.15 \text{ K}) = -407.103 \pm 8.4 \text{ kJ} \cdot \text{mol}^{-1}$ Δ_{ha}H° = -129 704 ± 41.8 kJ·mol⁻¹

 $S^{\circ}(298.15 \text{ K}) = 114.976 \pm 8.4 \text{ J·K}^{-1} \cdot \text{mol}^{-1}$ $T_{trs} = 2080 \pm 20 \text{ K}$

Pearson notation: mP10

Enthalpy of F

ia, which outlined based on Cub below. Auxiliar The adopted

f equilibrium data er's analysis are c		
is linear regression analysis of 8.15 K). The data used in Brew	T/K	
be critical review by Brewer. ¹ H both $\Delta_t H^o$ (298.15 K) and S^o (298 bles. ³	Reaction	
Formation central or the critical review by Brewer. ¹ His linear regression analysis of equilibrium data bicciotti's sigma-plot method, 2 yields both Δ_1H^2 (298.15 K) and S^2 (298.15 K). The data used in Brewer's analysis are cry data are taken from the JANAF tables. ³	Source	

	Source	Reaction	TIK
	McCabe*	<	1303 – 1425
	Isakova ⁵	B	1523 - 1738
	Hager and Elliott ⁶	U	1366 - 1612
	Stubbles and Richardson7	ပ	1119 – 1467
	Pouillard and Perrot	ပ	1030 - 1280
	Stubbles and Richardson7	Ω	1270 – 1470
	Pouillard and Perrot	Ω	1030 – 1280
eactions:	(A) 2 Mo(cr) + 3/2 S ₂ (g) = Mo ₂ S ₃ (cr) (B) 2 MoS ₂ (cr) = Mo ₂ S ₃ (cr) + 1/2S ₂ (g	Го ₂ S ₃ (ст) + 1/2S ₂ (g)	(C) 2 Mo(ct) + 3 H ₂ S(g) = Mo ₂ S ₃ (ct) + 3 H ₂ (g) (D) 2 MoS ₂ (ct) + H ₂ (g) = Mo ₂ S ₃ (ct) + H ₂ S(g)

69.317 52.108 52.108 52.108 52.1625 52.361 52.361 52.361 52.361 52.361 52.361 52.361 52.362 52.363 5

298.802 273.233 247.942

104.564 119.312 134.401 149.828 165.591 181.691

-222.920 -198.159

-574.954 -571.381 -567.668

193.781 201.898 209.695 217.195

145.762 149.186 152.582 155.957 159.317

-377.885 -370.204 -362.222 -350.811 -324.658

422.753 425.196 426.942 587.548 584.687 581.623

36.136 49.079 62.409 76.107 90.161

137.754 147.812 157.707 167.285 176.491

197.981 217.925 251.848 266.652 280.378 293.208 305.283 316.714

-407.116 -414.437 -419.287

15.653 (48.339 (75.164

298.15 88

127.399 135.162 138.775 142.297

-407.103

---> LIOUID

-- CRYSTAL -543.184 -538.867 -534.523 -530.172

-54.601

267.190 285.286 303.715 322.474

384,376 392,794 400,985 408,968

-173.650 -149.384 -125.354 -101.552 -77.970

-563.828 -559.873 -555.817 -551.674

224.421 231.396 238.138 244.667 250.996 255.927

337.978 347.940 357.523 366.768 375.709 382,663

162.666 166.006 169.339 172.666 175.989 178.645

Heat Capacity and Entropy

There are no experimental high temperature heat capacity or enthalpy studies. The adopted heat capacity, which is assumed to represent the high temperature crystal form, is based on the estimate of Gronvold and Westrum, 9 C, = 26.36 + 7.88 \times 10⁻³T = 2.30 \times 10³T. The value of S'(298.15 K) is taken from Brewer, refer above.

