

Thermodynamic Properties of Some Gaseous Halogen Compounds

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Tables of values of the heat of formation, ΔH_f° ; free energy of formation, ΔF_f° ; logarithm of the equilibrium constant of formation, $\log_{10} K_f$; free-energy function, $(F^\circ - H_0^\circ)/T$; heat-content function, $(H^\circ - H_0^\circ)/T$; entropy, S° ; heat content, $(H^\circ - H_0^\circ)$, and heat capacity, C_p° , are given from 0° K to high temperatures for the following gaseous substances: F, F₂, F₂O, Cl, Cl₂, ClO₂, Cl₂O, ClF, ClF₃, Br, Br₂, BrF, BrF₃, BrCl, I, I₂, IF, IF₅, IF₇, ICl and IBr. The data used in preparing the tables are discussed in detail.

1. Introduction

As part of the general program of the National Bureau of Standards on the collection, analysis, and compilation of data on the chemical thermodynamic properties of substances [1, 2]², the available information relating to the heats and free energies of formation and the thermodynamic functions of a number of gaseous halogen and oxyhalogen molecules has been assembled and reviewed. Tables of selected values of the heat of formation, ΔH_f° ; free energy of formation, ΔF_f° ; logarithm of the equilibrium constant of formation, $\log_{10} K_f$; free-energy function, $(F^\circ - H_0^\circ)/T$; heat-content function, $(H^\circ - H_0^\circ)/T$; entropy, S° ; heat content, $(H^\circ - H_0^\circ)$; and heat capacity, C_p° , are given from 0° K to high temperatures for the gaseous substances F, F₂, F₂O, Cl, Cl₂, ClO₂, ClF, ClF₃, Br, Br₂, BrF, BrF₃, BrCl, I, I₂, IF, IF₅, IF₇, ICl, and IBr. Some of the values reported here have been published [1], but no analysis of the data used to obtain the values was given. The present report not only includes a discussion of the sources and treatment of the data but also makes use of the available molecular and spectroscopic data to extend the tables to include values for high temperatures. It is this high-temperature region that is of great interest and importance to many engineers, chemists, and physicists working in the fields of reaction kinetics, fuels, propellants, and explosives.

2. Units and Standard States

The calorie used in these calculations is the thermochemical calorie, defined as 4.1840 abs j. The other constants used are those given by Wagman et al. [2]. The ice point, 0° C, is taken as 273.16° K [3]. The chemical atomic weights used are [4] O, 16; F, 19.00; Cl, 35.457; Br, 79.916; I, 126.91. The standard state chosen for all gases is the ideal gas at 1-atm pressure. As is customary, nuclear spin and isotopic mixing effects are omitted; all

values are for the naturally occurring isotopic mixture.

3. Calculations of the Thermodynamic Functions

3.1. Monatomic Gases

The translational contributions to the thermodynamic functions of the monatomic gases F, Cl, Br, and I were calculated by use of the equations given by Wagman et al. [2] (corrected for the new definition of the thermochemical calorie). The additional contributions due to electronic excitation were evaluated by direct summation [5]. The energy levels and multiplicities used were taken from Moore [6].

3.2. Diatomic Gases

The translational contributions to the thermodynamic functions for the diatomic molecules other than F₂ and ClF were evaluated with the same equations used for the monatomic gases [2]. The rotational and vibrational constants given in table 1 were used to calculate the thermodynamic functions for a rigid rotator [2] with moment of inertia I , equal to $h/[8\pi^2cB_e(1-\alpha_e/2)]$, and an independent harmonic oscillator [8] with a fundamental frequency $(\omega_e - 2x_e\omega_e)$.³ These constants have been adjusted to the usual isotopic mixture, using the product rule; isotopic masses were taken from Collins, Nier, and Johnson [9] (Cl), and Bainbridge and Nier [10] (Br).

Corrections for rotational stretching, vibrational anharmonicity, and rotational-vibrational interaction were calculated at 250°, 300°, 500°, 1,000°, and 1,500° K (and 2,000°, 2,500°, and 3,000° K for Cl₂, Br₂, and I₂), using equations [5] based on the treatment of the general diatomic molecule given by Mayer and Mayer [11]. Values at intermediate temperatures were obtained by graphical interpolation. Table 2 shows the magnitude of these corrections at 1,500° K.

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² Figures in brackets indicate the literature references at the end of this paper.

³ The spectroscopic notation is that used by Herzberg [14].

TABLE 1. Molecular constants used in calculating the thermodynamic functions for the diatomic halogen molecules

	P_e	α_e	ω_e	$x_e\omega_e$	$10^8 D_e$
F_2 -----	cm^{-1} 0.8901 [12,13]	cm^{-1} 0.0146 [7]	cm^{-1} 919.0 [12,13]	cm^{-1} 13.6 [7]	cm^{-1} 334. [7]
Cl_2 -----	0.2404 [14]	0.00166 [14]	561.0 [14]	3.94 [14]	^a 17.66
ClF -----	0.514012 [15]	0.0043272 [15]	784.43 [16,17]	6.20 [16,17]	86.9 [15]
Br_2 -----	0.08092 [14]	0.000275 [14]	323.2 [14]	1.07 [14]	2.03 [14]
BrF -----	0.356319 [18]	0.005206 [18]	673 [19,20]	4. [19,20]	^a 40.0
$BrCl$ -----	0.150797 [21]	0.0007597 [21]	443.1 [22,23]	1.8 [22]	^a 6.99
I_2 -----	0.037364 [24]	0.0001206 [24]	214.248 [24]	^b 0.6074 [24]	^a 0.455
IF -----	^d 0.2799	^e 0.00763	^c 612. [19]	^e 4. [19]	^a 23.42
ICl -----	0.112984 [25]	0.0005275 [25]	382.18 [14]	1.450 [14]	5.19 [14]
IBr -----	^d 0.05634	^e 0.000193	267.4 [14]	0.77 [14]	^a 1.00

^a Calculated from the relationship $D_e = (4F_e^2/\omega_e^2)$ [27].

^b $y_{e\omega_e} = 0.00130$; $x_e\omega_e = 0.0000525$.

^c Recalculated from Durie's data [19].

^d Calculated from the constants of the other halogen molecules, using Schomaker and Stevenson's relation [26].

^e Calculated from the relationship $\alpha_e = \frac{6B_e^2}{\omega_e} \left[\left(\frac{x_e\omega_e}{B_e} \right)^{1/2} - 1 \right]$ [27]

The thermodynamic functions of F_2 and ClF were taken from unpublished calculations made by the Heat and Power Division of the Bureau [7]. These were calculated in essentially the way outlined above.

TABLE 2. Corrections added to the thermodynamic functions obtained by the rigid rotator-harmonic oscillator approximation at 1,500° K, cal deg mole

	$-(F^0 - H_0^0)/T$	$(H^0 - H_0^0)/T$	C_p^0
F_2 -----	0.0696	0.1083	0.247
Cl_2 -----	.0628	.0860	.182
ClF -----	.0487	.0709	.156
Br_2 -----	.0629	.0762	.155
BrF -----	.0646	.0894	.190
$BrCl$ -----	.0567	.0722	.149
I_2 -----	.0867	.0991	.200
IF -----	.0563	.0780	.166
ICl -----	.0625	.0776	.159
IBr -----	.0710	.0833	.169

3.3. Polyatomic Gases

The thermodynamic functions for the polyatomic molecules, except ClO_2 , were calculated by using the rigid rotator-harmonic oscillator approximation [2,8]. The molecular data used, summarized in table 3, are as follows:

F_2O (table 9). The infrared spectrum has been measured by Bernstein and Powling [28]; Jones, Kirby-Smith, Woltz, and Nielsen [29]; Hettner, Pohlman, and Schumacher [30]; and Sutherland and Penney [31]. From their data the three nondegenerate fundamental frequencies were taken as 461, 828, and 929 cm^{-1} . The structural parameters nec-

essary to calculate the moments of inertia were calculated by Bernstein and Powling [28] from a combination of their infrared data and various electron diffraction data;⁴ they obtained a F-O-F angle of $101.5 \pm 1.5^\circ$ and a F-O distance of 1.38 Å. The symmetry of the molecule is C_{2v} . The product $I_A I_B I_C$ from these data is $88.65 \times 10^{-117} g^3 cm^6$.

TABLE 3. Molecular constants used in calculating the thermodynamic functions for the polyatomic halogen and oxyhalogen molecules

Molecule	Frequencies	Moments of inertia
	cm^{-1}	$10^{-30} g cm^2$
F_2O -----	461; 828; 929	7.211; 1.424; 8.635
ClO_2 ^a -----	450.1; 958.0; 1128.2	8.411; 1.749; 10.160
Cl_2O -----	320; 684; 971	23.028; 2.032; 25.060
ClF_3 -----	247; 318; 426; 508; 710; 750	6.1129; 18.1803; 24.3148
BrF_3 -----	244 b; 315; 365; 415 b; 481; 536; 572; 626 b; 683.	33.77; 28.16; 28.16
IF_5 -----	192 b; 275; 317; 375 b; 572; 605; 645 b; 693; 710.	39.53; 33.03; 33.03
IF_7 -----	250 b; 313 b; 350 b; 360 b; 426 b; 511 b; 547 b; 635; 638; 670; 678.	52.82; 47.54; 47.54

^a Anharmonicity terms also available.

^b Doubly degenerate frequencies.

ClO_2 (table 12). Nielsen and Woltz [33], by combining their infrared data with that of Bailey and Cassie [34], Hedberg [35], Coon [36, 37], and Coon and Ortiz [38], and with the Raman data of Kujumzelis [39], were able to obtain the harmonic fundamentals and the anharmonic constants for the ground state. Dunitz and Hedberg [40] and Coon [41] have measured the Cl-O distance as 1.487 Å and the O-Cl-O angle as 115.5° . The symmetry is C_{2v} . The product $I_A I_B I_C$ is then $149.46 \times 10^{-117} g^3 cm^6$.

