

## Sulfur (S)

## REFERENCE STATE

 $A_r = 32.06$  Sulfur (S) $S_1(\text{ref})$ 

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  $S_8(\text{g})$ ,  $S_7(\text{g})$ , and  $S_6(\text{g})$ . In our reference state for sulfur, we have arbitrarily chosen  $0.5 S_2(\text{g})$  to be the gas phase species.

T/K	Enthalpy Reference Temperature = $T_r = 298.15$ K				Standard State Pressure = $p^\circ = 0.1$ MPa			
	$C_p^\circ$	$S^\circ$	$-[G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$	
0	0.	0.	INFINITE	-4 412	0.	0.	0.	
100	12.770	12.522	49.744	-3.722	0.	0.	0.	
200	19.368	23.637	34.038	-2.080	0.	0.	0.	
298.15	22.698	32.056	32.056	0.	0.	0.	0.	
300	22.744	32.196	32.056	0.042	0.	0.	0.	
368.300	24.246	37.015	32.540	1.648	ALPHA <--> BETA			
368.300	24.773	38.103	32.540	2.049	TRANSITION			
388.360	25.167	39.427	32.861	2.550	BETA <--> LIQUID			
388.360	31.058	43.859	32.861	4.271	TRANSITION			
400	32.162	44.793	33.195	4.639	0.	0.	0.	
432.020	53.808	47.431	34.151	5.737	$C_p$ LAMBDA MAXIMUM			
432.020	53.806	47.431	34.151	5.737	TRANSITION			
500	37.986	53.532	36.398	8.567	0.	0.	0.	
600	34.308	60.078	39.825	12.152	0.	0.	0.	
700	32.681	65.241	43.099	15.499	0.	0.	0.	
800	31.699	69.530	46.143	18.710	0.	0.	0.	
882.117	31.665	72.624	48.467	21.310	LIQUID <--> IDEAL GAS			
882.117	18.454	133.077	48.467	74.636	FUGACITY = 1 bar			
900	18.483	133.448	50.152	74.967	0.	0.	0.	
1000	18.638	135.403	58.581	76.823	0.	0.	0.	
1100	18.792	137.187	65.647	78.694	0.	0.	0.	
1200	18.947	138.829	71.678	80.581	0.	0.	0.	
1300	19.103	140.352	76.903	82.484	0.	0.	0.	
1400	19.257	141.773	81.486	84.402	0.	0.	0.	
1500	19.409	143.107	85.550	86.335	0.	0.	0.	
1600	19.556	144.364	89.187	88.283	0.	0.	0.	
1700	19.697	145.554	92.468	90.246	0.	0.	0.	
1800	19.830	146.684	95.449	92.223	0.	0.	0.	
1900	19.956	147.759	98.174	94.212	0.	0.	0.	
2000	20.072	148.786	100.679	96.213	0.	0.	0.	
2100	20.176	149.768	102.993	98.226	0.	0.	0.	
2200	20.274	150.708	105.141	100.248	0.	0.	0.	
2300	20.364	151.612	107.142	102.280	0.	0.	0.	
2400	20.448	152.480	109.013	104.321	0.	0.	0.	
2500	20.526	153.316	110.769	106.370	0.	0.	0.	
2600	20.589	154.123	112.421	108.426	0.	0.	0.	
2700	20.650	154.901	113.980	110.488	0.	0.	0.	
2800	20.707	155.653	115.455	112.555	0.	0.	0.	
2900	20.762	156.381	116.853	114.629	0.	0.	0.	
3000	20.813	157.085	118.183	116.708	0.	0.	0.	
3100	20.855	157.768	119.449	118.791	0.	0.	0.	
3200	20.898	158.431	120.657	120.879	0.	0.	0.	
3300	20.940	159.075	121.811	122.971	0.	0.	0.	
3400	20.983	159.701	122.916	125.067	0.	0.	0.	
3500	21.025	160.310	123.976	127.167	0.	0.	0.	
3600	21.065	160.902	124.994	129.272	0.	0.	0.	
3700	21.106	161.480	125.972	131.380	0.	0.	0.	
3800	21.149	162.044	126.914	133.493	0.	0.	0.	
3900	21.194	162.594	127.822	135.610	0.	0.	0.	
4000	21.240	163.131	128.698	137.732	0.	0.	0.	
4200	21.337	164.169	130.362	141.989	0.	0.	0.	
4400	21.443	165.164	131.922	146.267	0.	0.	0.	
4600	21.558	166.120	133.388	150.567	0.	0.	0.	
4800	21.680	167.040	134.771	154.891	0.	0.	0.	
5000	21.810	167.928	136.080	159.240	0.	0.	0.	
5200	21.948	168.786	137.321	163.615	0.	0.	0.	
5400	22.090	169.617	138.502	168.019	0.	0.	0.	
5600	22.236	170.423	139.628	172.452	0.	0.	0.	
5800	22.385	171.206	140.703	176.914	0.	0.	0.	
6000	22.538	171.967	141.733	181.406	0.	0.	0.	