Rastogi and Ray ¹⁰ measured the low temperature $C_s^*(350 \text{ K})$ but report only $C_s^*(298.15 \text{ K}) = 33.2 \text{ cal·K}^{-1} \text{-mol}^{-1}$. This value apparently refers to the low temperature superstructure crystal form but is not expected to differ significantly from the high temperature form. The reason for the 7 cal·K⁻¹-mol⁻¹ discrepancy between the Rastogi-Ray value of $C_s^*(298.15 \text{ K})$ and that adopted here is not known but it should be mentioned that the Rastogi-Ray value is well above the classical limit of 15R. Insufficient information on sample preparation and calorimetric technique is available to assess the validity of the Rastogi-Ray data

Phase Data

The crystal structure of Mo₂S₃ is monoclinic and belongs to space group P2_i/m above 310 K.¹¹ Below 310 K all axes are doubled and a superstructure is formed. The heat of transition is reported to be 5 cal·K-1.mol-1.10

The stability region for Mo₂S₃ is from 900 \pm 40 K¹ to the melting point. Below 900 K the material is metastable with respect to disproportionation to Mo₂C₄C₃ and Mo₂S₄C₄C₅. However equilibrium is established very slowly below 1100 K^{11,12} and, once prepared, Mo₂S₃ may be quenched and stored indefinitely at room temperature. The enthalpy of decomposition at 900 K ($\Delta_{em}H$) for the reaction Mo₂S₁(cr) \rightarrow 1/2 Mo(ct) + 3/2 MoS₂(ct) is calculated from the JANAF tables.3

Fusion Data

We adopt the congruent melting point from Brewer.¹ The enthalpy of fusion is estimated assuming an entropy of fusion of \sim 3 cal·K⁻¹ g-atom⁻¹ as suggested by Kubaschewski et al.¹³ This gives a enthalpy of fusion of 31 kcal·mol⁻¹ and the uncertainty is estimated to be 10 kcal·mol-1

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JANAF Thermochemical Tables: Mo(cr) 3-31-78; MoS₂(cr) 6-30-78; S₂(g) 9-30-77; H₂S(g) 6-30-77.

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Molybdenum Sulfide (Mo₂S₃)

PREVIOUS:

1.389 0.972 0.498 0.498 0.110 -0.246 -1.139 -1.137

-55.846 -38.841 -21.915 -5053 11.763 28.548 45.321 62.101 79.010 98.290 117.506 117.506 117.506 117.506 117.506 117.506 117.506

-407.636 -407.546 -408.042 -481.053 -479.131

338.103 353.793 369.483 385.173 400.863

349.992 354.919 359.701 364.347 368.863

480.032 485.953 491.659 497.165 502.484

2100 2200 2300 2200 2200 2200 2200 2300 3300 3300 3300 3300

156.900 156.900 156.900 156.900 156.900

5.594 4.660 3.842 3.120 2.479 1.905

-142.743 -125.044 -107.527 -90.170 -72.949

-427.516 -424.305 -421.327 -418.594 -416.121

181.203 196.893 212.583 228.273 243.963 256.515

290.604 297.548 304.234 310.676 316.886

321.696

156.900

GLASS <--> LIQUID
TRANSITION

-160.649

-430.947

165.513

283,388

157.639 156.900 156.900 156.900 156.900 156.900 156.900 156.900

-234.816 -215.866 -197.195 -178.792

-444.824 -441.574 -438.155 -434.582

251.513 259.975 268.092 275.889 279.674 279.674

181.170 181.847 214.353 214.353 224.175 238.4119 318.042 335.402 335.402 335.402 338.410 338.410 338.410 338.410 338.410 338.410 348.413.42 433.88 443.88 443.88 443.88

-- CRYSTAL <---> LIQUID

-413.922 -412.011 -410.406 -409.124 -408.188

259.653 275.343 291.033 306.723 322.413

322.878 328.665 334.260 339.672 344.913

446.522 453.821 460.796 467.473 473.878

156.900 156.900 156.900 156.900 156.900 156.900 156.900 156.900

Mo₂S₃(1)

