

Sulfur (S)

REFERENCE STATE

- 0 to 368.3 K crystal, alpha
- 368.3 to 388.36 K crystal, beta
- 388.36 to 882.117 K liquid
- above 882.117 K ideal diatomic gas (see below)

The normal boiling point of sulfur at 1 atm, 717.824 K, is a secondary standard on the International Practical Temperature Scale of 1968. The vapor composition at this temperature is a mixture of several sulfur species, the predominant species being S<sub>2</sub>(g), S<sub>4</sub>(g), and S<sub>8</sub>(g). In our reference state for sulfur, we have arbitrarily chosen 0.5 S<sub>2</sub>(g) to be the gas phase species.

S<sub>1</sub>(ref)

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub>	S° - (C <sub>p</sub> - RT <sub>r</sub> )/T	H° - H°(T <sub>r</sub> )	Δ <sub>r</sub> H°	
0	0.	0.	INFINITE	0.	0.
100	12.770	12.522	49.744	0.	0.
200	19.368	23.637	34.038	-2.722	0.
298.15	22.698	32.056	32.056	-2.080	0.
300	22.744	32.196	32.056	0.	0.
368.300	24.246	37.015	32.540	0.042	0.
368.300	24.773	38.103	32.540	1.648	0.
				2.049	ALPHA <- -> BETA TRANSITION
388.360	25.167	39.427	32.861	2.550	0.
388.360	31.058	43.859	32.861	4.271	BETA <- -> LIQUID TRANSITION
400	32.162	44.793	33.195	4.639	0.
432.020	53.808	47.431	34.151	5.737	0.
432.020	53.806	47.431	34.151	5.737	C <sub>2</sub> LAMBDA MAXIMUM TRANSITION
500	37.986	53.532	36.398	8.567	0.
600	34.308	60.078	39.825	12.152	0.
700	32.681	65.241	43.099	15.499	0.
800	31.699	69.530	46.143	18.710	0.
882.117	31.665	72.624	48.467	21.310	LIQUID <- -> IDEAL GAS FUGACITY = 1 bar
882.117	18.454	133.077	48.467	74.636	0.
900	18.483	133.448	50.152	74.967	0.
1000	18.638	135.403	58.581	76.823	0.
1100	18.792	137.187	65.667	78.694	0.
1200	18.947	138.829	71.678	80.581	0.
1300	19.103	140.352	76.903	82.484	0.
1400	19.257	141.775	81.486	84.402	0.
1500	19.409	143.107	85.530	86.335	0.
1600	19.556	144.364	89.187	88.283	0.
1700	19.697	145.554	92.468	90.246	0.
1800	19.830	146.684	95.449	92.223	0.
1900	19.956	147.759	98.174	94.212	0.
2000	20.072	148.786	100.679	96.213	0.
2100	20.176	149.768	102.993	98.226	0.
2200	20.274	150.708	105.141	100.248	0.
2300	20.364	151.612	107.142	102.280	0.
2400	20.448	152.480	109.013	104.321	0.
2500	20.526	153.316	110.769	106.370	0.
2600	20.599	154.123	112.421	108.426	0.
2700	20.650	154.901	113.980	110.488	0.
2800	20.707	155.653	115.455	112.555	0.
2900	20.762	156.381	116.853	114.629	0.
3000	20.813	157.085	118.183	116.708	0.
3100	20.855	157.768	119.449	118.791	0.
3200	20.898	158.431	120.657	120.879	0.
3300	20.940	159.075	121.811	122.971	0.
3400	20.983	159.701	122.916	125.067	0.
3500	21.025	160.310	123.976	127.167	0.
3600	21.065	160.902	124.994	129.272	0.
3700	21.106	161.480	125.972	131.380	0.
3800	21.149	162.044	126.914	133.495	0.
3900	21.194	162.594	127.822	135.610	0.
4000	21.240	163.131	128.698	137.732	0.
4200	21.337	164.169	130.362	141.989	0.
4400	21.443	165.164	131.922	146.267	0.
4600	21.558	166.120	133.388	150.567	0.
4800	21.680	167.040	134.771	154.891	0.
5000	21.810	167.928	136.080	159.240	0.
5200	21.948	168.786	137.321	163.615	0.
5400	22.090	169.617	138.502	168.019	0.
5600	22.236	170.423	139.628	172.452	0.
5800	22.385	171.206	140.703	176.914	0.
6000	22.538	171.967	141.733	181.406	0.

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1977 (1 bar)

Sulfur (S)

S<sub>1</sub>(ref)

## CRYSTAL(β)

## Sulfur, Monoclinic (S)

$$S^{\circ}(298.15 \text{ K}) = 33.028 \pm 0.050 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_m = 368.3 \pm 0.3 \text{ K } (\alpha-\beta)$$

$$T_m = 388.36 \pm 0.1 \text{ K } (\beta-\beta)$$

## Enthalpy of Formation

The enthalpy formation of monoclinic sulfur at 298.15 K is calculated from that of orthorhombic sulfur by adding  $\Delta_{\alpha\beta}H^{\circ}$  and the difference is enthalpy,  $H^{\circ}(368.3) - H^{\circ}(298.15 \text{ K})$ , between orthorhombic and monoclinic sulfur.

## Heat Capacity and Entropy

Experimentally determined heat capacity values for monoclinic (β) sulfur have been reported by Eastman and McGavock (64.83–376.16 K),<sup>1</sup> West (368–388 K),<sup>2</sup> and Montgomery (12.41–386.83 K).<sup>3</sup> The thermochemical functions tabulated by Hultgren *et al.*<sup>4</sup> are based on work of Eastman and McGavock<sup>1</sup> and West.<sup>2</sup>

We adopt the heat capacity values tabulated (in 10 K increments) by Montgomery.<sup>3</sup> The heat capacity values above  $T_m = 388.36 \text{ K}$  are obtained by linear extrapolation of the tabulated heat capacity values<sup>3</sup> above 360 K. Using  $S^{\circ}(10 \text{ K}) = 0.063 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  and integrating the heat capacity values, we calculate  $S^{\circ}(298.15 \text{ K}) = 7.893 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ . The  $S^{\circ}(10)$  value contains a contribution of  $0.007 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  which is needed to make  $S^{\circ}(S, \text{cr}, \beta, T) = S^{\circ}(S, \text{cr}, \alpha, T) + \Delta_{\alpha\beta}H^{\circ}/T_m$ . Since both forms of sulfur are perfectly ordered crystals at 0 K,<sup>5</sup> the  $S^{\circ}(0 \text{ K})$  value should be zero, by definition. The contribution of  $0.007 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  is arbitrarily added at 10 K although it could appear in any temperature region at or below 368.3 K. Part of this entropy may be in the region of the lambda anomaly at 198.3 K. This contribution is comparable to the uncertainty expected from this adiabatic calorimeter.

## Phase Data

The  $\alpha$ - $\beta$  transition at 368.3 K is discussed on the orthorhombic sulfur table.<sup>5</sup> The heat capacity data of Montgomery<sup>3</sup> did not support the transition at 374 K reported by West.<sup>2</sup>

Montgomery<sup>3</sup> reported a  $\lambda$  anomaly in the heat capacity of monoclinic sulfur with a peak at 198.3 K. The entropy change in the lambda anomaly was  $0.052 \pm 0.005 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , this was interpreted as due to the disordering of the structure of monoclinic sulfur on heating.<sup>7</sup>

## Fusion Data

The melting of sulfur has been studied by many workers. An excellent review by Meyer<sup>6</sup> summarizes these studies. In addition, Hultgren *et al.*<sup>4</sup> tabulated numerous enthalpy of melting determinations. We adopt the results obtained by Montgomery<sup>3</sup> via adiabatic calorimetry:  $T_m = 388.36 \pm 0.02 \text{ K}$  and  $\Delta_{\text{fus}}H^{\circ} = 0.4128 \pm 0.0006 \text{ kcal}\cdot\text{mol}^{-1}$ . The only other precise study reported in the literature is that of West<sup>2</sup> who obtained  $\Delta_{\text{fus}}H^{\circ} = 0.41051 \pm 0.0005 \text{ kcal}\cdot\text{mol}^{-1}$  by adiabatic calorimetry.

## References

- <sup>1</sup>E. D. Eastman and W. C. McGavock, *J. Am. Chem. Soc.* **59**, 145 (1937).
- <sup>2</sup>E. D. West, *J. Am. Chem. Soc.* **81**, 29 (1959).
- <sup>3</sup>R. L. Montgomery, Ph.D. Dissertation, Oklahoma State University, 1976 [Diss. Abst. 76-09730].
- <sup>4</sup>R. Hultgren *et al.*, "Selected Values of the Thermodynamic Properties of the Elements," American Society for Metals, Metals Park, Ohio, (1973).
- <sup>5</sup>JANAF Thermochemical Tables: S(cr, α), 9-30-77.
- <sup>6</sup>B. Meyer, *Chem. Rev.* **76**, 367 (1976).
- <sup>7</sup>R. L. Montgomery, *Science* **184**, 562 (1974).

## Sulfur, Monoclinic (S)

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

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S° - [C <sub>p</sub> - H(T <sub>r</sub> )]/T <sub>r</sub>	H° - H(T <sub>r</sub> )	Δ <sub>r</sub> H°	
0	0	0	-4.525	0.247	INFINITE
100	12.874	12.964	-3.825	0.257	0.247
198.300	21.966	24.242	-2.162	0.313	0.213
198.300	21.966	24.242	-2.162	0.313	0.213
200	20.154	24.421	-2.127	0.313	0.157
250	21.736	29.066	-1.084	0.336	0.115
298.15	23.225	33.028	0	0.360	0.070
300	23.276	33.172	0.043	0.361	0.068
350	24.414	36.849	1.237	0.388	0.017
368.300	24.773	38.103	1.687	0.388	0.017
388.360	25.167	39.477	2.188	0.388	0.017
400	25.397	40.173	2.482	-1.797	0.050
450	26.380	43.222	3.776	-2.428	0.310
500	27.363	46.052	5.120	-3.087	0.653
600	29.330	51.215	7.955	-3.838	1.481
700	31.296	55.884	10.986	-4.153	2.397
800	33.263	60.191	14.214	-4.136	3.335

PREVIOUS:

CURRENT: September 1977

## Sulfur, Monoclinic (S)

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

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

Sulfur, Orthorhombic (S)

CRYSTAL(α)

Sulfur, Orthorhombic (S)

$\Delta_f H^\circ(0\text{ K}) = 0\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = 0\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{cr}} H^\circ = 0.4004 \pm 0.0029\text{ kJ}\cdot\text{mol}^{-1}$

T/K	Enthalpy Reference Temperature - T <sub>r</sub> = 298.15 K		Standard State Pressure - P° = 0.1 MPa		log K <sub>t</sub>
	C <sub>p</sub> <sup>o</sup>	S° - (G° - H°(T <sub>r</sub> ))/T	H° - H°(T <sub>r</sub> )	Δ <sub>r</sub> H°	
0	0	INFINITE	0	0	0
100	12.770	12.522	-4.412	0	0
200	19.368	21.637	-3.722	0	0
250	21.297	28.179	-2.080	0	0
298.15	22.698	32.422	-1.061	0	0
300	22.744	32.056	0	0	0
350	23.870	32.337	0.042	0	0
368.300	24.246	32.540	1.208	0	0
400	24.895	32.975	1.648	0	0
450	25.920	33.818	2.427	0.088	-0.011
500	26.945	44.819	3.698	-2.867	-0.047
500	26.945	44.819	5.019	-3.548	-0.084
600	28.995	49.913	7.816	-4.336	-0.154
700	31.045	54.537	10.818	-4.680	-0.210
800	33.095	58.816	14.025	-4.685	-0.254

--- ALPHA <---> BETA

$\Delta_f H^\circ(0\text{ K}) = 0\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = 0\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{cr}} H^\circ = 0.4004 \pm 0.0029\text{ kJ}\cdot\text{mol}^{-1}$

**Enthalpy of Formation**  
 Zero by definition.

**Heat Capacity and Entropy**

Experimentally determined heat capacity values for orthorhombic (α) sulfur have been reported by Nemst,<sup>1</sup> 23–202 K), Eastman and McGavock,<sup>2</sup> 12.68–365.60 K), West,<sup>3</sup> 2981–368 K), Mal'tsev and Demidenko,<sup>4</sup> 53–305 K), Finke,<sup>5</sup> 12–432 K), Montgomery,<sup>6</sup> 12.34–360.99 K), and Paukov.<sup>7</sup> The thermochemical functions tabulated by Hultgren *et al.*<sup>8</sup> are based primarily on the work of Eastman and McGavock<sup>2</sup> and unpublished work of Finke,<sup>5</sup> the latter presumably being the preliminary results of Montgomery.<sup>6</sup> The tentative values reported by CODATA<sup>9</sup> for S°(298.15 K) and H°(298.15 K) - H°(0 K) are based on Eastman and McGavock,<sup>2</sup> Montgomery,<sup>6</sup> and Paukov.<sup>7</sup> We adopt the heat capacity values tabulated (in 10 K increments) by Montgomery,<sup>6</sup> Using S°(10) = 0.036 cal·K<sup>-1</sup>·mol<sup>-1</sup>, and integrating the heat capacity values, we calculate S°(298.15 K) = 7.661 cal·K<sup>-1</sup>·mol<sup>-1</sup>, in agreement with CODATA.<sup>9</sup> The heat capacity values above T<sub>m</sub> = 368.3 K are obtained by linear extrapolation of the tabulated values<sup>6</sup> above 340 K.

The various heat capacity studies are in reasonably good agreement. The values recommended by Eastman and McGavock,<sup>2</sup> West,<sup>3</sup> and Mal'tsev and Demidenko<sup>4</sup> agree with Montgomery<sup>6</sup> to within 0.5% except for the ranges 15–50 K<sup>2</sup> and 53–80 K.<sup>3</sup> The smoothed value at 190 K reported by Mal'tsev and Demidenko<sup>4</sup> is undoubtedly a typographical error. The selected values of Hultgren *et al.*<sup>8</sup> agree within 0.5% with the data of Montgomery<sup>6</sup> except below 35 K.

**Fusion Data**

The orthorhombic-monoclinic (α-β) phase change has been studied by many workers. An excellent review by Meyer<sup>10</sup> summarizes these studies. We adopt the results obtained by Montgomery<sup>6</sup> via adiabatic calorimetry: T<sub>m</sub> = 368.3 ± 0.3 K and Δ<sub>m</sub>H° = 0.0957 ± 0.0007 kcal·mol<sup>-1</sup>. The only other precise study reported in the literature is that of West<sup>3</sup> who obtained Δ<sub>m</sub>H° = 0.0960 ± 0.0005 kcal·mol<sup>-1</sup> by adiabatic calorimetry. Other drop calorimetric<sup>11,12</sup> and vapor pressure<sup>13,14</sup> studies are much less precise with an uncertainty of ± 5 cal·mol<sup>-1</sup> or greater.

**Sublimation Data**

Since the reference state of sulfur involves 0.5 S<sub>2</sub>(g) rather than S(g), we define the enthalpy of sublimation (at 298.15 K) of orthorhombic sulfur as the process S(cr, α) = 0.5 S<sub>2</sub>(g). Thus the enthalpy of sublimation of orthorhombic sulfur is one-half the enthalpy of formation of S<sub>2</sub>(g). Since the dominant gaseous sulfur species at room temperature is actually S<sub>2</sub>(g), the enthalpy of sublimation to the equilibrium gas is significantly smaller.

**References**

<sup>1</sup>W. Nemst, Ann. Physik, **36**, 395 (1911).  
<sup>2</sup>E. D. Eastman and W. C. McGavock, J. Am. Chem. Soc. **59**, 145 (1937).  
<sup>3</sup>E. D. West, J. Am. Chem. Soc. **81**, 29 (1959).  
<sup>4</sup>A. K. Mal'tsev and A. F. Demidenko, Tr. Mosk. Khim.-Tekhnol. Inst., No. 51, 136 (1967).  
<sup>5</sup>H. L. Finke, U. S. Bureau of Mines, Unpublished Work. Quoted in reference.<sup>8</sup>  
<sup>6</sup>R. L. Montgomery, Ph.D. Dissertation, Oklahoma State University, (1976).  
<sup>7</sup>I. E. Paukov, to be published, 1977; mentioned in reference.<sup>8</sup>  
<sup>8</sup>R. Hultgren *et al.*, "Selected Values of the Thermodynamic Properties of the Elements," American Society for Metals, Metals Park, Ohio, (1973).  
<sup>9</sup>ICUS-CODATA Task Group Key Values for Thermodynamics, CODATA Special Report 4, (March, 1977).  
<sup>10</sup>B. Meyer, Chem. Rev. **76**, 367 (1976).  
<sup>11</sup>P. Mondain-Monval, Bull. Soc. Chim. France **39**, 1349 (1926).  
<sup>12</sup>J. N. Bronsted, Z. Physik. Chem. **55**, 371 (1906).  
<sup>13</sup>M. Thackray, Nature **203**, 1278 (1964); J. Chem. Eng. Data **15**, 495 (1970).  
<sup>14</sup>K. Neumann, Z. Physik. Chem. **A171**, 416 (1934).

PREVIOUS: December 1965

CURRENT: September 1977

Sulfur, Orthorhombic (S)

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

Sulfur (S) S<sub>1</sub>(l)

## LIQUID

$$A_r = 32.06$$

$$S^{\circ}(298.15 \text{ K}) = [36.825] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$T_m = 432.02 \pm 0.2 \text{ K}$$

$$T_{\text{fus}} = 388.36 \pm 0.2 \text{ K}$$

$$\Delta_f H^{\circ}(298.15 \text{ K}) = [1.854] \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta_{\text{sub}} H^{\circ} = 0 \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta_{\text{liq}} H^{\circ} = 1.7272 \pm 0.0025 \text{ kJ} \cdot \text{mol}^{-1}$$

## Enthalpy of Formation

The enthalpy of formation of liquid sulfur at 298.15 K is calculated from that of monoclinic sulfur by adding  $\Delta_{\text{liq}} H^{\circ}$  and the difference in enthalpy,  $H^{\circ}(388.6 \text{ K}) - H^{\circ}(298.15 \text{ K})$ , between the monoclinic crystal and the liquid.

