

Revised and Updated Thermochemical Properties of the Gases Mercapto (HS), Disulfur Monoxide (S₂O), Thiazyl (NS), and Thioxophosphino (PS)

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Computations were done to correct erroneous data tables given in the 4th edition of the NIST-JANAF Thermochemical Tables. Updated enthalpies of formation were included to compute the thermochemical tables for four ideal gases: mercapto (HS), disulfur monoxide (S₂O), thiazyl (NS), and thioxophosphino (PS). © 2004 American Institute of Physics. [DOI: 10.1063/1.1611178]

Key words: disulfur monoxide; enthalpy of formation; hydrogen monosulfide; mercapto; nitrogen monosulfide; phosphorus monosulfide; thermochemical properties; thiazyl; thionitrosyl; thioxophosphino

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1. Introduction

The third and fourth editions of the JANAF tables [Chase *et al.* (1985), Chase (1998)] combined the JANAF Thermochemical Data Tables published in the 2nd edition [Stull and Prophet (1971)] and the four supplements to the 2nd edition. In the third edition of JANAF Thermochemical Tables, all data were converted to SI units, calculations involving the fundamental constants, atomic/molecular weights, and formation properties (as calculated from the reference states) were recalculated, many compounds were updated, and new compounds were included as well. Unfortunately the thermochemical properties of HS(g) and S₂O(g) given correctly in the second edition of the JANAF Thermochemical Tables and its 1982 supplement [Stull and Prophet (1971), Chase *et al.* (1982)] were transferred erroneously to the third and fourth edition of the JANAF Thermochemical Tables. The data of two other sulfides, NS(g) and PS(g), were not changed since the second edition but the enthalpies of formation of NS and PS given in the second edition are erroneous and thus remained wrong in the 3rd and 4th edition. Therefore revised tables were computed in this paper, using updated enthalpies of formation for these four compounds.

Henceforth the following abbreviations are used for the various JANAF editions:

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TABLE I. Auxiliary data

Monatomic gas	$-[H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})]$ (kJ mol ⁻¹)	$\Delta_f H^\circ(298.15\text{ K})$ (kJ mol ⁻¹)	Reference ^a state	$-[H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})]$ (kJ mol ⁻¹)	Source
H(g)	6.197	217.986	H ₂ (g)	8.468	JANAF 2nd
H(g)	6.197	217.999	H ₂ (g)	8.468	JANAF 2nd S82
H(g)	6.197	217.999	H ₂ (g)	8.467	JANAF 4th
H(g)	6.197	217.998	H ₂ (g)	8.467	Gurvich <i>et al.</i> (1989)
N(g)	6.197	472.646	N ₂ (g)	8.669	JANAF 2nd
N(g)	6.197	472.687	N ₂ (g)	8.669	JANAF 2nd S82
N(g)	6.197	472.683	N ₂ (g)	8.670	JANAF 4th
N(g)	6.197	472.680	N ₂ (g)	8.670	Gurvich <i>et al.</i> (1989)
O(g)	6.728	249.195	O ₂ (g)	8.682	JANAF 2nd
O(g)	6.724	249.174	O ₂ (g)	8.682	JANAF 2nd S82
O(g)	6.725	249.173	O ₂ (g)	8.683	JANAF 4th
O(g)	6.725	249.180	O ₂ (g)	8.680	Gurvich <i>et al.</i> (1989)
S(g)	6.657	278.989	S(cr.)	4.406	JANAF 2nd
S(g)	6.657	276.981	S(cr.)	4.410	JANAF 2nd S82
S(g)	6.657	276.980	S(cr.)	4.412	JANAF 4th
S(g)	6.657	277.180	S(cr.)	4.412	Gurvich <i>et al.</i> (1989)
P(g)	6.197	316.402	P(wh., cr.)	5.360	JANAF 2nd
P(g)	6.197	316.390	P(wh., cr.)	5.360	JANAF 4th
P(g)	6.197	316.500	P(wh., cr.)	5.360	Gurvich <i>et al.</i> (1989)

^aThe reference state for sulfur is S(cr, α), S(cr, β), S(1), and 1/2 S₂(g). The reference state for phosphorus is P(cr, white), P(1), 1/2 P₂(g).

JANAF 2nd Stull and Prophet (1971)
 JANAF 2nd S82 Chase *et al.* (1982); supplement to Stull and Prophet (1971)
 JANAF 3rd Chase *et al.* (1985)
 NIST-JANAF 4th Chase (1998).
 In order to facilitate the data discussion, some general

information is given in this section. Auxiliary data necessary to compute the enthalpy of formation at $T=298.15\text{ K}$, $\Delta_f H^\circ(298.15\text{ K})$ from the dissociation energy at $T=0\text{ K}$, $D^\circ(0\text{ K})$, are given in Table 1. In general, for a molecule AB composed of atoms A and B, the equation used for this purpose is

$$\begin{aligned} \Delta_f H^\circ(\text{AB}, \text{g}, 298.15\text{ K}) = & -D^\circ(\text{AB}, \text{g}, 0\text{ K}) + \Delta_f H^\circ(\text{A}, \text{g}, 298.15\text{ K}) + \Delta_f H^\circ(\text{B}, \text{g}, 298.15\text{ K}) \\ & - [H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})](\text{AB}, \text{g}) + [H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})](\text{A}, \text{g}) \\ & + [H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})](\text{B}, \text{g}). \end{aligned} \quad (1)$$

Here $\Delta_f H^\circ(298.15\text{ K})$ is the enthalpy of formation of the gases - AB, A, and B - at $T=298.15\text{ K}$ from the constituent elements in their reference state; $H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})$, are the enthalpy differences between $T=0\text{ K}$ and $T=298.15\text{ K}$ for molecule AB and the monatomic gases A and B, respectively; $D^\circ(0\text{ K})$ is the dissociation energy of molecule AB at $T=0\text{ K}$. This equation together with appropriate stoichiometric coefficients is also used to calculate atomization energies for S₂O(g).

In some instances it is necessary to convert the enthalpy of formation at $T=0\text{ K}$ to that at $T=298.15\text{ K}$. This is done by adding respective enthalpy increment terms of the compound

and of the elements in their reference state to the enthalpy of formation at $T=0\text{ K}$:

$$\begin{aligned} \Delta_f H^\circ(\text{AB}, \text{g}, 298.15\text{ K}) = & \Delta_f H^\circ(\text{AB}, \text{g}, 0\text{ K}) \\ & - [H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})](\text{AB}, \text{g}) \\ & + [H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})](\text{A}, \text{ref}) \\ & + [H^\circ(0\text{ K}) - H^\circ(298.15\text{ K})](\text{B}, \text{ref}). \end{aligned} \quad (2)$$