Standard State Pressure = $p^* = 0.1$ MPa

Enthalpy Reference Temperature = T, = 29&15 K

J.K - 'mol - '

kJ·mol-1

H*-H*(T,) A.H*

 $S^* - [G^* - H^*(T_t)]/T$

ţ

log Kr

δç

48.808 48.516 48.516 29.395 24.446 20.874 18.873 13.270 11.150 9.396 7.923 6.671

-278.590 -278.641 -281.032 -281.374 -280.802 -279.740 -278.377 -278.377 -273.586 -254.052

-270.316 -277.637 -282.487 -285.953 -288.396 -290.142 -450.748

181.170 181.172 185.575 194.129 203.948 214.006 223.901 233.479 242.685

109.294 117.464 117.464 122.926 127.399 131.405 135.162 138.775 145.762 145.762 145.762 145.762

CURRENT: June 1978

PREVIOUS:

M _r = 288.06 Molybdenum Sulfide (Mo ₂ S ₃)	
LIQUID	
Molybdenum Sulfide (Mo ₂ S ₃)	

 $S^{\circ}(298.15 \text{ K}) = [181.170] \text{ J·K}^{-1} \cdot \text{mol}^{-1}$ $T_{\text{tat}} = 2080 \pm 20 \text{ K}$

 $\Delta_{\rm rd}$ "(298.15 K) = [-270.304] kJ·mol⁻¹ $\Delta_{\rm lm}$ H° = 129.704 ± 41.8 kJ·mol⁻¹ ΔH°(Mo₂S₃, I, 298.15 K) is calculated from that of the crystal by adding the enthalpy fusion, of Δt_wH°, and the difference in enthalpy, H°(2080 K)-H°(298.15 K), between the crystal and liquid. Enthalpy of Formation

A constant liquid C, of 7.5 cal·K-1·g-atom-1 is assumed which yields a C, value of 37.5 cal·K-1·mol-1. This value is adopted above an assumed glass transition at 1450 K. The heat capacity of the crystal' is assumed below the glass transition. S'(Mo₂S, 1, 298.15 K) in calculated by a manner analogous to that used for the enthalpy of formation. Heat Capacity and Entropy

Fusion Data

Refer to the crystal table for details.

Decomposition Data

According to Brewer's phase diagram, Mo₂S₂ has a very short liquid range at 1 atm S₂(g). We adopt a decomposition temperature of 2140 ± 30 K based on the phase diagram. Above this temperature Mo₂S₃(l) decomposes to S₂(g) plus a liquid poorer in sulfur than Mo₂S₃.

At higher sulfur pressures, the liquid range is much more extensive.

¹4ANAF Thermochemical Tables: Mo₂S₃(cr) 6–30–78.

²L. Brewer, Materials Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, personal communication of preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy Agency, Vienna, Austria; (September 29, 1978)

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

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(Mo ₂ S ₃)
olybdenum Sulfide
M,=288.06 M