## Heat Capacity and Entropy

The adopted heat capacity values are based on the studies by Montgomery,<sup>4</sup> 05.79–433.31 K) and West (373–678 K).<sup>2</sup> Liquid sulfur undergoes a second order transition with a maximum reported at 432.02  $\pm$  0.20 K and 432.25  $\pm$  0.30 K;<sup>2</sup> this has been attributed to the depolymerization of S<sub>8</sub> molecules.<sup>3</sup> We adopt the tabulated heat capacity values of Montgomery<sup>4</sup> up to 434 K and those of West<sup>2</sup> above 434 K. The heat capacity is assumed to be constant at 7.568 cal·K<sup>-1</sup>·mol<sup>-1</sup> above 810 K. Below T<sub>m</sub> = 388.36 K, the heat capacity values are obtained by linear extrapolation using the slope of the values in the region T<sub>m</sub> to 420 K. The entropy at 298.15 K is calculated in a manner analogous to that used for the enthalpy of formation.

## Vaporization Data

The normal boiling point of sulfur, T<sub>vap</sub>(1 atm) = 717.834 K is a secondary reference on the International Practical Temperature Scale of 1968. At this temperature, equilibrium sulfur vapor contains monomeric and several polymeric sulfur species: S<sub>2</sub>(g) and S<sub>8</sub>(g) predominate above 1000 K while S<sub>6</sub>(g), S<sub>7</sub>(g) and S<sub>4</sub>(g) dominate at T<sub>vap</sub>.

Since our reference state for sulfur is arbitrarily defined to involve 0.5 S<sub>2</sub>(g) as the vapor species, we calculate the arbitrary normal boiling point, T<sub>vap</sub>(1 bar), for the process S(l) = 0.5 S<sub>2</sub>(g). The brackets are used to indicate the arbitrary nature of this value. Since we only consider S<sub>2</sub>(g) in this vaporization, note that the boiling point is considerably different from the secondary reference IPTS value. If all n-mers of sulfur are considered in the vaporization process, then a normal boiling point (1 atm) is closely reproduced.

## References

- <sup>1</sup>R. L. Montgomery, Ph.D. Dissertation, Oklahoma State University, (1976).  
<sup>2</sup>E. D. West, J. Am. Chem. Soc. 81, 29 (1959).  
<sup>3</sup>B. Meyer, Chem. Rev. 76, 367 (1976).

T/K	C <sub>p</sub> <sup>a</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
		S <sup>b</sup> - [C <sub>p</sub> - H(T <sub>r</sub> )]/T	H <sup>c</sup> - H(T <sub>r</sub> )	Δ <sub>sub</sub> H <sup>d</sup>	Δ <sub>liq</sub> H <sup>e</sup>	
100	0					
200						
250						
298.15	22.531	36.825	0.	1.854	0.432	-0.076
300	22.707	36.965	0.042	1.854	0.423	-0.074
350	27.434	40.821	1.295	1.941	0.180	-0.027
388.360	31.058	43.859	2.417	---	BETA <- -> LIQUID	---
400	32.162	44.793	2.785	0.	0.	0.
432.020	53.829	47.431	38.442	3.884	C <sub>p</sub> LAMBDA MAXIMUM	---
432.020	53.808	47.431	38.442	3.884	TRANSITION	---
450	43.046	49.308	38.840	4.711	0.	0.
500	37.986	53.532	40.106	6.713	0.	0.
600	34.308	60.078	42.915	10.298	0.	0.
700	32.681	65.241	45.748	13.645	0.	0.
800	31.699	69.530	48.460	16.856	0.	0.
882.117	31.665	72.624	50.568	19.456	---	---
900	31.665	73.260	51.012	20.023	-53.090	-0.063
1000	31.665	76.596	53.407	23.189	-51.780	-0.367
1100	31.665	79.614	55.654	26.356	-50.485	-0.610
1200	31.665	82.369	57.767	29.522	-49.205	-0.807
1300	31.665	84.904	59.758	32.689	-47.941	-0.970
1400	31.665	87.250	61.639	35.855	-46.693	-1.106
1500	31.665	89.435	63.420	39.021	-45.460	-1.220

PREVIOUS: December 1965

CURRENT: September 1977

## Sulfur (S)

S<sub>1</sub>(l)

Sulfur (S)

$A_r = 32.06$  Sulfur (S)

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

0 to 368.3 K crystal, alpha  
368.3 to 388.36 K crystal, beta  
above 388.36 K liquid

Refer to the individual tables for details.

$S_1(\text{cr,l})$

T/K	Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $p^\circ = 0.1$ MPa	
	$C_p^\circ$	$S^\circ - [C_p^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f G^\circ$
0	0	INFINITE	-4.412	0
100	12.770	49.744	-3.772	0
200	19.368	34.038	-2.080	0
250	21.297	28.179	-1.061	0
298.15	22.698	32.056	0	0
300	22.744	32.196	0.042	0
350	23.870	35.789	1.208	0
368.300	24.246	37.015	1.648	ALPHA <--> BETA TRANSITION
368.300	24.773	38.103	2.049	
388.360	25.167	39.427	2.550	BETA <--> LIQUID TRANSITION
388.360	31.062	43.859	4.271	
400	32.162	44.793	4.639	0
432.020	53.808	47.431	5.737	$C_p$ LAMBDA MAXIMUM TRANSITION
432.020	53.806	47.431	5.737	
450	43.046	49.308	6.564	0
500	37.986	53.532	8.567	0
600	34.308	60.078	12.152	0
700	32.681	65.241	15.499	0
800	31.659	69.530	18.710	0
882.117	31.655	72.624	21.310	FUGACITY = 1 bar
900	31.665	73.260	21.877	-53.090 1.079 -0.063
1000	31.665	76.596	25.043	-51.780 7.028 -0.367
1100	31.665	79.614	28.209	-50.485 12.846 -0.610
1200	31.665	82.369	31.376	-49.205 18.546 -0.807
1300	31.665	84.904	34.542	-47.941 24.141 -0.970
1400	31.665	87.250	37.709	-46.693 29.639 -1.106
1500	31.665	89.435	40.875	-45.460 35.048 -1.220

PREVIOUS:

CURRENT: September 1977

Sulfur (S)

$S_1(\text{cr,l})$

## Sulfur (S)

IP(S, g) = 83558.0 ± 1 cm<sup>-1</sup>  $\Delta_f H^\circ(0 \text{ K}) = 274.73 \pm 0.25 \text{ kJ} \cdot \text{mol}^{-1}$   $\Delta_f H^\circ(298.15 \text{ K}) = 276.98 \pm 0.25 \text{ kJ} \cdot \text{mol}^{-1}$   $A_1 = 32.06$  Sulfur (S)  $S_1(\text{g})$

State	$\epsilon$ , cm <sup>-1</sup>	Quantum Weights	$g$
<sup>1</sup> P <sub>2</sub>	0.00	5	5
<sup>3</sup> P <sub>1</sub>	396.09	3	3
<sup>1</sup> P <sub>0</sub>	573.65	1	1
<sup>1</sup> D <sub>2</sub>	9238.58	5	5
<sup>1</sup> S <sub>0</sub>	22179.99	1	1

## Enthalpy of Formation

The enthalpy of formation is based on the dissociation energy for S<sub>2</sub>(g) as recommended by CODATA.<sup>1</sup> The adopted value for  $\Delta_f H^\circ(\text{S}, \text{g}, 298.15 \text{ K})$  is calculated using  $D^\circ(\text{S}_2) = 35216.4 \pm 2.5 \text{ cm}^{-1}$  (421.282 ± 0.03 kJ·mol<sup>-1</sup>) from the study of Ricks and Barrow.<sup>2</sup>

The selected dissociation energy, obtained from precise spectroscopic measurements,<sup>2</sup> is supported by additional studies on thermochemical cycles,<sup>3</sup> photoionization<sup>4</sup> and torsion-effusion measurements.<sup>6</sup> Earlier measurements have been reviewed by Herzberg,<sup>7</sup> Gaydon,<sup>8</sup> Brewer,<sup>9</sup> and Drowart and Goldfinger.<sup>3</sup>

## Heat Capacity and Entropy

The electronic levels for S(g) are given in the compilation by Moore.<sup>10,11</sup> Our calculations indicate that, except for the five levels lying below 23000 cm<sup>-1</sup>, the inclusion of levels up to  $n = 10$  has no effect on the thermodynamic function to 6000 K. This is a result of the high energy of these levels; the fifth excited state lies at 52623.88 cm<sup>-1</sup> above the ground state. Since the inclusion of these upper levels has no effect on the thermodynamic function (to 6000 K) we list only the lowest lying states ( $\epsilon < 23000 \text{ cm}^{-1}$ ). The reported uncertainty is  $S^\circ(298.15 \text{ K})$  is due to uncertainties in the relative atomic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states and utilization of proper fill and cutoff procedures.<sup>12</sup> In fact, the inclusion of these higher excited states and consideration of various cutoff procedures leads to calculational differences in the Gibbs energy function of  $\sim 0.4 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  or greater at temperatures in excess of 11500 K. The thermal functions at 298.15 K agree with CODATA recommendation<sup>1</sup> except for two minor differences. First, the entropy differs by 0.1094 J·K<sup>-1</sup>·mol<sup>-1</sup> because this table uses a standard state pressure of 1 bar, whereas the CODATA recommendations are based on 1 atm. Second, an entropy difference of 0.004 J·K<sup>-1</sup>·mol<sup>-1</sup> arises due to the use of slightly different values for the fundamental constants.

## References

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T/K	Enthalpy Reference Temperature = T <sub>1</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S° - (C <sub>p</sub> <sup>o</sup> - H°(T <sub>1</sub> ))/T	H° - H°(T <sub>1</sub> )	Δ <sub>r</sub> H°	
0	0	0	INFINITE	274.735	INFINITE
100	21.356	142.891	188.580	274.735	-137.427
200	23.388	138.392	169.994	276.133	-65.238
250	23.696	163.653	168.218	276.899	-50.779
298.15	23.673	167.828	167.828	276.980	-41.434
300	23.669	167.974	167.828	276.982	-41.135
350	23.480	171.610	168.116	276.985	-34.245
400	23.233	174.789	168.152	277.037	-29.069
450	22.979	177.451	169.571	277.062	-25.107
500	22.741	179.859	170.481	277.102	-20.938
600	22.338	183.968	172.398	277.170	-17.188
700	22.031	187.388	174.302	277.264	-13.815
800	21.800	190.314	176.125	277.351	-11.295
900	21.624	192.871	177.847	277.422	-9.405
1000	21.489	195.142	179.465	277.477	-8.154
1100	21.386	197.185	180.984	277.516	-7.128
1200	21.307	199.042	182.413	277.543	-6.272
1300	21.249	200.745	183.758	277.579	-5.548
1400	21.209	202.318	185.029	277.614	-4.926
1500	21.186	203.781	186.231	277.670	-4.386
1600	21.178	205.148	187.371	277.740	-3.914
1700	21.184	206.432	188.455	277.825	-3.497
1800	21.203	207.643	189.487	277.925	-3.126
1900	21.234	208.790	190.473	278.040	-2.793
2000	21.276	209.880	191.417	278.169	-2.494
2100	21.327	210.920	192.321	278.312	-2.224
2200	21.386	211.913	193.189	278.470	-1.977
2300	21.452	212.865	194.024	278.643	-1.752
2400	21.523	213.780	194.828	278.832	-1.546
2500	21.598	214.660	195.604	279.036	-1.356
2600	21.676	215.508	196.353	279.255	-1.180
2700	21.756	216.328	197.078	279.487	-1.018
2800	21.837	217.121	197.780	279.732	-0.867
2900	21.919	217.889	198.460	279.990	-0.726
3000	21.999	218.633	199.120	280.260	-0.595
3100	22.078	219.355	199.761	280.542	-0.472
3200	22.155	220.058	200.384	280.836	-0.357
3300	22.230	220.740	200.991	281.142	-0.248
3400	22.303	221.405	201.582	281.459	-0.146
3500	22.372	222.053	202.157	281.787	-0.050
3600	22.439	222.684	202.719	282.126	0.041
3700	22.502	223.300	203.267	282.476	0.127
3800	22.561	223.900	203.802	282.837	0.209
3900	22.618	224.487	204.325	283.209	0.286
4000	22.670	225.061	204.836	283.592	0.360
4100	22.720	225.621	205.336	283.986	0.430
4200	22.766	226.169	205.826	284.391	0.497
4300	22.808	226.705	206.305	284.807	0.561
4400	22.847	227.230	206.774	285.234	0.622
4500	22.884	227.744	207.235	285.672	0.680
4600	22.917	228.247	207.686	286.120	0.736
4700	22.947	228.740	208.129	286.577	0.789
4800	22.974	229.224	208.563	287.044	0.840
4900	22.999	229.698	208.990	287.520	0.890
5000	23.021	230.163	209.409	288.005	0.937
5100	23.040	230.619	209.820	288.500	0.982
5200	23.057	231.066	210.224	289.005	1.026
5300	23.072	231.505	210.622	289.520	1.068
5400	23.085	231.937	211.013	290.045	1.108
5500	23.096	232.361	211.397	290.580	1.147
5600	23.105	232.777	211.775	291.125	1.185
5700	23.112	233.186	212.147	291.680	1.221
5800	23.117	233.588	212.513	292.245	1.256
5900	23.121	233.983	212.874	292.820	1.290
6000	23.124	234.372	213.229	293.405	1.323

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1982 (1 bar)

S(g)

M<sub>r</sub> = 32.05945 Sulfur, Ion (S<sup>+</sup>)

IDEAL GAS

Sulfur, Ion (S<sup>+</sup>)

$\Delta_f H^\circ(\text{O K}) = 1274.311 \pm 0.4 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15 \text{ K}) = [1282.293] \text{ kJ}\cdot\text{mol}^{-1}$

$IP(\text{S}^+, \text{g}) = 188200 \pm 100 \text{ cm}^{-1}$   
 $S^\circ(298.15 \text{ K}) = 163.627 \pm 0.03 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

State	$\epsilon$ , cm <sup>-1</sup>	Quantum Weights	g
<sup>4</sup> S <sub>3/2</sub>	0.0	4	4
<sup>2</sup> D <sub>3/2</sub>	14853.0	4	4
<sup>2</sup> D <sub>5/2</sub>	14884.8	6	6
<sup>2</sup> P <sub>1/2</sub>	24524.9	2	2
<sup>2</sup> P <sub>3/2</sub>	24571.6	4	4

**Enthalpy of Formation**  
 $\Delta_f H^\circ(\text{S}^+, \text{g}, 0 \text{ K})$  is calculated from  $\Delta_f H^\circ(\text{S}, \text{g}, 0 \text{ K})$  using the spectroscopic value of  $IP(\text{S}) = 83558.0 \pm 1 \text{ cm}^{-1}$  (238.904 ± 0.01 kJ·mol<sup>-1</sup>) from Moore.<sup>2</sup> The ionization limit is converted from cm<sup>-1</sup> to kJ·mol<sup>-1</sup> using the factor, 1 cm<sup>-1</sup> = 0.01196266 kJ·mol<sup>-1</sup>, which is derived from the 1973 CODATA fundamental constants.<sup>3</sup> Rosenstock *et al.*<sup>4</sup> and Levin and Lias<sup>5</sup> have summarized additional ionization and appearance potential data.  
 $\Delta_f H^\circ(\text{S}^+, \text{g}, 298.15 \text{ K})$  is calculated from  $\Delta_f H^\circ(\text{S}, \text{g}, 0 \text{ K})$  by using  $IP(\text{S})$  with JANAF<sup>1</sup> enthalpies,  $H^\circ(\text{O K}) - H^\circ(298.15 \text{ K})$ , for S(g), S<sup>+</sup>(g), and e<sup>-</sup>(ref).  $\Delta_f H^\circ(\text{S} \rightarrow \text{S}^+ + e^-)$  differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*<sup>4</sup>  $\Delta_f H^\circ(298.15 \text{ K})$  should be changed by -6.197 kJ·mol<sup>-1</sup> if it is to be used in the ion convention that excludes the enthalpy of the electron.