These data were used to compute the thermodynamic functions for a rigid rotator-anharmonic oscillator by the method of Stockmayer, Kavanagh, and Mickley [42]. At 1,500° K the corrections to the harmonic oscillator approximation were 0.043, 0.080, and 0.174 cal/deg mole for $-(F^0 - H_0^0)/T$, $(H^0 - H_0^0)/T$, and C_p^0 , respectively.

Cl_2O (table 13). The infrared spectrum has been studied by Hedberg [35], Bailey and Cassie [43], Pohlman and Schumacher [44], and Sutherland and Penney [31]. From their data the three nondegenerate frequencies were taken as 320, 684, and 971 cm^{-1} . Dunitz and Hedberg [40] obtained the molecular structure from electron diffraction measurements. The symmetry is C_{2v} . Their values lead to a product $I_A I_B I_C$ of $1,173 \times 10^{-117} g^3 cm^6$.

ClF_3 (table 15). Jones, Parkinson, and Murray [45] have measured the Raman spectrum of the liquid and the infrared spectrum of the gas; Schäfer and Wicke [46] have also measured the Raman spectrum of the liquid. Unfortunately their assignments were based upon a pyramidal C_{3v} structure. Recently, Smith [47], from microwave measurements, and Burbank and Bensey [125], from X-ray diffraction measurements on the solid, have

⁴ After these calculations had been completed, Ibers and Schomaker [32] reported new electron diffraction data. They selected as the "best" values, based upon their own and upon other data, a F-O distance of 1.418 Å and a F-O-F angle of 103.2° . Use of these values would increase the values of $-(F^0 - H_0^0)/T$ and S^0 in table 9 by 0.16 cal/deg mole, and make the values of ΔF^0 more negative by (0.16T/1000) kcal/mole.

shown that the structure is a planar distorted "T" with C_{2v} symmetry. Such a molecule has six nondegenerate fundamental frequencies, all of which are both infrared and Raman active. On the basis of the C_{2v} symmetry a selection of the apparent fundamental frequencies was made from the spectral data: 247, 318, 426, 508, 710, and 750 cm^{-1} . The microwave data of Smith [47] give a product $I_A I_B I_C$ of $2702.2 \times 10^{-117} \text{ g}^3 \text{ cm}^6$.

BrF₅ (table 19). The Raman spectrum of BrF₅ has been measured by Stephenson and Jones [48]; with the aid of the infrared data of Burke and Jones [49], they have assigned the fundamental frequencies based upon a C_{4v} structure. In the absence of experimental data on the structure of BrF₅ it was assumed that the bromine atom is located at the center of mass and that the Br—F distance is 1.69 Å. This distance is based on Pauling's tetrahedral radii [50] and a value for F of 0.55 Å, based on CF₄. (See Allen and Sutton [51].) The product $I_A I_B I_C$ is then $26.78 \times 10^{-114} \text{ g}^3 \text{ cm}^6$.

IF₅ (table 24). Lord, Lynch, Schumb, and Slowinski [52] have measured the Raman and infrared spectra and assigned the fundamental frequencies on the basis of a C_{4v} structure. The I—F distance used, 1.83 Å, was obtained in the same way as the Br—F distance in BrF₅. The product $I_A I_B I_C$ is then $43.13 \times 10^{-114} \text{ g}^3 \text{ cm}^6$.

IF₇ (table 25). The Raman and infrared spectra were measured by Lord, Lynch, Schumb, and Slowinski [52]; they have assigned the fundamentals on the basis of a pentagonal bipyramidal D_{5h} structure. Slutsky and Bauer [53] report provisional electron diffraction data that lead to 1.93 Å for the two I—F bonds along the principal rotation axis and 1.83 Å for the radial bonds. These give a product $I_A I_B I_C$ of $131.62 \times 10^{-114} \text{ g}^3 \text{ cm}^6$.

4. Calculation of the Heats and Free Energies of Formation

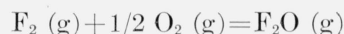
The heats of formation of gaseous O₂, F₂, Cl₂, Br₂, and I₂ are taken as zero (reference state); for bromine and iodine this differs from the liquid and solid states customarily used at 25° C [1]. Auxiliary data, except where noted otherwise, have been taken from Rossini et al. [1].

F (g). The dissociation energy of F₂ (g) has been the subject of much discussion in recent years. (See the reviews by Nathans [54], Evans, Warhurst, and Whittle [55], and Herzberg [14].) From the recent experimental measurements, summarized in table 4, we have selected the heat of dissociation of F₂ as $36.7 \pm 1.0\text{ kcal}.$ ⁵ This gives

$$\frac{1}{2} \text{F}_2 (\text{g}) = \text{F} (\text{g})$$

$$\Delta H_0^\circ = 18.4 \pm 0.5 \text{ kcal.}$$

F₂O (g). Von Wartenberg and Klinkott [61] have measured the heat of reaction of fluorine oxide with an aqueous solution of potassium iodide containing hydrofluoric acid to give a solution of potassium triiodide and potassium fluoride; they obtained $\Delta H_{291} = -176.6\text{ kcal/mole}$. When combined with the necessary auxiliary heats of formation their data give $\Delta H_{298.16}^\circ \text{F}_2\text{O} (\text{g}) = 6.0\text{ kcal/mole}$. They also measured the heat of reaction of fluorine oxide with aqueous potassium hydroxide to form oxygen gas and aqueous potassium fluoride, and obtained $\Delta H_{291} = -135.8\text{ kcal/mole}$. This gives $\Delta H_{298.16}^\circ \text{F}_2\text{O} (\text{g}) = 7.1\text{ kcal/mole}$. In a third experiment they measured the heat of reaction of fluorine oxide with aqueous hydrobromic acid to form a solution of bromine and hydrofluoric acid, obtaining $\Delta H_{291} = -134.4\text{ kcal/mole}$. If corrections are applied for the heats of solution of HBr and HF in aqueous hydrobromic acid (see Ruff and Menzel [62]), this value gives $\Delta H_{298.16}^\circ \text{F}_2\text{O} (\text{g}) = 9.7\text{ kcal/mole}$. The average was selected as the "best" value:



$$\Delta H_{298.16}^\circ = 7.6 \pm 2.0 \text{ kcal.}$$

Cl (g). Gaydon [63] calculated from various spectral data $D_0^\circ = 19,969\text{ cm}^{-1}$, or 57.08 kcal. This gives

$$1/2 \text{Cl}_2 (\text{g}) = \text{Cl} (\text{g})$$

$$\Delta H_0^\circ = 28.54 \pm 0.05 \text{ kcal.}$$

⁵ All uncertainties, unless otherwise indicated, represent our estimate of the over-all uncertainty.

TABLE 4. Dissociation energy of F₂

Observer	Method	Temperature range	Number of experiments	H_0° ^a
		° K		kcal
Wicke and Friz [56].....	H ₂ +F ₂ explosion.....	Approx. 1,000....	5	36.36±1.34
Gilles and Margrave [57]....	Gas density.....	815 to 869.....	3	32.07±0.76
Doescher [58].....	do.....	760 to 1,115.....	24	36.75±0.03
Wise [59].....	Effusion.....	508 to 676.....	9	38.36±0.28
Barrow and Caunt [60].....	Dissociation of alkali halides.....	^b 36.6±3.5

^a Probable error of the mean.

^b Over-all uncertainty as given by authors.

Attempts have been made to measure the dissociation of Cl_2 at high temperatures. Because of the difficulties of working at the high temperatures necessary to obtain measurable pressure changes, the results are not too concordant. Von Wartenberg and Henglein [64, 65] obtained gas-density data in the range 955° to $1,151^\circ$ K, which lead to $D_0^\circ=53.0$ kcal. Wohl [66], from measurements of the pressure rise during explosions of $\text{H}_2\text{-Cl}_2$ gas mixtures, calculated $D_0^\circ=59.1$ kcal. Trautz and Geissler [67] measured gas densities between $1,425^\circ$ and $1,537^\circ$ K; their data give $D_0^\circ=49.9$ kcal. These last measurements were questioned by von Wartenberg and Weigel [68], who obtained data at $1,478^\circ$ K that give $D_0^\circ=56.4$ kcal. Except for the value from Trautz and Geissler, the results agree with the spectroscopic value within their estimated uncertainties of ± 2 to 3 kcal.

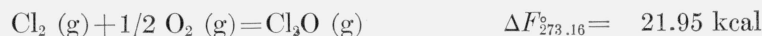
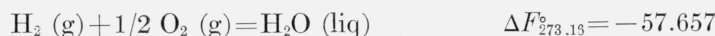
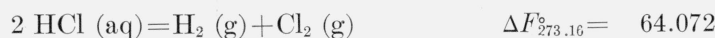
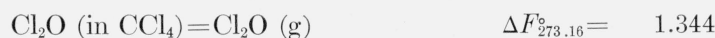
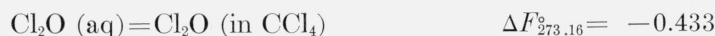
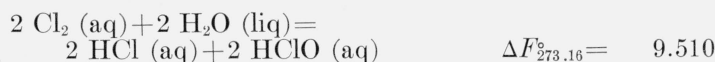
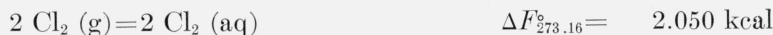
ClO_2 (g). Wallace and Goodeve [69] measured the heat of explosion of chlorine dioxide gas into the elements; their data give $\Delta H_{298.16}^\circ \text{ClO}_2$ (g) = 26.3 kcal. Booth and Bowen [70] also studied this decomposition and obtained $\Delta H_{298.16}^\circ \text{ClO}_2$ (g) = 23.5 kcal. Mayer [71], from spectroscopic measurements of predissociation, obtained $\Delta H_0^\circ=3.6$ kcal for the reaction ClO_2 (g) = Cl (g) + O_2 (g). This gives $\Delta H_{298.16}^\circ \text{ClO}_2$ (g) = 24.4 kcal. Finkelnburg and Schumacher [72] measured spectroscopically the

ionization dissociation energy of ClO_2 (g) to ClO (g) and O^+ (g) as 111 kcal. If this is combined with the dissociation energy of ClO (g) given by Parker and Wright [73], $D_0^\circ=60.7$ kcal, then $\Delta H_{298.16}^\circ \text{ClO}_2$ (g) = 18.7 kcal is obtained. However, Finkelnburg and Schumacher state that their value for the dissociation energy is probably high by 5 or 6 kcal because of predissociation; this correction would give a value of about 24.5 kcal for $\Delta H_{298.16}^\circ \text{ClO}_2$ (g). A value based primarily on the heats of explosion was selected:



$$\Delta H_{298.16}^\circ = 25.0 \pm 1.5 \text{ kcal.}$$

Cl_2O (g). Jakowkin [74] measured the solubility of chlorine gas in water and the hydrolysis equilibrium of aqueous chlorine to give aqueous hydrochloric and hypochlorous acids. Goldschmidt [75] studied the hydrolysis equilibrium of Cl_2O (aq) to give hypochlorous acid, and the equilibrium distribution of Cl_2O between water and carbon tetrachloride; his data have been recalculated by Roth [76]. Yost and Felt [77] measured the solubility of Cl_2O (g) in carbon tetrachloride. These data give the following series of free-energy equations:



From the thermodynamic functions $\Delta S_{273.16}^\circ = -14.06$ cal/deg mole for this reaction. Combining these gives $\Delta H_{273.16}^\circ \text{Cl}_2\text{O}$ (g) = 18.10 kcal; corrected to 298.16° K, this becomes 18.08 kcal.

Thomsen [78] measured the heat of hydrolysis of Cl_2O (g) to HClO (aq) as $\Delta H_{291} = -9.44$ kcal, which becomes -9.51 kcal at 298.16° K. He also measured the heat of the reaction of chlorine gas with aqueous sodium hydroxide to give an aqueous solution of sodium chloride and sodium hypochlorite, and the heats of neutralization of hydrochloric and hypochlorous acids with aqueous sodium hydroxide. Combining these data gives $\Delta H_{298.13}^\circ \text{Cl}_2\text{O}$ (g) = 18.3 kcal.

Wallace and Goodeve [69] obtained the heat of explosion of Cl_2O (g); their data give $\Delta H_{298.16}^\circ \text{Cl}_2\text{O}$ (g) = 21.4 kcal. Günther and Wekua [79] also measured the heat of explosion; their data give $\Delta H_{298.16}^\circ \text{Cl}_2\text{O}$ (g) = 24.7 kcal.

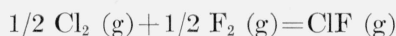
For the "best" value we have taken



$$\Delta H_{298.16}^\circ = 18.1 \pm 0.3 \text{ kcal.}$$

ClF (g). Wicke and Friz [56, 80] measured the heat evolved in the adiabatic explosion of $\text{Cl}_2\text{-F}_2$ mixtures; their results give $\Delta H_{298}^\circ \text{ClF}$ (g) = -11.7

kcal. Schmitz and Schumacher [81] measured the heat of the reaction $\text{NaCl (c)} + \text{ClF (g)} = \text{NaF (c)} + \text{Cl}_2 \text{(g)}$ at 18°C . Their value of ΔH , -24.5 kcal, gives $\Delta H_f^\circ \text{ ClF (g)} = -13.3$ kcal. They also measured the heat of the reaction $1/2 \text{F}_2 \text{(g)} + \text{NaCl (c)} = \text{NaF (c)} + 1/2 \text{Cl}_2 \text{(g)}$; if this heat, $\Delta H = -39.5$ kcal, is combined with that given above for the reaction of ClF, then $\Delta H_f^\circ \text{ ClF (g)} = -15.0$ kcal. Schmitz and Schumacher [82], Schumacher, Schmitz, and Brodersen [83], and Warhaftig [84] obtained the dissociation limit of ClF (g) from spectroscopic measurements. Two combinations of dissociation products are possible: $\text{Cl}(^2\text{P}_{1/2}) + \text{F}(^2\text{P}_{3/2})$ or $\text{Cl}(^2\text{P}_{3/2}) + \text{F}(^2\text{P}_{1/2})$. After reducing the measured dissociation energies to the atomic ground states, using energies from Moore [6], the values in table 5 are obtained. These data give $\Delta H_f^\circ \text{ ClF (g)} = -12.0$ or -13.4 kcal. The data for IBr (g) and ICl (g) (see below) show that in these molecules the lighter atom is in the excited $^2\text{P}_{1/2}$ state; by analogy the fluorine should be in the excited state. This choice also agrees somewhat better with the data for ClF_3 (g). (See also, the discussion by Slutsky and Bauer [53].) The "best" value appears to be



$$\Delta H_f^\circ = -13.4 \pm 0.5 \text{ kcal.}$$

TABLE 5. Dissociation energy of ClF

Observer	D_0° , kcal, if products of dissociation are—	
	$\text{Cl}(^2\text{P}_{1/2}) + \text{F}(^2\text{P}_{3/2})$	$\text{Cl}(^2\text{P}_{3/2}) + \text{F}(^2\text{P}_{1/2})$
Schmitz and Schumacher [82]-----	59.00	60.37
Schumacher, Schmitz, and Brodersen [83]-----	58.97	60.34
Warhaftig [84]-----	58.96	60.33

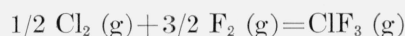
Ruff and Laass [85] measured the heat of reduction of ClF (g) by hydrogen. The data they report are self-consistent, but give a much too negative value of -27.6 kcal for $\Delta H_f^\circ \text{ ClF (g)}$.

ClF₃ (g). Schmitz and Schumacher [86] reported three measurements of the equilibrium constant for the reaction $\text{ClF}_3 \text{(g)} = \text{ClF (g)} + \text{F}_2 \text{(g)}$; their data give $\Delta H_0^\circ = 24.50$ kcal for this reaction. Schäfer and Wicke [46] reported 13 measurements of the same equilibrium; their results as read from a graph give $\Delta H_0^\circ = 24.6$ kcal. The value $\Delta H_0^\circ = 24.5$ kcal was selected for this reaction. Two possible values of $\Delta H_f^\circ \text{ ClF (g)}$ may be combined with this value of ΔH_0° to calculate the heat of formation of ClF_3 . If $\Delta H_f^\circ \text{ ClF (g)}$ is taken as -12.0 kcal, $\Delta H_f^\circ \text{ ClF}_3 \text{(g)} = -36.5$ kcal; if $\Delta H_f^\circ \text{ ClF (g)}$ is -13.4 kcal, the value for ClF_3 becomes -37.9 kcal.

Schmitz and Schumacher [81] also obtained, at 18°C , for the reaction $\text{ClF}_3 \text{(g)} + 3 \text{NaCl (c)} = 3 \text{NaF (c)} + 2 \text{Cl}_2 \text{(g)}$, $\Delta H = -76.5$ kcal. A number of different values of $\Delta H_f^\circ \text{ ClF}_3 \text{(g)}$ can be calculated from this value, depending upon the auxiliary data used. If the heats of formation of NaCl and NaF are taken as the selected "best" values [1], $\Delta H_f^\circ \text{ ClF}_3 \text{(g)} =$

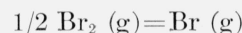
-35.9 kcal. A second value can be obtained by using Schmitz and Schumacher's [81] data for the reaction, at 18°C , $1/2 \text{F}_2 \text{(g)} + \text{NaCl (c)} = 1/2 \text{Cl}_2 \text{(g)} + \text{NaF (c)}$, $\Delta H = -39.5$ kcal, and the selected heat of formation of NaCl. From these data we calculate $\Delta H_f^\circ \text{ ClF}_3 \text{(g)} = -41.9$ kcal. The third and fourth values are obtained by combining Schmitz and Schumacher's [81] data for the reaction $\text{ClF (g)} + \text{NaCl (c)} = \text{NaF (c)} + \text{Cl}_2 \text{(g)}$, $\Delta H = -24.5$ kcal at 18°C , with the data for the similar reaction with ClF_3 given above, to get $\text{ClF}_3 \text{(g)} + \text{Cl}_2 \text{(g)} = 3 \text{ClF (g)}$, $\Delta H = -3.0$ kcal. Depending upon the value chosen for $\Delta H_f^\circ \text{ ClF (g)}$, -12.0 or -13.4 kcal, this gives $\Delta H_f^\circ \text{ ClF}_3 \text{(g)} = -32.1$ or -36.3 kcal, respectively.

The value most consistent with all of the data summarized above, and also with the data for ClF, seems to be that from the equilibrium measurements. We have selected as the "best" value



$$\Delta H_0^\circ = -37.9 \pm 1.0 \text{ kcal.}$$

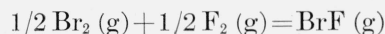
Br (g). Herzberg [14] and Gaydon [63] give the dissociation energy $D_0^\circ \text{ (Br}_2)$ as 1.971 eV, or 45.456 kcal. This was used to obtain the selected value



$$\Delta H_0^\circ = 22.73 \pm 0.05 \text{ kcal.}$$

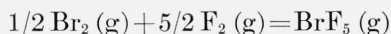
Vapor-density measurements have been made at high temperatures by von Wartenberg and Henglein [64, 65] (833° to $1,003^\circ \text{K}$), Perman and Atkinson [87, 88] ($1,175^\circ$ to $1,330^\circ \text{K}$), Cramer [87] ($1,056^\circ$ to $1,558^\circ \text{K}$), and Bodenstern and Schmidt [126] ($1,495^\circ \text{K}$). Their data give, respectively, 46.33, 44.92, 46.04, and 45.20 kcal for $D_0^\circ \text{ (Br}_2)$, in agreement with the spectroscopic value within the estimated uncertainty of ± 1.0 kcal. DeVries and Rodebush [90] have also reported data in the range 923° to $1,173^\circ \text{K}$; their data give values of D_0° , approximately 5 kcal more positive, which show a pronounced trend with temperature.