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1977 (1 bar)

## Sulfur, Monoclinic (S)

CRYSTAL( $\beta$ ) $A_r = 32.06$  Sulfur, Monoclinic (S) $S_1(\text{cr})$ 

$S^\circ(298.15 \text{ K}) = 33.028 \pm 0.050 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{tr}} = 368.3 \pm 0.3 \text{ K}$  ( $\alpha$ - $\beta$ )  
 $T_{\text{fm}} = 388.36 \pm 0.1 \text{ K}$  ( $\beta$ -l)

## Enthalpy of Formation

The enthalpy formation of monoclinic sulfur at 298.15 K is calculated from that of orthorhombic sulfur by adding  $\Delta_{\text{tr}}H^\circ$  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 ( $\beta$ ) 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  $T_{\text{fm}} = 388.36 \text{ K}$  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  $S^\circ(\text{S, cr, } \beta, T) = S^\circ(\text{S, cr, } \alpha, T) + \Delta_{\text{tr}}H^\circ/T_{\text{tr}}$ . 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:  $T_{\text{fm}} = 388.36 \pm 0.02 \text{ K}$  and  $\Delta_{\text{fm}}H^\circ = 0.4128 \pm 0.0006 \text{ kcal}\cdot\text{mol}^{-1}$ . The only other precise study reported in the literature is that of West<sup>2</sup> who obtained  $\Delta_{\text{fm}}H^\circ = 0.41051 \pm 0.0005 \text{ kcal}\cdot\text{mol}^{-1}$  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,  $\alpha$ ), 9-30-77.
- <sup>6</sup>B. Meyer, *Chem. Rev.* **76**, 367 (1976).
- <sup>7</sup>R. L. Montgomery, *Science* **184**, 562 (1974).

$\Delta_f H^\circ(0 \text{ K}) = 0.247 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15 \text{ K}) = 0.360 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{tr}} H^\circ = 0.4004 \pm 0.0029 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{fm}} H^\circ = 1.721 \pm 0.008 \text{ kJ}\cdot\text{mol}^{-1}$

T/K	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$			Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$			log $K_f$
	$C_p^\circ$	$S^\circ$	$-[G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.	0.	INFINITE	-4.525	0.247	0.247	INFINITE
100	12.874	12.964	51.217	-3.825	0.257	0.213	-0.111
198.300	21.966	24.242	35.146	-2.162	C <sub>p</sub> LAMBDA MAXIMUM	TRANSITION	
198.300	21.966	24.242	35.146	-2.162			
200	20.154	24.421	35.054	-2.127	0.313	0.157	-0.041
250	21.736	29.066	33.402	-1.084	0.336	0.115	-0.024
298.15	23.225	33.028	33.028	0.	0.360	0.070	-0.012
300	23.276	33.172	33.028	0.043	0.361	0.068	-0.012
350	24.414	36.849	33.316	1.237	0.388	0.017	-0.003
368.300	24.773	38.103	33.523	1.687	---- ALPHA <--> BETA ----		
388.360	25.167	39.427	33.794	2.188	---- BETA <--> LIQUID ----		
400	25.397	40.173	33.969	2.482	-1.797	0.050	-0.007
450	26.380	43.222	34.830	3.776	-2.428	0.310	-0.036
500	27.363	46.052	35.812	5.120	-3.087	0.653	-0.068
600	29.330	51.215	37.957	7.955	-3.838	1.481	-0.129
700	31.296	55.884	40.189	10.986	-4.153	2.397	-0.179
800	33.263	60.191	42.424	14.214	-4.136	3.335	-0.218

PREVIOUS:

CURRENT: September 1977

## Sulfur, Orthorhombic (S)

CRYSTAL( $\alpha$ ) $A_r = 32.06$  Sulfur, Orthorhombic (S) $S_1(\text{cr})$ 

$S^\circ(298.15 \text{ K}) = 32.056 \pm 0.050 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_m = 368.3 \pm 0.3 \text{ K} (\alpha\text{-}\beta)$

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

## Enthalpy of Formation

Zero by definition.