**Heat Capacity and Entropy**  
 The information on electronic energy levels and quantum weights, given by Moore,<sup>2,6</sup> is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels and cutting off the summation in the partition function<sup>7</sup> has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of all levels other than the ground state and the first four excited states; the next excited state is approximately 79000 cm<sup>-1</sup> above the ground state. Since inclusion of these excited states has no effect on the thermodynamic functions (to 6000 K), we list only the ground state and the first four excited states. The reported uncertainty in S<sup>o</sup>(298.15 K) is due to uncertainties in the relative ionic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the excited states and use of different fill and cutoff procedures.<sup>7</sup>

**References**  
<sup>1</sup>JANAF Thermochemical Tables: S(g), 9-30-82; e<sup>-</sup>(ref), 3-31-82.  
<sup>2</sup>C. E. Moore, U. S. Nat. Bur. Stand., NSRDS-NBS-34, 8 pp. (1970).  
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<sup>4</sup>H. M. Rosenstock, K. Draxl *et al.*, J. Phys. Chem. Ref. Data 6, Supp. 1, 783 pp. (1977).  
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<sup>6</sup>C. E. Moore, U. S. Nat. Bur. Stand., NSRDS-NBS-35, Volume I, (1971) [Reprinted from NBS Circular 467, Volume 1, 1949].  
<sup>7</sup>J. R. Downey, Jr., The Dow Chemical Company, AFOSR-TR-78-0960, Contract No. F44620-75-1-0048, (1978).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>t</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	Δ <sub>f</sub> H <sup>o</sup>	
0	0	INFINITE	-6.197	1274.311	-216.684
100	20.786	140.970	-4.119	1282.328	-215.299
200	20.786	155.378	-2.040	1283.241	-183.392
250	20.786	159.966	-1.001	1281.888	-159.456
298.15	20.786	163.627	0	1282.042	-140.854
300	20.786	163.627	0	1282.118	-125.973
350	20.786	166.960	0.038	1282.690	-103.645
400	20.786	169.736	1.078	1283.500	-87.698
450	20.786	172.184	2.117	1284.446	-75.711
500	20.786	174.374	3.156	1285.347	-66.457
550	20.786	176.164	4.196	1286.247	-59.293
600	20.786	177.568	5.241	1287.148	-53.425
650	20.786	178.588	6.271	1288.050	-48.576
700	20.786	179.216	7.293	1288.954	-44.373
750	20.786	179.576	8.315	1289.859	-40.807
800	20.786	179.692	9.338	1290.765	-37.711
850	20.786	179.576	10.361	1291.671	-34.997
900	20.786	179.216	11.384	1292.577	-32.598
1000	20.786	178.588	12.407	1293.483	-30.462
1100	20.786	177.568	13.430	1294.389	-28.547
1200	20.786	176.164	14.453	1295.295	-26.821
1300	20.786	174.374	15.476	1296.201	-25.256
1400	20.786	172.184	16.500	1297.107	-23.832
1500	20.786	169.736	17.523	1298.013	-22.532
1600	20.792	166.960	18.546	1298.919	-21.350
1700	20.797	163.627	19.569	1299.825	-20.280
1800	20.806	160.293	20.592	1300.731	-19.210
1900	20.820	156.959	21.615	1301.637	-18.265
2000	20.840	153.627	22.638	1302.543	-17.385
2100	20.867	150.293	23.661	1303.449	-16.565
2200	20.904	146.959	24.684	1304.355	-15.798
2300	20.951	143.627	25.707	1305.261	-15.080
2400	21.009	140.293	26.730	1306.167	-14.405
2500	21.080	136.959	27.753	1307.073	-13.770
2600	21.164	133.627	28.776	1307.979	-13.171
2700	21.262	130.293	29.800	1308.885	-12.606
2800	21.374	126.959	30.823	1309.791	-12.071
2900	21.500	123.627	31.846	1310.697	-11.564
3000	21.640	120.293	32.869	1311.603	-11.083
3100	21.795	116.959	33.892	1312.509	-10.626
3200	21.962	113.627	34.915	1313.415	-10.191
3300	22.142	110.293	35.938	1314.321	-9.776
3400	22.332	106.959	36.961	1315.227	-9.381
3500	22.538	103.627	37.984	1316.133	-9.003
3600	22.751	100.293	39.007	1317.039	-8.641
3700	22.973	96.959	40.030	1317.945	-8.296
3800	23.204	93.627	41.053	1318.851	-7.964
3900	23.441	90.293	42.076	1319.757	-7.646
4000	23.684	86.959	43.100	1320.663	-7.341
4100	23.931	83.627	44.123	1321.569	-7.047
4200	24.182	80.293	45.146	1322.475	-6.765
4300	24.436	76.959	46.169	1323.381	-6.494
4400	24.694	73.627	47.192	1324.287	-6.232
4500	24.946	70.293	48.215	1325.193	-5.980
4600	25.201	66.959	49.238	1326.099	-5.736
4700	25.464	63.627	50.261	1327.005	-5.501
4800	25.735	60.293	51.284	1327.911	-5.274
4900	25.993	56.959	52.307	1328.817	-5.055
5000	26.197	53.627	53.330	1329.723	-4.842
5100	26.436	50.293	54.353	1330.629	-4.637
5200	26.671	46.959	55.376	1331.535	-4.437
5300	26.899	43.627	56.400	1332.441	-4.242
5400	27.121	40.293	57.423	1333.347	-4.053
5500	27.337	36.959	58.446	1334.253	-3.870
5600	27.545	33.627	59.470	1335.159	-3.693
5700	27.746	30.293	60.493	1336.065	-3.522
5800	27.940	26.959	61.516	1336.971	-3.357
5900	28.125	23.627	62.540	1337.877	-3.200
6000	28.302	20.293	63.563	1338.783	-3.050

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1982 (1 bar)

Sulfur, Ion (S<sup>+</sup>)

S(g)

S<sup>-</sup>(g)Sulfur, ion (S<sup>-</sup>)

IDEAL GAS

Sulfur, ion (S<sup>-</sup>)

EA(S, g) = 2.077120 ± 0.000001 eV  
 S<sup>-</sup>(298.15 K) = 164.918 ± 0.001 J·K<sup>-1</sup>·mol<sup>-1</sup>

Δ<sub>f</sub>H<sup>0</sup>(0 K) = 74.325 ± 0.25 kJ·mol<sup>-1</sup>  
 Δ<sub>f</sub>H<sup>0</sup>(298.15 K) = [70 180] kJ·mol<sup>-1</sup>

Electronic Levels and Quantum Weights	
State	g <sub>i</sub>
2 <sup>1</sup> P <sub>1</sub>	4
2 <sup>3</sup> P <sub>1</sub>	2

### Enthalpy of Formation

Δ<sub>f</sub>H<sup>0</sup>(S<sup>-</sup>, g, 0 K) is calculated from Δ<sub>f</sub>H<sup>0</sup>(S, g, 0 K)<sup>1</sup> using the adopted electron affinity of EA(S) = 2.077120 ± 0.000001 eV (200.4100 ± 0.0001 kJ·mol<sup>-1</sup>). This value, recommended by Hotop and Lineberger,<sup>2</sup> is based on a tunable laser photodetachment threshold study.<sup>3</sup> Additional information on S<sup>-</sup>(g) may be obtained in the critical discussions of Hotop and Lineberger,<sup>2</sup> Rosenstock *et al.*,<sup>4</sup> and Massey.<sup>6</sup>

Δ<sub>f</sub>H<sup>0</sup>(S<sup>-</sup>, g, 298.15 K) is obtained from Δ<sub>f</sub>H<sup>0</sup>(S, g, 0 K) by using EA(S) with JANAF<sup>1</sup> enthalpies, H<sup>0</sup>(0 K) - H<sup>0</sup>(298.15 K), for S<sup>-</sup>(g), S(g), and e<sup>-</sup>(ref). Δ<sub>f</sub>H<sup>0</sup>(S<sup>-</sup>, g, 298.15 K) differs from a room-temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*,<sup>4</sup> Δ<sub>f</sub>H<sup>0</sup>(298.15 K) should be changed by +6.197 kJ·mol<sup>-1</sup> if it is to be used in the ion convention that excludes the enthalpy of the electron.

### Heat Capacity and Entropy

The ground state and the fine-structure separation (483.54 ± 0.01 cm<sup>-1</sup>) for S<sup>-</sup>(g) has been experimentally determined,<sup>5</sup> a discussion of the relevant work is given by Hotop and Lineberger<sup>2</sup> and Massey.<sup>6</sup> Lacking any experimental evidence as to the stability of any excited states, we assume no stable excited states exist.

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T/K	C <sub>p</sub> <sup>0</sup>	Enthalpy Reference Temperature = T <sub>1</sub> = 298.15 K		Standard State Pressure = P <sup>0</sup> = 0.1 MPa		log K <sub>i</sub>
		S <sup>0</sup> - [G <sup>0</sup> - H <sup>0</sup> (T)]/T	H <sup>0</sup> - H <sup>0</sup> (T <sub>1</sub> )	ΔG <sup>0</sup>	ΔG <sup>0</sup>	
0	0	INFINITE	-6.465	74.325		
100	20.977	140.952	-4.383	70.180	36.822	-6.451
200	22.291	155.895	-2.220	70.142	36.615	-6.375
250	22.660	160.914	-1.095	69.075	31.111	-4.643
298.15	22.783	164.918	0	65.741	25.851	-3.376
300	22.784	165.059	0.042	63.905	20.966	-2.434
350	22.757	168.571	1.181	61.965	16.500	-1.703
400	22.653	171.603	2.317	58.545	7.492	-0.652
450	22.515	174.264	3.446	55.317	-0.760	0.057
500	22.370	176.628	4.568	52.205	-8.538	0.559
600	22.096	180.682	6.791	47.166	-14.889	0.864
700	21.868	184.071	8.989	41.476	-21.007	0.836
800	21.687	186.978	11.166	35.171	-26.947	0.701
900	21.543	189.524	13.327	28.714	-32.833	0.434
1000	21.429	191.788	15.476	21.716	-38.617	0.156
1100	21.338	193.826	17.614	14.716	-44.391	0.081
1200	21.264	195.679	19.744	7.716	-50.156	0.067
1300	21.203	197.378	21.867	0.716	-55.911	0.058
1400	21.153	198.948	23.985	-13.140	-61.656	0.052
1500	21.112	200.406	26.098	-19.146	-67.381	0.048
1600	21.076	201.767	28.207	-25.146	-73.086	0.045
1700	21.047	203.044	30.313	-31.146	-78.771	0.043
1800	21.021	204.246	32.417	-37.146	-84.436	0.042
1900	20.999	205.382	34.518	-43.146	-90.081	0.041
2000	20.980	206.459	36.617	-49.146	-95.706	0.040
2100	20.963	207.482	38.714	-55.146	-101.311	0.039
2200	20.949	208.457	40.809	-61.146	-106.896	0.038
2300	20.936	209.388	42.904	-67.146	-112.461	0.037
2400	20.924	210.279	44.997	-73.146	-118.006	0.036
2500	20.914	211.133	47.089	-79.146	-123.531	0.035
2600	20.905	211.953	49.180	-85.146	-129.036	0.034
2700	20.897	212.742	51.270	-91.146	-134.521	0.033
2800	20.890	213.501	53.359	-97.146	-140.006	0.032
2900	20.883	214.234	55.448	-103.146	-145.481	0.031
3000	20.877	214.942	57.536	-109.146	-150.946	0.030
3100	20.871	215.627	59.623	-115.146	-156.401	0.029
3200	20.866	216.289	61.710	-121.146	-161.846	0.028
3300	20.862	216.931	63.796	-127.146	-167.281	0.027
3400	20.858	217.554	65.882	-133.146	-172.706	0.026
3500	20.854	218.158	67.968	-139.146	-178.121	0.025
3600	20.850	218.746	70.053	-145.146	-183.526	0.024
3700	20.847	219.317	72.138	-151.146	-188.921	0.023
3800	20.844	219.873	74.222	-157.146	-194.306	0.022
3900	20.841	220.414	76.307	-163.146	-199.681	0.021
4000	20.838	220.942	78.391	-169.146	-205.046	0.020
4100	20.836	221.457	80.474	-175.146	-210.401	0.019
4200	20.834	221.959	82.558	-181.146	-215.746	0.018
4300	20.832	222.449	84.641	-187.146	-221.081	0.017
4400	20.830	222.928	86.724	-193.146	-226.406	0.016
4500	20.828	223.396	88.807	-199.146	-231.721	0.015
4600	20.826	223.854	90.890	-205.146	-237.026	0.014
4700	20.824	224.301	92.972	-211.146	-242.321	0.013
4800	20.823	224.740	95.055	-217.146	-247.606	0.012
4900	20.821	225.169	97.137	-223.146	-252.881	0.011
5000	20.820	225.590	99.219	-229.146	-258.146	0.010
5100	20.819	226.002	101.301	-235.146	-263.401	0.009
5200	20.818	226.406	103.383	-241.146	-268.646	0.008
5300	20.816	226.803	105.464	-247.146	-273.881	0.007
5400	20.815	227.192	107.546	-253.146	-279.106	0.006
5500	20.814	227.574	109.627	-259.146	-284.321	0.005
5600	20.813	227.949	111.709	-265.146	-289.526	0.004
5700	20.812	228.317	113.790	-271.146	-294.721	0.003
5800	20.811	228.679	115.871	-277.146	-299.906	0.002
5900	20.811	229.035	117.952	-283.146	-305.081	0.001
6000	20.810	229.385	120.033	-289.146	-310.246	0.000

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1982 (1 bar)

Sulfur, ion (S<sup>-</sup>)S<sup>-</sup>(g)



S<sub>2</sub>Si(g)

M<sub>r</sub> = 60.1455 Silicon Sulfide (SiS)

IDEAL GAS

Silicon Sulfide (SiS)

$\Delta_f H^\circ(0 \text{ K}) = 104.6 \pm 12.6 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15 \text{ K}) = 106.0 \pm 12.6 \text{ kJ}\cdot\text{mol}^{-1}$

$S^\circ(298.15 \text{ K}) = 223.80 \pm 2.0 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

Electronic State	Quantum Weights	g <sub>e</sub>
X <sup>1</sup> Σ <sup>+</sup>	0	1
[a <sup>1</sup> Π]	[24700]	6
D <sup>1</sup> Π	35029	2
[e <sup>1</sup> Σ <sup>+</sup> ]	[35140]	3
F	37114	2
I <sup>1</sup> Σ <sup>+</sup>	[37290]	1
Σ <sup>1</sup> Σ <sup>+</sup>	41924	1

$\omega_e = 740.34 \text{ cm}^{-1}$   
 $B_e = 0.29930 \text{ cm}^{-1}$   
 $\omega_e x_e = 2.544 \text{ cm}^{-1}$   
 $\alpha_e = 0.00145 \text{ cm}^{-1}$   
 $\sigma = 1$   
 $r_e = 1.92932$

**Enthalpy of Formation**

Herzberg<sup>7</sup> suggests a dissociation energy for SiS(g) of 6.6 eV. This result was derived from a spectroscopic analysis of the D-X and E-X band systems by Barrow and Jevons,<sup>4</sup> Vago and Barrow,<sup>5</sup> and Barrow.<sup>6</sup> Robinson and Barrow<sup>8</sup> extended the work of Vago and Barrow<sup>5</sup> and arrived at a value of 147.4 ± 3.0 kcal·mol<sup>-1</sup> (6.39 eV). In this latter work, a graphical Birge-Sponner extrapolation was made using 28 vibrational levels of the E state. The highest level is quite near the convergence limit and thus only a short extrapolation is necessary. The extrapolation graphically indicates the absolute minimum and maximum to be 6.28 eV and 6.57 eV, respectively. This amounts to a range of maximum uncertainty of approximately 7 kcal·mol<sup>-1</sup>. The products of the dissociation must be Si(<sup>3</sup>P) and S(<sup>3</sup>P) but it is not certain as to which of the sublevels of the <sup>3</sup>p states are involved. This leads to an uncertainty of ±1.2 kcal·mol<sup>-1</sup>. The result is in agreement with a rotational analysis of the D<sup>1</sup>Π-X<sup>1</sup>Σ<sup>+</sup> system by Lagerqvist, Nilheden, and Barrow<sup>9</sup> which led to a value of 6.47 eV (149.2 kcal·mol<sup>-1</sup>). The value of the dissociation energy chosen is 147.4 ± 3.0 kcal·mol<sup>-1</sup>, based on the work by Robinson and Barrow,<sup>5</sup> Gaydon<sup>1</sup> and Vedenev *et al.*<sup>3</sup> suggest a similar value, based on the work by Robinson and Barrow<sup>5</sup> and others. This value is also consistent with the tabulated dissociation energies of Gaydon<sup>1</sup> as far as trends which might be expected in the oxides, sulfides, and selenides of C, Si, Ge, Sn, and Pb. The resulting enthalpy of formation is Δ<sub>f</sub>H<sup>0</sup>(0 K) = 25.01 ± 3.00 kcal·mol<sup>-1</sup>.

Rosenqvist and Tunesvik<sup>13</sup> studied two reaction systems by a transportation method. By combining these two systems, the standard free energy of the reaction 2 Si(s) + S<sub>2</sub>(g) = 2 SiS(g) was calculated. Using JANAF values<sup>14</sup> for Si(s) and S<sub>2</sub>(g), ΔG<sup>0</sup> (1 atm) values for SiS(g) at 0 K and 300 K are 27.652 kcal·mol<sup>-1</sup> and 15.933 kcal·mol<sup>-1</sup>, respectively. These values are within the error range of the values in this tabulation.

**Heat Capacity and Entropy**

The spectroscopic constants, corrected for the natural abundances of Si and S, are from Hoeft,<sup>9</sup> and Lagerqvist, Nilheden, and Barrow.<sup>7</sup> Herzberg<sup>7</sup> tabulates the X<sup>1</sup>Σ<sup>+</sup>, D<sup>1</sup>Π, and E states and comments on unresolved bands at 16000-29000 cm<sup>-1</sup>. The a<sup>1</sup>Π state is predicted by an interpolation of similar a<sup>1</sup>Π X<sup>1</sup>Σ<sup>+</sup> splittings in the sulfides and oxides of C, Ge, Sn,<sup>10,11</sup> The remaining states are deduced by a rotational analysis of the E-X system of SiS.<sup>7,12</sup> It is not known conclusively whether the F state is <sup>1</sup>Π or <sup>1</sup>Δ. The energy of the e and I states are upper bound estimates.

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- JANAF Thermochemical Tables: Si(s), 12-31-66; S<sub>2</sub>(g), 12-31-65.