C\$** = \(C ^2 - H(T_1) \) \) \(H^* - H^* T_1 \) \(A ^4 \) \(T/K C; S' -[G"-H(T)] T H"-H(T) Ath" AG" In the third AG"	<u></u>	Enthalpy Reference		Temperature =	- T, = 298.15 K		Standard State Pressure		p = 0.1 MPa
0 0 -407.103 -955.654 20% 288.15 109.294 114.976 114.976 0. -407.103 -395.654 30 109.489 115.553 114.978 10.202 -407.116 -395.333 40 117.464 148.339 119.381 -131.33 -414.437 -391.314 50 127.925 177.924 127.924 -21.615 -419.287 -395.333 70 131.405 217.925 177.724 45.156 -370.204 80 135.162 235.719 157.707 62.409 -425.105 -370.204 80 135.162 235.719 176.491 90.161 -384.687 -342.222 100 142.297 236.233 201.898 114.401 -578.322 -302.222 100 142.707 26.6625 171.912 -31.638 -31.233 -31.233 110 145.762 23.708 185.319 114.431 -31.536 -31.222 110	100 298.15 109.294 114.976 114.976 0407.103 -395.654 300 117.459 115.35 114.978 0.0407.110 -395.654 400 117.459 115.35 114.978 0.0407.110 -395.654 500 127.295 175.164 127.394 137734 35.136 -412.273 -377.835 700 131.402 217.295 177.394 137.794 35.136 -427.173 -377.835 700 131.402 217.295 177.394 137.794 -427.105 -427.273 -377.835 700 131.402 217.295 177.394 137.794 -427.105 -370.204 800 135.102 23.794 137.794 -427.105 -370.204 800 135.102 23.794 137.794 -427.105 -370.204 800 135.102 23.794 137.797 -425.105 -370.204 800 135.102 23.208 193.784 1193.12 -578.374 -370.204 8100 145.762 230.208 193.784 1193.12 -578.377 -273.233 8100 152.582 30.208 193.784 1193.12 -578.377 -273.233 8100 152.582 30.208 193.784 134.401 -578.377 -273.233 8100 152.582 30.208 231.396 144.822 -571.381 -273.826 8200000 175.696 347.990 231.396 198.124 -559.277 -107.334 8200000 175.696 347.990 231.396 198.124 -559.277 -107.334 820000 176.600 445.021 255.977 399.314 -115.20 8200000 186.500 445.021 255.977 399.314 -115.20 820000 186.500 467.021 255.977 440.246 -51.624 8200 186.500 467.791 282.672 -441.212 -421.322 8200 186.500 467.791 282.672 -441.212 -421.322 8200 186.500 467.791 282.672 -441.212 -421.342 8200 186.500 467.791 282.672 -441.242 -471.322 8200 186.500 467.791 282.672 -471.322 -471.342 8200 186.500 467.791 282.672 -471.342 -471.343 8200 186.500 467.791 282.672 -471.343 -471.344 8200 186.500 467.791 282.672 -471.343 -471.344 8200 186.500 467.791 382.673 -471.342 -471.343 8200 186.500 467.791 382.673 -471.342 -471.343 8200 186.500 467.791 380.242 -471.343 -471.344 8200 186.500 473.783 200.193 447.972 -471.343 155.756 8200 186.500 473.783 200.193 447.972 -471.343 155.756 8200 186.500 473.783 200.193 447.972 -471.343 155.756 8200 186.500 473.783 200.193 447.973 -471.343 155.756 8200 186.500 473.783 200.193 447.973 -471.343 155.756 8200 186.500 473.783 200.193 447.973 -471.343 155.756 8200 186.500 473.783 200.193 447.973 -471.343 155.778 8200 186.500 572.473 572.873 -471.344 177.778 177.778 8200 186.500 572.473 572.778 -471.343 17		7/K	រូ	-	-H'(T,)]/T	H*-H*(T,)	A.H.	∇^{Q}	log Kr
