

Sulfur (S)

A_r = 32.06 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 S₂(g), S₄(g), and S₈(g). In our reference state for sulfur, we have arbitrarily chosen 0.5 S₂(g) to be the gas phase species.

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p	S° - (C _p - RT _r)/T	H° - H°(T _r)	Δ _r H°	
0	0.	0.	INFINITE	0.	0.
100	12.770	12.522	49.744	0.	0.
200	19.368	23.637	34.038	-2.080	0.
298.15	22.698	32.056	32.056	0.	0.
300	22.744	32.196	32.056	0.042	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.
432.020	53.808	47.431	34.151	5.737	C ₂ LAMBDA MAXIMUM
432.020	53.806	47.431	34.151	5.737	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
882.117	18.454	133.077	48.467	74.636	FUGACITY = 1 bar
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)

S₁(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),¹ West (368–388 K),² and Montgomery (12.41–386.83 K).³ The thermochemical functions tabulated by Hultgren *et al.*⁴ are based on work of Eastman and McGavock¹ and West.²

We adopt the heat capacity values tabulated (in 10 K increments) by Montgomery.³ The heat capacity values above $T_m = 388.36 \text{ K}$ are obtained by linear extrapolation of the tabulated heat capacity values³ 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,⁵ 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 α-β transition at 368.3 K is discussed on the orthorhombic sulfur table.⁵ The heat capacity data of Montgomery³ did not support the transition at 374 K reported by West.²

Montgomery³ reported a λ 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.⁷

Fusion Data

The melting of sulfur has been studied by many workers. An excellent review by Meyer⁶ summarizes these studies. In addition, Hultgren *et al.*⁴ tabulated numerous enthalpy of melting determinations. We adopt the results obtained by Montgomery³ 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 West² who obtained $\Delta_{\text{fus}}H^{\circ} = 0.41051 \pm 0.0005 \text{ kcal} \cdot \text{mol}^{-1}$ by adiabatic calorimetry.

References

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

Sulfur, Monoclinic (S)

S₁(cr)

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p ^o	S° - [C _p - H(T _r)]/T _r	H° - H(T _r)	Δ _r 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)

S₁(cr)

S₁(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 _r = 298.15 K		Standard State Pressure - P° = 0.1 MPa		log K _t
	C _p ^o	S° - (G° - H°(T _r))/T	H° - H°(T _r)	Δ _r 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	-2.212	-0.011
500	26.945	44.035	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,¹ 23–202 K), Eastman and McGavock,² 12.68–365.60 K), West,³ 2981–368 K), Mal'tsev and Demidenko,⁴ 53–305 K), Finke,⁵ 12–432 K), Montgomery,⁶ 12.34–360.99 K), and Paukov.⁷ The thermochemical functions tabulated by Hultgren *et al.*⁸ are based primarily on the work of Eastman and McGavock² and unpublished work of Finke,⁵ the latter presumably being the preliminary results of Montgomery.⁶ The tentative values reported by CODATA⁹ for S°(298.15 K) and H°(298.15 K) - H°(0 K) are based on Eastman and McGavock,² Montgomery,⁶ and Paukov.⁷ We adopt the heat capacity values tabulated (in 10 K increments) by Montgomery,⁶ Using S°(10) = 0.036 cal·K⁻¹·mol⁻¹, and integrating the heat capacity values, we calculate S°(298.15 K) = 7.661 cal·K⁻¹·mol⁻¹, in agreement with CODATA.⁹ The heat capacity values above T_m = 368.3 K are obtained by linear extrapolation of the tabulated values⁶ above 340 K.

The various heat capacity studies are in reasonably good agreement. The values recommended by Eastman and McGavock,² West,³ and Mal'tsev and Demidenko⁴ agree with Montgomery⁶ to within 0.5% except for the ranges 15–50 K² and 53–80 K.³ The smoothed value at 190 K reported by Mal'tsev and Demidenko⁴ is undoubtedly a typographical error. The selected values of Hultgren *et al.*⁸ agree within 0.5% with the data of Montgomery⁶ except below 35 K.

Fusion Data

The orthorhombic-monoclinic (α-β) phase change has been studied by many workers. An excellent review by Meyer¹⁰ summarizes these studies. We adopt the results obtained by Montgomery⁶ via adiabatic calorimetry: T_m = 368.3 ± 0.3 K and Δ_mH° = 0.0957 ± 0.0007 kcal·mol⁻¹. The only other precise study reported in the literature is that of West³ who obtained Δ_mH° = 0.0960 ± 0.0005 kcal·mol⁻¹ by adiabatic calorimetry. Other drop calorimetric^{11,12} and vapor pressure^{13,14} studies are much less precise with an uncertainty of ± 5 cal·mol⁻¹ or greater.