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (C <sub>p</sub> <sup>o</sup> - RT <sub>r</sub> )/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	Δ <sub>f</sub> H <sup>o</sup>	
0	0	INFINITE	INFINITE	104.650	INFINITE
100	29.129	190.877	251.180	106.603	89.151
200	30.303	211.317	226.691	106.738	-46.568
300	31.355	218.191	224.325	106.410	-18.683
298.15	32.332	223.799	223.799	105.960	-13.115
300	32.368	223.999	223.799	105.941	-9.531
350	33.259	229.066	224.197	105.380	-9.417
400	33.953	233.542	225.090	104.583	-6.788
450	34.531	237.576	226.257	103.543	-4.539
500	34.996	241.239	227.575	102.206	-3.259
600	35.681	247.684	230.404	99.789	-2.193
700	36.148	253.222	233.277	97.364	-1.476
800	36.478	258.072	236.080	95.162	-0.772
900	36.722	262.383	238.767	93.074	-0.676
1000	36.908	266.262	241.326	91.131	-0.722
1100	37.054	269.787	243.755	89.302	-0.772
1200	37.173	273.016	246.061	87.584	-0.826
1300	37.271	275.995	248.251	85.968	-0.883
1400	37.355	278.761	250.332	84.450	-0.942
1500	37.427	281.340	252.315	83.029	-1.002
1600	37.491	283.758	254.205	81.698	-1.062
1700	37.548	286.033	256.011	80.457	-1.122
1800	37.600	288.180	257.739	79.293	-1.182
1900	37.647	290.214	259.395	78.203	-1.242
2000	37.692	292.147	260.985	77.184	-1.302
2100	37.733	293.987	262.510	76.234	-1.362
2200	37.773	295.743	263.984	75.344	-1.422
2300	37.811	297.423	265.409	74.514	-1.482
2400	37.848	299.033	266.789	73.742	-1.542
2500	37.885	300.579	268.091	73.026	-1.602
2600	37.923	302.065	269.328	72.364	-1.662
2700	37.960	303.497	270.507	71.752	-1.722
2800	37.996	304.878	271.630	71.188	-1.782
2900	38.040	306.212	272.700	70.670	-1.842
3000	38.084	307.503	273.710	70.198	-1.902
3100	38.132	308.752	274.660	69.770	-1.962
3200	38.185	309.964	275.560	69.384	-2.022
3300	38.243	311.140	276.400	69.042	-2.082
3400	38.308	312.282	277.180	68.742	-2.142
3500	38.380	313.394	277.900	68.482	-2.202
3600	38.460	314.476	278.560	68.262	-2.262
3700	38.549	315.531	279.160	68.082	-2.322
3800	38.648	316.560	279.710	67.942	-2.382
3900	38.758	317.566	280.210	67.842	-2.442
4000	38.880	318.548	280.660	67.782	-2.502
4100	39.013	319.510	281.060	67.762	-2.562
4200	39.160	320.452	281.410	67.782	-2.622
4300	39.320	321.375	281.710	67.842	-2.682
4400	39.493	322.281	282.000	67.942	-2.742
4500	39.681	323.171	282.290	68.082	-2.802
4600	39.884	324.045	282.580	68.262	-2.862
4700	40.101	324.905	282.870	68.482	-2.922
4800	40.334	325.752	283.160	68.742	-2.982
4900	40.582	326.586	283.450	69.042	-3.042
5000	40.844	327.408	283.740	69.384	-3.102
5100	41.122	328.220	284.030	69.762	-3.162
5200	41.415	329.021	284.320	70.182	-3.222
5300	41.723	329.813	284.610	70.642	-3.282
5400	42.045	330.596	284.900	71.142	-3.342
5500	42.381	331.370	285.190	71.682	-3.402
5600	42.730	332.137	285.480	72.262	-3.462
5700	43.092	332.897	285.770	72.882	-3.522
5800	43.467	333.649	286.060	73.542	-3.582
5900	43.853	334.396	286.350	74.242	-3.642
6000	44.251	335.136	286.640	74.982	-3.702

PREVIOUS: December 1971 (1 atm)

CURRENT: December 1971 (1 bar)

Silicon Sulfide (SiS)

S<sub>2</sub>Si(g)

## Strontium Sulfide (SrS)

## CRYSTAL

 $M_r = 119.68$ 

## Strontium Sulfide (SrS)

 $S_1Sr_1(cr)$  $S^{\circ}(298.15\text{ K}) = 68.41 \pm 0.8\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  $\Delta_f H^{\circ}(10\text{ K}) = -467.4 \pm 17\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^{\circ}(298.15\text{ K}) = -468.6 \pm 17\text{ kJ}\cdot\text{mol}^{-1}$ 

## Enthalpy of Formation

Sabatier<sup>1</sup> measured the enthalpy of solution of SrS in hydrochloric acid solution as  $\Delta_f H^{\circ}(283.6\text{ K}) = -26.9 \pm 1.0\text{ kcal}\cdot\text{mol}^{-1}$  for SrS(cr) + 2 HCl(aq, 100 H<sub>2</sub>O)  $\rightarrow$  SrCl<sub>2</sub>(aq, 100 H<sub>2</sub>O) + H<sub>2</sub>S(aq). We derive  $\Delta_f H^{\circ}(SrS, cr, 298.15\text{ K}) = -113.1 \pm 2.0\text{ kcal}\cdot\text{mol}^{-1}$  based on the following auxiliary data:  $\Delta_f H^{\circ}(HCl, aq, 100\text{ H}_2\text{O}, 298.15\text{ K}) = -39.657\text{ kcal}\cdot\text{mol}^{-1}$  (3),  $\Delta_f H^{\circ}(H_2S, aq, 298.15\text{ K}) = -9.5\text{ kcal}\cdot\text{mol}^{-1}$ ,<sup>2</sup> and  $\Delta_f H^{\circ}(SrCl_2, aq, 200\text{ H}_2\text{O}, 298.15\text{ K}) = -209.78\text{ kcal}\cdot\text{mol}^{-1}$ .<sup>3</sup> The uncertainty reflects the correction to 298.15 K and the ambiguity of the exact solution composition. Mourlot<sup>4</sup> also measured the enthalpy of solution of SrS in hydrochloric acid solution as  $\Delta_f H^{\circ} = -27.1 \pm 1.0\text{ kcal}\cdot\text{mol}^{-1}$  from which we calculate  $\Delta_f H^{\circ}(SrS, cr, 298.15\text{ K}) = -112.8 \pm 2.0\text{ kcal}\cdot\text{mol}^{-1}$ , using the same auxiliary data.

Cater and Johnson<sup>5</sup> determined that SrS sublimes congruently and derived partial pressures of the various gaseous species Sr(g), S(g), and SrS(g) in an effusion and mass-spectrometric study. We analyze their data and the equilibrium study of Schenck and Hammerschmidt<sup>6</sup> below. Other mass-spectrometric studies of Berkowitz and Marquart<sup>7</sup> and Collin *et al.*<sup>8</sup> are also listed. The calculated 3rd law  $\Delta_f H^{\circ}(298.15\text{ K})$  may have an uncertainty of 0.5 kcal·mol<sup>-1</sup> since the JANAF Gibbs energy functions are partially based on the estimated  $C_p^{\circ}$  data (above 300 K).

The enthalpy of solution studies<sup>1,4</sup> show wide disagreement from the mass spectrometric studies.<sup>3,7,8</sup> Our experience tends to indicate that mass spectrometric experiments provide very good data on gas phase species for homogeneous reactions, but are not as reliable for condensed phases in heterogeneous reactions. A weighted average of the equilibrium and enthalpy of solution studies,  $\Delta_f H^{\circ}(SrS, cr, 298.15\text{ K}) = -112.0 \pm 4\text{ kcal}\cdot\text{mol}^{-1}$  is adopted in the tabulation.

Source	Method	Reaction*	T/K	Data Points	$\delta S$ cal·K <sup>-1</sup> ·mol <sup>-1</sup>	$\Delta_f H^{\circ}(298.15\text{ K})$ kcal·mol <sup>-1</sup>	$\Delta_f H^{\circ}(298.15\text{ K})$ kcal·mol <sup>-1</sup>
5	Knudsen mass spec.	A	1825–2181	Equation	1.26	212.70	210.18 ± 0.38
5	Knudsen mass spec.	B	1825–2181	Equation	0.23	131.75	131.29 ± 0.08
6	Equilibrium	C	1237–1383	3	8.8 ± 1.8	-53.0 ± 2.4	-105.43 ± 2
7	Mass spec.	B	1809	1			-64.55 ± 1.3
8	Mass spec.	D	1857–2170	9			210.18 ± 1.0
9	Vaporization	B	1400–1700	Equation	-3.3	102.6	-3.3 ± 5.5
							21.8 ± 2.4
							-119.8 ± 16
							82 ± 30

A) SrS(cr) = Sr(g) + S(g)  
B) SrS(cr) = SrS(g)  
C) SrS(cr) + 2 SO<sub>2</sub>(g) = SrSO<sub>4</sub>(cr) + S<sub>2</sub>(g)  
D) SrS(cr) + 3 S(g) = Sr(g) + 2 S<sub>2</sub>(g)

## Heat Capacity and Entropy

King and Weller<sup>10</sup> measured the low temperature heat capacities from 53–296 K. Their smooth values are adopted in the tabulation. The entropy,  $S^{\circ}(298.15\text{ K}) = 16.3 \pm 0.2\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , is based on  $S^{\circ}(51\text{ K}) = 1.59\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  as extrapolated by King and Weller using Debye and Einstein functions ( $\theta_D = 208, \theta_E = 311$ ). The  $C_p^{\circ}$  values above 300 K are estimated by graphical extrapolation combined with method B of Kubaschewski *et al.*<sup>11</sup>

## Fusion Data

Literature melting data for SrS(cr) are not available. The value quoted by Mills<sup>12</sup> for the melting point, 2275 K, seems too low when compared to the alkaline earth oxide melting points.<sup>13</sup>

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- <sup>13</sup>JANAF Thermochemical Tables: BaO(cr), 6–30–74; CaO(cr), 6–30–73; SrO(cr), 12–31–72.

T/K	Enthalpy Reference Temperature = T <sub>1</sub> = 298.15 K			Standard State Pressure = P <sup>o</sup> = 0.1 MPa		
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - H <sup>o</sup> (T <sub>1</sub> )]/T <sub>1</sub>	H <sup>o</sup> - H <sup>o</sup> (T <sub>1</sub> )	Δ <sub>f</sub> H <sup>o</sup>	Δ <sub>f</sub> G <sup>o</sup>	log K <sub>f</sub>
0	0	0	INFINITE	-467.438	-467.438	INFINITE
100	32.008	22.471	108.640	-468.434	-468.434	243.739
200	44.936	49.669	72.763	-468.566	-468.566	121.575
298.15	48.702	68.410	68.410	-468.608	-468.608	81.088
300	48.727	68.711	68.411	-468.609	-468.609	80.582
400	50.208	82.977	70.339	-470.990	-460.763	60.169
500	51.882	94.318	74.032	-472.639	-488.026	47.850
600	53.179	103.897	78.232	-473.897	-454.979	39.609
700	54.099	112.165	82.503	-474.913	-451.744	33.710
800	54.894	119.443	86.674	-475.813	-448.372	29.276
900	55.522	125.944	90.683	-476.653	-445.737	25.754
1000	56.233	131.832	94.508	-477.424	-443.143	22.677
1100	56.771	137.217	98.149	-478.146	-440.625	20.146
1200	57.820	142.180	101.614	-478.820	-414.010	18.021
1300	57.870	146.790	104.914	-479.059	-403.756	16.223
1400	58.469	151.099	108.061	-479.150	-393.496	14.682
1500	58.937	155.146	111.066	-479.162	-383.235	13.345
1600	59.455	158.967	113.942	-479.137	-372.974	12.176
1700	59.951	162.586	116.698	-479.070	-362.700	11.109
1800	60.439	166.027	119.343	-478.932	-352.421	9.960
1900	60.982	169.310	121.887	-478.724	-342.142	8.955
2000	61.505	172.451	124.338	-478.457	-331.861	8.015
2100	62.028	175.465	126.701	-478.132	-321.576	7.186
2200	62.551	178.362	128.984	-477.750	-311.287	6.434
2300	63.074	181.154	131.192	-477.312	-300.994	5.750
2400	63.597	183.850	133.330	-476.810	-290.698	5.124
2500	64.120	186.456	135.403	-476.252	-280.401	4.551
2600	64.643	188.981	137.416	-475.634	-270.104	4.023
2700	65.166	191.431	139.371	-474.957	-260.807	3.546
2800	65.689	193.810	141.273	-474.221	-251.510	3.086
2900	66.212	196.124	143.125	-473.424	-242.213	2.667
3000	66.735	198.378	144.929	-472.567	-232.916	2.278

PREVIOUS:

CURRENT: September 1977

## Strontium Sulfide (SrS)

 $S_1Sr_1(cr)$

Strontium Sulfide (SrS)

IDEAL GAS

M<sub>r</sub> = 119.68 Strontium Sulfide (SrS)

S<sub>2</sub>Sr(g)

S<sup>o</sup>(298.15 K) = 243.107 ± 0.42 J·K<sup>-1</sup>·mol<sup>-1</sup> Δ<sub>f</sub>H<sup>o</sup>(0 K) = 109.6 ± 8.4 kJ·mol<sup>-1</sup> Δ<sub>f</sub>H<sup>o</sup>(298.15 K) = 108.2 ± 8.4 kJ·mol<sup>-1</sup>

State	ε <sub>1</sub> , cm <sup>-1</sup>	g	ω <sub>1-6</sub> , cm <sup>-1</sup>	ω <sub>7-8</sub> , cm <sup>-1</sup>	B <sub>0</sub> , cm <sup>-1</sup>	α <sub>1-6</sub> , cm <sup>-1</sup>	r <sub>0</sub> , Å	Source
X <sup>1</sup> Σ <sup>+</sup>	0.0	1	388.38	1.310	0.12072	0.00044	2.4405	7
<sup>1</sup> π	[7800.]	6	[1.1]	[1.1]	[0.0943]	[0.0005]	[2.76]	6
<sup>3</sup> Σ <sup>+</sup>	[8000.]	3	[3.0]	[1.2]	[0.114]	[0.0005]	[2.51]	6
<sup>1</sup> π	[8100.]	2	[2.0]	[1.1]	[0.0943]	[0.0005]	[2.76]	6
<sup>3</sup> Σ <sup>+</sup>	[11000.]	1	[3.0]	[1.2]	[0.114]	[0.0005]	[2.51]	6
B <sup>1</sup> Σ <sup>+</sup>	26531.2	1	286.8	0.84	0.10566	0.00032	2.609	7 <sup>a</sup>

Enthalpy of Formation

The adopted value for the enthalpy of formation, Δ<sub>f</sub>H<sup>o</sup>(SrS, g, 298.15 K) = 25.86 ± 2 kcal·mol<sup>-1</sup>, is based on the Knudsen mass spectrometric studies analyzed below. The three independent studies are in very good agreement and we have chosen the average of the measurements. Our value is in very good agreement with Δ<sub>f</sub>H<sup>o</sup>(298.15 K) = 25.0 kcal·mol<sup>-1</sup> adopted by NBS<sup>4</sup> and is slightly greater than Δ<sub>f</sub>H<sup>o</sup>(298.15 K) = 24.1 ± 4 kcal·mol<sup>-1</sup> obtained by Mills<sup>5</sup> (using different Gibbs energy functions) in a recent critical compilation. Using auxiliary JANAF data<sup>6</sup> and a recommended value for D<sub>0</sub><sup>o</sup>(S<sub>2</sub>, g) = 100.69 ± 0.01 kcal·mol<sup>-1</sup>, we calculate D<sub>0</sub><sup>o</sup>(SrS, g) = 78.8 ± 2.0 kcal·mol<sup>-1</sup>.

Source Method	Reaction <sup>a</sup>	T/K	Data Points	ΔS cal·K <sup>-1</sup> ·mol <sup>-1</sup>	Δ <sub>f</sub> H <sup>o</sup> (298.15 K), kcal·mol <sup>-1</sup>	D <sub>0</sub> <sup>o</sup> , kcal·mol <sup>-1</sup>	
1	Mass spec	A	2010-2170	4	17.42 ± 17.9	25.06 ± 1.66	79.63 ± 2.0
2	Mass spec	A	1809-1934	2	34.19	25.12 ± 1.3	79.56 ± 1.5
3	Mass spec	A	1825-2181	Equation	20.85	23.07 ± 0.34	77.87 ± 1.0
3	Mass spec	B	1825-2181	Equation	-80.95	-78.89 ± 0.31	78.09 ± 0.3

<sup>a</sup>A) Sr(g) + S<sub>2</sub>(g) = SrS(g) + S(g) B) Sr(g) + S(g) = SrS(g)

Heat Capacity and Entropy

Electronic levels (T<sub>0</sub>) and vibrational-rotational constants for the observed states are from the optical study of Barrow.<sup>7,8</sup> Other low-lying electronic states and their vibrational-rotational constants are estimated in isoelectronic groups by analogy with SrO<sup>9</sup> and from trends observed in the known states of the other alkaline-earth oxides and sulfides.<sup>6</sup> Uncertainty in the energy and constants for the estimated states may contribute as much as 2-3 cal·K<sup>-1</sup>·mol<sup>-1</sup> to S<sup>o</sup> at 3000 K. The molecular constants have been corrected to the natural isotopic abundances. The thermodynamic functions are calculated using first-order anharmonic corrections to Q<sub>v</sub> and Q<sub>r</sub> in the partition function Q = Q<sub>tr</sub>Q<sub>v</sub>Q<sub>r</sub>Q<sub>e</sub>exp(-ε<sub>0</sub>/T).