298.15 109.294 114.976 114.976 0. -407.103 -395.654 300 109.483 115.553 114.978 0.02 -407.116 -395.533 400 117.464 177.144 177.14 3.01 -407.117 -91.374 500 127.296 177.164 177.14 3.05 -40.217 -31.314 700 131.405 177.724 3.05 -40.273 -377.224 800 135.162 23.771 157.707 6.2490 -405.22 -30.222 900 135.162 23.771 167.215 -40.10 -375.38 -30.222 100 135.162 167.218 167.218 167.218 -415.218 -32.222 100 145.166 29.208 119.311 -518.63 -32.222 100 145.167 20.208 119.4401 -518.63 -32.223 100 145.266 37.378 117.135 144.61 -518.63 -713.23 100 157	298.15 109.294 114.976 114.978 0. -407.103 -395.654 300 109.489 115.553 114.978 0.020 -407.116 -395.333 400 117.464 177.144 27.013 -395.654 -395.331 500 127.296 177.164 177.144 27.015 -407.173 -397.314 700 127.295 177.724 40.70 -40.217 -377.224 -30.2024 900 135.162 23.771 167.249 -40.217 -30.2024 -30.2024 900 135.162 23.771 167.249 -40.549 -30.2022 -30.2022 900 135.162 137.741 40.161 -30.175 -30.2022 -30.2022 100 135.762 23.773 116.491 90.161 -34.648 -34.648 -30.2022 100 147.762 26.573 116.491 90.161 -34.648 -37.333 100 157.762 26.773 114.471 -30.2273		0 0 0 200 0							
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16.7.62 20.378 18.5.19 104.564 - 581.623 - 298.820 15.18.6 29.32.08 19.3781 119.312 - 578.373 - 273.233 15.2.5. 30.2.38 13.4401 - 574.594 - 273.233 15.3.7. 31.5.71 20.6895 14.401 - 574.594 - 272.230 15.3.7. 31.7.38 21.7.11 18.531 - 571.381 - 272.290 16.0.60 37.7.39 224.421 18.631 - 561.688 - 172.290 16.0.39 37.7.39 231.396 188.124 - 553.887 - 118.50 17.509 37.7.30 244.667 231.992 - 551.674 - 101.53 17.599 375.709 250.996 249.425 - 547.48 - 115.334 17.590 375.709 250.996 249.425 - 547.48 - 115.334 17.590 445.021 255.977 253.610 - 77.970 - 17.970 15.580 445.021 257.735 396.425 - 411.2011 - 18.334 <tr< td=""><td>145.762 280.378 185.319 104.564 -581.623 -288.822 181.518 259.208 193.781 119.312 -578.373 -273.233 115.314 205.958 114.401 -574.594 -2773.233 115.314 205.958 114.401 -574.594 -2773.233 115.314 205.958 114.401 -574.594 -2773.233 115.314 205.958 114.401 -574.594 -2773.233 115.314 205.958 114.401 -574.594 -2773.233 115.314 117.668 237.978 224.41 181.691 -563.828 -173.500 117.598 237.592 231.396 125.314 -1015.324 117.598 237.572 231.396 125.314 -1015.324 117.598 237.572 231.396 125.314 -1015.334 117.598 2375.792 235.977 235.510 -574.487 -1015.334 117.598 235.592 255.577 255.510 -77.570 117.598 255.592 255.577 255.510 -77.570 117.593 115.590 445.572 257.315 396.452 -471.201 -38.841 115.590 460.796 71.573 396.432 -401.504 -1015.32 117.693 115.590 491.629 310.844 506.232 -407.546 22.101 116.590 491.629 310.844 506.232 -407.546 22.101 116.590 115.59</td><td></td><td>85</td><td>138.775</td><td>251.848</td><td>167.285</td><td>76.107</td><td>-587.548</td><td>-324 658</td><td>20.361</td></tr<>	145.762 280.378 185.319 104.564 -581.623 -288.822 181.518 259.208 193.781 119.312 -578.373 -273.233 115.314 205.958 114.401 -574.594 -2773.233 115.314 205.958 114.401 -574.594 -2773.233 115.314 205.958 114.401 -574.594 -2773.233 115.314 205.958 114.401 -574.594 -2773.233 115.314 205.958 114.401 -574.594 -2773.233 115.314 117.668 237.978 224.41 181.691 -563.828 -173.500 117.598 237.592 231.396 125.314 -1015.324 117.598 237.572 231.396 125.314 -1015.324 117.598 237.572 231.396 125.314 -1015.334 117.598 2375.792 235.977 235.510 -574.487 -1015.334 117.598 235.592 255.577 255.510 -77.570 117.598 255.592 255.577 255.510 -77.570 117.593 115.590 445.572 257.315 396.452 -471.201 -38.841 115.590 460.796 71.573 396.432 -401.504 -1015.32 117.693 115.590 491.629 310.844 506.232 -407.546 22.101 116.590 491.629 310.844 506.232 -407.546 22.101 116.590 115.59		85	138.775	251.848	167.285	76.107	-587.548	-324 658	20.361