BrF (g). Durie [19] has obtained the spectroscopic dissociation limit of BrF as $21,190 \text{ cm}^{-1}$. As in the case of ClF, there are two possible sets of dissociation products: $\text{Br}(^2\text{P}_{1/2}) + \text{F}(^2\text{P}_{3/2})$ or $\text{Br}(^2\text{P}_{3/2}) + \text{F}(^2\text{P}_{1/2})$. Correcting the observed dissociation limit to the ground states of the atoms gives two values for $D_0^\circ \text{ (BrF)}$; if fluorine is the excited atom ($\text{F}(^2\text{P}_{1/2})$), $D_0^\circ = 59.42$ kcal; if bromine is excited, $D_0^\circ = 50.04$ kcal. By analogy with ClF and IF (see below) the "best" value seems to be the higher one: this gives



$$\Delta H_0^\circ = -18.3 \pm 0.5 \text{ kcal.}$$

BrF₅ (g). Experimental data leading to a heat of formation for BrF₅(g) are not available. Slutsky and Bauer [53] have estimated average bond energies that give



$$\Delta H_0^\circ = -122 \pm 10 \text{ kcal.}$$

BrCl (g). The equilibrium $2 \text{BrCl}(\text{g}) = \text{Br}_2(\text{g}) + \text{Cl}_2(\text{g})$ has been studied by several investigators; their results are summarized in table 6. The average of all, except Jost's, gives

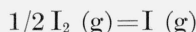


$$\Delta H_0^\circ = -0.20 \pm 0.05 \text{ kcal.}$$

TABLE 6. Heat of dissociation of BrCl (g)

Observer	ΔH_0°
	<i>kcal</i>
Mattraw, Pachucki, and Hawkins [22].....	0.150
Braune and Victor [92].....	.105
Vesper and Rollefson [93].....	.245
Gray and Style [94].....	.233
Beeson and Yost [95].....	.265
Jost [96].....	.378

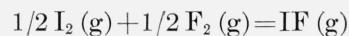
I (g). Gaydon [63] and Herzberg [14] give the dissociation limit of I₂ to I(²P_{1/2}) + I(²P_{3/2}) as 20,037 cm⁻¹. When corrected to the ground state this becomes 12,434 cm⁻¹, or 35.543 kcal, for D₀⁰ (I₂). High-temperature gas-density measurements have been made by Braune and Ramstetter [87] (915° to 1,385° K), Starck and Bodenstern [98] (1,073° to 1,473° K), DeVries and Rodebush [90] (732° to 898° K), Bodenstern and Schmidt [126] (1,495° K), and Perlman and Rollefson [99] (872° to 1,274° K). Their data give values of D₀⁰ (I₂) of 35.95, 35.49, 35.68, 35.17, and 35.534 kcal, respectively. We have taken 35.538 kcal as the "best" value for D₀⁰ (I₂); this is the average of the values from the very careful work of Perlman and Rollefson and from the spectroscopic data. Consequently,



$$\Delta H_0^\circ = 17.77 \pm 0.03 \text{ kcal}$$

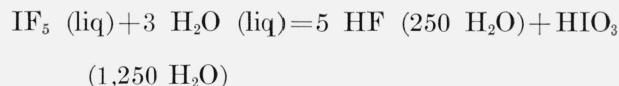
IF (g). Durie [19] has obtained the dissociation limit of IF as 23,570 cm⁻¹. As in the case of the other interhalogen compounds, two sets of dissociation products are possible: I(²P_{1/2}) + F(²P_{3/2}) or I(²P_{3/2}) + F(²P_{1/2}). When corrected to the normal atoms, this limit gives D₀⁰ (IF) as 45.64 or 66.22 kcal, respectively. Durie and Gaydon [91], arguing from the much higher stability of IF₅, as compared with IF, favored the lower value. However, Slutsky and Bauer [53] have pointed out a numerical error in their calculations, which removes the chief support for the low value, and presented additional evidence favoring the high value. The data for ICl (g) and

IBr (g) also support this value. At present the "best" value seems to be the higher one. This gives



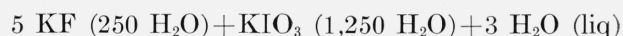
$$\Delta H_0^\circ = -30.0 \pm 0.5 \text{ kcal.}$$

IF₅ (g). Woolf [100] measured the heat of hydrolysis of liquid IF₅:



$$\Delta H_{291} = -22.05 \text{ kcal.}$$

Correcting this to 298° K gives $\Delta H_{298.16} = -23.55$ kcal. From this, $\Delta H_f^\circ_{298.16} \text{IF}_5 (\text{liq}) = -212.3$ kcal. Woolf also measured the alkaline heat of hydrolysis:



$$\Delta H_{291} = -118.9 \text{ kcal;}$$

at 298° K this becomes -118.7 kcal. From this, $\Delta H_f^\circ_{298.16} \text{IF}_5 (\text{liq}) = -212.5$ kcal. The average, -212.4 ± 1.5 kcal, was taken as the "best" value.

The heat of vaporization of IF₅ (liq) at 10° C is 10.12 kcal [1]; correction to 25° C makes this 9.85 kcal. When added to the value for the liquid this gives



$$\Delta H^\circ_{298.16} = -202.6 \pm 1.6 \text{ kcal.}$$

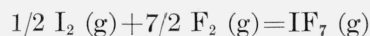
IF₇ (g). Bernstein and Katz [101] have measured the dissociation equilibrium of IF₇ (g) between 450° and 550° K. Their data give



$$\Delta H_0^\circ = 28.0 \pm 0.5 \text{ kcal}$$

$$\Delta H^\circ_{298.16} = 29.1 \pm 0.5 \text{ kcal.}$$

Combining this with $\Delta H_f^\circ_{298.16} \text{IF}_5 (\text{g})$ gives



$$\Delta H^\circ_{298.16} = -231.7 \pm 1.8 \text{ kcal.}$$

ICl (g). Brown and Gibson [102] obtained the dissociation limits of ICl going to both I(²P_{3/2}) + Cl(²P_{3/2}) and I(²P_{3/2}) + Cl(²P_{1/2}). Their data give D₀⁰ (ICl) as 49.64 and 49.65 kcal, respectively; from these $\Delta H_f^\circ \text{ICl} (\text{g})$ is -3.33 and -3.34 kcal. McMorris and Yost [103] measured the dissociation equilibrium of ICl (g); their data give $\Delta H_f^\circ \text{ICl} (\text{g}) = -3.32$ kcal. The average was taken as the "best" value:



$$\Delta H_0^\circ = -3.33 \pm 0.05 \text{ kcal.}$$

IBr (g). McMorris and Yost [104] measured the dissociation equilibrium of IBr (g); their data give $\Delta H_f^\circ = -1.42$ kcal. Brown [105] obtained the dissociation limits of IBr going to $I(^2P_{3/2}) + Br(^2P_{1/2})$ and to $I(^2P_{3/2}) + Br(^2P_{3/2})$; both limits give D_0° (IBr) = 41.91 kcal and ΔH_f° IBr (g) = -1.41 kcal.



$$\Delta H_0^\circ = -1.41 \pm 0.06 \text{ kcal.}$$

Bodenstein and Schmidt [126] obtained ΔH_f° IBr (g) = -1.48 kcal from gas-density measurements at 1,495° K; Müller [127] calculated -1.73 kcal from his kinetic studies. The agreement between the equilibrium data and the spectroscopic dissociation limits, in which the lighter atom is in the excited state in the normal dissociation process, furnishes additional support for the selection of the dissociation products assumed for ClF, BrF, and IF.

5. Discussion

The thermodynamic functions calculated, as outlined in section 3, are given in tables 7 to 27. The uncertainties in the functions are estimated to be not more than about 20 in the last figure given; the heat contents, $H^\circ - H_0^\circ$, however, as quantities derived directly from the heat-content functions, may retain one additional significant figure.

Tables 7 to 27 also include values of the heat of formation, ΔH_f° , free energy of formation, ΔF_f° , and logarithm of the equilibrium constant of formation, $\log K_f$, as a function of temperature. These were calculated from the relations

$$\Delta H_f^\circ = \Delta H_{f_0}^\circ + \Delta(H^\circ - H_0^\circ)$$

$$\Delta F_f^\circ = \Delta H_{f_0}^\circ + T\Delta[(F^\circ - H_0^\circ)/T]$$

$$\log_{10} K_f = -\Delta F_f^\circ / 4.57567 T.$$

The values of $\Delta H_{f_0}^\circ$ used were those selected in section 4; where $\Delta \bar{H}_{298.16}^\circ$ has been selected, this was corrected to $\Delta H_{f_0}^\circ$ for the calculations. The values of ΔH_f° and ΔF_f° are often given to more significant figures than the basic value at 0° K or 298.16° K to retain differences that are more precise than the basic value. As a derived quantity, $\log K_f$ is given to one more decimal place than is ΔF_f° .

Cole, Farber, and Elverum [106], Murphy and Vance [107], and Butkov and Rozenbaum [108] have calculated the thermodynamic functions for F (g); our calculations agree closely with those of Cole, Farber, and Elverum, and of Murphy and Vance, when allowance is made for the different values used for the fundamental constants. They have also calculated the thermodynamic functions for F₂ (g). Because of different choices for molecular and fundamental constants, none of these calculations agrees exactly with the present one. Recently Hu, White, and Johnston [109] have calculated the entropy of F₂ (g) at 85.02° K from low-temperature heat-

capacity data and heats of transition, fusion, and vaporization; their value, 39.58 ± 0.16 cal/deg mole, agrees very closely with one calculated from the data used in the present calculation, 39.57 ± 0.03 cal/deg mole.

Potter [110] has calculated thermodynamic functions for F₂O (g), using a different frequency assignment. His values differ from ours and have a different temperature dependence.