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T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T)]/T	H <sup>o</sup> - H <sup>o</sup> (T)	Δ <sub>f</sub> H <sup>o</sup>	log K <sub>r</sub>
0	0	INFINITE	0	109.642	INFINITE
100	30.117	207.226	-9.536	109.642	109.642
200	33.694	229.274	-6.608	110.381	93.716
250	34.778	236.918	-4.906	109.463	77.367
300	35.477	243.107	-3.692	108.845	69.410
350	35.999	248.108	0.066	108.198	61.878
400	36.343	252.659	1.854	107.441	53.884
450	36.601	257.965	3.663	106.443	45.450
500	36.796	263.032	5.486	105.247	36.774
600	37.072	268.567	11.016	98.266	18.642
700	37.262	274.296	14.723	93.863	10.415
800	37.414	279.282	18.167	92.246	6.469
900	37.578	283.688	22.216	90.864	3.070
1000	37.811	287.668	25.983	89.743	1.070
1100	38.185	291.288	29.783	88.808	-0.808
1200	38.773	294.634	33.629	88.044	-2.334
1300	39.639	297.770	37.547	87.430	-3.616
1400	40.828	300.749	41.568	86.953	-4.681
1500	42.357	303.616	45.724	86.581	-5.556
1600	44.211	306.407	50.050	86.306	-6.281
1700	46.345	309.150	54.576	86.118	-6.866
1800	48.689	311.865	59.326	86.000	-7.333
1900	51.155	314.563	64.318	85.958	-7.698
2000	53.642	317.250	69.558	85.989	-8.000
2100	56.053	319.926	75.044	86.088	-8.255
2200	58.297	322.586	80.776	86.244	-8.466
2300	60.298	325.226	86.750	86.458	-8.632
2400	62.001	327.836	92.954	86.721	-8.761
2500	63.372	330.386	99.384	87.032	-8.851
2600	64.399	332.893	105.947	87.389	-8.903
2700	65.086	335.357	112.642	87.789	-8.925
2800	65.456	337.772	119.468	88.229	-8.917
2900	65.538	340.011	126.426	88.706	-8.881
3000	65.370	342.231	133.518	89.219	-8.817
3100	64.991	344.369	140.742	89.762	-8.727
3200	64.443	346.424	148.100	90.332	-8.614
3300	63.762	348.397	155.593	90.924	-8.479
3400	62.983	350.289	163.219	91.534	-8.326
3500	62.136	352.102	170.974	92.151	-8.158
3600	61.248	353.840	178.856	92.772	-7.978
3700	60.339	355.506	186.861	93.397	-7.786
3800	59.427	357.103	194.986	94.024	-7.583
3900	58.576	358.635	203.226	94.651	-7.369
4000	57.645	360.106	211.577	95.278	-7.147
4100	56.793	361.519	220.034	95.902	-6.917
4200	55.975	362.877	228.592	96.521	-6.680
4300	55.195	364.183	237.254	97.134	-6.437
4400	54.455	365.446	246.014	97.740	-6.190
4500	53.756	366.661	254.866	98.339	-5.940
4600	53.098	367.836	263.804	98.930	-5.688
4700	52.481	368.971	272.822	99.512	-5.434
4800	51.903	370.070	281.914	100.084	-5.178
4900	51.364	371.134	291.074	100.646	-4.920
5000	50.861	372.167	300.296	101.198	-4.661
5100	50.394	373.169	309.566	101.740	-4.401
5200	49.960	374.144	318.879	102.272	-4.141
5300	49.560	375.091	328.229	102.794	-3.881
5400	49.183	376.014	337.614	103.306	-3.621
5500	48.837	376.913	347.022	103.808	-3.361
5600	48.517	377.790	356.448	104.300	-3.101
5700	48.221	378.647	365.886	104.782	-2.841
5800	47.948	379.483	375.330	105.254	-2.581
5900	47.696	380.300	384.774	105.716	-2.321
6000	47.464	381.100	394.212	106.168	-2.061

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1977 (1 bar)

Strontium Sulfide (SrS)

S<sub>2</sub>Sr(g)

Sulfur (S<sub>2</sub>)

## IDEAL GAS

M<sub>r</sub> = 64.12 Sulfur (S<sub>2</sub>)S<sub>2</sub>(g)

$$S^{\circ}(298.15 \text{ K}) = 228.165 \pm 0.05 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$\Delta H^{\circ}(0 \text{ K}) = 128.30 \pm 0.30 \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta H^{\circ}(298.15 \text{ K}) = 128.60 \pm 0.30 \text{ kJ} \cdot \text{mol}^{-1}$$

State	$g$	$\epsilon$ , cm <sup>-1</sup>	$\omega_e$ , cm <sup>-1</sup>	$\omega_e x_e$ , cm <sup>-1</sup>	$B_e$ , cm <sup>-1</sup>	$\alpha_e$ , cm <sup>-1</sup>	$D_e$ , cm <sup>-1</sup>	$r_e$ , Å
X <sup>1</sup> Σ <sub>g</sub> <sup>+</sup>	3	0	724.67	2.836	0.2946	0.00157	$2.134 \times 10^{-7}$	1.889
a <sup>1</sup> Δ <sub>g</sub>	2	4700	702.35	3.09	0.2923	0.0017	$2.040 \times 10^{-7}$	1.889
b <sup>1</sup> Δ <sub>g</sub>	1	8500	700.87	3.47	[0.29]	[0.0016]	$[2.0 \times 10^{-7}]$	—
A <sup>1</sup> Δ	6	21855	488.6	2.63	0.2284	0.0014	$1.996 \times 10^{-7}$	2.148

## Enthalpy of Formation

The adopted enthalpy of formation is that selected by CODATA.<sup>1</sup> The value was calculated from measurements of the equilibrium H<sub>2</sub>S(g) = H<sub>2</sub>(g) + 0.05 S<sub>2</sub>(g) reported by Randall and Bichowsky,<sup>2</sup> Preuner,<sup>3</sup> and Preuner and Schupp,<sup>4</sup> and from measurements of the partial pressure of S<sub>2</sub>(g) over sulfur reported by Drowart *et al.*<sup>5</sup>

The dissociation energy,  $D_0^{\circ} = 35216.4 \pm 2.5 \text{ cm}^{-1}$  (100.689 ± 0.021 kcal·mol<sup>-1</sup>) is from the spectroscopic study by Ricks and Barrow.<sup>12</sup>

## Heat Capacity and Entropy

The thermal functions above 600 K are calculated using the program of McBride and Gordon.<sup>6</sup> The contribution of vibrational anharmonicity, rotation-vibration interaction, and centrifugal stretching are calculated via the procedures given by Pennington and Kobe.<sup>7</sup> The electronic and molecular constant data in the above table are that summarized by Rosen<sup>8</sup> and Suchard<sup>9</sup> with the exception that the position of the a<sup>1</sup>Δ<sub>g</sub> state at 4700 cm<sup>-1</sup> is from the more recent absorption study by Carlier and Collin.<sup>10</sup> The thermal functions below 600 K are calculated by direct summation over vibrational-rotational energy levels of the ground state (including the proper treatment of the splitting of this level, i.e.  $\alpha = -0.0066 \text{ cm}^{-1}$  and  $\beta = 11.84 \text{ cm}^{-1}$ , and three excited states. We performed the direct summation with a program written by W. H. Evans of the U. S. Bureau of Standards. The direct summation results are not extended to temperatures above 600 K since the energy levels derived from the reported vibrational-rotational constants do not converge to the dissociation energy. For these higher temperatures, the program of McBride and Gordon is used, as in the case of gaseous O<sub>2</sub>.<sup>11</sup>

The value of  $S^{\circ}(298.15 \text{ K})$  agrees exactly with the CODATA recommended value.<sup>1</sup> The uncertainty in  $S^{\circ}(298.15 \text{ K})$  is due to uncertainties in fundamental constants, the atomic weight, and the ground state molecular constants. The contributions of the excited states above 22000 cm<sup>-1</sup> do not affect the thermal functions below 2000 K but do become significant at higher temperatures. However, these states are not included for two reasons. First, the electronic and molecular constants are not all well-defined. Second, many of these levels have a sufficiently shallow potential energy well, which would lead to unreasonably large heat capacity values at high temperatures.

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T/K	C <sub>v</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
		J·K <sup>-1</sup> ·mol <sup>-1</sup>	S <sup>o</sup> - (G <sup>o</sup> - H(T)) / T	H <sup>o</sup> - H(T)	ΔH <sup>o</sup>	
0	0	INFINITE	INFINITE	128.300	128.300	INFINITE
100	29.367	195.067	255.684	-1.024	129.583	-59.015
200	30.452	215.621	231.077	-1.062	129.670	-25.073
250	31.513	222.529	228.693	-1.541	129.180	87.637
298.15	32.490	228.165	228.165	0	128.600	79.687
300	32.525	228.366	228.166	0.060	128.576	79.384
350	33.387	233.447	228.565	1.709	127.892	71.238
400	34.090	237.953	229.462	3.396	127.118	60.632
450	34.656	242.034	230.634	5.115	126.063	48.275
500	35.111	245.678	231.958	6.860	118.376	31.019
600	35.781	252.142	234.798	10.407	114.703	15.511
700	36.260	257.695	237.681	14.009	111.612	-3.092
800	36.637	262.562	240.493	17.653	108.835	-12.684
882.117	36.908	266.155	242.717	20.674	106.333	-20.655
900	36.966	266.896	243.191	21.335	0	0
1000	37.277	270.807	245.760	25.047	0	0
1100	37.584	274.374	248.201	28.790	0	0
1200	37.894	277.658	250.521	32.564	0	0
1300	38.205	280.703	252.727	36.366	0	0
1400	38.514	283.546	254.828	40.205	0	0
1500	38.818	286.213	256.832	44.072	0	0
1600	39.112	288.728	258.748	47.968	0	0
1700	39.394	291.108	260.582	51.894	0	0
1800	39.661	293.367	262.341	55.847	0	0
1900	39.911	295.518	264.031	59.825	0	0
2000	40.144	297.571	265.657	63.828	0	0
2100	40.352	299.535	267.224	67.853	0	0
2200	40.547	301.417	268.736	71.898	0	0
2300	40.729	303.223	270.196	75.962	0	0
2400	40.897	304.960	271.609	80.044	0	0
2500	41.052	306.633	272.977	84.141	0	0
2600	41.179	308.246	274.302	88.253	0	0
2700	41.299	309.802	275.588	92.377	0	0
2800	41.414	311.306	276.837	96.512	0	0
2900	41.523	312.761	278.051	100.659	0	0
3000	41.626	314.171	279.232	104.817	0	0
3100	41.711	315.537	280.381	108.984	0	0
3200	41.795	316.863	281.500	113.159	0	0
3300	41.880	318.150	282.592	117.343	0	0
3400	41.966	319.402	283.656	121.535	0	0
3500	42.051	320.619	284.695	125.736	0	0
3600	42.130	321.805	285.709	129.945	0	0
3700	42.212	322.960	286.700	134.162	0	0
3800	42.298	324.087	287.669	138.387	0	0
3900	42.388	325.187	288.617	142.622	0	0
4000	42.481	326.261	289.545	146.865	0	0
4100	42.575	327.312	290.454	151.118	0	0
4200	42.675	328.339	291.343	155.380	0	0
4300	42.778	329.344	292.215	159.653	0	0
4400	42.886	330.329	293.070	163.936	0	0
4500	42.997	331.294	293.909	168.230	0	0
4600	43.115	332.240	294.722	172.536	0	0
4700	43.236	333.169	295.520	176.853	0	0
4800	43.361	334.080	296.341	181.183	0	0
4900	43.488	334.975	297.115	185.525	0	0
5000	43.619	335.855	297.879	189.881	0	0
5100	43.757	336.721	298.632	194.250	0	0
5200	43.897	337.572	299.373	198.632	0	0
5300	44.038	338.409	300.102	203.029	0	0
5400	44.181	339.234	300.819	207.440	0	0
5500	44.325	340.046	301.525	211.865	0	0
5600	44.472	340.845	302.220	216.305	0	0
5700	44.620	341.634	302.904	220.760	0	0
5800	44.770	342.411	303.579	225.229	0	0
5900	44.922	343.178	304.243	229.714	0	0
6000	45.075	343.934	304.899	234.213	0	0

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1977 (1 bar)

Sulfur (S<sub>2</sub>)S<sub>2</sub>(g)

Silicon Sulfide (SiS<sub>2</sub>) **M<sub>r</sub> = 92.2055 Silicon Sulfide (SiS<sub>2</sub>)** **S<sub>2</sub>Si<sub>1</sub>(cr)**

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa	
	C <sub>p</sub> <sup>o</sup>	S° - [G° - H°(T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	Δ <sub>r</sub> G°
0	0	0	-213.384	-212.609
100	77.488	80.333	-213.362	-212.605
200	78.617	83.387	-216.872	-212.329
250	79.789	89.189	-219.092	-210.962
298.15	81.714	95.737	-220.548	-209.185
300	82.006	96.363	-221.511	-207.211
400	83.136	108.804	-222.185	-205.119
500	84.266	114.970	-228.891	-200.795
600	85.395	120.842	-232.297	-186.677
700	86.525	126.423	-234.534	-172.778
800	87.655	131.730	-237.021	-159.081
900	88.784	136.783	-239.021	-145.571
1000	89.496	141.603	-240.722	-132.239
1363.000	89.915	146.208	---	---
1400	91.044	150.618	---	---
1500	92.154	154.847	---	---
1600	93.291	158.912	---	---
1700	94.370	162.824	---	---
1800	95.318	166.597	---	---
1900	96.650	170.269	---	---
2000			---	---

$\Delta_r H^\circ(0\text{ K}) = \text{Unknown}$   
 $\Delta_r H^\circ(298.15\text{ K}) = -213.384 \pm 20.9\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{ref}} H^\circ = [8.4 \pm 4.2]\text{ kJ}\cdot\text{mol}^{-1}$

**CRYSTAL**

**Silicon Sulfide (SiS<sub>2</sub>)**

$S^\circ(298.15\text{ K}) = [80.333 \pm 4.2]\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}} = 1363\text{ K}$

**Enthalpy of Formation**  
 Rocquet and Ancy-*Maret*<sup>1</sup> determined the enthalpy of reaction for the following:  
 $\text{SiS}_2(\text{cr}) + 6\text{ HF}(20\%) \rightarrow \text{H}_2\text{SiF}_6(<20\%\text{HF}) + 2\text{ H}_2\text{S}(\text{g}), \Delta_r H^\circ(298.15\text{ K}) = -72.8 \pm 2.2\text{ kcal}\cdot\text{mol}^{-1}$ .

A related system was examined by Kilday and Prosen:<sup>2</sup>  
 $\text{SiO}_2(\alpha\text{-quartz}) + 6\text{ HF}(20.0\%) \rightarrow \text{H}_2\text{SiF}_6(<20.0\%\text{HF}) + 2\text{ H}_2\text{O}(\text{l}), \Delta_r H^\circ(298.15\text{ K}) = -32.65 \pm 0.02\text{ kcal}\cdot\text{mol}^{-1}$ .

Combining these two systems mathematically yields approximately the following:  
 $\text{SiO}_2(\alpha\text{-quartz}) + 2\text{ H}_2\text{S}(\text{g}) \rightarrow \text{SiS}_2(\text{cr}) + 2\text{ H}_2\text{O}(\text{l}), \Delta_r H^\circ(298.15\text{ K}) = 40.2 \pm 3.0\text{ kcal}\cdot\text{mol}^{-1}$ .

Using JANAF<sup>3</sup> and NBS<sup>4</sup> auxiliary data,  $\Delta_r H^\circ(\text{SiS}_2, \text{cr}, 298.15\text{ K})$  is equal to  $-51.1 \pm 3.0\text{ kcal}\cdot\text{mol}^{-1}$ . In addition to the normal experimental error in each study, another source of error arises from the saturated solution of H<sub>2</sub>S in the former work but not the latter. Emmons and Theisen<sup>5</sup> measured the equilibrium vapor pressures for the system 1/2 SiS<sub>2</sub>(cr) + 1/2 S<sub>2</sub>(g) → SiS(g) and presented graphically log P(SiS) vs 1/T data. Using these data, a 3rd law analysis yields  $\Delta_r H^\circ(298.15\text{ K}) = 55.27\text{ kcal}\cdot\text{mol}^{-1}$ , with a drift of  $5.1 \pm 1.2\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ . A 2nd law analysis yields  $\Delta_r H^\circ(298.15\text{ K}) = 50.09\text{ kcal}\cdot\text{mol}^{-1}$ . These results lead, respectively, to  $\Delta_r H^\circ(\text{SiS}_2, \text{cr}, 298.15\text{ K}) = -59.84\text{ kcal}\cdot\text{mol}^{-1}$  and  $\Delta_r H^\circ(\text{SiS}_2, \text{cr}, 298.15\text{ K}) = -49.53\text{ kcal}\cdot\text{mol}^{-1}$ , with JANAF<sup>3</sup> auxiliary data. Fruehan and Turkdogan<sup>6</sup> studied the same reaction by means of a silica Knudsen cell-mass spectrometer combination. A 2nd law analysis of their graphical data for two different orifice sizes yields values of  $\Delta_r H^\circ(298.15\text{ K}) = 53.74\text{ kcal}\cdot\text{mol}^{-1}$  and  $46.9\text{ kcal}\cdot\text{mol}^{-1}$ . Again, using JANAF auxiliary data,  $\Delta_r H^\circ(\text{SiS}_2, \text{cr}, 298.15\text{ K}) = -56.83\text{ kcal}\cdot\text{mol}^{-1}$  and  $-42.33\text{ kcal}\cdot\text{mol}^{-1}$ , respectively, or an average value of  $-49.58\text{ kcal}\cdot\text{mol}^{-1}$ .

The value chosen for the enthalpy of formation is  $\Delta_r H^\circ(\text{SiS}_2, \text{cr}, 298.15\text{ K}) = -51.0 \pm 5.0\text{ kcal}\cdot\text{mol}^{-1}$ . This value is a rounded value of the work of Rocquet and Ancy-*Maret*<sup>1</sup>. Berezhnoi<sup>7</sup> references five reported values for the enthalpy of formation (through 1954) and recommended the work of Rocquet and Ancy-*Maret*<sup>1</sup> as the most accurate. Kubaschewski *et al.*<sup>8</sup> in their compilation of enthalpies of formation (through 1965) also rely on the data from Rocquet and Ancy-*Maret*<sup>1</sup>.

**Heat Capacity and Entropy**  
 The heat capacity is assumed to be given by the relation  $C_p^\circ(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = 17.72 \pm 2.96 \times 10^{-3} T$  for  $298 < T < 1363\text{ K}$ . This relation was suggested by Rasch<sup>9</sup> following procedures described by Kubaschewski *et al.*<sup>8</sup> This equation was linearly extrapolated to yield C<sub>p</sub><sup>o</sup> values up to 2000 K. Kubaschewski *et al.*<sup>8</sup> suggested  $S^\circ(298.15\text{ K}) = 19.2\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ .

**Fusion Data**  
 The melting point of SiS<sub>2</sub>(cr) was determined to be  $T_{\text{fus}} = 1363\text{ K}$  by Tiede and Thimann.<sup>10</sup>  $\Delta_{\text{ref}} H^\circ$  was estimated, based on the entropy of melting for SiO<sub>2</sub> (quartz and cristobolite).

**References**  
<sup>1</sup>P. Rocquet and H. F. Ancy-*Maret*, Bull. Soc. Chim. France **1954**, 1038.  
<sup>2</sup>M. V. Kilday and E. J. Prosen, U. S. Nat. Bur. Stand., personal communication, (July 26, 1972).  
<sup>3</sup>H. H. Emmons and L. Theisen, Monats. Chem. **103**, 62 (1972).  
<sup>4</sup>JANAF Thermochemical Tables: SiS(g), 12-31-71, SiO<sub>2</sub>(cr), 6-30-67, H<sub>2</sub>S(g), 12-31-65.  
<sup>5</sup>R. J. Fruehan and E. T. Turkdogan, Met. Trans. **2**, 895 (1971).  
<sup>6</sup>U. S. Nat. Bur. Stand. Tech. Note 270-3, 264 pp. (1968).  
<sup>7</sup>A. S. Berezhnoi, "Silicon and its Binary Systems," Consultants Bureau, New York, 1960 (Russian trans.).  
<sup>8</sup>O. Kubaschewski, E. L. Evans, and C. B. Alcock, "Metallurgical Thermochemistry," Pergamon Press, New York, (1967).  
<sup>9</sup>R. Rasch, Glas-Email-Keram.-Tech. **20**, 297 (1969).  
<sup>10</sup>E. Tiede and H. Thimann, Ber. **59**, II B, 1703 (1926).