## Heat Capacity and Entropy

Experimentally determined heat capacity values for orthorhombic ( $\alpha$ ) sulfur have been reported by Nernst,<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  $S^\circ(298.15 \text{ K})$  and  $H^\circ(298.15 \text{ K}) - H^\circ(0 \text{ K})$  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  $S^\circ(10) = 0.036 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  and integrating the heat capacity values, we calculate  $S^\circ(298.15 \text{ K}) = 7.661 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , in agreement with CODATA<sup>9</sup>. The heat capacity values above  $T_m = 368.3 \text{ K}$  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 ( $\alpha\text{-}\beta$ ) 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:  $T_m = 368.3 \pm 0.3 \text{ K}$  and  $\Delta_{\text{cr}} H^\circ = 0.0957 \pm 0.0007 \text{ kcal}\cdot\text{mol}^{-1}$ . The only other precise study reported in the literature is that of West<sup>3</sup> who obtained  $\Delta_{\text{cr}} H^\circ = 0.0960 \pm 0.0005 \text{ kcal}\cdot\text{mol}^{-1}$  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  $\pm 5 \text{ cal}\cdot\text{mol}^{-1}$  or greater.

## Sublimation Data

Since the reference state of sulfur involves 0.5  $S_2(\text{g})$  rather than  $S(\text{g})$ , we define the enthalpy of sublimation (at 298.15 K) of orthorhombic sulfur as the process  $S(\text{cr}, \alpha) = 0.5 S_2(\text{g})$ . Thus the enthalpy of sublimation of orthorhombic sulfur is one-half the enthalpy of formation of  $S_2(\text{g})$ . Since the dominant gaseous sulfur species at room temperature is actually  $S_2(\text{g})$ , the enthalpy of sublimation to the equilibrium gas is significantly smaller.

## References

- W. Nernst, Ann. Physik. 36, 395 (1911).
- E. D. Eastman and W. C. McGavock, J. Am. Chem. Soc. 59, 145 (1937).
- E. D. West, J. Am. Chem. Soc. 81, 29 (1959).
- A. K. Mal'tsev and A. F. Demidenko, Tr. Mosk. Khim.-Tekhnol. Inst., No. 51, 136 (1967).
- H. L. Finke, U. S. Bureau of Mines, Unpublished Work, Quoted in reference.<sup>3</sup>
- R. L. Montgomery, Ph.D. Dissertation, Oklahoma State University, (1976).
- I. E. Paukov, to be published, 1977; mentioned in reference.<sup>9</sup>
- R. Hultgren *et al.*, "Selected Values of the Thermodynamic Properties of the Elements," American Society for Metals, Metals Park, Ohio, (1973).
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- J. N. Bronsted, Z. Physik. Chem. 55, 371 (1906).
- M. Thackray, Nature 203, 1278 (1964); J. Chem. Eng. Data 15, 495 (1970).
- K. Neumann, Z. Physik. Chem. A171, 416 (1934).

T/K	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$			Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ $\text{kJ}\cdot\text{mol}^{-1}$			
	$C_p^\circ$	$S^\circ$	$-[G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_r G^\circ$	$\log K_r$
0	0.	0.	INFINITE	-4.412	0.	0.	0.
100	12.770	12.522	49.744	-3.722	0.	0.	0.
200	19.368	23.637	34.038	-2.080	0.	0.	0.
250	21.297	28.179	32.422	-1.061	0.	0.	0.
298.15	22.698	32.056	32.056	0.	0.	0.	0.
300	22.744	32.196	32.056	0.042	0.	0.	0.
350	23.870	35.789	32.337	1.208	0.	0.	0.
368.300	24.246	37.015	32.540	1.648	----	ALPHA <--> BETA	----
400	24.895	39.044	32.975	2.427	-2.212	0.088	-0.011
450	25.920	42.035	33.818	3.698	-2.867	0.406	-0.047
500	26.945	44.819	34.780	5.019	-3.548	0.809	-0.084
600	28.995	49.913	36.886	7.816	-4.336	1.764	-0.154
700	31.045	54.537	39.082	10.818	-4.680	2.812	-0.210
800	33.095	58.816	41.284	14.025	-4.685	3.887	-0.254