Giauque and Overstreet [111] have calculated the free-energy function for Cl (g), using fundamental constants from the International Critical Tables; when revised to the constants used in this paper their values agree with ours. Giauque and Overstreet also calculated the free-energy functions for Cl₂ (g) by a semidirect summation method. Their values, as corrected to new constants [113] by Sherman and Giauque [112], agree with the present results. Giauque and Powell [114] calculated the entropy of Cl₂ (g) from low-temperature calorimetric data to be 51.56 ± 0.10 cal/deg mole at 239.05° K; the present calculations give 51.54 ± 0.03 cal/deg mole.

Thermodynamic functions for ClF (g) were calculated by Schäfer and Wicke [46], using the rigid rotator-harmonic oscillator approximation, and by Potter [110] (revised by Cole and Elverum [115] for new fundamental constants). When converted to the same fundamental constants used here, the latter calculations agree with the present ones.

Previous calculations of the thermodynamic functions for ClF₃ (g) by Schäfer and Wicke [46] and Scheer [116] were based upon structural parameters and frequency assignments for the incorrect pyramidal structures.

Grisard, Bernhardt, and Oliver [117] measured the heat capacity of solid and liquid ClF₃ from 14° to 278° K and the vapor pressure of the liquid from 226° to 303° K. The calculation of the entropy of the gas from these data is complicated by the presence of the dimer (ClF₃)₂ in the vapor. The data of Schmitz and Schumacher [123] on the monomer-dimer equilibrium were used to obtain the partial pressure of the monomer for each reported total pressure. From a $\log P - 1/T$ plot of these partial pressures the normal boiling point of monomeric ClF₃ was obtained as 285.74° K. Calculation of the heat of vaporization from the vapor pressure data by use of the Clapeyron equation requires the molar volumes of the gas and liquid. The volume of the gas was obtained from the Berthelot equation of state, using the critical constants estimated by Grisard, Bernhardt, and Oliver. The liquid volume was taken from the data of Banks and Rudge [124]. With dP/dT obtained from the slope of the monomer vapor-pressure curve, these data gave 6,490 cal/mole for the heat of vaporization of ClF₃ at its boiling point and an entropy of vaporization of 22.71 cal/deg mole.

The entropy of liquid ClF₃, 43.74 cal/deg mole, was obtained by correcting the value given by Grisard, Bernhardt, and Oliver at 284.91° K to the boiling point 285.74° K. The entropy change in going from the real to the ideal gas was calculated

from the Berthelot equation to be 0.11 cal/deg mole.

The entropy of ClF_3 as an ideal gas at 285.74°K and 1 atm calculated from these data is 66.56 cal/deg mole. The value calculated statistically is 67.38 cal/deg mole. The reason for the difference is not known at present. The vibrational frequency assignment used is not certain and may be in error; however, it seems to be consistent with all the available spectroscopic data. (cf. Weber and Ferigle [118].) On the other hand, Burbank and Bensey [125] have obtained some evidence that there is a random arrangement within the crystal that would lead to a residual entropy in the solid at 0°K .

Gordon and Barnes [119] and Zeise [120] have calculated the functions for Br_2 (g). The more precise calculations of Gordon and Barnes, when converted to the new fundamental constants, agree with the present ones within 0.005 cal/deg mole.

The thermodynamic functions for BrF (g) and BrCl (g) have been calculated by Cole and Elverum [115]. Different choices of molecular constants, based in part upon more recent data, lead to small differences between the present calculations and theirs.

Stephenson and Jones [48] have calculated the functions for BrF_5 (g); as they assumed different molecular dimensions, their values of $-(F^\circ - H_0^\circ)/T$ and S° should differ from the present ones by a con-

stant amount; this is nearly true. Their value for the free-energy function at $1,000^\circ\text{K}$ is in error.

Murphy [121] and Zeise [122] have calculated free-energy functions for I (g); Murphy's values, corrected to the new constants, agree with the present ones. They have also calculated the free-energy function for I_2 (g); again, Murphy's calculations agree.

Cole and Elverum [115] have calculated the functions for IF (g). Their tabulated values of $-(F^\circ - H_0^\circ)/T$ are seriously in error for some reason; their other functions are in good agreement with the present ones.

Cole and Elverum also calculated the functions for ICl (g) and IBr (g); Zeise [120] has calculated free-energy functions for IBr (g). The calculations, corrected for constants, of Cole and Elverum agree with ours.

Gaydon has recently [128] revised many of his previous selections [63] of the values of gaseous diatomic dissociation energies. These values differ in part from those selected here. Because of a different choice of decomposition products, the values of D_0° that Gaydon selects for ClF , BrF , and IF differ from ours; this is discussed under the individual compounds. The other difference is for BrCl ; in this case Gaydon does not give details sufficient to locate the source of the discrepancy.

TABLE 7. Thermodynamic properties of F (g)

T	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	S°	$H^\circ - H_0^\circ$	C_p°	ΔH_f°	ΔF_f°	log K_f
$^\circ\text{K}$	cal/deg mole	cal/deg mole	cal/deg mole	cal/mole	cal/deg mole	kcal/mole	kcal/mole	
0	0	0	0	0	0	18.4	18.4	
250	-31.7750	5.1834	36.9584	1295.8	5.4454	18.819	15.472	-13.5257
273.16	-32.2352	5.2057	37.4409	1422.0	5.4452	18.861	15.161	-12.1298
298.16	-32.6919	5.2254	37.9173	1558.0	5.4365	18.903	14.820	-10.8631
300	-32.7241	5.2267	37.9508	1568.0	5.4355	18.906	14.794	-10.7779
400	-34.2348	5.2703	39.5051	2108.1	5.3612	19.06	13.40	-7.322
500	-35.4123	5.2804	40.6927	2640.2	5.2819	19.19	11.97	-5.232
600	-36.3747	5.2751	41.6498	3165.1	5.2180	19.30	10.51	-3.830
700	-37.1871	5.2633	42.4504	3684.3	5.1692	19.40	9.04	-2.823
800	-37.8889	5.2491	43.1380	4199.3	5.1324	19.48	7.56	-2.065
900	-38.5063	5.2345	43.7408	4711.0	5.1043	19.55	6.06	-1.472
1,000	-39.0571	5.2204	44.2775	5220.4	5.0826	19.62	4.56	-0.997
1,100	-39.5540	5.2070	44.7610	5727.7	5.0655	19.69	3.05	-0.606
1,200	-40.0065	5.1946	45.2011	6233.5	5.0519	19.75	1.53	-0.280
1,300	-40.4218	5.1832	45.6050	6738.2	5.0409	19.80	0.01	-0.002
1,400	-40.8056	5.1727	45.9783	7241.8	5.0319	19.86	-1.51	.235
1,500	-41.1622	5.1631	46.3253	7744.6	5.0244	19.91	-3.04	.442
1,600	-41.4951	5.1542	46.6493	8246.7	5.0182	19.96	-4.57	.624
1,700	-41.8073	5.1460	46.9533	8748.2	5.0129	20.00	-6.10	.784
1,800	-42.1012	5.1385	47.2397	9249.3	5.0084	20.05	-7.64	.927
1,900	-42.3788	5.1316	47.5104	9750.0	5.0045	20.09	-9.18	1.056
2,000	-42.6419	5.1252	47.7671	10250.4	5.0012	20.13	-10.72	1.171
2,100	-42.8918	5.1192	48.0110	10750.3	4.9983	20.17	-12.26	1.276
2,200	-43.1298	5.1136	48.2434	11249.9	4.9958	20.21	-13.81	1.372
2,300	-43.3571	5.1084	48.4655	11749.3	4.9936	20.25	-15.36	1.459
2,400	-43.5744	5.1036	48.6780	12248.6	4.9916	20.29	-16.91	1.539
2,500	-43.7826	5.0991	48.8817	12747.8	4.9898	20.32	-18.46	1.613
2,750	-44.2681	5.0890	49.3571	13994.8	4.9862	20.41	-22.34	1.775
3,000	-44.7105	5.0803	49.7908	15240.9	4.9834	20.49	-26.23	1.911
3,250	-45.1168	5.0728	50.1896	16486.6	4.9812	-----	-----	-----
3,500	-45.4925	5.0662	50.5587	17731.7	4.9794	-----	-----	-----
3,750	-45.8419	5.0604	50.9023	18976.5	4.9780	-----	-----	-----
4,000	-46.1683	5.0552	51.2235	20220.8	4.9768	-----	-----	-----
4,250	-46.4746	5.0505	51.5251	21464.6	4.9758	-----	-----	-----
4,500	-46.7632	5.0463	51.8095	22708.4	4.9750	-----	-----	-----
4,750	-47.0359	5.0426	52.0785	23952.4	4.9743	-----	-----	-----
5,000	-47.2945	5.0392	52.3337	25196.0	4.9737	-----	-----	-----

TABLE 8. *Thermodynamic properties of F₂ (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> [°]	<i>H</i> [°] - <i>H</i> ₀ [°]	<i>C</i> _p [°]	ΔH_f°	ΔF_f°	log <i>Kf</i>
^{°K}	cal/deg mole	cal/deg mole	cal/deg mole	cal/mole	cal/deg mole	kcal/mole	kcal/mole	
0	0	0	0	0	0	0	0	-----
250	-40.129	7.017	47.146	1754.2	7.28	0	0	0
273.16	-40.755	7.033	47.788	1921.1	7.38	0	0	0
298.16	-41.371	7.076	48.447	2109.8	7.49	0	0	0
300	-41.415	7.078	48.493	2123.4	7.49	0	0	0
400	-43.472	7.233	50.705	2893.2	7.89	0	0	0
500	-45.103	7.396	52.499	3698.0	8.19	0	0	0
600	-46.464	7.547	54.011	4528.2	8.41	0	0	0
700	-47.639	7.682	55.321	5377.4	8.56	0	0	0
800	-48.672	7.800	56.472	6240.0	8.68	0	0	0
900	-49.598	7.903	57.501	7112.7	8.77	0	0	0
1,000	-50.435	7.992	58.427	7992.0	8.84	0	0	0
1,100	-51.200	8.074	59.274	8881.4	8.90	0	0	0
1,200	-51.905	8.144	60.049	9772.8	8.94	0	0	0
1,300	-52.559	8.207	60.766	10669.1	8.99	0	0	0
1,400	-53.171	8.265	61.436	11571.0	9.02	0	0	0
1,500	-53.744	8.316	62.060	12474.0	9.06	0	0	0
1,600	-54.280	8.362	62.642	13379.2	9.08	0	0	0
1,700	-54.789	8.406	63.195	14290.2	9.11	0	0	0
1,800	-55.272	8.446	63.718	15202.8	9.13	0	0	0
1,900	-55.729	8.483	64.212	16117.7	9.15	0	0	0
2,000	-56.164	8.517	64.681	17034.0	9.18	0	0	0
2,100	-56.581	8.549	65.130	17952.9	9.20	0	0	0
2,200	-56.979	8.579	65.558	18873.8	9.22	0	0	0
2,300	-57.350	8.607	65.967	19796.1	9.23	0	0	0
2,400	-57.728	8.634	66.362	20721.6	9.25	0	0	0
2,500	-58.082	8.658	66.740	21645.0	9.27	0	0	0
2,750	-58.908	8.715	67.623	23966.2	9.31	0	0	0
3,000	-59.669	8.767	68.436	26301.0	9.34	0	0	0