PREVIOUS: December 1960

CURRENT: June 1972

Silicon Sulfide (SiS<sub>2</sub>)

S<sub>2</sub>Si<sub>1</sub>(cr)

S<sub>2</sub>Si<sub>1</sub>(l)Silicon Sulfide (SiS<sub>2</sub>)

LIQUID

Silicon Sulfide (SiS<sub>2</sub>)

$$S^{\circ}(298.15 \text{ K}) = [84.687] \text{ J K}^{-1} \cdot \text{mol}^{-1}$$

$$T_{\text{fus}} = 1363 \text{ K}$$

$$\Delta H^{\circ}(298.15 \text{ K}) = [-206.924] \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta_{\text{liq}} H^{\circ} = [8.4 \pm 4.2] \text{ kJ} \cdot \text{mol}^{-1}$$

## Enthalpy of Formation

$\Delta H^{\circ}(cr, 298.15 \text{ K})$  is calculated from  $\Delta H^{\circ}(cr, 298.15 \text{ K})$  and the difference in enthalpy,  $H^{\circ}(1363 \text{ K}) - H^{\circ}(298.15 \text{ K})$ , between the crystal and the liquid.

## Heat Capacity and Entropy

Using methods suggested by Kubaschewski *et al.*,<sup>1</sup> the heat capacity of the liquid is assumed to be a constant  $21.75 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  from 1363 K to 1403 K.  $S^{\circ}(l, 298.15 \text{ K})$  is calculated in a manner similar to that used for the enthalpy of formation. A glass transition is assumed at 900 K.

## Fusion Data

Refer to the crystal table for details.

## References

<sup>1</sup>O. Kubaschewski, E. L. Evans, and C. B. Alcock, "Metallurgical Thermochemistry," Pergamon Press, New York, (1967).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>f</sub>
	C <sub>p</sub> <sup>o</sup>	S° - (G° - H°(T <sub>r</sub> ))/T	H° - H°(T <sub>r</sub> )	Δ <sub>liq</sub> H°	
0					
100					
200					
250					
298.15	77.488	84.687	84.687	0	-206.924
300	77.508	85.166	84.688	0.143	-206.902
400	78.617	107.614	87.742	7.949	-207.451
500	79.789	125.269	93.543	15.863	-210.412
600	81.714	140.011	100.091	23.952	-212.632
700	82.006	152.619	106.717	32.131	-214.089
800	83.136	163.643	113.158	40.388	-215.051
900	84.266	173.500	119.324	48.758	-215.723
900.000	84.266	173.500	119.324	48.758	-215.723
900.000	91.002	173.500	119.324	48.758	-215.723
1000	91.002	183.088	125.230	57.858	-319.654
1100	91.002	191.762	130.890	66.958	-316.952
1200	91.002	199.480	136.297	76.059	-314.325
1300	91.002	206.964	141.457	85.159	-311.770
1363.000	91.002	211.270	144.585	90.892	-311.770
1400	91.002	213.708	146.380	94.259	-309.288
1500	91.002	219.986	151.080	103.359	-306.879
1600	91.002	225.859	155.572	112.459	-304.541
1700	91.002	231.376	159.871	121.560	-302.279
1800	91.002	236.578	163.989	130.660	-300.074
1900	91.002	241.498	167.940	139.760	-297.922
2000	91.002	246.166	171.756	148.860	-295.822

PREVIOUS: December 1960

CURRENT: June 1972

Silicon Sulfide (SiS<sub>2</sub>)S<sub>2</sub>Si<sub>1</sub>(l)

Silicon Sulfide (SiS<sub>2</sub>)

CRYSTAL-LIQUID

0 to 1363 K crystal  
above 1363 K liquid

Refer to the individual tables for details.

M<sub>r</sub> = 92.2055 Silicon Sulfide (SiS<sub>2</sub>)

S<sub>2</sub>Si<sub>1</sub>(cr,l)

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa	
	C <sub>p</sub> <sup>o</sup> J·K <sup>-1</sup> ·mol <sup>-1</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - f(T <sub>r</sub> )]/T <sub>r</sub> J·K <sup>-1</sup> ·mol <sup>-1</sup>	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> ) kJ·mol <sup>-1</sup>	Δ <sub>f</sub> G <sup>o</sup> kJ·mol <sup>-1</sup>
0			0	
100	77.488	80.333	-213.384	-212.609
200	77.598	80.334	-213.362	-212.605
300	78.617	83.387	-216.872	-212.329
400	79.789	89.189	-219.092	-210.962
500	81.714	95.737	-220.548	-209.185
600	82.006	102.363	-221.511	-207.211
700	83.136	108.804	-222.185	-205.119
800	84.266	114.970	-222.891	-200.795
900	85.395	120.842	-223.534	-186.677
1000	86.525	126.423	-224.219	-172.778
1100	87.655	131.730	-224.946	-159.081
1200	88.784	136.783	-225.714	-145.571
1300	89.496	139.846	-226.523	-132.247
1363.000	91.002	141.766	-227.373	-119.921
1400	91.002	146.773	-228.263	-107.534
1500	91.002	151.535	-229.192	-94.844
1600	91.002	156.071	-229.160	-81.811
1700	91.002	160.400	-229.169	-68.481
1800	91.002	164.540	-229.210	-54.811
1900	91.002	168.506	-229.282	-40.788
2000	91.002	172.300	-229.385	-26.344

PREVIOUS:

CURRENT: June 1972

Silicon Sulfide (SiS<sub>2</sub>)

S<sub>2</sub>Si<sub>1</sub>(cr,l)

Sulfur (S<sub>2</sub>) IDEAL GAS M<sub>r</sub> = 96.18 Sulfur (S<sub>2</sub>) S<sub>2</sub>(g)

$S^{\circ}(298.15\text{ K}) = [269.5 \pm 4] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$   $\Delta_f H^{\circ}(298.15\text{ K}) = [141.5 \pm 8] \text{ kJ} \cdot \text{mol}^{-1}$

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T)]/T	H <sup>o</sup> - H <sup>o</sup> (T)	Δ <sub>f</sub> H <sup>o</sup>	Δ <sub>f</sub> G <sup>o</sup>	log K <sub>r</sub>	S <sub>2</sub> (g)
0			0.	141.461	89.777		-15.729
100	47.664	269.517	304.899	141.461	89.777		-15.729
200	47.862	269.813	269.518	141.423	89.456		-15.576
250	47.996	270.109	239.518	140.375	87.877		-12.070
300	48.140	271.405	210.518	139.327	86.298		-9.496
350	48.284	272.701	181.518	138.279	84.719		-6.916
400	48.428	274.000	152.518	137.230	83.140		-4.336
450	48.572	275.296	123.518	136.181	81.561		-1.756
500	48.716	276.592	94.518	135.132	79.982		0.824
550	48.860	277.888	65.518	134.083	78.403		2.403
600	49.004	279.184	36.518	133.034	76.824		3.982
650	49.148	280.480	7.518	131.985	75.245		5.561
700	49.292	281.776	-21.482	130.936	73.666		7.140
750	49.436	283.072	-50.482	129.887	72.087		8.719
800	49.580	284.368	-79.482	128.838	70.508		10.298
850	49.724	285.664	-108.482	127.789	68.929		11.877
900	49.868	286.960	-137.482	126.740	67.350		13.456
950	49.999	288.256	-166.482	125.691	65.771		15.035
1000	50.143	289.552	-195.482	124.642	64.192		16.614
1100	50.432	293.827	-299.851	120.193	59.743		21.763
1200	50.721	300.899	-404.260	115.744	55.294		26.912
1300	51.010	309.971	-508.669	111.295	50.845		32.061
1400	51.299	320.043	-613.078	106.846	46.396		37.210
1500	51.588	331.115	-717.487	102.397	41.947		42.359
1600	51.877	343.187	-821.896	97.948	37.498		47.508
1700	52.166	356.259	-926.305	93.499	33.049		52.657
1800	52.455	370.331	-1030.714	89.000	28.600		57.806
1900	52.744	385.403	-1135.123	84.501	24.151		62.955
2000	53.033	401.475	-1239.532	80.002	19.702		68.104
2100	53.322	418.547	-1343.941	75.503	15.253		73.253
2200	53.611	436.619	-1448.350	70.904	10.804		78.402
2300	53.900	455.691	-1552.759	66.405	6.355		83.551
2400	54.189	475.763	-1657.168	61.906	1.906		88.700
2500	54.478	496.835	-1761.577	57.407	-2.543		93.849
2600	54.767	518.907	-1865.986	52.908	-7.994		98.998
2700	55.056	541.979	-1970.395	48.409	-13.445		104.147
2800	55.345	566.051	-2074.804	43.910	-18.896		109.296
2900	55.634	591.123	-2179.213	39.411	-24.347		114.445
3000	55.923	617.195	-2283.622	34.912	-29.798		119.594
3100	56.212	644.267	-2388.031	30.413	-35.249		124.743
3200	56.501	672.339	-2492.440	25.914	-40.700		129.892
3300	56.790	701.411	-2596.849	21.415	-46.151		135.041
3400	57.079	731.483	-2701.258	16.916	-51.602		140.190
3500	57.368	762.555	-2805.667	12.417	-57.053		145.339
3600	57.657	794.627	-2910.076	7.918	-62.504		150.488
3700	57.946	827.699	-3014.485	3.419	-67.955		155.637
3800	58.235	861.771	-3118.894	-1.080	-73.406		160.786
3900	58.524	896.843	-3223.303	-6.581	-78.857		165.935
4000	58.813	932.915	-3327.712	-12.082	-84.308		171.084
4100	59.102	969.987	-3432.121	-17.583	-89.759		176.233
4200	59.391	1008.059	-3536.530	-23.084	-95.210		181.382
4300	59.680	1047.131	-3640.939	-28.585	-100.661		186.531
4400	59.969	1087.203	-3745.348	-34.086	-106.112		191.680
4500	60.258	1128.275	-3849.757	-39.587	-111.563		196.829
4600	60.547	1170.347	-3954.166	-45.088	-117.014		201.978
4700	60.836	1213.419	-4058.575	-50.589	-122.465		207.127
4800	61.125	1257.491	-4162.984	-56.090	-127.916		212.276
4900	61.414	1302.563	-4267.393	-61.591	-133.367		217.425
5000	61.703	1348.635	-4371.802	-67.092	-138.818		222.574
5100	62.000	1395.707	-4476.211	-72.593	-144.269		227.723
5200	62.289	1443.779	-4580.620	-78.094	-149.720		232.872
5300	62.578	1492.851	-4685.029	-83.595	-155.171		238.021
5400	62.867	1542.923	-4789.438	-89.096	-160.622		243.170
5500	63.156	1593.995	-4893.847	-94.597	-166.073		248.319
5600	63.445	1645.067	-5000.000	-100.098	-171.524		253.468
5700	63.734	1697.139	-5106.153	-106.099	-176.975		258.617
5800	64.023	1750.211	-5212.306	-112.100	-182.426		263.766
5900	64.312	1804.283	-5318.459	-118.101	-187.877		268.915
6000	64.601	1859.355	-5424.612	-124.102	-193.328		274.064

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

**Sulfur (S<sub>2</sub>) IDEAL GAS**  $M_r = 96.18$  **Sulfur (S<sub>2</sub>)**  $S_2(g)$

$S^{\circ}(298.15\text{ K}) = [269.5 \pm 4] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$   $\Delta_f H^{\circ}(298.15\text{ K}) = [141.5 \pm 8] \text{ kJ} \cdot \text{mol}^{-1}$

**Enthalpy of Formation**  
 The enthalpy of formation for each vapor phase sulfur species S<sub>2</sub> to S<sub>8</sub> is calculated by a third law calculation using the thermal functions described below and assuming that the vapor pressure data given by Hultgren *et al.*<sup>1</sup> and Rau *et al.*<sup>2</sup> are correct. These values for the enthalpy of formation are dependent on the somewhat arbitrary thermal functions adopted for the polyatomic sulfur gases.

**Heat Capacity and Entropy**  
 The thermal functions for the polyatomic species, S<sub>2</sub> to S<sub>8</sub>, are estimated following the suggestion of *et al.*<sup>2</sup> Using thermal functions calculated for S(g), S<sub>2</sub>(g), and S<sub>8</sub>(g), the heat capacity values for the remaining species were calculated by Rau *et al.*<sup>2</sup> assuming that the vibrational heat capacity per degree of freedom is the same for all sulfur polyatomic species. The resulting heat capacity equations are given by Rau *et al.*<sup>2</sup>

The use of the procedure of Rau *et al.*<sup>2</sup> leads to a set of thermal functions and associated enthalpies of formation which reproduce the observed sulfur vapor pressure data. That is, the sum of the calculated partial pressures of all eight sulfur vapor species, S<sub>2</sub>(g) to S<sub>8</sub>(g), does closely reproduce the observed vapor pressure. [A difference between the calculated boiling point (at 1 atm) and the secondary reference temperature boiling point is due to the difference between the ideal gas calculation and the real observed value.]

The thermal functions for S<sub>2</sub>(g) were calculated<sup>3</sup> by adjusting the low valued vibrational frequencies such that S(298.15 K) and Δ<sub>f</sub>H<sup>o</sup>(298.15 K) values could be found which reproduced the partial pressure of the octamer. The entropy of S<sub>2</sub>(g) is well-known,<sup>3</sup> being based on reliable data and sound statistical mechanical calculations.

The thermal functions which would result from the use of the available structural and vibrational information for the remaining polyatomic species, are biased in the same way as for S<sub>2</sub>(g). Some of the necessary information is derived from condensed phase spectra (rather than gas phase spectra), as with the octamer, the low-valued vibrational frequencies (and possibly the structure) may need to be adjusted. In any event, the use of the existing spectroscopic data (unaltered) leads to calculated entropies which are unreasonable when used in a 3rd law analysis to mesh in the vapor pressure with these thermal functions.

**References**

<sup>1</sup>R. Hultgren, P. D. Desai, *et al.*, "Selected Values of the Thermodynamic Properties of the Elements", American Society for Metals, Metals Park, Ohio, (1973).

<sup>2</sup>H. Rau, R. N. Kuty and J. R. F. Guedes de Carvalho, *J. Chem. Thermodyn.* **5**, 833 (1973).

<sup>3</sup>JANAF Thermochemical Tables: S<sub>2</sub>(g), 9-30-77.

**Sulfur (S<sub>2</sub>)**



S<sub>4</sub>(g)

M<sub>r</sub> = 128.24 Sulfur (S<sub>4</sub>)

IDEAL GAS

Sulfur (S<sub>4</sub>)

$\Delta_f H^\circ(298.15\text{ K}) = [310.6 \pm 4] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$

$\Delta_f H^\circ(298.15\text{ K}) = [145.8 \pm 8] \text{ kJ} \cdot \text{mol}^{-1}$

**Enthalpy of Formation**  
 The enthalpy of formation for each vapor phase sulfur species S<sub>2</sub> to S<sub>7</sub> is calculated by a third law using the thermal functions described below and assuming that the vapor pressure data given by Hultgren *et al.*<sup>1</sup> and Rau *et al.*<sup>2</sup> are correct. These values for the enthalpy of formation are dependent on the somewhat arbitrary thermal functions adopted for the polyatomic sulfur gases.

**Heat Capacity and Entropy**  
 The thermal functions for the polyatomic species, S<sub>2</sub> to S<sub>7</sub>, are estimated following the suggestion of Rau *et al.*<sup>2</sup> Using thermal functions calculated for S(g), S<sub>2</sub>(g), and S<sub>4</sub>(g), the heat capacity values for the remaining species were calculated by Rau *et al.*<sup>2</sup> assuming that the vibrational heat capacity per degree of freedom is the same for all sulfur polyatomic species. The resulting heat capacity equations are given by Rau *et al.*<sup>2</sup>

The use of the procedure of Rau *et al.*<sup>2</sup> leads to a set of thermal functions and associated enthalpies of formation which reproduce the observed sulfur vapor pressure data. That is, the sum of the calculated partial pressures of all eight sulfur vapor species, S<sub>2</sub>(g) to S<sub>8</sub>(g), does closely reproduce the observed vapor pressure. [A difference between the calculated boiling point (at 1 atm) and the secondary reference temperature boiling point is due to the difference between the ideal gas calculation and the real observed value.]

The thermal functions for S<sub>4</sub>(g) were calculated<sup>3</sup> by adjusting the low valued vibrational frequencies such that S(298.15 K) and  $\Delta_f H^\circ(298.15\text{ K})$  values could be found which reproduced the partial pressure of the octamer. The entropy of S<sub>4</sub>(g) is well-known,<sup>2</sup> being based on reliable data and sound statistical mechanical calculations.

The thermal functions which would result from the use of the available structural and vibrational information for the remaining polyatomic species, are biased in the same way as for S<sub>4</sub>(g). Some of the necessary information is derived from condensed phase spectra (rather than gas phase spectra). As with the octamer, the low-valued vibrational frequencies (and possibly the structure) may need to be adjusted. In any event, the use of the existing spectroscopic data (unaltered) leads to calculated entropies which are unreasonable when used in a 3rd law analysis to mesh in the vapor pressure with these thermal functions.

**References**  
<sup>1</sup>R. Hultgren, P. D. Desai, *et al.*, "Selected Values of the Thermodynamic Properties of the Elements," American Society for Metals, Metals Park, Ohio, (1973).  
<sup>2</sup>H. Rau, R. N. Kuttly and J. R. F. Guedes de Carvalho, *J. Chem. Thermodyn.* **5**, 833 (1973).  
<sup>3</sup>JANAF Thermochemical Tables: S<sub>2</sub>(g), 9-30-77.