In Eq. (2), stoichiometric coefficients have to be taken into

TABLE 2. Some thermochemical properties for HS(g) at $T=0$ K and $T=298.15$ K^a

D° (kJ mol ⁻¹)	$\Delta_f H^{\circ}(0$ K) (kJ mol ⁻¹)	$\Delta_f H^{\circ}(298.15$ K) (kJ mol ⁻¹)	$-[H^{\circ}(0$ K) $- H^{\circ}(298.15$ K)] (kJ mol ⁻¹)	$S^{\circ}(298.15$ K) (J K ⁻¹ mol ⁻¹)	Sources and Notes
{346.7±16.7}	+144.139±16.7	+144.766±16.7	(9.098)	195.628	Mackle (1963)
340.6±11.6	{+150.9±12}	{+151.4±12}	(9.098)	—	Gaydon (1968)
352.3±4.2	+138.3±4.2	+138.9±4.2	9.088	195.71	Mills (1974)
{350.8±4.6}	+140.0±4.6	+140.6±4.6	(9.098)	—	Hwang and Benson (1979)
{348.75}	+142.00	+142.67	9.083	195.67	Wagman <i>et al.</i> (1982)
351.0±3.5	+139.970±3.5	+140.422±3.5	9.098	195.552	Gurvich <i>et al.</i> (1989)
346.4	{+144.5}	{+145.0}	(9.098)	—	Curtiss <i>et al.</i> (1991)
350.5±1.2	{+140.37±1.2}	{+140.82±1.2}	(9.098)	—	Morley <i>et al.</i> (1993)
{348.68±6.28}	+141.84±6.28	{+142.29±6.28}	(9.098)	—	Nourbakhsh <i>et al.</i> (1991)
348.23±3.26	+142.55±3.0	+143.01±2.85	{9.106}	—	Nicovich <i>et al.</i> (1992)
348.6±0.6	{+142.3±0.6}	{+142.8±0.6}	(9.098)	—	Wilson <i>et al.</i> (1996)
350.0±4.3	{+140.97±4.3}	{+141.42±4.3}	(9.098)	—	Rempala and Erwin (2000)
348.4±0.5	{+142.5±0.5}	{+143.0±0.5}	(9.098)	—	Shiell <i>et al.</i> (2000)
—	+144.135±16.7	+144.766±16.7	9.272	195.623	JANAF 2nd
352.4±5.0	+138.695±16.7	+139.327±5.0	9.272	195.627	JANAF 2nd S82
—	+136.493±5.0	+139.327±5.0	9.273	195.628	JANAF 3rd, 4th
{351.930±6.3}	+138.841±6.3	+139.467±6.3	9.273	—	recalc. from JANAF 4th
348.50±0.78	+142.47±0.78	+142.92±0.78	9.098	195.552	selected value

^aData in italics may not be correct and are given only for comparison. Entropies are for 1 bar. Data for enthalpy increments $-[H^{\circ}(0$ K) $- H^{\circ}(298.15$ K)] given in parentheses indicate the value used to compute enthalpies of formation at 298.15 from 0 K data or from dissociation energies. Data in curly braces are computed here using auxiliary data from Table 1 if not noted otherwise.

account if the reference state is a diatomic gas such as H₂, N₂, and O₂. The enthalpy increments and enthalpies of formation used as auxiliary data are taken from Gurvich *et al.* (1989) and are given in Table 1. The respective data from the various editions of JANAF Thermochemical Tables are listed there for comparison.

The following conversion factors from NIST-JANAF 4th were used: 1 kcal mol⁻¹ = 4.184 kJ mol⁻¹; 1 eV = 96.4846 kJ mol⁻¹; 1 cm⁻¹ = 0.011 962 66 kJ mol⁻¹. Entropy units are given with reference to 1 bar and when necessary, literature data were converted using S^{atm} (J K⁻¹ mol⁻¹) + 0.109 442 = S^{bar} (J K⁻¹ mol⁻¹), as recommended in NIST-JANAF 4th.

An earlier article by Lodders (1999) dealt with revised thermochemical tables for four phosphorus compounds: PH(g), PH₃(g), PN(g), and Mg₃P₂O₈(cr,l).

2. Thermochemical Data Tables

2.1. Hydrogen Monosulfide Gas, Mercapto Gas, HS(g)

The last data revision of HS in the JANAF Tables was performed in 1977, which was published in JANAF 2nd S82. In the transfer of this data table to the JANAF 3rd, the columns for $\Delta_f H^{\circ}$, $\Delta_f G^{\circ}$, and $\log K_f$ were computed incorrectly. The introductory text to JANAF 4th states that the table for HS(g), which was incorrect in JANAF 3rd, was corrected. Unfortunately, the corrected table was not printed and the same table for HS(g) appeared again in the 4th edition. Thus, except for $\Delta_f H^{\circ}(298.15$ K), the data in the columns for $\Delta_f H^{\circ}$, $\Delta_f G^{\circ}$, and $\log K_f$ remain erroneous. The reason for these incorrect data columns is unclear and is not easily traced.

2.1.1. Enthalpy of Formation

Before computing the table correcting the $\Delta_f H^{\circ}$, $\Delta_f G^{\circ}$, and $\log K_f$ columns for HS(g), the enthalpy of formation is updated. Table 2 summarizes some properties at $T=0$ K and $T=298.15$ K for HS(g). In JANAF 2nd, the enthalpy of formation was based on Mackle's (1963) data from photoionization studies. The properties of HS(g) were updated in JANAF 2nd S82 and these data remained in JANAF 3rd and 4th. The reaction enthalpy of $\Delta_R H^{\circ}(0$ K) = 89.02 ± 1.15 kcal mol⁻¹ for H₂S(g) = HS(g) + H(g) was used to derive $\Delta_f H^{\circ}(\text{HS,g}, 298.15$ K) = 33.30 ± 1.2 kcal mol⁻¹ (139.327 ± 5.0 kJ mol⁻¹) in JANAF 2nd S82. Using the same reaction enthalpy and all auxiliary data from JANAF 4th, essentially the same $\Delta_f H^{\circ}(298.15$ K) = 139.467 ± 6.3 kJ mol⁻¹ is derived. The corresponding dissociation energy is $D^{\circ}(\text{HS,g}) = 352 \pm 6.3$ kJ mol⁻¹. Gurvich *et al.* (1989) select $D^{\circ}(\text{HS,g}) = 351.0 \pm 3.5$ kJ mol⁻¹ based on photoionization measurements by Dibeler and Liston (1968), the ionization potential of HS(g), and the atomization energy of H₂S(g).

Here the dissociation energy of HS(g) is derived from more recent studies (Table 2). Wilson *et al.* (1996) and Shiell *et al.* (2000) determined $D^{\circ}(\text{H-SH,g}) = 376.106 \pm 0.239$ and 376.238 ± 0.048 kJ mol⁻¹, respectively. These data, combined with data for the atomization of H₂S(g) from Gurvich *et al.* (1989) yield an average dissociation energy of $D^{\circ}(\text{HS,g}) = 348.50 \pm 0.78$ kJ mol⁻¹, which is selected here. This value compares well to the direct determination of the HS(g) dissociation energy of $D^{\circ}(\text{HS,g}) = 350.0 \pm 4.3$ kJ mol⁻¹ by Rempala and Erwin (2000).

The selected dissociation energy yields $\Delta_f H^{\circ}(298.15$ K) = 142.92 ± 0.78 kJ mol⁻¹ which is adopted to compute thermochemical properties for HS(g) listed in Table 3.

2.1.2. Entropy and Heat Capacity

The entropy at 298.15 K and heat capacity functions are from Gurvich *et al.* (1989) because they used a more exact statistical mechanical calculation (a direct sum over the rotation–vibrational energy levels) for the thermal functions, which increases the heat capacity by $0.032 \text{ J K}^{-1} \text{ mol}^{-1}$ at 298.15 K and $0.707 \text{ J K}^{-1} \text{ mol}^{-1}$ at 6000 K by comparison to the JANAF table.

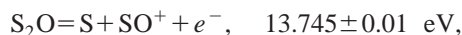
2.2. Disulfur Monoxide Gas, S₂O(g)

The data analysis for the S₂O(g) JANAF Thermochemical Table was performed in 1965; no data updates were made since it was published in JANAF 2nd. As in the case for HS, the data transfer from the second to third edition introduced errors in the data columns for $\Delta_f H^\circ$, $\Delta_f G^\circ$, and $\log K_f$. The introductory text to JANAF 4th states that the table for S₂O(g) was corrected from the previous edition, but the erroneous table for S₂O(g) was printed again in the 4th edition so the data in the columns for $\Delta_f H^\circ$, $\Delta_f G^\circ$, and $\log K_f$ remain erroneous [except for $\Delta_f H^\circ(298.15 \text{ K})$]. The reason for the incorrect data columns is not easily traced.