TABLE 9. *Thermodynamic properties of F₂O (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> [°]	<i>H</i> [°] - <i>H</i> ₀ [°]	<i>C</i> _p [°]	ΔH_f°	ΔF_f°	log <i>Kf</i>
^{°K}	cal/deg mole	cal/deg mole	cal/deg mole	cal/mole	cal/deg mole	kcal/mole	kcal/mole	
0	0	0	0	0	0	8.14	8.14	-----
250	-48.73	8.48	57.21	2120	9.75	7.64	11.09	-9.698
273.16	-49.49	8.60	58.09	2349	10.05	7.62	11.41	-9.132
298.16	-50.25	8.74	58.99	2306	10.35	7.6	11.8	-8.65
300	-50.30	8.75	59.05	2325	10.38	7.60	11.79	-8.589
400	-52.89	9.29	62.18	3716	11.38	7.57	13.20	-7.209
500	-55.02	9.78	64.80	4890	12.06	7.57	14.60	-6.382
600	-55.84	10.20	66.04	6120	12.53	7.59	16.00	-5.830
700	-58.44	10.56	69.00	7392	12.84	7.63	17.40	-5.434
800	-59.87	10.86	70.73	8688	13.07	7.66	18.80	-5.136
900	-61.16	11.11	72.27	9999	13.23	7.69	20.19	-4.904
1,000	-62.35	11.33	73.68	11330	13.35	7.73	21.57	-4.715
1,100	-63.44	11.52	74.96	12672	13.44	7.76	22.95	-4.560
1,200	-64.44	11.68	76.12	14016	13.51	7.79	24.34	-4.432
1,300	-65.38	11.82	77.20	15366	13.57	7.82	25.72	-4.325
1,400	-66.27	11.95	78.22	16730	13.61	7.85	27.09	-4.230
1,500	-67.09	12.06	79.15	18090	13.65	7.87	28.47	-4.149

TABLE 10. *Thermodynamic properties of Cl (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> [°]	<i>H</i> [°] - <i>H</i> ₀ [°]	<i>C</i> _p [°]	ΔH_f°	ΔF_f°	log <i>Kf</i>
^{°K}	cal/deg mole	cal/deg mole	cal/deg mole	cal/mole	cal/deg mole	kcal/mole	kcal/mole	-----
0	0	0	0	0	0	28.54	28.54	-----
250	-33.5460	4.9996	38.5456	1249.9	5.1275	28.886	25.735	-22.4968
273.16	-33.9984	5.0123	39.0107	1369.2	5.1946	28.913	25.439	-20.3531
298.16	-34.4291	5.0278	39.4569	1499.1	5.2203	28.942	25.122	-18.4144
300	-34.4600	5.0290	39.4890	1508.7	5.2237	28.943	25.099	-18.2843
400	-35.9161	5.0977	41.0138	2039.1	5.3705	29.06	23.80	-13.003
500	-37.0605	5.1601	42.2206	2580.0	5.4363	29.17	22.47	-9.822
600	-38.0058	5.2074	43.2132	3124.4	5.4448	29.28	21.12	-7.693
700	-38.8111	5.2400	44.0517	3668.0	5.4232	29.39	19.75	-6.166
800	-39.5123	5.2608	44.7731	4208.6	5.3887	29.49	18.37	-5.018
900	-40.1327	5.2729	45.4056	4745.6	5.3506	29.58	16.97	-4.121
1,000	-40.6886	5.2788	45.9674	5278.8	5.3133	29.66	15.57	-3.402
1,100	-41.1918	5.2804	46.4722	5808.4	5.2788	29.74	14.15	-2.812
1,200	-41.6512	5.2789	46.9301	6334.7	5.2477	29.82	12.73	-2.319
1,300	-42.0736	5.2754	47.3490	6858.0	5.2201	29.89	11.31	-1.901
1,400	-42.4644	5.2706	47.7350	7378.8	5.1958	29.96	9.88	-1.542
1,500	-42.8278	5.2649	48.0927	7897.4	5.1745	30.02	8.44	-1.229
1,600	-43.1674	5.2586	48.4260	8413.8	5.1557	30.09	7.00	-0.956
1,700	-43.4860	5.2521	48.7381	8928.6	5.1392	30.15	5.55	-0.713
1,800	-43.7860	5.2454	49.0314	9441.7	5.1246	30.21	4.10	-0.498
1,900	-44.0695	5.2387	49.3082	9953.5	5.1117	30.26	2.65	-0.304
2,000	-44.3380	5.2320	49.5700	10464.0	5.1002	30.31	1.20	-0.131
2,100	-44.5931	5.2255	49.8186	10973.6	5.0900	30.37	-0.26	.027
2,200	-44.8361	5.2192	50.0553	11482.2	5.0809	30.42	-1.87	.186
2,300	-45.0679	5.2130	50.2809	11989.9	5.0727	30.46	-3.18	.302
2,400	-45.2896	5.2070	50.4966	12496.8	5.0654	30.51	-4.65	.423
2,500	-45.5021	5.2012	50.7033	13003.0	5.0588	30.56	-6.12	.535
2,750	-45.9972	5.1876	51.1848	14265.9	5.0449	30.67	-9.86	.783
3,000	-46.4480	5.1752	51.6232	15525.6	5.0339	30.76	-13.47	.981
3,250	-46.8618	5.1640	52.0258	16783.0	5.0251	-----	-----	-----
3,500	-47.2441	5.1538	52.3979	18038.3	5.0179	-----	-----	-----
3,750	-47.5994	5.1445	52.7439	19291.9	5.0120	-----	-----	-----
4,000	-47.9311	5.1361	53.0672	20544.4	5.0070	-----	-----	-----
4,250	-48.2422	5.1284	53.3706	21795.7	5.0028	-----	-----	-----
4,500	-48.5352	5.1213	53.6565	23045.8	4.9993	-----	-----	-----
4,750	-48.8119	5.1148	53.9237	24295.3	4.9964	-----	-----	-----
5,000	-49.0744	5.1088	54.1832	25544.0	4.9941	-----	-----	-----

TABLE 11. *Thermodynamic properties of Cl₂ (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> [°]	<i>H</i> [°] - <i>H</i> ₀ [°]	<i>C</i> _p [°]	ΔH_f°	ΔF_f°	log <i>Kf</i>
^{°K}	cal/deg mole	cal/deg mole	cal/deg mole	cal/mole	cal/deg mole	kcal/mole	kcal/mole	-----
0	0	0	0	0	0	0	0	-----
250	-44.649	7.233	51.882	1808.2	7.88	0	0	0
273.16	-45.292	7.293	52.585	1992.2	8.00	0	0	0
298.16	-45.934	7.357	53.291	2193.6	8.11	0	0	0
300	-45.979	7.362	53.341	2208.6	8.12	0	0	0
400	-48.130	7.595	55.725	3038.0	8.44	0	0	0
500	-49.847	7.783	57.630	3891.5	8.62	0	0	0
600	-51.278	7.935	59.213	4761.0	8.74	0	0	0
700	-52.511	8.057	60.568	5639.9	8.82	0	0	0
800	-53.594	8.156	61.750	6524.8	8.88	0	0	0
900	-54.560	8.238	62.798	7414.2	8.92	0	0	0
1,000	-55.432	8.309	63.741	8309.0	8.96	0	0	0
1,100	-56.226	8.370	64.596	9207.0	8.99	0	0	0
1,200	-56.956	8.423	65.379	10107.6	9.02	0	0	0
1,300	-57.633	8.469	66.102	11009.7	9.04	0	0	0
1,400	-58.263	8.510	66.773	11914.0	9.06	0	0	0
1,500	-58.851	8.548	67.399	12822.0	9.08	0	0	0
1,600	-59.404	8.581	67.985	13729.6	9.10	0	0	0
1,700	-59.925	8.611	68.536	14638.7	9.11	0	0	0
1,800	-60.418	8.640	69.058	15552.0	9.13	0	0	0
1,900	-60.885	8.665	69.550	16463.5	9.14	0	0	0
2,000	-61.331	8.690	70.021	17380.0	9.16	0	0	0
2,100	-61.756	8.712	70.468	18295.2	9.17	0	0	0
2,200	-62.162	8.734	70.896	19214.8	9.19	0	0	0
2,300	-62.550	8.754	71.304	20134.2	9.20	0	0	0
2,400	-62.923	8.773	71.696	21055.2	9.22	0	0	0
2,500	-63.281	8.791	72.072	21977.5	9.23	0	0	0
2,750	-64.069	8.824	72.893	24266.0	9.26	0	0	0
3,000	-64.891	8.870	73.761	26610.0	9.30	0	0	0