PREVIOUS: December 1965

CURRENT: September 1977

## Sulfur (S)

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

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

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

## Enthalpy of Formation

The enthalpy of formation of liquid sulfur at 298.15 K is calculated from that of monoclinic sulfur by adding  $\Delta_{\text{tr}}H^{\circ}$  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  $432.02 \pm 0.20 \text{ K}^1$  and  $432.25 \pm 0.30 \text{ K}$ ;<sup>2</sup> this has been attributed to the depolymerization of  $S_8$  molecules.<sup>3</sup> We adopt the tabulated heat capacity values of Montgomery<sup>1</sup> up to 434 K and those of West<sup>2</sup> above 434 K. The heat capacity is assumed to be constant at  $7.568 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  above 810 K. Below  $T_m = 388.36 \text{ K}$ , the heat capacity values are obtained by linear extrapolation using the slope of the values in the region  $T_m$  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,  $T_{\text{vap}}(1 \text{ atm}) = 717.834 \text{ K}$  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:  $S_2(\text{g})$  and  $S(\text{g})$  predominate above 1000 K while  $S_6(\text{g})$ ,  $S_7(\text{g})$  and  $S_8(\text{g})$  dominate at  $T_{\text{vap}}$ .

Since our reference state for sulfur is arbitrarily defined to involve  $0.5 S_2(\text{g})$  as the vapor species, we calculate the arbitrary normal boiling point,  $T_{\text{vap}}(1 \text{ bar})$ , for the process  $S(\text{l}) = 0.5 S_2(\text{g})$ . The brackets are used to indicate the arbitrary nature of this value. Since we only consider  $S_2(\text{g})$  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).

## LIQUID

 $A_r = 32.06$  Sulfur (S)

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

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

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

T/K	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$			Standard State Pressure = $p^{\circ} = 0.1 \text{ MPa}$			
	$C_p^{\circ}$	$S^{\circ}$	$-[G^{\circ} - H^{\circ}(T_r)]/T$	$H^{\circ} - H^{\circ}(T_r)$	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	$\log K_r$
0							
100							
200							
250							
298.15	22.531	36.825	36.825	0.	1.854	0.432	-0.076
300	22.707	36.965	36.826	0.042	1.854	0.423	-0.074
350	27.434	40.821	37.120	1.295	1.941	0.180	-0.027
388.360	31.058	43.859	37.635	2.417	-----	BETA <---> LIQUID	-----
400	32.162	44.793	37.829	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.	0.
500	37.986	53.532	40.106	6.713	0.	0.	0.
600	34.308	60.078	42.915	10.298	0.	0.	0.
700	32.681	65.241	45.748	13.645	0.	0.	0.
800	31.699	69.530	48.460	16.856	0.	0.	0.
882.117	31.665	72.624	50.568	19.456	-----	FUGACITY = 1 bar	-----
900	31.665	73.260	51.012	20.023	-53.090	1.079	-0.063
1000	31.665	76.596	53.407	23.189	-51.780	7.028	-0.367
1100	31.665	79.614	55.654	26.356	-50.485	12.846	-0.610
1200	31.665	82.369	57.767	29.522	-49.205	18.546	-0.807
1300	31.665	84.904	59.758	32.689	-47.941	24.141	-0.970
1400	31.665	87.250	61.639	35.855	-46.693	29.639	-1.106
1500	31.665	89.435	63.420	39.021	-45.460	35.048	-1.220

PREVIOUS: December 1965

CURRENT: September 1977

## Sulfur (S)

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

Sulfur (S)

CRYSTAL( $\alpha$ - $\beta$ )-LIQUID $A_r = 32.06$  Sulfur (S) $S_1(\text{cr,l})$ 

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.