2.2.1. Enthalpy of Formation

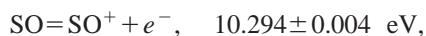
Before recalculating the thermochemical data table for S₂O, updates to the enthalpy of formation have been examined. Table 4 summarizes some properties at $T=0 \text{ K}$ and $T=298.15 \text{ K}$ for S₂O(g). The description in JANAF 2nd gives a selected value of $\Delta_f H^\circ(\text{S}_2\text{O}, \text{g}, 0 \text{ K}) = -13 \pm 8 \text{ kcal mol}^{-1}$ ($-54.392 \text{ kJ mol}^{-1}$) based on Blukis and Myers (1965). The enthalpy of formation at 298.15 K in JANAF 2nd is given as $-13.5 \text{ kcal mol}^{-1}$ ($-54.484 \text{ kJ mol}^{-1}$). This value is used in JANAF 3rd and 4th but the data for the enthalpy of formation at temperatures other than 298.15 K in JANAF 3rd and 4th are incorrect, as are the columns for $\Delta_f G^\circ$ and $\log K_f$.

Gurvich *et al.* (1989) base their selection of $\Delta_f H^\circ(\text{S}_2\text{O}, \text{g}, 298.15 \text{ K}) = -56.036 \pm 1.4 \text{ kJ mol}^{-1}$ on photodissociation studies by Berkowitz *et al.* (1977). The result of the latter study was not included in the evaluation by JANAF but is close to their selected value. The enthalpy of formation at $T=298.15 \text{ K}$ is computed here from the $T=0 \text{ K}$ reaction enthalpies of



Berkowitz *et al.* (1977)

and



Norwood and Ng (1989)

so that $\Delta_f H^\circ(\text{S}_2\text{O}, \text{g}, 0 \text{ K}) = -53.35 \pm 1.10 \text{ kJ mol}^{-1}$ is obtained. Using auxiliary functions from Gurvich *et al.* (1989), the adopted enthalpy of formation $\Delta_f H^\circ[(\text{S}_2\text{O}, \text{g}, 298.15 \text{ K}) = -55.39 \pm 1.10 \text{ kJ mol}^{-1}]$ is derived.

2.2.2. Entropy and Heat Capacity

As seen from Table 4, the entropy values given in JANAF 2nd and JANAF 3rd and 4th are inconsistent, as are those in JANAF 3rd and Gurvich *et al.* (1989). However, the fundamental constants, molecular weight, heat capacity functions are the same in JANAF 3rd and Gurvich *et al.* (1989). Here the thermal functions from Gurvich *et al.* (1989) are used to compute thermochemical properties of S₂O(g) in Table 5.

2.3. Nitrogen Monosulfide Gas, Thiazyl Gas, Thionitrosyl Gas, NS(g)

2.3.1. Enthalpy of Formation

Table 6 summarizes some properties at $T=0 \text{ K}$ and $T=298.15 \text{ K}$ for NS(g). The enthalpy of formation in JANAF 2nd to JANAF 4th was derived from the dissociation energy of $D^\circ(\text{NS}, \text{g}) = 5.0 \pm 0.7 \text{ eV}$ ($115.3 \pm 16,482.4 \pm 67.5 \text{ kJ mol}^{-1}$) as given by Gaydon (1953), (1968) from a linear Birge Spomer extrapolation for the ground state. However, something went wrong in JANAF when the enthalpy of formation was calculated from this dissociation energy. Using all auxiliary thermal data and $\Delta_f H^\circ(298.15 \text{ K})$ for N(g) and S(g) from JANAF 2nd, the dissociation energy yields $\Delta_f H^\circ(298.15 \text{ K}) = 265.778 \pm 67.5 \text{ kJ mol}^{-1}$ instead of the value of $263.592 \pm 105 \text{ kJ mol}^{-1}$ listed in JANAF 2nd. This erroneous value was kept in JANAF 3rd and 4th.

Furthermore, in JANAF 2nd S82 and following editions of JANAF, the enthalpy of formation of S(g) was changed to $\Delta_f H^\circ(298.15 \text{ K}) = 276.980 \text{ kJ mol}^{-1}$ from the previous value of $\Delta_f H^\circ(298.15 \text{ K}) = 278.989 \text{ kJ mol}^{-1}$ in JANAF 2nd. Similarly, the enthalpy of formation of N(g) was revised but the change was not as large as that for S(g), see Table 1. The enthalpies of formation should have been recomputed in JANAF 2nd S82 to 4th for all compounds that include sulfur and nitrogen and for which the enthalpy of formation was derived from the dissociation energy in JANAF 2nd, but this was not done for NS(g). Using all auxiliary data and $\Delta_f H^\circ(298.15 \text{ K})$ for N(g) and S(g) from JANAF 4th, Gaydon's dissociation energy, $D^\circ(\text{NS}, \text{g}) = 5.0 \pm 0.7 \text{ eV} = 115.3 \pm 16.1 \text{ kcal mol}^{-1}$ ($482.4 \pm 67.5 \text{ kJ mol}^{-1}$), yields $\Delta_f H^\circ(298.15 \text{ K}) = 263.806 \pm 67.5 \text{ kJ mol}^{-1}$ for NS(g).

Gurvich *et al.* (1989) selected the dissociation energy of 479 kJ mol^{-1} in part based on Gaydon (1968) and they derived $\Delta_f H^\circ(\text{NS}, \text{g}, 298.15 \text{ K}) = 267.399 \text{ kJ mol}^{-1}$. The difference in the enthalpy of formation from Gurvich and the recalculated value from JANAF is mainly due to the differences in the selected dissociation energy and the differences in $\Delta_f H^\circ(\text{S}, \text{g}, 298.15 \text{ K})$.

O'Hare (1970) analyzed the available spectroscopic data and deduced $D^\circ(\text{NS}, \text{g}) = 463 \pm 24 \text{ kJ mol}^{-1}$, which he compares to a theoretical *ab initio* value of $D^\circ(\text{NS}, \text{g}) = 502 \text{ kJ mol}^{-1}$. More recently, lower and upper bounds for the dissociation energy of NS(g) derived from experimental emission studies are reported as $\geq 476 \text{ kJ mol}^{-1}$ [Murai *et al.* (1979)] and $\leq 543 \text{ kJ mol}^{-1}$ [Chiu and Silvers (1975)].

TABLE 3. Ideal gas thermochemical properties of HS(g) at standard state pressure, $p^{\circ}=0.1$ MPa ($T_r=298.15$ K)