Sublimation Data

Since the reference state of sulfur involves 0.5 S₂(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 S₂(g). Thus the enthalpy of sublimation of orthorhombic sulfur is one-half the enthalpy of formation of S₂(g). Since the dominant gaseous sulfur species at room temperature is actually S₂(g), the enthalpy of sublimation to the equilibrium gas is significantly smaller.

References

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

PREVIOUS: December 1965

CURRENT: September 1977

Sulfur, Orthorhombic (S)

S₁(cr)

Sulfur (S) S₁(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,⁴ 05.79–433.31 K) and West (373–678 K).² 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;² this has been attributed to the depolymerization of S₈ molecules.³ We adopt the tabulated heat capacity values of Montgomery⁴ up to 434 K and those of West² above 434 K. The heat capacity is assumed to be constant at 7.568 cal·K⁻¹·mol⁻¹ above 810 K. Below T_m = 388.36 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_{vap}(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: S₂(g) and S₈(g) predominate above 1000 K while S₆(g), S₇(g) and S₄(g) dominate at T_{vap}.

Since our reference state for sulfur is arbitrarily defined to involve 0.5 S₂(g) as the vapor species, we calculate the arbitrary normal boiling point, T_{vap}(1 bar), for the process S(l) = 0.5 S₂(g). The brackets are used to indicate the arbitrary nature of this value. Since we only consider S₂(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

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

T/K	C _p ^a	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p ^o = 0.1 MPa		log K _r
		S ^b - [G ^c - H ^d (T _r)]/T	H ^e - H ^d (T _r)	Δ _{sub} H ^o	Δ _{liq} H ^o	
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 _p 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)

S₁(l)

Sulfur (S)

$A_r = 32.06$ Sulfur (S)

CRYSTAL(α - β)-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°	$S^\circ - [C_p^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f G^\circ$
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 \leftarrow \rightarrow BETA TRANSITION
368.300	24.773	38.103	2.049	
388.360	25.167	39.427	2.550	BETA \leftarrow \rightarrow 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	63.241	13.499	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⁻¹ $\Delta_f H^\circ(0 \text{ K}) = 274.73 \pm 0.25 \text{ kJ} \cdot \text{mol}^{-1}$ $\Delta_f H^\circ(298.15 \text{ K}) = 276.98 \pm 0.25 \text{ kJ} \cdot \text{mol}^{-1}$ $\Delta_f G^\circ(298.15 \text{ K}) = 167.828 \pm 0.035 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ $A_1 = 32.06$ Sulfur (S) $S_1(\text{g})$

State	ϵ , cm ⁻¹	Quantum Weights	g
¹ S ₀	0.00	5	5
¹ P ₁	396.09	3	3
¹ P ₀	573.65	1	1
¹ D ₂	9238.58	5	5
¹ S ₀	22179.99	1	1

Enthalpy of Formation
The enthalpy of formation is based on the dissociation energy for S₂(g) as recommended by CODATA.¹ 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⁻¹) from the study of Ricks and Barrow.² The selected dissociation energy, obtained from precise spectroscopic measurements,³ is supported by additional studies on thermochemical cycles,⁴ photoionization⁵ and torsion-effusion measurements.⁶ Earlier measurements have been reviewed by Herzberg,⁷ Gaydon,⁸ Brewer,⁹ and Drowart and Goldfinger.³

Heat Capacity and Entropy
The electronic levels for S(g) are given in the compilation by Moore.^{10,11} Our calculations indicate that, except for the five levels lying below 23000 cm⁻¹, 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⁻¹ 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.¹² 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 recommendation¹³ except for two minor differences. First, the entropy differs by 0.1094 J·K⁻¹·mol⁻¹ 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⁻¹·mol⁻¹ arises due to the use of slightly different values for the fundamental constants.