TABLE 12. *Thermodynamic properties of ClO₂ (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> [°]	<i>H</i> [°] - <i>H</i> ₀ [°]	<i>C</i> _p [°]	ΔH_f°	ΔF_f°	log <i>Kf</i>
^{°K}	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/mole</i>	<i>cal/deg mole</i>	<i>kcal/mole</i>	<i>kcal/mole</i>	
0	0	0	0	0	0	25.500	25.500	
250	-49.910	8.431	58.341	2107.8	9.50	25.061	28.902	-25.2660
273.16	-50.661	8.531	59.192	2330.3	9.74	25.025	29.258	-23.4088
298.16	-51.413	8.642	60.055	2576.7	10.00	25.0	29.6	-21.73
300	-51.467	8.651	60.118	2595.3	10.02	24.998	29.678	-21.6204
400	-54.019	9.115	63.134	3646.0	10.96	24.92	31.25	-17.076
500	-56.101	9.561	65.662	4780.5	11.69	24.90	32.84	-14.354
600	-57.881	9.963	67.844	5977.8	12.22	24.91	34.42	-12.539
700	-59.444	10.316	69.760	7221.2	12.61	24.93	36.01	-11.242
800	-60.841	10.622	71.463	8497.6	12.90	24.97	37.59	-10.269
900	-62.108	10.888	72.996	9799.2	13.12	25.01	39.16	-9.510
1,000	-63.268	11.120	74.388	11120.0	13.29	25.06	40.74	-8.902
1,100	-64.338	11.323	75.661	12455.3	13.42	25.11	42.30	-8.404
1,200	-65.331	11.502	76.833	13802.4	13.53	25.16	43.86	-7.988
1,300	-66.258	11.661	77.919	15159.3	13.61	25.20	45.42	-7.635
1,400	-67.127	11.804	78.931	16525.6	13.68	25.25	46.97	-7.332
1,500	-67.946	11.932	79.878	17898.0	13.74	25.30	48.52	-7.070

TABLE 13. *Thermodynamic properties of Cl₂O (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> [°]	<i>H</i> [°] - <i>H</i> ₀ [°]	<i>C</i> _p [°]	ΔH_f°	ΔF_f°	log <i>Kf</i>
^{°K}	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/mole</i>	<i>cal/deg mole</i>	<i>kcal/mole</i>	<i>kcal/mole</i>	
0	0	0	0	0	0	18.61	18.61	
250	-52.94	8.84	61.78	2210	10.3	18.15	21.64	-18.919
273.16	-53.73	8.97	62.70	2450	10.6	18.12	21.97	-17.574
298.16	-54.52	9.12	63.64	2719	10.9	18.1	22.3	-16.36
300	-54.59	9.13	63.72	2739	10.9	18.10	22.34	-16.276
400	-57.28	9.68	66.96	3872	11.7	18.05	23.77	-12.989
500	-59.49	10.16	69.65	5080	12.3	18.04	25.21	-11.018
600	-61.38	10.55	71.93	6330	12.7	18.04	26.64	-9.704
700	-63.03	10.88	73.91	7616	13.0	18.06	28.07	-8.764
800	-64.50	11.16	75.66	8928	13.2	18.09	29.50	-8.060
900	-65.83	11.39	77.22	10251	13.3	18.11	30.93	-7.510
1,000	-67.04	11.59	78.63	11590	13.4	18.14	32.35	-7.070
1,100	-68.16	11.76	79.92	12936	13.5	18.17	33.76	-6.707
1,200	-69.19	11.91	81.10	14292	13.6	18.20	35.18	-6.406
1,300	-70.14	12.04	82.18	15652	13.6	18.23	36.60	-6.153
1,400	-71.04	12.16	83.20	17024	13.7	18.27	38.01	-5.934
1,500	-71.91	12.27	84.18	18405	13.7	18.31	39.39	-5.737

TABLE 14. *Thermodynamic properties of ClF (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> [°]	<i>H</i> [°] - <i>H</i> ₀ [°]	<i>C</i> _p [°]	ΔH_f°	ΔF_f°	log <i>Kf</i>
^{°K}	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/mole</i>	<i>cal/deg mole</i>	<i>kcal/mole</i>	<i>kcal/mole</i>	
0	0	0	0	0	0	-13.4	-13.4	
250	-43.672	7.060	50.732	1,765.0	7.44	-13.416	-13.721	11.9945
273.16	-44.300	7.098	51.398	1,938.9	7.55	-13.418	-13.749	11.0000
298.16	-44.922	7.140	52.062	2,128.9	7.67	-13.423	-13.779	10.0995
300	-44.966	7.144	52.110	2,143.2	7.68	-13.423	-13.781	10.0391
400	-47.047	7.329	54.376	2,931.6	8.07	-13.43	-13.90	7.594
500	-48.702	7.506	56.208	3,753.0	8.33	-13.44	-14.01	6.126
600	-50.085	7.659	57.744	4,595.4	8.51	-13.45	-14.13	5.146
700	-51.275	7.790	59.065	5,453.0	8.64	-13.46	-14.24	4.446
800	-52.323	7.902	60.225	6,321.6	8.73	-13.46	-14.35	3.921
900	-53.260	7.997	61.257	7,197.3	8.80	-13.47	-14.46	3.512
1,000	-54.107	8.080	62.187	8,080.0	8.85	-13.47	-14.57	3.185
1,100	-54.880	8.153	63.033	8,968.3	8.89	-13.48	-14.68	2.917
1,200	-55.592	8.216	63.808	9,859.2	8.93	-13.48	-14.79	2.694
1,300	-56.252	8.271	64.523	10,752.3	8.96	-13.49	-14.90	2.505
1,400	-56.867	8.320	65.187	11,648.0	8.98	-13.49	-15.01	2.343
1,500	-57.442	8.366	65.808	12,549.0	9.00	-13.50	-15.12	2.203

TABLE 15. *Thermodynamic properties of ClF₃ (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> ^o	$H^\circ - H_0^\circ$	<i>C_p</i> ^o	ΔH_f°	ΔF_f°	log <i>Kf</i>
^o K	cal/deg mole	cal/deg mole	cal/deg mole	cal/mole	cal/deg mole	kcal/mole	kcal/mole	-----
0	0	0	0	0	0	-37.9	-37.9	-----
250	-54.81	10.59	65.40	2,647.5	14.48	-38.79	-30.97	27.076
273.16	-55.76	10.94	66.70	2,988.4	15.03	-38.79	-30.24	24.193
298.16	-56.73	11.31	68.04	3,372.2	15.55	-38.79	-29.46	21.597
300	-56.80	11.33	68.13	3,399.0	15.58	-38.79	-29.41	21.422
400	-60.24	12.59	72.83	5,036	17.05	-38.72	-26.29	14.363
500	-63.16	13.58	76.74	6,790	17.92	-38.60	-23.19	10.138
600	-65.71	14.35	80.06	8,610	18.45	-38.46	-20.13	7.340
700	-67.97	14.96	82.93	10,472	18.80	-38.31	-17.09	5.332
800	-70.00	15.45	85.45	12,360	19.03	-38.16	-14.06	3.840
900	-71.84	15.86	87.70	14,274	19.20	-38.00	-11.05	2.682
1,000	-73.52	16.20	89.72	16,200	19.32	-37.84	-8.05	1.176
1,100	-75.08	16.49	91.57	18,139	19.41	-37.69	-5.08	1.010
1,200	-76.54	16.74	93.28	20,088	19.48	-37.53	-2.14	0.391
1,300	-77.90	16.95	94.85	22,035	19.54	-37.37	0.78	-.132
1,400	-79.16	17.13	96.29	23,982	19.59	-37.22	3.71	-.581
1,500	-80.34	17.30	97.64	25,950	19.63	-37.07	6.65	-.969

TABLE 16. *Thermodynamic properties of Br (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> ^o	$H^\circ - H_0^\circ$	<i>C_p</i> ^o	ΔH_f°	ΔF_f°	log <i>Kf</i>
^o K	cal/deg mole	cal/deg mole	cal/deg mole	cal/mole	cal/deg mole	kcal/mole	kcal/mole	-----
0	0	0	0	0	0	22.73	22.73	-----
250	-35.9620	4.9680	40.9300	1,242.0	4.9680	23.016	19.926	-17.4189
273.16	-36.4022	4.9680	41.3702	1,357.1	4.9680	23.032	19.639	-15.7125
298.16	-36.8372	4.9680	41.8052	1,481.3	4.9680	23.049	19.327	-14.1667
300	-36.8678	4.9680	41.8358	1,490.4	4.9680	23.050	19.305	-14.0633
400	-38.2970	4.9680	43.2650	1,987.2	4.9683	23.11	18.05	-9.860
500	-39.4057	4.9682	44.3739	2,484.1	4.9708	23.17	16.77	-7.332
600	-40.3115	4.9693	45.2808	2,981.6	4.9793	23.22	15.49	-5.642
700	-41.0776	4.9718	46.0494	3,480.3	4.9973	23.27	14.20	-4.432
800	-41.7418	4.9767	46.7185	3,981.4	5.0257	23.33	12.90	-3.523
900	-42.3285	4.9841	47.3125	4,485.7	5.0631	23.38	11.59	-2.814
1,000	-42.8541	4.9942	47.8483	4,994.2	5.1065	23.44	10.28	-2.246
1,100	-43.3306	5.0065	48.3371	5,507.2	5.1528	23.50	8.96	-1.780
1,200	-43.7669	5.0206	48.7875	6,024.7	5.1991	23.57	7.63	-1.390
1,300	-44.1693	5.0361	49.2054	6,546.9	5.2433	23.64	6.30	-1.060
1,400	-44.5431	5.0523	49.5954	7,073.2	5.2838	23.71	4.97	-0.975
1,500	-44.8922	5.0690	49.9612	7,603.5	5.3198	23.79	3.62	-.528
1,600	-45.2200	5.0857	50.3057	8,137.1	5.3509	23.87	2.28	-.311
1,700	-45.5288	5.1021	50.6309	8,673.6	5.3770	23.95	0.92	-.119
1,800	-45.8218	5.1180	50.9388	9,212.4	5.3983	24.03	-.43	-.052
1,900	-46.0979	5.1332	51.2311	9,753.1	5.4151	24.12	-1.79	-.206
2,000	-46.3616	5.1476	51.5092	10,295.2	5.4279	24.20	-3.16	-.345
2,100	-46.6131	5.1612	51.7743	10,838.5	5.4369	24.29	-4.53	-.471
2,200	-46.8535	5.1739	52.0274	11,382.6	5.4427	24.37	-5.90	-.586
2,300	-47.0838	5.1856	52.2694	11,923.9	5.4457	24.46	-7.28	-.692
2,400	-47.3047	5.1965	52.5012	12,471.6	5.4464	24.54	-8.66	-.789
2,500	-47.5170	5.2065	52.7235	13,016.3	5.4451	24.63	-10.05	-.878
2,750	-48.0143	5.2277	53.2420	14,376.2	5.4348	24.84	-13.52	1.075
3,000	-48.4999	5.2443	53.7142	15,732.9	5.4178	25.04	-17.02	1.240
3,250	-48.8902	5.2599	54.1471	17,084.9	5.3972	-----	-----	-----
3,500	-49.2801	5.2361	54.5462	18,431.4	5.3748	-----	-----	-----
3,750	-49.6437	5.2726	54.9163	19,772.3	5.3519	-----	-----	-----
4,000	-49.9841	5.2769	55.2610	21,107.6	5.3293	-----	-----	-----
4,250	-50.3041	5.2793	55.5834	22,437.0	5.3075	-----	-----	-----
4,500	-50.6059	5.2803	55.8862	23,761.4	5.2868	-----	-----	-----
4,750	-50.8914	5.2801	56.1715	25,080.5	5.2673	-----	-----	-----
5,000	-51.1622	5.2790	56.4412	26,395.0	5.2490	-----	-----	-----