T (K)	C_p° (J K ⁻¹ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	$-[G^{\circ}-H^{\circ}(298.15\text{ K})]/T$ (J K ⁻¹ mol ⁻¹)	$H^{\circ}-H^{\circ}(298.15\text{ K})$ (kJ mol ⁻¹)	$\Delta_f H^{\circ}$ (kJ mol ⁻¹)	$\Delta_f G^{\circ}$ (kJ mol ⁻¹)	$\log K_f$ (kJ mol ⁻¹)
298.15	32.479	195.552	195.552	0.000	142.920	113.659	-19.9123
300	32.466	195.753	195.553	0.060	142.911	113.477	-19.7579
350	32.102	200.730	195.947	1.674	142.635	108.592	-16.2063
400	31.769	204.994	196.817	3.271	140.065	103.840	-13.5600
450	31.512	208.721	197.937	4.852	138.991	99.367	-11.5341
500	31.346	212.031	199.184	6.424	137.822	95.029	-9.9275
550	31.274	215.015	200.490	7.989	136.821	90.799	-8.6233
600	31.287	217.736	201.815	9.552	135.905	86.657	-7.5440
650	31.371	220.243	203.138	11.119	135.041	82.588	-6.6367
700	31.507	222.573	204.444	12.690	134.228	78.584	-5.8639
750	31.686	224.752	205.726	14.270	133.467	74.636	-5.1980
800	31.897	226.804	206.980	15.859	132.717	70.738	-4.6187
850	32.129	228.745	208.203	17.460	131.975	66.887	-4.1103
900	32.372	230.588	209.396	19.072	78.194	64.158	-3.7236
950	32.621	232.345	210.558	20.697	78.142	63.379	-3.4848
1000	32.872	234.024	211.690	22.335	78.094	62.604	-3.2700
1100	33.366	237.181	213.866	25.647	78.010	61.059	-2.8994
1200	33.834	240.104	215.932	29.007	77.938	59.521	-2.5909
1300	34.270	242.830	217.897	32.412	77.873	57.989	-2.3300
1400	34.670	245.384	219.770	35.860	77.813	56.462	-2.1066
1500	35.037	247.789	221.559	39.345	77.753	54.939	-1.9131
1600	35.372	250.061	223.270	42.866	77.692	53.420	-1.7440
1700	35.679	252.215	224.910	46.419	77.628	51.905	-1.5948
1800	35.961	254.262	226.484	50.001	77.560	50.394	-1.4624
1900	36.221	256.214	227.998	53.610	77.486	48.886	-1.3440
2000	36.462	258.078	229.455	57.245	77.407	47.383	-1.2375
2100	36.687	259.862	230.861	60.902	77.324	45.884	-1.1413
2200	36.898	261.574	232.219	64.582	77.235	44.389	-1.0539
2300	37.097	263.218	233.531	68.281	77.142	42.898	-0.9742
2400	37.286	264.801	234.801	72.001	77.046	41.411	-0.9013
2500	37.467	266.327	236.032	75.738	76.945	39.928	-0.8342
2600	37.641	267.800	237.226	79.494	76.842	38.450	-0.7725
2700	37.809	269.224	238.384	83.266	76.737	36.975	-0.7153
2800	37.971	270.602	239.511	87.055	76.630	35.504	-0.6623
2900	38.129	271.937	240.606	90.860	76.521	34.038	-0.6131
3000	38.282	273.232	241.672	94.681	76.412	32.574	-0.5672
3100	38.431	274.490	242.710	98.517	76.301	31.115	-0.5243
3200	38.576	275.712	243.723	102.367	76.190	29.659	-0.4841
3300	38.716	276.902	244.710	106.232	76.078	28.207	-0.4465
3400	38.851	278.059	245.674	110.110	75.965	26.758	-0.4111
3500	38.982	279.187	246.616	114.002	75.851	25.312	-0.3778
3600	39.106	280.287	247.536	117.906	75.736	23.870	-0.3463
3700	39.224	281.360	248.435	121.823	75.618	22.431	-0.3167
3800	39.336	282.408	249.316	125.751	75.498	20.995	-0.2886
3900	39.439	283.431	250.177	129.690	75.374	19.562	-0.2620
4000	39.535	284.431	251.021	133.638	75.245	18.133	-0.2368
4100	39.621	285.408	251.848	137.596	75.112	16.707	-0.2128
4200	39.698	286.364	252.659	141.562	74.972	15.284	-0.1901
4300	39.765	287.299	253.453	145.536	74.824	13.865	-0.1684
4400	39.822	288.214	254.233	149.515	74.668	12.448	-0.1478
4500	39.868	289.109	254.998	153.500	74.502	11.036	-0.1281
4600	39.902	289.986	255.749	157.488	74.326	9.628	-0.1093
4700	39.926	290.844	256.487	161.480	74.137	8.223	-0.0914
4800	39.937	291.685	257.211	165.473	73.935	6.823	-0.0743
4900	39.937	292.508	257.923	169.467	73.719	5.427	-0.0579
5000	39.926	293.315	258.623	173.460	73.487	4.036	-0.0422
5100	39.903	294.106	259.311	177.451	73.239	2.649	-0.0271
5200	39.868	294.880	259.988	181.440	72.973	1.268	-0.0127
5300	39.822	295.639	260.653	185.425	72.689	-0.109	0.0011
5400	39.766	296.383	261.308	189.404	72.386	-1.480	0.0143
5500	39.698	297.112	261.952	193.377	72.062	-2.844	0.0270
5600	39.621	297.827	262.587	197.344	71.718	-4.203	0.0392
5700	39.533	298.527	263.211	201.301	71.352	-5.556	0.0509
5800	39.437	299.214	263.826	205.250	70.965	-6.901	0.0622
5900	39.331	299.887	264.431	209.188	70.555	-8.241	0.0730
6000	39.217	300.547	265.028	213.116	70.123	-9.572	0.0833

TABLE 4. Some thermochemical properties for S₂O(g) at T=0 K and T=298.15 K^a

<i>D</i> ^o (kJ mol ⁻¹)	$\Delta_f H^o(0\text{ K})$ (kJ mol ⁻¹)	$\Delta_f H^o(298.15\text{ K})$ (kJ mol ⁻¹)	$-[H^o(0\text{ K}) - H^o(298.15\text{ K})]$ (kJ mol ⁻¹)	<i>S</i> ^o (298.15 K) (J K ⁻¹ mol ⁻¹)	Sources and Notes
{851.057}	-54.392	{-56.428}	(11.128)	—	Blukis and Myers (1965)
{836.47±1.26}	{-39.87±1.26}	-41.84±1.26	11.192	268.388	Hagemann <i>et al.</i> (1967)
{850.011±1.100}	-53.346±1.100	{-55.382±1.100}	(11.128)	—	Berkowitz <i>et al.</i> (1977)
838.5±8.4	{-38.5±8.4}	-40.6±8.4	11.129	267.05	Mills (1974)
{850.665±1.4}	-54.000±1.4	-56.036±1.4	11.128	266.961	Gurvich <i>et al.</i> (1989)
—	-54.392±33.5	-56.484±33.5	11.129	267.049	JANAF 2nd
—	-58.859±33.5	-56.484±33.5	11.128	267.020	JANAF 3rd, 4th
850.00±1.10	-53.35±1.10	-55.39±1.10	11.128	266.961	selected value

^aData in italics may not be correct and are given only for comparison. Entropies are for 1 bar. Data for enthalpy increments $-[H^o(0\text{ K}) - H^o(298.15\text{ K})]$ given in parentheses indicate the value used to compute enthalpies of formation at 298.15 K from 0 K data or from dissociation energies. Data in curly braces are computed here using auxiliary data from Table 1 if not noted otherwise.

$D^o(\text{NS,g}) = 463 \pm 24 \text{ kJ mol}^{-1}$, as derived by O'Hare (1970), is selected here. This value and auxiliary data from Gurvich *et al.* (1989) listed in Table 1 lead to the adopted enthalpy of formation of $\Delta_f H^o(298.15\text{ K}) = 283.40 \pm 24 \text{ kJ mol}^{-1}$ which is used to compute thermodynamic properties for NS(g) listed in Table 7.

2.3.2. Entropy and Heat Capacity

The values for the entropy and heat capacity for NS(g) were taken directly from Gurvich *et al.* (1989).

2.4. Phosphorus Monosulfide Gas, Thioxophosphino Gas, PS(g)

2.4.1. Enthalpy of Formation

Table 8 summarizes some properties at T=0 K and T=298.15 K for PS(g). The descriptive text for PS in JANAF 2nd to 4th gives the enthalpy of formation of PS(g) as $\Delta_f H^o(298.15\text{ K}) = 156.063 \pm 105 \text{ kJ mol}^{-1}$. This value is reported with respect to the red phosphorus reference state. The $\Delta_f H^o(298.15\text{ K})$ is based on an estimated dissociation energy of $D^o(\text{PS,g}) = 140 \pm 25 \text{ kcal mol}^{-1}$ ($585.8 \pm 105 \text{ kJ mol}^{-1}$). In JANAF 3rd and 4th the reference state for phosphorus was changed from red to white phosphorus, which changes the enthalpy of formation at T=298.15 K by $\Delta_f H^o(\text{P,cr,white,298.15 K}) = \Delta_f H^o(\text{P,cr,red,298.15 K}) - 17.460 \text{ kJ mol}^{-1}$ per formula unit phosphorus. Thus, the tables in JANAF 3rd and 4th use $\Delta_f H^o(\text{PS,g,298.15 K}) = 138.603 \text{ kJ mol}^{-1}$. The uncertainty for the enthalpy of formation is given as $\pm 105 \text{ kJ mol}^{-1}$ in the text in JANAF 3rd and 4th and not $\pm 41.8 \text{ kJ mol}^{-1}$ as printed in the data summary on top of the descriptive text.