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T/K	C _p ^o	Enthalpy Reference Temperature = T ₂ = 298.15 K		Standard State Pressure = P ^o = 0.1 MPa		log K _r
		S ^o - (G ^o - H ^o (T ₂))/T	H ^o - H ^o (T ₂)/T	Δ _f H ^o	Δ _f G ^o	
0	0	INFINITE	0	274.735	274.735	INFINITE
100	21.356	142.891	-6.657	274.735	274.735	-137.427
200	23.388	138.392	-4.569	276.133	263.096	-65.238
250	23.696	163.653	-2.320	276.740	249.789	-65.237
298.15	23.673	167.828	-1.141	276.899	243.031	-50.779
300	23.669	167.828	0	276.980	236.500	-41.434
350	23.669	167.974	0.044	276.982	236.248	-41.135
400	23.480	171.610	1.223	276.985	236.458	-34.245
450	23.233	174.789	2.149	277.022	237.337	-29.069
500	22.979	177.451	3.146	277.062	238.197	-25.107
600	22.741	179.859	4.689	277.102	239.938	-21.932
700	22.538	183.968	6.942	277.170	241.436	-17.188
800	22.031	187.388	9.160	277.302	243.138	-13.815
900	21.800	190.314	11.351	269.621	247.994	-11.295
1000	21.624	192.871	13.522	215.535	215.535	-9.405
1100	21.489	195.142	15.677	215.834	156.096	-8.154
1200	21.386	197.185	17.821	216.106	150.109	-7.128
1300	21.307	199.042	19.955	216.354	144.098	-6.272
1400	21.249	200.745	22.083	216.579	138.067	-5.548
1500	21.209	202.318	24.205	216.784	132.020	-4.926
1600	21.186	203.781	26.325	216.970	125.959	-4.386
1700	21.178	205.148	28.445	217.140	119.886	-3.914
1800	21.184	206.432	30.561	217.295	113.803	-3.497
1900	21.204	207.643	32.680	217.438	107.711	-3.126
2000	21.234	208.790	34.802	217.570	101.611	-2.793
2100	21.276	209.880	36.927	217.694	95.503	-2.494
2200	21.327	210.920	39.058	217.812	89.392	-2.224
2300	21.386	211.913	41.193	217.925	83.275	-1.977
2400	21.452	212.865	43.335	218.035	77.152	-1.752
2500	21.523	213.780	45.484	218.143	71.024	-1.546
2600	21.598	214.660	47.640	218.250	64.892	-1.356
2700	21.676	215.508	49.803	218.358	58.755	-1.180
2800	21.756	216.328	51.975	218.467	52.615	-1.018
2900	21.837	217.121	54.155	218.579	46.470	-0.867
3000	21.919	217.889	56.343	218.690	40.321	-0.726
3100	22.005	218.633	58.538	218.811	34.169	-0.595
3200	22.078	219.355	60.742	218.931	28.012	-0.477
3300	22.155	220.058	62.954	219.055	21.851	-0.372
3400	22.230	220.740	65.173	219.183	15.697	-0.286
3500	22.302	221.405	67.400	219.315	9.518	-0.146
3600	22.372	222.053	69.634	219.447	3.346	-0.050
3700	22.439	222.684	71.874	219.583	-2.830	0.041
3800	22.502	223.300	74.121	219.721	-9.011	0.127
3900	22.561	223.900	76.375	219.862	-15.194	0.209
4000	22.618	224.487	78.634	220.003	-21.382	0.286
4100	22.670	225.061	80.898	220.146	-27.573	0.360
4200	22.720	225.621	83.167	220.289	-33.768	0.430
4300	22.766	226.169	85.442	220.432	-39.966	0.497
4400	22.808	226.705	87.720	220.575	-46.168	0.561
4500	22.847	227.230	90.003	220.716	-52.373	0.622
4600	22.884	227.744	92.290	220.856	-58.581	0.680
4700	22.917	228.247	94.580	220.993	-64.796	0.736
4800	22.947	228.740	96.873	221.127	-71.026	0.789
4900	22.974	229.224	99.169	221.258	-77.273	0.840
5000	22.999	229.698	101.468	221.386	-83.443	0.890
5100	23.021	230.163	103.769	221.509	-89.665	0.937
5200	23.040	230.619	106.072	221.628	-95.890	0.982
5300	23.072	231.066	108.377	221.741	-102.117	1.026
5400	23.085	231.503	110.683	221.849	-108.346	1.068
5500	23.096	231.937	112.991	221.952	-114.577	1.108
5600	23.106	232.361	115.300	222.048	-120.810	1.147
5700	23.112	232.777	117.610	222.138	-127.044	1.185
5800	23.117	233.186	119.921	222.222	-133.281	1.221
5900	23.121	233.588	122.232	222.299	-139.518	1.256
6000	23.124	233.983	124.544	222.368	-145.757	1.290
6100	23.124	234.372	126.857	222.431	-151.997	1.323

PREVIOUS: September 1977 (1 atm) CURRENT: September 1982 (1 bar)

Sulfur (S) $S_1(\text{g})$