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T)]/T	H <sup>o</sup> - H <sup>o</sup> (T)	Δ <sub>f</sub> H <sup>o</sup>	Δ <sub>f</sub> G <sup>o</sup>	log K <sub>f</sub>
0			0.			
100	67.585	310.646	388.341	145.771	91.381	-16.010
200	67.754	311.065	310.647	145.728	91.044	-15.852
300	67.854	311.803	311.487	145.728	91.044	-15.852
400	67.903	312.305	313.393	145.728	91.044	-15.852
500	67.929	312.630	314.093	145.728	91.044	-15.852
600	67.944	312.892	314.611	145.728	91.044	-15.852
700	67.951	313.107	315.000	145.728	91.044	-15.852
800	67.953	313.283	315.300	145.728	91.044	-15.852
900	67.953	313.417	315.530	145.728	91.044	-15.852
1000	67.953	313.503	315.611	145.728	91.044	-15.852
1100	67.953	313.549	315.646	145.728	91.044	-15.852
1200	67.953	313.567	315.663	145.728	91.044	-15.852
1300	67.953	313.573	315.667	145.728	91.044	-15.852
1400	67.953	313.570	315.660	145.728	91.044	-15.852
1500	67.953	313.559	315.643	145.728	91.044	-15.852
1600	67.953	313.541	315.617	145.728	91.044	-15.852
1700	67.953	313.518	315.582	145.728	91.044	-15.852
1800	67.953	313.491	315.539	145.728	91.044	-15.852
1900	67.953	313.461	315.488	145.728	91.044	-15.852
2000	67.953	313.428	315.431	145.728	91.044	-15.852
2100	67.953	313.392	315.369	145.728	91.044	-15.852
2200	67.953	313.354	315.302	145.728	91.044	-15.852
2300	67.953	313.313	315.231	145.728	91.044	-15.852
2400	67.953	313.270	315.156	145.728	91.044	-15.852
2500	67.953	313.225	315.077	145.728	91.044	-15.852
2600	67.953	313.178	315.000	145.728	91.044	-15.852
2700	67.953	313.129	314.925	145.728	91.044	-15.852
2800	67.953	313.078	314.852	145.728	91.044	-15.852
2900	67.953	313.025	314.781	145.728	91.044	-15.852
3000	67.953	312.970	314.712	145.728	91.044	-15.852
3100	67.953	312.913	314.646	145.728	91.044	-15.852
3200	67.953	312.854	314.583	145.728	91.044	-15.852
3300	67.953	312.793	314.523	145.728	91.044	-15.852
3400	67.953	312.730	314.466	145.728	91.044	-15.852
3500	67.953	312.665	314.412	145.728	91.044	-15.852
3600	67.953	312.600	314.360	145.728	91.044	-15.852
3700	67.953	312.533	314.311	145.728	91.044	-15.852
3800	67.953	312.466	314.265	145.728	91.044	-15.852
3900	67.953	312.400	314.222	145.728	91.044	-15.852
4000	67.953	312.333	314.182	145.728	91.044	-15.852
4100	67.953	312.267	314.144	145.728	91.044	-15.852
4200	67.953	312.201	314.109	145.728	91.044	-15.852
4300	67.953	312.136	314.077	145.728	91.044	-15.852
4400	67.953	312.070	314.048	145.728	91.044	-15.852
4500	67.953	312.005	314.021	145.728	91.044	-15.852
4600	67.953	311.940	313.997	145.728	91.044	-15.852
4700	67.953	311.875	313.975	145.728	91.044	-15.852
4800	67.953	311.810	313.955	145.728	91.044	-15.852
4900	67.953	311.745	313.937	145.728	91.044	-15.852
5000	67.953	311.680	313.921	145.728	91.044	-15.852
5100	67.953	311.615	313.907	145.728	91.044	-15.852
5200	67.953	311.550	313.895	145.728	91.044	-15.852
5300	67.953	311.485	313.885	145.728	91.044	-15.852
5400	67.953	311.420	313.877	145.728	91.044	-15.852
5500	67.953	311.355	313.871	145.728	91.044	-15.852
5600	67.953	311.290	313.867	145.728	91.044	-15.852
5700	67.953	311.225	313.864	145.728	91.044	-15.852
5800	67.953	311.160	313.862	145.728	91.044	-15.852
5900	67.953	311.095	313.861	145.728	91.044	-15.852
6000	67.953	311.030	313.861	145.728	91.044	-15.852

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

S<sub>4</sub>(g)

Sulfur (S<sub>4</sub>)

T/K	C <sub>v</sub>	S°	S° - [C <sub>v</sub> - R(T)]/T	H° - H°(T)	ΔH°	ΔG°	log K <sub>f</sub>	S <sub>2</sub> (g)
0				0				
100								
200								
250								
298.15	89.501	308.638	471.413		109.370	65.137	-11.412	
300	89.721	309.192	308.639		109.325	64.862	-11.294	
350	94.425	321.052	309.751	.166	108.107	57.548	-8.588	
400	97.607	336.226	312.722	4.778	105.756	50.851	-6.640	
450	99.419	352.859	315.589	9.261	103.160	43.475	-5.279	
500	101.155	368.419	319.531	14.512	100.688	40.689	-4.251	
600	103.187	377.057	321.458	19.539	97.959	32.370	-2.818	
700	104.456	393.065	325.714	29.759	95.218	25.218	-1.882	
800	105.316	409.515	331.514	40.146	92.637	18.690	-1.235	
900	105.939	427.515	338.883	51.201	90.262	12.690	-0.865	
1000	106.415	430.703	348.883	61.201	88.024	43.391	-2.266	
1100	106.795	440.864	363.881	71.820	85.981	67.959	-3.227	
1200	107.109	450.170	372.522	82.481	84.127	91.410	-4.022	
1300	107.377	458.754	378.830	93.177	82.450	116.758	-4.691	
1400	107.612	466.730	384.826	103.902	80.941	141.014	-5.261	
1500	107.821	474.152	390.537	114.651	79.568	165.190	-5.752	
1600	108.012	481.117	395.982	125.425	78.332	189.293	-6.180	
1700	108.188	487.670	401.185	147.025	77.213	213.333	-6.585	
1800	108.353	493.859	406.163	157.852	76.199	237.315	-6.887	
1900	108.509	499.722	410.934	168.695	75.287	261.247	-7.182	
2000	108.657	505.291	415.514	179.554	74.477	285.132	-7.447	
2100	108.800	510.596	419.917	190.427	73.765	308.975	-7.685	
2200	108.937	515.661	424.154	201.314	73.147	332.781	-7.901	
2300	109.071	520.506	428.239	212.214	72.618	356.553	-8.098	
2400	109.201	525.151	432.181	223.128	72.173	380.293	-8.277	
2500	109.329	529.611	435.989	234.054	71.802	404.003	-8.441	
2600	109.453	533.902	439.673	244.993	71.498	427.688	-8.592	
2700	109.576	538.055	443.240	255.945	71.254	451.347	-8.732	
2800	109.697	542.022	446.697	266.909	71.070	474.982	-8.861	
2900	109.817	545.573	450.051	277.884	70.941	498.596	-8.981	
3000	109.935	549.598	453.308	288.872	70.859	522.188	-9.092	
3100	110.052	553.205	456.472	299.871	70.814	545.762	-9.196	
3200	110.168	556.701	459.550	310.882	70.800	569.316	-9.293	
3300	110.283	560.093	462.546	321.905	70.814	592.853	-9.384	
3400	110.397	563.387	465.463	332.939	70.842	616.373	-9.469	
3500	110.511	566.588	468.307	343.984	70.885	639.877	-9.550	
3600	110.624	569.703	471.081	355.041	70.941	663.365	-9.625	
3700	110.736	572.736	473.787	366.109	71.009	686.839	-9.696	
3800	110.848	575.690	476.430	377.188	71.088	710.298	-9.764	
3900	110.959	578.571	479.013	388.279	71.178	733.748	-9.827	
4000	111.070	581.382	481.537	399.380	71.278	757.178	-9.888	
4100	111.181	584.126	484.006	410.493	71.388	780.599	-9.945	
4200	111.291	586.806	486.421	421.616	71.509	804.009	-9.999	
4300	111.401	589.426	488.787	432.751	71.641	827.407	-10.051	
4400	111.511	591.989	491.103	443.896	71.784	850.796	-10.100	
4500	111.620	594.496	493.373	455.053	71.938	874.174	-10.147	
4600	111.729	596.950	495.598	466.220	72.103	897.543	-10.192	
4700	111.838	599.354	497.780	477.399	72.278	920.904	-10.235	
4800	111.947	601.710	499.921	488.588	72.463	944.257	-10.276	
4900	112.056	604.019	502.022	499.788	72.658	967.603	-10.315	
5000	112.164	606.284	504.084	510.999	72.863	990.941	-10.352	
5100	112.273	608.507	506.110	522.221	73.078	1014.274	-10.388	
5200	112.381	610.688	508.100	533.454	73.303	1037.600	-10.423	
5300	112.489	612.829	510.056	544.697	73.538	1060.922	-10.456	
5400	112.597	614.933	511.979	555.952	73.783	1084.239	-10.488	
5500	112.705	617.000	513.870	567.217	74.038	1107.552	-10.519	
5600	112.812	619.032	515.730	578.492	74.303	1130.862	-10.548	
5700	112.920	621.030	517.559	589.779	74.578	1154.169	-10.577	
5800	113.027	622.994	519.360	601.076	74.863	1177.473	-10.604	
5900	113.135	624.927	521.133	612.385	75.158	1200.776	-10.631	
6000	113.242	626.830	522.879	623.703	75.463	1224.077	-10.657	

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1977 (1 bar)

## IDEAL GAS

Sulfur (S<sub>2</sub>)Sulfur (S<sub>2</sub>)S<sub>2</sub>(g)

$S^{\circ}(298.15\text{ K}) = [308.6 \pm 4] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$   $\Delta H^{\circ}(298.15\text{ K}) = [109.4 \pm 8] \text{ kJ} \cdot \text{mol}^{-1}$

**Enthalpy of Formation**  
The enthalpy of formation for each vapor phase sulfur species S<sub>2</sub> to S<sub>8</sub> is calculated by a third law using the thermal functions described below and assuming that the vapor pressure data given by Hultgren *et al.*<sup>1</sup> and Rau *et al.*<sup>2</sup> are correct. These values for the enthalpy of formation are dependent on the somewhat arbitrary thermal functions adopted for the polyatomic sulfur gases.

**Heat Capacity and Entropy**

The thermal functions for the polyatomic species, S<sub>2</sub> to S<sub>8</sub>, are estimated following the suggestion of Rau *et al.*<sup>2</sup> Using thermal functions calculated for S(g), S<sub>2</sub>(g), and S<sub>8</sub>(g), the heat capacity values for the remaining species were calculated by Rau *et al.*<sup>2</sup> assuming that the vibrational heat capacity per degree of freedom is the same for all sulfur polyatomic species. The resulting heat capacity equations are given by Rau *et al.*<sup>2</sup>

The use of the procedure of Rau *et al.*<sup>2</sup> leads to a set of thermal functions and associated enthalpies of formation which reproduce the observed sulfur vapor pressure data. That is, the sum of the calculated partial pressures of all eight sulfur vapor species, S<sub>2</sub>(g) to S<sub>8</sub>(g), does closely reproduce the observed vapor pressure. [A difference between the calculated boiling point (at 1 atm) and the secondary reference temperature boiling point is due to the difference between the ideal gas calculation and the real observed value.]

The thermal functions for S<sub>2</sub>(g) were calculated<sup>3</sup> by adjusting the low valued vibrational frequencies such that S(298.15 K) and ΔH°(298.15 K) values could be found which reproduced the partial pressure of the octamer. The entropy of S<sub>2</sub>(g) is well-known<sup>3</sup> being based on reliable data and sound statistical mechanical calculations.

The thermal functions which would result from the use of the available structural and vibrational information for the remaining polyatomic species, are biased in the same way as for S<sub>2</sub>(g). Some of the necessary information is derived from condensed phase spectra (rather than gas phase spectra). As with the octamer, the low-valued vibrational frequencies (and possibly the structure) may need to be adjusted. In any event, the use of the existing spectroscopic data (unaltered) leads to calculated entropies which are unreasonable when used in a 3rd law analysis to mesh in the vapor pressure with these thermal functions.

**References**

- R. Hultgren, P. D. Desai, *et al.*, "Selected Values of the Thermodynamic Properties of the Elements", American Society for Metals, Metals Park, Ohio, (1973).
- H. Rau, R. N. Kurty and J. R. F. Guedes de Carvalho, *J. Chem. Thermodyn.* 5, 833 (1973).
- JANAF Thermochemical Tables: S<sub>2</sub>(g), 9-30-77.

Sulfur (S<sub>2</sub>)S<sub>2</sub>(g)

Sulfur (S<sub>8</sub>) IDEAL GAS M<sub>r</sub> = 160.30 Sulfur (S<sub>2</sub>)

Standard State Pressure = p° = 0.1 MPa

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

Standard State Pressure = p° = 0.1 MPa

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - H(T <sub>r</sub> )]/T	H <sup>o</sup> - H(T <sub>r</sub> )	A <sub>1</sub> H <sup>o</sup>	A <sub>2</sub> G <sup>o</sup>	log K <sub>r</sub>
0			0.			
100						
200						
250						
298.15	111.571	354.076	522.879	101.922	53.699	-9.408
300	111.826	354.767	523.078	101.877	53.400	-9.298
350	117.278	372.446	555.462	100.618	50.419	-6.778
400	120.826	388.354	598.596	98.591	38.152	-4.982
450	123.265	402.735	652.715	80.544	32.445	-3.766
500	125.018	415.817	717.381	67.738	27.426	-2.865
550	127.318	428.833	779.424	58.838	18.838	-1.640
600	129.155	438.573	837.640	58.583	11.592	-0.865
650	130.556	445.826	891.608	62.575	5.237	-0.347
700	131.510	451.137	940.165	75.575	6.293	-0.365
750	132.016	454.893	983.262	88.631	37.144	-1.940
800	132.162	457.377	1020.895	101.729	67.806	-3.220
850	131.455	458.802	1052.083	114.861	98.300	-4.279
900	131.694	459.334	1077.858	128.019	128.646	-5.169
950	131.894	459.101	1108.245	141.198	158.861	-5.927
1000	132.066	458.207	1143.276	154.397	188.958	-6.580
1100	132.215	456.735	1212.979	167.611	218.951	-7.148
1200	132.347	454.755	1288.379	180.839	258.715	-7.646
1300	132.466	452.323	1369.501	194.080	297.668	-8.087
1400	132.575	449.488	1456.366	207.332	335.017	-8.479
1500	132.675	446.291	1549.094	220.594	370.864	-8.830
1600	132.768	442.766	1647.603	233.867	405.296	-9.146
1700	132.855	438.945	1751.818	247.148	439.325	-9.432
1800	132.936	434.852	1861.755	260.437	472.958	-9.692
1900	133.016	430.519	1977.435	273.735	506.218	-9.929
2000	133.091	425.943	2100.000	287.040	539.064	-10.147
2500	133.164	411.164	2515.644	300.353	615.010	-10.347
2600	133.234	406.191	2570.016	313.673	647.330	-10.531
2700	133.302	401.038	2624.252	327.000	679.049	-10.702
2800	133.368	395.717	2678.361	340.333	710.166	-10.860
2900	133.432	390.239	2732.348	353.673	740.686	-11.007
3000	133.496	384.616	2786.222	367.020	770.611	-11.144
3100	133.558	378.855	2840.000	380.373	800.049	-11.272
3200	133.619	373.055	2893.693	393.731	829.000	-11.392
3300	133.679	367.215	2947.311	407.096	857.466	-11.505
3400	133.738	361.336	3000.874	420.467	885.449	-11.611
3500	133.796	355.418	3054.391	433.844	912.950	-11.710
3600	133.854	349.461	3107.862	447.226	940.000	-11.804
3700	133.911	343.466	3161.297	460.615	966.619	-11.893
3800	133.968	337.431	3214.696	474.008	992.800	-11.977
3900	134.024	331.356	3268.060	487.408	1018.543	-12.056
4000	134.080	325.241	3321.389	500.813	1043.844	-12.132
4100	134.135	319.086	3374.683	514.224	1068.700	-12.205
4200	134.190	312.891	3427.941	527.640	1093.119	-12.271
4300	134.245	306.656	3481.164	541.062	1117.100	-12.336
4400	134.299	300.381	3534.361	554.489	1140.643	-12.398
4500	134.353	294.066	3587.531	567.922	1163.750	-12.457
4600	134.407	287.711	3640.683	581.360	1186.421	-12.513
4700	134.461	281.316	3693.818	594.803	1208.656	-12.567
4800	134.514	274.881	3746.937	608.252	1230.466	-12.619
4900	134.567	268.406	3800.041	621.706	1251.851	-12.668
5000	134.621	261.891	3853.130	635.165	1272.821	-12.716
5100	134.673	255.336	3906.203	648.630	1293.376	-12.761
5200	134.726	248.741	3959.261	662.100	1313.516	-12.805
5300	134.779	242.106	4012.304	675.575	1333.241	-12.847
5400	134.831	235.429	4065.333	689.056	1352.551	-12.888
5500	134.884	228.711	4118.347	702.542	1371.446	-12.927
5600	134.936	221.956	4171.346	716.033	1389.926	-12.965
5700	134.988	215.166	4224.330	729.529	1408.000	-13.001
5800	135.040	208.331	4277.300	743.030	1425.676	-13.036
5900	135.092	201.451	4330.256	756.537	1442.951	-13.070
6000	135.144	194.526	4383.200	770.040	1459.826	-13.103

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

S<sup>o</sup>(298.15 K) = [354.1 ± 4] J·K<sup>-1</sup>·mol<sup>-1</sup> Δ<sub>f</sub>H<sup>o</sup>(298.15 K) = [101.9 ± 8] kJ·mol<sup>-1</sup>

**Enthalpy of Formation**  
 The enthalpy of formation for each vapor phase sulfur species S<sub>2</sub> to S<sub>8</sub> is calculated by a third law using the thermal functions described below and assuming that the vapor pressure data given by Hultgren *et al.*<sup>1</sup> and Rau *et al.*<sup>2</sup> are correct. These values for the enthalpy of formation are dependent on the somewhat arbitrary thermal functions adopted for the polyatomic sulfur gases.

**Heat Capacity and Entropy**  
 The thermal functions for the polyatomic species, S<sub>2</sub> to S<sub>8</sub>, are estimated following the suggestion of Rau *et al.*<sup>2</sup> Using thermal functions calculated for S(g), S<sub>2</sub>(g), and S<sub>8</sub>(g), the heat capacity values for the remaining species were calculated by Rau *et al.*<sup>2</sup> assuming that the vibrational heat capacity per degree of freedom is the same for all sulfur polyatomic species. The resulting heat capacity equations are given by Rau *et al.*<sup>2</sup>

The use of the procedure of Rau *et al.*<sup>2</sup> leads to a set of thermal functions and associated enthalpies of formation which reproduce the observed sulfur vapor pressure data. That is, the sum of the calculated partial pressures of all eight sulfur vapor species, S<sub>2</sub>(g) to S<sub>8</sub>(g), does closely reproduce the observed vapor pressure. [A difference between the calculated boiling point (at 1 atm) and the secondary reference temperature boiling point is due to the difference between the ideal gas calculation and the real observed value.]