However, the dissociation energy of $140 \pm 25 \text{ kcal mol}^{-1}$ combined with auxiliary data for P(g), S(g), and PS(g) from JANAF 4th results in an enthalpy of formation of $\Delta_f H^o(298.15\text{ K}) = +4.37 \text{ kJ mol}^{-1}$ for formation of PS(g) from white P and orthorhombic sulfur, which is quite different than the $\Delta_f H^o(298.15\text{ K}) = 138.60 \text{ kJ mol}^{-1}$ used in JANAF 4th. In contrast, the given $\Delta_f H^o(298.15\text{ K})$ corresponds to $D^o(\text{PS,g}) = 541.5 \text{ kJ mol}^{-1}$ ($108 \text{ kcal mol}^{-1}$), also obviously different than the $140 \text{ kcal mol}^{-1}$ used in all

JANAF editions. A calculation using all auxiliary data from JANAF 2nd and red P as reference state also shows this mismatch. Thus, something went wrong in the derivation of the enthalpy of formation for PS in all JANAF editions.

Mills (1974) included the $D^o(\text{PS,g}) = 140 \text{ kcal mol}^{-1}$ from JANAF in his evaluation, but he adopted the value of Gaydon (1968) of $D^o(\text{PS,g}) = 120 \text{ kcal mol}^{-1}$ (502 kJ mol^{-1}). From this dissociation energy value, the enthalpy of formation is $\Delta_f H^o(\text{PS,g,298.15 K}) = 88.4 \text{ kJ mol}^{-1}$, while Mills lists an enthalpy of formation of $238.5 \pm 105 \text{ kJ mol}^{-1}$ which is much too high for reasons that are unclear.

Theoretical quantum chemical computations yield dissociation energies of $D^o(\text{PS,g}) = 550 \text{ kJ mol}^{-1}$ [Lakshman and Venkataramanaiah (1980)] and $D^o(\text{PS,g}) = 482 \text{ kJ mol}^{-1}$ [Moussaoui *et al.* (1998)] from which the corresponding $\Delta_f H^o(\text{PS,g,298.15 K})$ are calculated as +40.4 and +108.4 kJ mol^{-1} , respectively. The only experimental value for the dissociation energy of PS(g) was obtained by Drowart *et al.* (1973) yielding $D^o(\text{PS,g}) = 438 \pm 10 \text{ kJ mol}^{-1}$. Using auxiliary data from Gurvich *et al.* (1989), this corresponds to $\Delta_f H^o(\text{PS,g,298.15 K}) = +152.44 \pm 10 \text{ kJ mol}^{-1}$ (from white P). Based on this experimental study, Gurvich *et al.* (1989) adopted a dissociation energy of $440 \pm 12 \text{ kJ mol}^{-1}$ and gave the corresponding enthalpy of formation as $\Delta_f H^o(\text{PS,g,298.15 K}) = 150.442 \text{ kJ mol}^{-1}$ (white P reference state).

The enthalpy of formation $\Delta_f H^o(\text{PS,g,298.15 K}) = 152.44 \pm 10 \text{ kJ mol}^{-1}$ derived from experimental data by Drowart *et al.* (1973) is adopted for computation of Table 9.

2.4.2. Entropy and Heat Capacity

The values for the heat capacity and entropy for Table 9 are taken directly from Gurvich *et al.* (1989) because they included more recent experimental data in addition to those of Dressler (1955) whose data were the only source for this used in the JANAF Tables.

TABLE 5. Ideal gas thermochemical properties of S₂O(g) at standard state pressure, $p^{\circ}=0.1$ MPa ($T_r=298.15$ K)

T (K)	C_p° (J K ⁻¹ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	$-[G^{\circ}-H^{\circ}(298.15\text{ K})]/T$ (J K ⁻¹ mol ⁻¹)	$H^{\circ}-H^{\circ}(298.15\text{ K})$ (kJ mol ⁻¹)	$\Delta_f H^{\circ}$ (kJ mol ⁻¹)	$\Delta_f G^{\circ}$ (kJ mol ⁻¹)	$\log K_f$ (kJ mol ⁻¹)
298.15	44.114	266.961	266.961	0.000	-55.390	-85.279	14.9403
300	44.191	267.234	266.962	0.082	-55.420	-85.464	14.8804
350	46.133	274.196	267.507	2.341	-56.231	-90.408	13.4924
400	47.797	280.467	268.742	4.690	-61.504	-95.057	12.4131
450	49.201	286.181	270.367	7.116	-63.688	-99.139	11.5076
500	50.379	291.427	272.214	9.607	-65.987	-102.949	10.7549
550	51.368	296.277	274.184	12.151	-67.894	-106.551	10.1192
600	52.201	300.783	276.215	14.741	-69.594	-109.989	9.5753
650	52.905	304.990	278.268	17.369	-71.167	-113.291	9.1040
700	53.497	308.933	280.319	20.029	-72.626	-116.476	8.6914
750	54.003	312.641	282.352	22.717	-73.975	-119.560	8.3268
800	54.436	316.141	284.355	25.429	-75.303	-122.556	8.0020
850	54.809	319.452	286.323	28.160	-76.619	-125.469	7.7103
900	55.131	322.595	288.252	30.909	-184.023	-126.149	7.3214
950	55.411	325.583	290.139	33.672	-183.978	-122.935	6.7593
1000	55.656	328.432	291.983	36.449	-183.935	-119.723	6.2536
1100	56.061	333.756	295.542	42.036	-183.855	-113.306	5.3804
1200	56.379	338.648	298.933	47.658	-183.788	-106.895	4.6530
1300	56.632	343.171	302.164	53.309	-183.741	-100.490	4.0377
1400	56.836	347.376	305.245	58.983	-183.720	-94.087	3.5104
1500	57.004	351.303	308.186	64.675	-183.725	-87.684	3.0534
1600	57.143	354.987	310.997	70.383	-183.761	-81.281	2.6535
1700	57.259	358.454	313.688	76.103	-183.826	-74.874	2.3006
1800	57.358	361.730	316.267	81.834	-183.921	-68.462	1.9867
1900	57.442	364.834	318.742	87.574	-184.046	-62.045	1.7057
2000	57.514	367.782	321.121	93.322	-184.200	-55.620	1.4526
2100	57.576	370.590	323.410	99.077	-184.381	-49.186	1.2234
2200	57.630	373.269	325.616	104.837	-184.589	-42.744	1.0149
2300	57.678	375.832	327.744	110.603	-184.823	-36.291	0.8242
2400	57.720	378.288	329.799	116.373	-185.080	-29.828	0.6492
2500	57.757	380.645	331.786	122.146	-185.361	-23.353	0.4879
2600	57.790	382.911	333.709	127.924	-185.663	-16.867	0.3389
2700	57.819	385.092	335.572	133.704	-185.986	-10.369	0.2006
2800	57.846	387.195	337.378	139.488	-186.329	-3.858	0.0720
2900	57.869	289.226	339.131	145.273	-186.691	2.665	-0.0480
3000	57.891	391.188	340.834	151.061	-187.071	9.201	-0.1602
3100	57.910	393.087	342.489	156.851	-187.469	15.750	-0.2654
3200	57.928	394.925	344.099	162.643	-187.884	22.312	-0.3642
3300	57.944	396.708	345.667	168.437	-188.316	28.887	-0.4572
3400	57.959	398.438	347.193	174.232	-188.764	35.476	-0.5450
3500	57.972	400.118	348.682	180.029	-189.229	42.078	-0.6280
3600	57.985	401.752	350.133	185.827	-189.711	48.693	-0.7065
3700	57.996	403.341	351.550	191.626	-190.208	55.322	-0.7810
3800	58.007	404.887	352.933	197.426	-190.722	61.965	-0.8518
3900	58.017	406.394	354.285	203.227	-191.253	68.622	-0.9191
4000	58.026	407.863	355.606	209.029	-191.801	75.292	-0.9832
4100	58.034	409.296	356.898	214.832	-192.366	81.977	-1.0444
4200	58.042	410.695	358.162	220.636	-192.947	88.675	-1.1028
4300	58.049	412.061	359.400	226.440	-193.547	95.387	-1.1587
4400	58.056	413.395	360.612	232.246	-194.164	102.113	-1.2122
4500	58.062	414.700	361.800	238.052	-194.799	108.854	-1.2635
4600	58.068	415.976	362.964	243.858	-195.453	115.609	-1.3128
4700	58.074	417.225	364.105	249.665	-196.125	122.379	-1.3601
4800	58.079	418.448	365.224	255.473	-196.815	129.163	-1.4056
4900	58.084	419.645	366.323	261.281	-197.524	135.961	-1.4493
5000	58.088	420.819	367.401	267.090	-198.252	142.775	-1.4915
5100	58.093	421.969	368.460	272.899	-198.998	149.602	-1.5322
5200	58.097	423.097	369.500	278.708	-199.764	156.445	-1.5715
5300	58.101	424.204	370.521	284.518	-200.548	163.303	-1.6094
5400	58.104	425.290	371.526	290.328	-201.351	170.175	-1.6461
5500	58.108	426.356	372.513	296.139	-202.173	177.063	-1.6816
5600	58.111	427.403	373.484	301.950	-203.014	183.966	-1.7159
5700	58.114	428.432	374.439	307.761	-203.873	190.883	-1.7492
5800	58.117	429.443	375.378	313.573	-204.750	197.817	-1.7815
5900	58.120	430.436	376.303	319.385	-205.645	204.765	-1.8128
6000	58.123	431.413	377.214	325.197	-206.558	211.729	-1.8432