149,18 293,208 193,781 119,312 -773,333 153,28 292,208 193,781 119,311 -5718,343 -273,233 153,937 316,714 200,695 149,823 -571,831 -221,292 165,091 377,892 217,195 165,591 -567,668 -198,139 165,039 377,892 213,136 148,233 -118,139 -148,239 165,039 377,242 213,136 -148,232 -18,139 -148,232 -18,138 -148,232 -18,138 -148,232 -18,138 -148,232 -18,138 -148,232 -18,138 -148,232 -18,138 -148,232 -18,138 -148,232 -18,138 -148,232 -119,334 -101,334 -101,334 -101,334 -101,334 -101,334 -101,334 -101,334 -101,334 -101,334 -101,334 -101,334 -11,334 -11,334 -11,334 -11,334 -11,334 -11,334 -11,334 -11,334 -11,334 -11,334 -11,334 -11,334 -11,334 <t< td=""><td> 149.18 293.208 193.781 119431</td><td></td><td>8 8</td><td>145.762</td><td>280.378</td><td>185.319</td><td>104.564</td><td>-581.623</td><td>-298.802</td><td>14.189</td></t<>	149.18 293.208 193.781 119431		8 8	145.762	280.378	185.319	104.564	-581.623	-298.802	14.189
153.957 157.24 167.24 147.25	153.957 157.24 167.25 149.82		021	149.186	293.208	193.781	119.312	-578.373	-273.233	11.894
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166,006 377,918 274,411 181,591 -25.0.4281 -15.0.509 175.0.509 377,542 231,396 198,1124 -55.0.4281 -16.0.509 377,543 231,396 231,396 -15.0.4281 -16.0.334 -16.0.33	166,006 37,978 274,411 181,891 -25,04,283 -14,530 166,006 37,978 274,441 181,891 -25,04,283 -14,530 117,666 37,934 37,940 231,996 231,997 -551,674 -101,533 175,799 375,799 250,996 249,425 -551,674 -101,533 175,890 375,799 250,996 249,425 -551,674 -101,530 175,890 445,021 255,927 256,410 -27,478 -17,970 155,800 445,021 255,927 256,410 -27,478 -17,970 155,800 445,021 255,927 256,410 -27,410,406 -21,915 155,800 457,473 256,424 471,221 -412,011 -38,841 155,800 467,473 282,677 447,822 -400,124 -23,033 155,800 467,473 282,677 447,822 -400,124 -23,033 11,625 -23,033 -23,033 -24,034 -23,033 -23,034 -23,033 -23,034 -23,033 -23,034		1200	159317	327.589	217.195	165.591	-567.668	-198,159	1063
17.589 35.723 238.138 21.482 -515.817 -115.334	17.500 37.51 37.51 31.		<u>8</u>	65.68 165.006	337.978	231.396	181.691	-563.828 -559.873	-173.650	5.88 5.88
175.989 387.769 249.84 249.425 249.84 249.84 249.425 249.84	175.989 382.68 249.89 249.42 249.14 249.09 249.42	_	0081	169.339	357.523	238.138	214.892	-555.817	-125.354	3,638
178.645 382.653 255.971 255.610 — CRYSTAL <>LIQUI 156.900 445.01 255.977 395.44 TRANSTIRON 156.900 456.22 257.735 395.34 TRANSTIRON 156.900 456.72 257.735 396.45 -412.01 -38.84 156.900 467.74 247.72 -415.01 -38.84 156.900 467.47 282.67 443.52 -400.16 -1915 156.900 467.47 282.67 443.52 -400.16 -5.033 156.900 485.95 397.37 440.52 -407.66 11.75 156.900 485.95 397.37 440.52 -407.56 45.31 156.900 485.95 317.175 440.52 -407.56 45.31 156.900 502.44 32.24 502.82 -407.56 45.31 156.900 502.44 32.24 32.34 -407.36 45.31 156.900 502.44 32.24 45.38 45.31 45.3	178,645 382,653 255,977 255,510		88	175.989	375.709	250.996	249.425		-71.970	2036
165,900 445,202 253,241 359,514 100,000 165,900 445,822 256,434 411,322 411,302 165,900 445,822 266,434 411,212 -410,011 -38,841 165,900 467,73 282,672 441,202 -10,841 -5,834 165,900 467,473 282,672 441,202 -40,114 -5,033 165,900 467,473 282,672 -40,114 -5,033 -5,033 165,900 483,583 290,193 493,212 -407,164 -11,753 165,900 485,953 304,257 490,592 -407,546 45,311 165,900 487,163 317,175 490,592 -407,546 45,311 165,900 487,163 317,175 490,592 -407,546 45,311 165,900 502,484 33,244 350,247 -407,131 982,90 165,900 507,484 33,244 35,332 -407,131 982,90 165,900 517,610 4	165.900 445.321 253.241 395.344 INAVASITION INFORMATION INFORMATIO		2080.000		382.663	255.927	263.610	S	[AL <> Li	dino