The thermal functions for S<sub>2</sub>(g) were calculated<sup>3</sup> by adjusting the low valued vibrational frequencies such that S(298.15 K) and Δ<sub>f</sub>H<sup>o</sup>(298.15 K) values could be found which reproduced the partial pressure of the octamer. The entropy of S<sub>2</sub>(g) is well-known,<sup>3</sup> being based on reliable data and sound statistical mechanical calculations.

The thermal functions which would result from the use of the available structural and vibrational information for the remaining polyatomic species, are biased in the same way as for S<sub>2</sub>(g). Some of the necessary information is derived from condensed phase spectra (rather than gas phase spectra). As with the octamer, the low-valued vibrational frequencies (and possibly the structure) may need to be adjusted. In any event, the use of the existing spectroscopic data (unaltered) leads to calculated entropies which are unreasonable when used in a 3rd law analysis to mesh in the vapor pressure with these thermal functions.

**References**  
 1R. Hultgren, P. D. Desai, *et al.*, "Selected Values of the Thermodynamic Properties of the Elements", American Society for Metals, Metals Park, Ohio, (1973).  
 2H. Rau, R. N. Kuttly and J. R. F. Guedes de Carvalho, *J. Chem. Thermodyn.* 5, 833 (1973).  
 3JANAF Thermochemical Tables: S<sub>2</sub>(g), 9-30-77.

Sulfur (S <sub>2</sub> )	T/K	C <sub>p</sub> <sup>a</sup>	S <sup>b</sup>	S <sup>c</sup> - [C <sub>p</sub> - H(T <sub>2</sub> )/T]	H <sup>c</sup> - H(T <sub>2</sub> )	ΔH <sup>c</sup>	log K <sub>f</sub>	S <sub>T</sub> (g)
	0				0.			
	100							
	200							
	250							
	298.15	133.502	407.673	617.165	0.	113.679	59.034	-10.342
	300	133.780	408.500	407.675	2.47	113.632	58.695	-10.270
	350	139.733	429.603	409.328	7.096	112.318	49.641	-9.691
	400	143.642	448.534	413.067	14.867	110.877	41.999	-9.066
	450	146.363	465.619	417.972	21.441	109.169	34.960	-8.352
	500	148.147	481.147	423.525	28.811	107.250	29.310	-7.661
	600	151.017	508.450	435.467	43.790	104.656	19.665	-6.712
	700	152.729	531.867	447.605	58.983	102.411	11.583	-5.86
	800	153.931	552.344	459.445	74.319	100.479	5.572	-5.293
	900	154.836	570.579	470.706	89.759	98.759	3.919	-4.844
	1000	155.556	586.881	481.600	105.280	97.280	4.144	-4.201
	1100	156.155	601.736	491.857	120.867	96.000	78.117	-3.709
	1200	156.672	615.346	501.588	136.508	94.881	113.867	-4.956
	1300	157.132	627.904	510.828	152.199	93.808	149.416	-6.004
	1400	157.549	639.565	519.612	167.934	92.784	184.784	-6.894
	1500	157.936	650.448	527.976	183.708	91.800	219.990	-7.661
	1600	158.299	660.652	535.953	199.520	90.850	255.049	-8.376
	1700	158.643	670.260	543.573	215.367	90.000	289.974	-9.010
	1800	158.974	679.337	550.866	231.248	89.200	324.776	-9.582
	1900	159.293	687.941	557.856	247.161	88.450	359.466	-10.119
	2000	159.603	696.119	564.566	263.106	87.750	394.053	-10.629
	2100	159.905	703.914	571.018	279.082	87.100	428.545	-11.119
	2200	160.201	711.359	577.229	295.087	86.500	462.947	-11.592
	2300	160.492	718.487	583.127	311.122	85.950	497.267	-12.050
	2400	160.779	725.374	588.996	327.185	85.450	531.508	-12.500
	2500	161.063	731.893	594.852	343.278	85.000	565.675	-12.950
	2600	161.343	738.215	599.985	359.398	84.600	599.774	-13.400
	2700	161.621	744.310	605.218	375.546	84.250	633.805	-13.850
	2800	161.896	750.192	610.292	391.722	83.950	667.774	-14.300
	2900	162.170	755.878	615.214	407.925	83.700	701.682	-14.750
	3000	162.442	761.381	619.995	424.156	83.500	735.532	-15.200
	3100	162.712	766.711	624.643	440.414	83.350	769.326	-15.650
	3200	162.981	771.882	629.163	456.698	83.250	803.066	-16.100
	3300	163.249	776.901	633.565	473.010	83.200	836.754	-16.550
	3400	163.516	781.778	637.832	489.348	83.200	870.390	-17.000
	3500	163.782	786.522	642.033	505.713	83.200	903.980	-17.450
	3600	164.048	791.140	646.111	522.105	83.200	937.521	-17.900
	3700	164.312	795.638	650.091	538.523	83.200	971.016	-18.350
	3800	164.576	800.074	653.980	554.967	83.200	1004.466	-18.800
	3900	164.840	804.302	657.779	571.438	83.200	1037.873	-19.250
	4000	165.103	808.479	661.495	587.935	83.200	1071.237	-19.700
	4100	165.365	812.559	665.130	604.458	83.200	1104.560	-20.150
	4200	165.627	816.547	668.688	621.008	83.200	1137.844	-20.600
	4300	165.889	820.447	672.172	637.584	83.200	1171.088	-21.050
	4400	166.150	824.264	675.985	654.186	83.200	1204.296	-21.500
	4500	166.411	828.000	678.931	670.814	83.200	1237.466	-21.950
	4600	166.672	831.661	682.211	687.468	83.200	1270.601	-22.400
	4700	166.932	835.248	685.429	704.148	83.200	1303.702	-22.850
	4800	167.192	838.765	688.587	720.854	83.200	1336.770	-23.300
	4900	167.452	842.215	691.688	737.587	83.200	1369.806	-23.750
	5000	167.712	845.601	694.732	754.345	83.200	1402.810	-24.200
	5100	167.971	848.925	697.723	771.129	83.200	1435.785	-24.650
	5200	168.231	852.189	700.662	787.939	83.200	1468.730	-25.100
	5300	168.490	855.396	703.552	804.775	83.200	1501.647	-25.550
	5400	168.749	858.548	706.393	821.637	83.200	1534.538	-26.000
	5500	169.008	861.646	709.187	838.525	83.200	1567.401	-26.450
	5600	169.267	864.694	711.937	855.439	83.200	1600.240	-26.900
	5700	169.525	867.692	714.644	872.378	83.200	1633.055	-27.350
	5800	169.784	870.643	717.308	889.344	83.200	1665.846	-27.800
	5900	170.042	873.547	719.931	906.335	83.200	1698.615	-28.250
	6000	170.301	876.408	722.516	923.352	83.200	1731.361	-28.700

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1977 (1 bar)

Sulfur (S<sub>2</sub>)S<sub>T</sub>(g)

## IDEAL GAS

Sulfur (S<sub>2</sub>)

M<sub>r</sub> = 224.42

S<sup>c</sup>(298.15 K) = (407.7 ± 4) J·K<sup>-1</sup>·mol<sup>-1</sup>

ΔH<sup>c</sup>(298.15 K) = [113.7 ± 8] kJ·mol<sup>-1</sup>

## Enthalpy of Formation

The enthalpy of formation for each vapor phase sulfur species S<sub>2</sub> to S<sub>8</sub> is calculated by a third law using the thermal functions described below and assuming that the vapor pressure data given by Hultgren *et al.*<sup>1</sup> and Rau *et al.*<sup>2</sup> are correct. These values for the enthalpy of formation are dependent on the somewhat arbitrary thermal functions adopted for the polyatomic sulfur gases.

## Heat Capacity and Entropy

The thermal functions for the polyatomic species, S<sub>2</sub> to S<sub>8</sub>, are estimated following the suggestion of Rau *et al.*<sup>2</sup> Using thermal functions calculated for S(g), S<sub>2</sub>(g), and S<sub>8</sub>(g), the heat capacity values for the remaining species were calculated by Rau *et al.*<sup>2</sup> assuming that the vibrational heat capacity per degree of freedom is the same for all sulfur polyatomic species. The resulting heat capacity equations are given by Rau *et al.*<sup>2</sup>

The use of the procedure of Rau *et al.*<sup>2</sup> leads to a set of thermal functions and associated enthalpies of formation which reproduce the observed sulfur vapor pressure data. That is, the sum of the calculated partial pressures of all eight sulfur vapor species, S<sub>2</sub>(g) to S<sub>8</sub>(g), does closely reproduce the observed vapor pressure. [A difference between the calculated boiling point (at 1 atm) and the secondary reference temperature boiling point is due to the difference between the ideal gas calculation and the real observed value.]

The thermal functions for S<sub>2</sub>(g) were calculated<sup>3</sup> by adjusting the low valued vibrational frequencies such that S(298.15 K) and ΔH<sup>c</sup>(298.15 K) values could be found which reproduced the partial pressure of the octamer. The entropy of S<sub>2</sub>(g) is well-known,<sup>3</sup> being based on reliable data and sound statistical mechanical calculations.

The thermal functions which would result from the use of the available structural and vibrational information for the remaining polyatomic species, are biased in the same way as for S<sub>2</sub>(g). Some of the necessary information is derived from condensed phase spectra (rather than gas phase spectra). As with the octamer, the low-valued vibrational frequencies (and possibly the structure) may need to be adjusted. In any event, the use of the existing spectroscopic data (unaltered) leads to calculated entropies which are unreasonable when used in a 3rd law analysis to mesh in the vapor pressure with these thermal functions.

## References

- <sup>1</sup>R. Hultgren, P. D. Desai, *et al.*, "Selected Values of the Thermodynamic Properties of the Elements", American Society for Metals, Metals Park, Ohio, (1973).
- <sup>2</sup>H. Rau, R. N. Kuty and J. R. F. Guedes de Carvalho, *J. Chem. Thermodyn.* **5**, 833 (1973).
- <sup>3</sup>JANAF Thermochemical Tables: S<sub>2</sub>(g), 9-30-77.

Sulfur (S<sub>8</sub>)

M<sub>r</sub> = 256.48 Sulfur (S<sub>8</sub>)

IDEAL GAS

S<sub>8</sub>(g)

S°(298.15 K) = 430.31 ± 0.05 J·K<sup>-1</sup>·mol<sup>-1</sup>

Δ<sub>f</sub>H°(0 K) = 104.39 ± 0.63 kJ·mol<sup>-1</sup>  
 Δ<sub>f</sub>H°(298.15 K) = 100.42 ± 0.63 kJ·mol<sup>-1</sup>

Vibrational Frequencies and Degeneracies	
$\nu$ , cm <sup>-1</sup>	$\nu$ , cm <sup>-1</sup>
475(1)	243(1)
218(1)	437(2)
471(2)	56(2)
191(2)	411(1)

Ground State Quantum Weight: [1]  
 Point Group: D<sub>4h</sub>  
 Bond Distance: S-S = 2.059 ± 0.002 Å  
 Bond Angle S-S-S = 107.9 ± 0.6°  
 Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = 3.90326 × 10<sup>-111</sup> g<sup>3</sup>·cm<sup>6</sup>  
 σ = 8

Enthalpy of Formation

The vapor pressure of S(cr) has been measured by many investigators. Using the seven more recent vapor pressure data, the respective enthalpy of sublimation was calculated by both the 2nd and 3rd law methods. The values obtained are tabulated as follows:

Source	T/K	Δ <sub>sub</sub> H°(298.15), kcal·mol <sup>-1</sup>	
		3rd law	2nd law
West-Menzies <sup>1</sup>	376.6 - 448.8	24.29	21.29
Neumann <sup>2</sup>	312.6 - 362.1	24.35	26.47
Fouretier <sup>3</sup>	304.1 - 351.6	24.36	24.10
Taillade <sup>4</sup>	303.6 - 352.5	24.29	24.87
Bradley <sup>5</sup>	288.3 - 305.7	24.29	23.80
Magée <sup>6</sup>	331.9 - 368.0	24.11	24.44
	332.7 - 367.4	24.12	23.88
Briske <sup>7</sup>	273.2 - 313.2	24.28	24.00

Due to the presence of S<sub>8</sub>(g) in S<sub>8</sub>(l), the measured total pressures were corrected to give the partial pressures of S<sub>8</sub>(g) for the first five sets of vapor pressure data, according to Scott.<sup>8</sup> However, the magnitude of the correction is only 0.1-0.2 kcal·mol<sup>-1</sup>. The adopted value is the weighted average of both the 2nd and 3rd law values.

Heat Capacity and Entropy

The vibrational frequencies were taken from Scott *et al.*<sup>9</sup> Four of the eighteen frequencies, i.e. 86(2) and 218(2) cm<sup>-1</sup>, were changed to 56(2) and 248(2) cm<sup>-1</sup>, respectively, as suggested by Scott.<sup>10</sup> The molecular structure and bond distance and angle were reported by Donohur *et al.*<sup>11</sup> The principle moments of inertia are: I<sub>A</sub> = I<sub>B</sub> = 1.28594 × 10<sup>-37</sup>, and I<sub>C</sub> = 2.36042 × 10<sup>-37</sup> g·cm<sup>2</sup>.

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T/K	C <sub>p</sub> J·K <sup>-1</sup> ·mol <sup>-1</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>r</sub>
		S° - [G° - H°(T <sub>r</sub> )]/T J·K <sup>-1</sup> ·mol <sup>-1</sup>	H° - H°(T <sub>r</sub> ) kJ·mol <sup>-1</sup>	Δ <sub>f</sub> H° kJ·mol <sup>-1</sup>	Δ <sub>f</sub> G° kJ·mol <sup>-1</sup>	
0	0	0	0	0	0	0
100	87.155	722.516	-31.324	104.388	104.388	-44.377
200	134.162	522.031	-25.698	104.495	104.495	-17.258
250	147.427	372.007	-14.381	102.677	102.677	-11.920
298.15	156.043	430.311	-7.319	101.582	101.582	-8.511
300	156.314	430.311	0	100.416	100.416	-8.511
350	162.400	431.277	0.289	100.369	100.369	-8.402
400	166.689	432.241	8.266	99.016	99.016	-8.071
450	169.799	436.591	16.499	79.803	79.803	-4.179
500	172.113	447.662	24.915	72.816	72.816	-3.062
600	175.248	474.358	33.466	65.345	65.345	-2.260
700	177.206	517.531	50.847	54.048	54.048	-1.220
800	178.306	598.284	86.477	44.903	44.903	-0.603
900	179.411	619.364	104.165	37.003	37.003	-0.220
1000	180.064	638.302	122.140	30.265	30.265	-0.079
1100	180.552	655.488	140.172	24.500	24.500	-0.026
1200	180.925	671.215	158.247	19.859	19.859	-0.011
1300	181.216	685.709	176.355	15.939	15.939	-0.006
1400	181.448	699.147	194.488	12.510	12.510	-0.003
1500	181.636	711.672	212.643	8.922	8.922	-0.001
1600	181.790	723.400	230.814	4.722	4.722	0.000
1700	181.918	734.425	249.000	0.318	0.318	0.000
1800	182.025	744.826	267.197	-3.722	-3.722	0.000
1900	182.116	754.670	285.404	-7.787	-7.787	0.000
2000	182.194	764.013	303.620	-11.657	-11.657	0.000
2100	182.261	772.904	321.843	-15.248	-15.248	0.000
2200	182.319	781.384	340.072	-18.579	-18.579	0.000
2300	182.370	789.490	358.306	-21.667	-21.667	0.000
2400	182.414	797.253	376.546	-24.521	-24.521	0.000
2500	182.453	804.789	394.789	-27.152	-27.152	0.000
2600	182.488	811.857	413.036	-29.572	-29.572	0.000
2700	182.519	818.744	431.287	-31.798	-31.798	0.000
2800	182.547	825.383	449.540	-33.833	-33.833	0.000
2900	182.572	831.789	467.796	-35.681	-35.681	0.000
3000	182.595	837.979	486.054	-37.351	-37.351	0.000
3100	182.615	843.966	504.315	-38.762	-38.762	0.000
3200	182.634	849.764	522.577	-39.934	-39.934	0.000
3300	182.651	855.385	540.841	-40.888	-40.888	0.000
3400	182.666	860.838	559.107	-41.637	-41.637	0.000
3500	182.680	866.133	577.375	-42.197	-42.197	0.000
3600	182.693	871.279	595.643	-42.584	-42.584	0.000
3700	182.705	876.285	613.913	-42.722	-42.722	0.000
3800	182.716	881.158	632.184	-42.738	-42.738	0.000
3900	182.726	885.904	650.456	-42.638	-42.638	0.000
4000	182.736	890.530	668.729	-42.434	-42.434	0.000
4100	182.744	895.042	687.003	-42.137	-42.137	0.000
4200	182.752	899.446	705.278	-41.751	-41.751	0.000
4300	182.760	903.747	723.554	-41.288	-41.288	0.000
4400	182.767	907.948	741.830	-40.759	-40.759	0.000
4500	182.774	912.056	760.107	-40.166	-40.166	0.000
4600	182.780	916.073	778.385	-39.521	-39.521	0.000
4700	182.786	920.004	796.663	-38.834	-38.834	0.000
4800	182.791	923.852	814.942	-38.114	-38.114	0.000
4900	182.796	927.621	833.221	-37.371	-37.371	0.000
5000	182.801	931.314	851.501	-36.614	-36.614	0.000
5100	182.805	934.934	869.782	-35.842	-35.842	0.000
5200	182.808	938.484	888.062	-35.056	-35.056	0.000
5300	182.811	941.966	906.343	-34.256	-34.256	0.000
5400	182.817	945.383	924.625	-33.442	-33.442	0.000
5500	182.821	948.738	942.907	-32.614	-32.614	0.000
5600	182.824	952.032	961.189	-31.772	-31.772	0.000
5700	182.828	955.268	979.472	-30.917	-30.917	0.000
5800	182.831	958.448	997.755	-30.049	-30.049	0.000
5900	182.834	961.573	1016.038	-29.168	-29.168	0.000
6000	182.836	964.646	1034.321	-28.275	-28.275	0.000

PREVIOUS: September 1977 (1 atm) CURRENT: September 1977 (0.1 MPa)

Sulfur (S<sub>8</sub>)

S<sub>8</sub>(g)