TABLE 6. Some thermochemical properties for NS(g) at $T=0$ K and $T=298.15$ K^a

D° (kJ mol ⁻¹)	$\Delta_f H^{\circ}(0$ K) (kJ mol ⁻¹)	$\Delta_f H^{\circ}(298.15$ K) (kJ mol ⁻¹)	$-[H^{\circ}(0$ K) $-H^{\circ}(298.15$ K)] (kJ mol ⁻¹)	$S^{\circ}(298.15$ K) (J K ⁻¹ mol ⁻¹)	Sources and Notes
482.4±67.5	{+263.4±67.5}	{+264.0±67.5}	(9.393)	—	Gaydon (1953), (1968)
463±24	{+282.75±24}	{+283.40±24}	(9.393)	—	O'Hare (1970), from spectroscopy
502	{+243.7}	{+244.4}	(9.393)	—	O'Hare (1970), theoretical value
462.8±25.1	+286.4±25.1	+287.0±25.1	9.397	222.11	Mills (1974)
≤543	{≥202.7}	{≥203.4}	(9.393)	—	Chiu and Silvers (1975)
≥476	{≤269.7}	{≤270.4}	(9.393)	—	Murai <i>et al.</i> (1979)
479±50	+266.753±50	+267.399±50	9.393	222.093	Gurvich <i>et al.</i> (1989)
452.7	{+293.1}	{+293.7}	(9.393)	—	Curtiss <i>et al.</i> (1991)
481.2±104.6	+262.935±105	+263.592±105	9.397	222.092	JANAF 2nd
482.4±67.5	+265.122±67.5	+265.778±67.5	9.397	—	JANAF 2nd recalculated, see text
482.4±67.5	+262.942±105	+263.592±105	9.397	222.087	JANAF 3rd, 4th
482.4±67.5	+263.806±67.5	+263.783±67.5	9.397	—	JANAF 4th recalculated, see text
463±24	+282.75±24	+283.40±24	9.393	222.093	selected value

^aData in italics may not be correct and are given only for comparison. Entropies are given for 1 bar. Data for enthalpy increments $-[H^{\circ}(0$ K) $-H^{\circ}(298.15$ K)] given in parentheses indicate the value used to compute enthalpies of formation at 298.15 from 0 K data or from dissociation energies. Data in curly braces are computed here using auxiliary data from Table 1 if not noted otherwise.

TABLE 7. Ideal gas thermochemical properties of NS(g) at standard state pressure, $p^{\circ}=0.1$ MPa ($T_r=298.15$ K)

T (K)	C_p° (J K ⁻¹ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	$-[G^{\circ}-H^{\circ}(298.15$ K)]/ T (J K ⁻¹ mol ⁻¹)	$H^{\circ}-H^{\circ}(298.15$ K) (kJ mol ⁻¹)	$\Delta_f H^{\circ}$ (kJ mol ⁻¹)	$\Delta_f G^{\circ}$ (kJ mol ⁻¹)	$\log K_f$ (kJ mol ⁻¹)
298.15	31.795	222.093	222.093	0.000	283.400	255.308	-44.7284
300	31.799	222.290	222.094	0.059	283.390	255.134	-44.4222
350	32.024	227.206	222.481	1.654	283.090	250.448	-37.3768
400	32.393	231.505	223.346	3.264	280.532	245.896	-32.1102
450	32.825	235.345	224.470	4.894	279.504	241.619	-28.0460
500	33.269	238.827	225.734	6.546	278.410	237.470	-24.8080
550	33.694	242.018	227.071	8.220	277.508	233.421	-22.1682
600	34.083	244.966	228.441	9.915	276.707	229.449	-19.9750
650	34.433	247.708	229.819	11.628	275.967	225.541	-18.1245
700	34.753	250.272	231.189	13.358	275.282	221.688	-16.5424
750	35.035	252.680	232.543	15.103	274.650	217.883	-15.1745
800	35.285	254.949	233.873	16.861	274.026	214.118	-13.9803
850	35.508	257.095	235.176	18.631	273.406	210.393	-12.9290
900	35.706	259.130	236.451	20.411	272.740	207.782	-12.0592
950	35.883	261.065	237.696	22.201	272.095	207.116	-11.3879
1000	36.041	262.910	238.911	23.999	271.447	206.448	-10.7836
1100	36.312	266.358	241.252	27.617	270.937	205.103	-9.7394
1200	36.535	269.528	243.478	31.260	220.008	203.752	-8.8690
1300	36.721	272.460	245.596	34.923	220.059	202.395	-8.1322
1400	36.878	275.187	247.613	38.603	220.092	201.034	-7.5006
1500	37.014	277.736	249.537	42.298	220.108	199.673	-6.9531
1600	37.132	280.129	251.375	46.005	220.107	198.310	-6.4741
1700	37.236	282.383	253.134	49.724	220.090	196.948	-6.0514
1800	37.330	284.514	254.818	53.452	220.059	195.588	-5.6757
1900	37.145	286.535	256.435	57.190	220.014	194.229	-5.3397
2000	37.493	288.456	257.988	60.935	219.957	192.874	-5.0373
2100	37.565	290.287	259.783	64.688	219.889	191.521	-4.7638
2200	37.633	292.036	260.923	68.448	219.811	190.172	-4.5152
2300	37.697	293.710	262.313	72.214	219.724	188.827	-4.2883
2400	37.758	295.316	263.655	75.987	219.629	187.486	-4.0805
2500	37.816	296.858	264.952	79.766	219.526	186.148	-3.8893
2600	37.873	298.343	266.208	83.550	219.418	184.815	-3.7129
2700	37.928	299.773	267.425	87.340	219.304	183.487	-3.5497
2800	37.983	301.153	268.605	91.136	219.186	182.162	-3.3982
2900	38.037	302.487	269.750	94.937	219.064	180.842	-3.2573

TABLE 7. Ideal gas thermochemical properties of NS(g) at standard state pressure, $p^\circ=0.1$ MPa ($T_r=298.15$ K)—Continued