T/K	Enthalpy Reference Temperature = $T_r = 298.15$ K			Standard State Pressure = $p^\circ = 0.1$ MPa			
	$C_p^\circ$	$S^\circ$	$-(G^\circ - H^\circ(T_r))/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
	J·K <sup>-1</sup> ·mol <sup>-1</sup>			kJ·mol <sup>-1</sup>			
0	0.	0.	INFINITE	-4.412	0.	0.	0.
100	12.770	12.522	49.744	-3.722	0.	0.	0.
200	19.368	23.637	34.038	-2.080	0.	0.	0.
250	21.297	28.179	32.422	-1.061	0.	0.	0.
298.15	22.698	32.056	32.056	0.	0.	0.	0.
300	22.744	32.196	32.056	0.042	0.	0.	0.
350	23.870	35.789	32.337	1.208	0.	0.	0.
368.300	24.246	37.015	32.540	1.648	ALPHA <- -> BETA TRANSITION		
368.300	24.773	38.103	32.540	2.049			
388.360	25.167	39.427	32.861	2.550	BETA <- -> LIQUID TRANSITION		
388.360	31.062	43.859	32.861	4.271			
400	32.162	44.793	33.195	4.639	0.	0.	0.
432.020	53.808	47.431	34.151	5.737	C <sub>2</sub> LAMBDA MAXIMUM TRANSITION		
432.020	53.806	47.431	34.151	5.737			
450	43.046	49.308	34.720	6.564	0.	0.	0.
500	37.986	53.532	36.398	8.567	0.	0.	0.
600	34.308	60.078	39.825	12.152	0.	0.	0.
700	32.681	65.241	43.099	15.499	0.	0.	0.
800	31.699	69.530	46.143	18.710	0.	0.	0.
882.117	31.665	72.624	48.467	21.310	----- FUGACITY = 1 bar -----		
900	31.665	73.260	48.952	21.877	-53.090	1.079	-0.063
1000	31.665	76.596	51.553	25.043	-51.780	7.028	-0.367
1100	31.665	79.614	53.969	28.209	-50.485	12.846	-0.610
1200	31.665	82.369	56.222	31.376	-49.205	18.546	-0.807
1300	31.665	84.904	58.332	34.542	-47.941	24.141	-0.970
1400	31.665	87.250	60.315	37.709	-46.693	29.639	-1.106
1500	31.665	89.435	62.185	40.875	-45.460	35.048	-1.220

PREVIOUS:

CURRENT: September 1977

Sulfur (S)

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

## Sulfur (S)

## IDEAL GAS

A<sub>r</sub> = 32.06 Sulfur (S)S<sub>2</sub>(g)

IP(S, g) = 83558.0 ± 1 cm<sup>-1</sup>  
 S°(298.15 K) = 167.828 ± 0.035 J·K<sup>-1</sup>·mol<sup>-1</sup>

Δ<sub>f</sub>H°(0 K) = 274.73 ± 0.25 kJ·mol<sup>-1</sup>  
 Δ<sub>f</sub>H°(298.15 K) = 276.98 ± 0.25 kJ·mol<sup>-1</sup>