155,000	155,000 453,821 256,484 412,142 -412,011 -38,381 155,000 453,821 256,000 453,821 -21915 155,000 453,473 413,522 -4010,466 -21915 156,900 473,473 473,522 -409,174 -203,31 156,900 473,873 -409,174 -409,174 -203,31 156,900 473,873 -409,174 -409,174 -409,174 -210,31		2080.000		445.021	357.736	305.453		-55 846	1 180
15,500 460,775 274,782 473,827 471,824 473,821 471,913 -21,913 15,6500 471,878 290,193 459,212 -409,134 -5.053 15,6500 480,032 297,377 479,922 -407,636 28.548 15,6500 4815,923 297,377 479,922 -407,636 28.548 15,6500 491,639 310,844 506,292 -481,635 79,010 15,690 571,65 317,175 231,972 -481,633 79,010 15,690 577,684 315,175 231,972 -481,633 79,010 15,690 577,684 312,136 533,462 -47,131 98,290 15,690 577,682 329,128 559,022 -47,231 13,566 15,690 512,610 34,785 569,022 -47,321 13,566 15,690 512,610 34,785 569,022 -47,341 13,794 15,690 512,12 345,238 600,422 -47,341 147,	156,500 460779 274.72 473.82 470.40 -21913 156,500 460779 274.73 473.22 -409.14 -5.053 156,500 473.878 290.193 459.212 -409.184 -5.053 156,500 487.473 274.72 -409.184 -5.053 156,500 487.52 304.25 490.52 -407.656 28.548 156,500 491.659 310.844 505.22 -407.656 473.11 156,500 691.659 310.844 537.65 -407.656 62.101 156,500 502.484 323.264 537.652 -407.131 82.290 156,500 517.48 323.264 537.652 -407.313 82.290 156,500 517.48 340.247 584.732 117.506 156,500 517.48 340.247 584.732 -473.217 156,500 522.122 345,528 600.422 -473.217 114.794 156,500 526.671 350.639 616.112 -469.716 193.778		2200	156.900	453.821	266.484	412.142	-412.011	-38.841	0.922
156,500 473,878 200,193 459,212 -408,187 1,755 156,500 460,012 273,377 474,902 -407,656 28,548 156,500 461,659 310,844 506,232 -407,646 45,213 156,500 491,659 310,844 506,232 -481,053 79,010 156,500 576,423 271,775 271,972 -481,053 79,010 156,500 576,423 271,775 271,7	156,500 473,578 250,193 459,212 -408,187 11.763 156,500 480,032 297,377 474,992 -407,656 28,548 156,900 481,592 304,232 474,992 -407,656 28,548 156,900 491,659 310,844 506,232 -408,042 156,900 570,629 329,128 531,972 -479,131 156,900 570,639 329,128 559,042 -479,213 156,900 572,612 345,528 600,422 -475,377 156,900 522,122 345,528 600,422 -475,377 156,900 526,671 350,639 616,112 -469,716 193,778	_	2300	26.900	460.796	274.782	427.832	-410.406	-21915	0.498
156,900 48,0021 297,377 474,902 -447,636 28,548 156,900 485,935 39,425 490,592 -407,546 45,321 156,900 497,165 317,175 521,972 -481,053 79,010 156,900 497,165 317,175 521,972 -481,053 79,010 156,900 507,629 329,128 533,352 -477,222 117,506 156,900 512,610 334,785 569,042 -477,222 115,506 156,900 512,610 334,785 569,042 -471,347 155,766 156,900 522,122 345,528 600,042 -471,347 157,794	156,000		8 8 8 8 8 8	156.900	473.878	290.193	459.212	-408.187	11.763	-0.246