T (K)	C_p° (J K ⁻¹ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	$-[G^\circ - H^\circ(298.15 \text{ K})]/T$ (J K ⁻¹ mol ⁻¹)	$H^\circ - H^\circ(298.15 \text{ K})$ (kJ mol ⁻¹)	$\Delta_f H^\circ$ (kJ mol ⁻¹)	$\Delta_f G^\circ$ (kJ mol ⁻¹)	$\log K_f$ (kJ mol ⁻¹)
3000	38.091	303.778	270.863	98.743	218.939	179.526	-3.1258
3100	38.145	305.027	271.945	102.555	218.810	178.215	-3.0029
3200	38.200	306.239	272.998	106.372	218.680	176.907	-2.8877
3300	38.257	307.416	274.023	110.195	218.548	175.604	-2.7795
3400	38.316	308.559	275.022	114.024	218.414	174.304	-2.6778
3500	38.376	309.670	275.996	117.859	218.279	173.009	-2.5820
3600	38.440	310.752	276.947	121.699	218.144	171.717	-2.4915
3700	38.507	311.806	277.875	125.547	218.008	170.430	-2.4060
3800	38.577	312.834	278.781	129.401	217.872	169.146	-2.3250
3900	38.652	313.837	279.667	133.262	217.737	167.865	-2.2483
4000	38.731	314.817	280.534	137.131	217.602	166.588	-2.1754
4100	38.815	315.774	281.382	141.009	217.468	165.314	-2.1061
4200	38.905	316.711	282.212	144.894	217.336	164.044	-2.0402
4300	39.000	317.627	283.025	148.790	217.205	162.777	-1.9773
4400	39.100	318.525	283.822	152.695	217.076	161.512	-1.9174
4500	39.206	319.405	284.603	156.610	216.950	160.251	-1.8601
4600	39.319	320.268	285.369	160.536	216.826	158.992	-1.8054
4700	39.438	321.114	286.120	164.474	216.706	157.737	-1.7530
4800	39.562	321.946	286.858	168.424	216.590	156.483	-1.7029
4900	39.693	322.763	287.582	172.387	216.477	155.232	-1.6548
5000	39.830	323.566	288.294	176.363	216.370	153.983	-1.6086
5100	39.972	324.357	288.993	180.353	216.267	152.736	-1.5643
5200	40.120	325.134	289.681	184.357	216.170	151.492	-1.5217
5300	40.273	325.900	290.357	188.377	216.079	150.249	-1.4808
5400	40.431	326.654	291.022	192.412	215.994	149.008	-1.4413
5500	40.593	327.397	291.677	196.463	215.916	147.768	-1.4034
5600	40.760	328.130	292.321	200.531	215.845	146.529	-1.3668
5700	40.930	328.853	292.956	204.615	215.782	145.292	-1.3314
5800	41.103	329.567	293.581	208.717	215.726	144.056	-1.2973
5900	41.279	330.271	294.197	212.836	215.678	142.821	-1.2644
6000	41.457	330.966	294.804	216.973	215.639	141.586	-1.2326

TABLE 8. Some thermochemical properties for PS(g) at $T=0$ K and $T=298.15$ K^a

D° (kJ mol ⁻¹)	$\Delta_f H^\circ(0 \text{ K})$ (kJ mol ⁻¹)	$\Delta_f H^\circ(298.15 \text{ K})$ (kJ mol ⁻¹)	$-[H^\circ(0 \text{ K}) - H^\circ(298.15 \text{ K})]$ (kJ mol ⁻¹)	$S^\circ(298.15 \text{ K})$ (J K ⁻¹ mol ⁻¹)	Sources and Notes
502±96	{+88.6±96}	{+88.4±96}	(9.616)	—	Gaydon (1968)
438±10	{+152.60±10}	{+152.44±10}	(9.616)	—	Drowart <i>et al.</i> (1973)
502±105	—	+238.5±105	9.611	234.41	Mills 1974
502±105	—	+88±105	9.611	234.41	Mills (1974), $\Delta_f H$ recal. from $D^\circ(0)$
550	{40.6}	{+40.4}	(9.616)	—	Lakshman and Venkataramanaiah (1980)
440±12	+150.598±12	+150.442±12	9.616	234.065	Gurvich <i>et al.</i> (1989)
413.8	{+176.8}	{+176.6}	(9.616)	—	Curtiss <i>et al.</i> (1991)
482	{+108.6}	{+108.4}	(9.616)	—	Moussaoui <i>et al.</i> (1998)
585.8±105	+154.465±41.8	+156.063±41.8	9.611	234.238	JANAF 2nd, $\Delta_f H$ for P _{red}
585.8±105	—	+156.063±105	9.610	—	Text to table in JANAF 3rd, 4th, $\Delta_f H$ for P _{red}
—	+138.765±41.8	+138.603±41.8	9.610	234.241	Tables in JANAF 3rd, 4th
438±10	+152.60±10	+152.44±10	9.616	234.065	selected value

^aData in italics may not be correct and are given only for comparison. Entropies are given for 1 bar. If not noted otherwise, data for the enthalpy of formation for PS (g) are in reference to P(white). Data for enthalpy increments, $-[H^\circ(0 \text{ K}) - H^\circ(298.15 \text{ K})]$, given in parentheses indicate the value used to compute enthalpies of formation at 298.15 from 0 K data or from dissociation energies. Data in curly braces are computed here using auxiliary data from Table 1 if not noted otherwise.

TABLE 9. Ideal gas thermochemical properties of PS(g) at standard state pressure, $p^{\circ}=0.1$ MPa ($T_r=298.15$ K)