Electronic Levels and Quantum Weights		
State	ε, cm <sup>-1</sup>	g <sub>r</sub>
<sup>3</sup> P <sub>2</sub>	0.00	5
<sup>3</sup> P <sub>1</sub>	396.09	3
<sup>3</sup> P <sub>0</sub>	573.65	1
<sup>1</sup> D <sub>2</sub>	9238.58	5
<sup>1</sup> S <sub>0</sub>	22179.99	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 Δ<sub>f</sub>H°(S, g, 298.15 K) is calculated using D<sub>0</sub>(S<sub>2</sub>) = 35216.4 ± 2.5 cm<sup>-1</sup> (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>4,5</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 (ε < 23000 cm<sup>-1</sup>). The reported uncertainty is S°(298.15 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 ~0.4 J·K<sup>-1</sup>·mol<sup>-1</sup> 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>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>f</sub> H°	Δ <sub>f</sub> G°	log K <sub>r</sub>
0	0	0	INFINITE	-6.657	274.735	274.735	INFINITE
100	21.356	142.891	188.580	-4.569	276.133	263.096	-137.427
200	23.388	158.392	169.994	-2.320	276.740	249.789	-65.238
250	23.696	163.653	168.218	-1.141	276.899	243.031	-50.779
298.15	23.673	167.828	167.828	0	276.980	236.500	-41.434
300	23.669	167.974	167.828	0.044	276.982	236.248	-41.135
350	23.480	171.610	168.116	1.223	276.995	229.458	-34.245
400	23.233	174.729	168.752	2.391	274.732	222.757	-29.089
450	22.979	177.451	169.571	3.546	273.962	216.297	-25.107
500	22.741	179.859	170.481	4.689	273.102	209.938	-21.932
600	22.338	183.968	172.398	6.942	271.770	197.436	-17.188
700	22.031	187.388	174.302	9.160	270.641	185.138	-13.815
800	21.800	190.314	176.125	11.351	269.621	172.994	-11.295
900	21.624	192.871	177.847	13.522	215.535	162.055	-9.405
1000	21.489	195.142	179.465	15.677	215.834	156.096	-8.154
1100	21.386	197.185	180.984	17.821	216.106	150.109	-7.128
1200	21.307	199.042	182.413	19.955	216.354	144.098	-6.272
1300	21.249	200.745	183.758	22.083	216.579	138.067	-5.548
1400	21.209	202.318	185.029	24.205	216.784	132.020	-4.926
1500	21.186	203.781	186.231	26.325	216.970	125.959	-4.386
1600	21.178	205.148	187.371	28.443	217.140	119.886	-3.914
1700	21.184	206.432	188.455	30.561	217.295	113.803	-3.497
1800	21.203	207.643	189.487	32.680	217.438	107.711	-3.126
1900	21.234	208.790	190.473	34.802	217.570	101.611	-2.793
2000	21.276	209.880	191.417	36.927	217.694	95.505	-2.494
2100	21.327	210.920	192.321	39.058	217.812	89.392	-2.224
2200	21.386	211.913	193.189	41.193	217.925	83.275	-1.977
2300	21.452	212.865	194.024	43.335	218.035	77.152	-1.752
2400	21.523	213.780	194.828	45.484	218.143	71.024	-1.546
2500	21.598	214.660	195.604	47.640	218.250	64.892	-1.356
2600	21.676	215.508	196.353	49.803	218.358	58.755	-1.180
2700	21.756	216.328	197.078	51.975	218.467	52.615	-1.018
2800	21.837	217.121	197.780	54.155	218.579	46.470	-0.867
2900	21.919	217.888	198.460	56.343	218.694	40.321	-0.726
3000	21.999	218.633	199.120	58.538	218.811	34.169	-0.595
3100	22.078	219.355	199.761	60.742	218.931	28.012	-0.472
3200	22.155	220.058	200.384	62.954	219.055	21.851	-0.357
3300	22.230	220.740	200.991	65.173	219.183	15.687	-0.248
3400	22.303	221.405	201.582	67.400	219.313	9.518	-0.146
3500	22.372	222.053	202.157	69.634	219.447	3.346	-0.050
3600	22.439	222.684	202.719	71.874	219.583	-2.830	0.041
3700	22.502	223.300	203.267	74.121	219.721	-9.011	0.127
3800	22.561	223.900	203.802	76.375	219.862	-15.194	0.209
3900	22.618	224.487	204.325	78.634	220.003	-21.382	0.286
4000	22.670	225.061	204.836	80.898	220.146	-27.573	0.360
4100	22.720	225.621	205.336	83.167	220.289	-33.768	0.430
4200	22.766	226.169	205.826	85.442	220.432	-39.966	0.497
4300	22.808	226.705	206.305	87.720	220.575	-46.168	0.561
4400	22.847	227.230	206.775	90.003	220.716	-52.373	0.622
4500	22.884	227.744	207.235	92.290	220.856	-58.581	0.680
4600	22.917	228.247	207.686	94.580	220.993	-64.792	0.736
4700	22.947	228.740	208.129	96.873	221.127	-71.006	0.789
4800	22.974	229.224	208.563	99.169	221.258	-77.223	0.840
4900	22.999	229.698	208.990	101.468	221.386	-83.443	0.890
5000	23.021	230.163	209.409	103.769	221.509	-89.665	0.937
5100	23.040	230.619	209.820	106.072	221.628	-95.890	0.982
5200	23.057	231.066	210.224	108.377	221.741	-102.117	1.026
5300	23.072	231.505	210.622	110.683	221.849	-108.346	1.068
5400	23.085	231.937	211.013	112.991	221.952	-114.577	1.108
5500	23.096	232.361	211.397	115.300	222.048	-120.810	1.147
5600	23.105	232.777	211.775	117.610	222.138	-127.044	1.185
5700	23.112	233.186	212.147	119.921	222.222	-133.281	1.221
5800	23.117	233.588	212.513	122.232	222.299	-139.518	1.256
5900	23.121	233.983	212.874	124.544	222.368	-145.757	1.290
6000	23.124	234.372	213.229	126.857	222.431	-151.997	1.323

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1982 (1 bar)