156,900 452,925 344,224 450,222 446,124 452,111 456,900 457,165 457,165 457,165 456,900 457,165 457,165 456,900 457,165 457,165 456,900 457,165 456,900 457,165 456,900 457,165 456,900 457,165 456,900 457,165 456,900 457,165 456,900 457,165 456,900 457,165 456,900 457,165 456,900 457,165 456,900 457,165 457,165 456,900 457,165 457,165 457,165 456,900 457,165 457,	156,900 482,523 364,224 470,232 446,124 456,500 456,501 456,500 471,654 471,		2600	156.900	480.032	297.377	474.902	407,636	28.548	-0.574
156,900 497 165 317,175 311,972 -481,053 79,010 156,900 502,481 321,245 531,662 -479,131 98,290 156,900 512,610 334,785 589,042 -473,272 115,665 156,900 517,481 340,281 584,732 -471,443 155,756 156,900 522,122 345,528 600,422 -471,443 147,794	156,900 497 165 317,175 311,972 -481,653 79,010 156,900 502,484 312,124 531,562 -479,131 98,290 156,900 512,610 334,785 559,023 -477,327 117,506 156,900 511,438 340,247 584,72 -473,477 156,600 156,900 526,671 350,639 616,112 -469,716 193,778	-	2,00 2,00 2,00 2,00 2,00 2,00 2,00 2,00	156.900	485,953	310 844	490.592 506.282	-407.546	62,101	-1.159
156,900 507,629 339,128 553,352 -477,222 117,306 156,900 512,610 334,785 569,042 -475,327 136,600 156,900 517,438 349,247 584,732 -471,343 155,756 156,900 522,122 345,238 600,422 -471,547 114,794	156.900 577.629 329.128 553.352 -477.222 117.506 115.690 512.610 334.785 559.024 -475.327 115.660 115.690 512.112 345.218 650.412 -471.343 115.756 115.590 512.112 345.218 650.412 -471.343 115.756 115.590 512.112 345.218 650.412 -469.716 1191.778		2805	156.900	507 165	317.175	521.972	-481.053	98.290	-1.43
156,000 512,610 334,785 569,042 47.327 136,660 156,000 517,488 340,234 584,732 473,443 155,756 156,000 522,122 345,528 600,422 471,573 174,794	156.900 512.610 334.785 569.042 -475.327 136.660 156.900 517.438 340.247 584.732 -473.441 155.756 156.900 522.122 535.539 616.112 -469.716 193.778 156.500 526.671 350.639 616.112 -469.716 193.778	_	3100	156 900	507.629	329.128	553.352	-411222	117.506	-1.980
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10:500 SEC. 141.240 SEC. 141.240 SEC. 151.340 SEC. 151.34	156.500 526.671 350.639 616.112 –469.716 193.778	-	3300	156.900	517.438	340.247	584.732	-473.443	174 794	2.45
156.900 526 671 350.639 616.112469.716 193.778		-	350	156.900	526 671	350.639	616.112	-469.716	193.778	-2892

This material is reported to be metastable with respect to disproportionation to Mo(cr) and MoS₂(cr) below 900 K. However, disproportion ation is very slow and the material may be quenched and stored at room temperature indefinitely. Refer to the individual tables for details. 2080 K crystal 2080 K liquid

CRYSTAL-LIQUID

Molybdenum Sulfide (Mo₂S₃)

Continuation of discussions of selected Mo species

Molybdenum

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The ground state is assumed to be ³A₁ and the first excited level is assumed to lie close to the observed transitions at 7890 Å and 7806 Å in WO₂. Since both these states are presumed to be triplet, we have assigned a total degeneracy The electronic levels and quantum weights are estimated from the data reported by Weltner and McLeod¹⁰ on WO₂.

of 6. In addition, we expect from the electronic levels of $Mo^{4}(g)^{11}$ that other electronic states will also be found and these are arbitrarily estimated in the level at 25000 cm⁻¹. The principal moments of inertia are: $I_A = 3.3489 \times 10^{-39}$. $I_B = 11.4373 \times 10^{-39}$, and $I_C = 14.7862 \times 10^{-39}$ ccm⁻².

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