T (K)	C_p° (J K ⁻¹ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	$-[G^{\circ}-H^{\circ}(298.15\text{ K})]/T$ (J K ⁻¹ mol ⁻¹)	$H^{\circ}-H^{\circ}(298.15\text{ K})$ (kJ mol ⁻¹)	$\Delta_f H^{\circ}$ (kJ mol ⁻¹)	$\Delta_f G^{\circ}$ (kJ mol ⁻¹)	$\log K_f$ (kJ mol ⁻¹)
298.15	35.242	234.065	234.065	0.000	152.440	104.466	-18.3018
300	35.259	234.283	234.066	0.065	152.419	104.169	-18.1371
350	35.672	239.750	234.497	1.839	151.098	96.245	-14.3635
400	36.002	244.536	235.459	3.631	148.146	88.546	-11.5628
450	36.262	248.792	236.708	5.438	146.721	81.172	-9.4221
500	36.469	252.624	238.111	7.256	145.225	73.972	-7.7277
550	36.638	256.108	239.591	9.084	143.912	66.911	-6.3546
600	36.779	259.302	241.103	10.920	142.695	59.965	-5.2203
650	36.898	262.251	242.617	12.762	141.535	53.118	-4.2686
700	36.995	264.989	244.119	14.609	140.426	46.359	-3.4593
750	37.080	267.544	245.596	16.461	139.368	39.677	-2.7633
800	37.154	269.940	247.044	18.317	138.318	33.065	-2.1589
850	37.219	272.194	248.457	20.176	137.272	26.519	-1.6296
900	37.277	274.323	249.836	22.039	83.180	21.112	-1.2253
950	37.329	276.340	251.178	23.904	82.811	17.674	-0.9718
1000	37.376	278.256	252.485	25.772	82.440	14.255	-0.7446
1100	37.458	281.822	254.992	29.513	81.693	7.473	-0.3548
1200	37.529	285.085	257.366	33.263	17.057	1.842	-0.0802
1300	37.592	288.091	259.615	37.019	17.045	0.575	-0.0231
1400	37.649	290.879	261.750	40.781	17.017	-0.691	0.0258
1500	37.701	293.479	263.780	44.549	16.975	-1.955	0.0681
1600	37.751	295.913	265.713	48.321	16.919	-3.215	0.1050
1700	37.798	298.203	267.557	52.099	16.851	-4.471	0.1374
1800	37.844	300.365	269.320	55.881	16.770	-5.723	0.1661
1900	37.889	302.412	271.009	59.667	16.678	-6.970	0.1916
2000	37.933	304.357	272.628	63.458	16.577	-8.212	0.2145
2100	37.978	306.209	274.183	67.254	16.466	-9.449	0.2350
2200	38.023	307.977	275.679	71.054	16.348	-10.680	0.2536
2300	38.069	309.668	277.121	74.859	16.222	-11.906	0.2704
2400	38.117	311.289	278.511	78.668	16.090	-13.126	0.2857
2500	38.168	312.846	279.853	82.482	15.953	-14.341	0.2996
2600	38.223	314.344	281.151	86.302	15.810	-15.550	0.3124
2700	38.281	315.788	282.407	90.127	15.664	-16.753	0.3241
2800	38.344	317.181	283.625	93.958	15.514	-17.951	0.3349
2900	38.413	318.528	284.805	97.796	15.361	-19.144	0.3448
3000	38.488	319.831	285.951	101.641	15.206	-20.331	0.3540
3100	38.570	321.095	287.064	105.494	15.048	-21.513	0.3625
3200	38.661	322.321	288.147	109.355	14.888	-22.690	0.3704
3300	38.759	323.512	289.201	113.226	14.727	-23.862	0.3777
3400	38.867	324.670	290.227	117.107	14.564	-25.028	0.3845
3500	38.984	325.799	291.227	121.000	14.400	-26.191	0.3909
3600	39.111	326.899	292.203	124.904	14.234	-27.348	0.3968
3700	39.249	327.972	293.155	128.822	14.068	-28.501	0.4024
3800	39.397	329.021	294.085	132.755	13.901	-29.649	0.4075
3900	39.556	330.046	294.994	136.702	13.732	-30.793	0.4124
4000	39.725	331.050	295.883	140.666	13.562	-31.932	0.4170
4100	39.905	332.033	296.753	144.647	13.390	-33.068	0.4213
4200	40.096	332.997	297.604	148.647	13.217	-34.199	0.4253
4300	40.297	333.943	298.439	152.667	13.042	-35.325	0.4291
4400	40.508	334.871	299.256	156.707	12.865	-36.448	0.4327
4500	40.728	335.784	300.058	160.769	12.685	-37.567	0.4361
4600	40.958	336.682	300.844	164.853	12.502	-38.682	0.4392
4700	41.196	337.565	301.616	168.961	12.317	-39.792	0.4422
4800	41.442	338.435	302.374	173.093	12.127	-40.899	0.4451
4900	41.695	339.292	303.119	177.249	11.934	-42.002	0.4477
5000	41.955	340.137	303.851	181.432	11.737	-43.100	0.4503
5100	42.221	340.971	304.570	185.641	11.535	-44.195	0.4526
5200	42.492	341.793	305.278	189.876	11.327	-45.286	0.4549
5300	42.768	342.605	305.975	194.139	11.115	-46.373	0.4570
5400	43.047	343.407	306.661	198.430	10.896	-47.455	0.4590
5500	43.329	344.199	307.336	202.749	10.671	-48.534	0.4609
5600	43.613	344.983	308.001	207.096	10.439	-49.608	0.4627
5700	43.897	345.757	308.657	211.471	10.200	-50.678	0.4644
5800	44.183	346.523	309.303	215.875	9.954	-51.744	0.4660
5900	44.468	347.281	309.941	220.308	9.700	-52.806	0.4675
6000	44.751	348.031	310.569	224.769	9.438	-53.863	0.4689

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4. References

- Berkowitz, J., Eland, J. H. D., and Appelman, E. H., *J. Chem. Phys.* **66**, 2183–2186 (1977).
- Blukis, U., and Myers, R., *J. Phys. Chem.* **69**, 1154–1156 (1965).
- Chase, M. W., *NIST-JANAF Thermochemical Tables*, 4th ed. [J. Phys. Chem. Ref. Data Monograph No. 9 (1998)].
- Chase, M. W., Curnutt, J. L., Downey, J. R., McDonald, R. A., Syverud, A. N., and Valenzuela, E. A., *JANAF Thermochemical Tables*, Supplement [J. Phys. Chem. Ref. Data **11**, 695–940 (1982)].
- Chase, M. W., Davis, C. A., Downey, J. R., Frurip, D. J., McDonald, R. A., and Syverud, A. N., *JANAF Thermochemical Tables*, 3rd ed., [J. Phys. Chem. Ref. Data, Suppl. **14** (1985)].
- Chiu, C. L., and Silvers, S. J., *J. Chem. Phys.* **63**, 1095–1098 (1975).
- Curtiss, L. A., Raghavachari, K., Trucks, G. W., and Pople, J. A., *J. Chem. Phys.* **94**, 7221–7229 (1991).
- Dibeler, V. H., and Liston, S. K., *J. Chem. Phys.* **49**, 482–485 (1968).
- Dressler, K., *Helv. Chim. Acta* **28**, 563–590 (1955).
- Drowart, J., Myers, C. E., Swarc, R., Vander Auwera-Mahieu, A., and Uy, O. M., *High Temp. Sci.* **5**, 482–488 (1973).
- Gaydon, A. G., *Dissociation Energies and Spectra of Diatomic Molecules* (Chapman and Hall, London, 1953).
- Gaydon, A. G., *Dissociation Energies and Spectra of Diatomic Molecules*, 3rd ed. (Chapman and Hall, London, 1968).
- Gurvich, L. V., Veyts, I. V., and Alcock, C. B., *Thermodynamic Properties of Individual Substances*, 4th ed. (Hemisphere, New York, 1989), Vol. 1, Parts 1 and 2.
- Hagemann, R., Botter, R., Nief, G., and Roth, E., *Ann. Genie Chim.* **3**, 33–41 (1967).
- Hwang, R. J., and Benson, S. W., *Int. J. Chem. Kinet.* **11**, 579–583 (1979).
- Lakshman, S. V. J., and Venkataramanaiah, M., *Curr. Sci.* **15**, 579–581 (1980).
- Lodders, K., *J. Phys. Chem. Ref. Data* **28**, 1705–1712 (1999).
- Mackle, H., *Tetrahedron* **19**, 1159–1170 (1963).
- Mills, K. C., *Thermodynamic Data for Inorganic Sulphides, Selenides and Tellurides* (Butterworth, London, 1974).
- Morley, G. P., Lambert, I. R., Mordaunt, D. H., Wilson, H. S., Ashfold, M. N. R., Dixon, R. N., and Western, C. M., *J. Chem. Soc. Faraday Trans.* **89**, 3865–3875 (1993).
- Moussaoui, Y., Ouamerali, O., and De Mare, G. R., *J. Mol. Struct.* **425**, 237–247 (1998).
- Murai, H., Yagi, T., Obi, K., and Tanaka, I., *Chem. Phys. Lett.* **61**, 513–517 (1979).
- Nicovich, J. M., Kreutter, K. D., van Dijk, C. A., and Wine, P. H., *J. Phys. Chem.* **96**, 2518–2528 (1992).
- Norwood, K., and Ng, C. Y., *Chem. Phys. Lett.* **156**, 145–150 (1989).
- Nourbakhsh, S., Norwood, K., Yin, H. M., Liao, C. L., and Ng, C. Y., *J. Chem. Phys.* **95**, 946–954 (1991).
- O'Hare, P. A. G., *J. Chem. Phys.* **52**, 2292–2996 (1970).
- Rempala, K., and Ervin, K. M., *J. Chem. Phys.* **112**, 4579–4590 (2000).
- Shiell, R. C., Hu, X. K., Hu, Q. J., and Hepburn, J. W., *J. Phys. Chem.* **104**, 4339–4342 (2000).
- Stull, D. R., and Prophet, H., *JANAF Thermochemical Tables*, 2nd ed. [NSRDS-NBS **37**, 1141 pp. (1971)].
- Wagman, D. D., Evans, W. H., Parker, V. B., Schumm, R. H., Halow, I., Bailey, S. M., Churney, K. L., and Nuttall, R. L., *The NBS Tables of Chemical Thermodynamic Properties*, [J. Chem. Phys. Ref. Data **11**, Suppl. 2 (1982)].
- Wilson, S. H. S., Howe, J. D., and Ashfold, M. N. R. *Mol. Phys.* **88**, 841–858 (1996).