TABLE 17. *Thermodynamic properties of Br₂ (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	S°	$H^\circ - H_0^\circ$	C_p°	ΔH_f°	ΔF_f°	$\log K_f$
$^\circ K$	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/mole</i>	<i>cal/deg mole</i>	<i>kcal/mole</i>	<i>kcal/mole</i>	-----
0	0	0	0	0	0	0	0	0
250	-49.491	7.650	57.141	1,912.5	8.48	0	0	0
273.16	-50.172	7.724	57.896	2,109.9	8.55	0	0	0
298.16	-50.851	7.796	58.647	2,324.5	8.62	0	0	0
300	-50.899	7.801	58.700	2,340.3	8.62	0	0	0
400	-53.176	8.028	61.204	3,211.2	8.78	0	0	0
500	-54.986	8.186	63.172	4,093.0	8.86	0	0	0
600	-56.489	8.303	64.792	4,981.8	8.91	0	0	0
700	-57.776	8.392	66.168	5,874.4	8.94	0	0	0
800	-58.901	8.462	67.363	6,769.6	8.97	0	0	0
900	-59.901	8.520	68.421	7,668.0	8.99	0	0	0
1,000	-60.801	8.568	69.369	8,568.0	9.01	0	0	0
1,100	-61.620	8.609	70.229	9,469.9	9.03	0	0	0
1,200	-62.371	8.644	71.015	10,372.8	9.04	0	0	0
1,300	-63.064	8.676	71.740	11,278.8	9.06	0	0	0
1,400	-63.708	8.703	72.411	12,184.2	9.07	0	0	0
1,500	-64.309	8.728	73.037	13,092.0	9.08	0	0	0
1,600	-64.873	8.750	73.623	14,000.0	9.09	0	0	0
1,700	-65.404	8.770	74.174	14,909.0	9.11	0	0	0
1,800	-65.906	8.790	74.696	15,822.0	9.12	0	0	0
1,900	-66.382	8.807	75.189	16,733.3	9.13	0	0	0
2,000	-66.834	8.824	75.658	17,648.0	9.14	0	0	0
2,100	-67.265	8.839	76.104	18,561.9	9.15	0	0	0
2,200	-67.677	8.853	76.530	19,476.6	9.16	0	0	0
2,300	-68.071	8.867	76.938	20,394.1	9.17	0	0	0
2,400	-68.448	8.880	77.328	21,312.0	9.18	0	0	0
2,500	-68.811	8.892	77.703	22,230.0	9.20	0	0	0
2,750	-69.662	8.921	78.583	24,532.8	9.22	0	0	0
3,000	-70.436	8.947	79.383	26,841.0	9.25	0	0	0

TABLE 18. *Thermodynamic properties of BrF (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	S°	$H^\circ - H_0^\circ$	C_p°	ΔH_f°	ΔF_f°	$\log K_f$
$^\circ K$	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/mole</i>	<i>cal/deg mole</i>	<i>kcal/mole</i>	<i>kcal/mole</i>	-----
0	0	0	0	0	0	-18.3	-18.3	0
250	-46.206	7.128	53.334	1,782.0	7.63	-18.353	-18.649	16.3028
273.16	-46.839	7.176	54.015	1,960.2	7.76	-18.355	-18.676	14.9419
298.16	-47.470	7.230	54.700	2,155.7	7.88	-18.361	-18.705	13.7107
300	-47.514	7.234	54.748	2,170.2	7.88	-18.362	-18.707	13.6279
400	-49.625	7.446	57.071	2,978.4	8.25	-18.37	-18.82	10.283
500	-51.307	7.633	58.940	3,816.5	8.49	-18.38	-18.93	8.275
600	-52.713	7.789	60.502	4,673.4	8.64	-18.38	-19.04	6.936
700	-53.924	7.918	61.842	5,542.6	8.74	-18.38	-19.15	5.980
800	-54.989	8.027	63.016	6,421.6	8.82	-18.38	-19.26	5.262
900	-55.940	8.118	64.058	7,306.2	8.88	-18.38	-19.37	4.704
1,000	-56.790	8.196	64.995	8,196.0	8.92	-18.38	-19.48	4.258
1,100	-57.584	8.264	65.848	9,090.4	8.96	-18.39	-19.59	3.892
1,200	-58.305	8.323	66.628	9,987.6	8.99	-18.39	-19.70	3.588
1,300	-58.974	8.376	67.350	10,888.8	9.02	-18.39	-19.81	3.330
1,400	-59.596	8.423	68.019	11,792.2	9.04	-18.39	-19.92	3.109
1,500	-60.178	8.465	68.643	12,697.5	9.07	-18.39	-20.03	2.918

TABLE 19. *Thermodynamic properties of BrF₅(g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	S°	$H^\circ - H_0^\circ$	C_p°	ΔH_f°	ΔF_f°	$\log K_f$
$^\circ K$	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/mole</i>	<i>cal/deg mole</i>	<i>kcal/mole</i>	<i>kcal/mole</i>	-----
0	0	0	0	0	0	-122	-122	0
250	-58.93	13.48	72.41	3,370	21.78	-124.0	-105.5	92.20
273.16	-60.15	14.24	74.39	3,890	22.90	-124.0	-103.7	83.00
298.16	-61.43	15.01	76.44	4,475	23.93	-124.0	-101.9	74.69
300	-61.53	15.06	76.59	4,518	24.00	-124.0	-101.8	74.13
400	-66.23	17.68	83.91	7,072	26.82	-123.8	-94.4	51.57
500	-70.41	19.68	90.09	9,840	28.41	-123.5	-87.1	38.06
600	-74.14	21.22	95.36	12,732	29.36	-123.1	-79.8	29.08
700	-77.50	22.43	99.93	15,701	29.96	-122.7	-72.7	22.69
800	-80.50	23.40	103.96	18,720	30.37	-122.3	-65.5	17.91
900	-83.37	24.19	107.56	21,771	30.66	-121.8	-58.5	14.20
1,000	-85.95	24.85	110.80	24,850	30.87	-121.4	-51.5	11.25
1,100	-88.35	25.41	113.76	27,951	31.03	-121.0	-44.5	8.84
1,200	-90.58	25.88	116.46	31,056	31.15	-120.6	-37.6	6.84
1,300	-92.66	26.29	118.95	34,177	31.24	-120.1	-30.7	5.16
1,400	-94.62	26.64	121.26	37,296	31.31	-119.7	-23.8	3.71
1,500	-96.47	26.96	123.43	40,440	31.38	-119.3	-16.9	2.47

TABLE 20. Thermodynamic properties of BrCl (g)

T	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	S°	$H^\circ - H_0^\circ$	C_p°	ΔH_f°	ΔF_f°	$\log K_f$
$^\circ K$	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/mole</i>	<i>cal/deg mole</i>	<i>kcal/mole</i>	<i>kcal/mole</i>	
0	0	0	0	0	0	-0.20	-0.20	-----
250	-48.485	7.396	55.881	1849.0	8.17	-213	-554	0.4841
273.16	-49.144	7.466	56.610	2039.4	8.27	-212	-586	.4686
298.16	-49.800	7.538	57.338	2247.5	8.36	-212	-620	.4544
300	-49.847	7.543	57.390	2262.9	8.37	-212	-623	.4535
400	-52.051	7.783	59.834	3113.2	8.61	-21	-76	.415
500	-53.808	7.963	61.771	3981.5	8.74	-21	-91	.392
600	-55.272	8.100	63.372	4860.0	8.83	-21	-1.03	.376
700	-56.528	8.208	64.736	5745.6	8.88	-21	-1.17	.365
800	-57.631	8.295	65.926	6636.0	8.92	-21	-1.31	.357
900	-58.613	8.366	66.979	7529.4	8.95	-21	-1.44	.350
1,000	-59.498	8.426	67.924	8426.0	8.98	-21	-1.58	.346
1,100	-60.303	8.477	68.780	9324.7	9.00	-21	-1.72	.341
1,200	-61.043	8.521	69.564	10225.2	9.02	-22	-1.86	.338
1,300	-61.726	8.560	70.286	11128.0	9.03	-22	-1.99	.335
1,400	-62.362	8.594	70.956	12031.6	9.05	-22	-2.13	.332
1,500	-62.956	8.625	71.581	12937.5	9.06	-22	-2.26	.330

TABLE 21. Thermodynamic properties of I (g)

T	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	S°	$H^\circ - H_0^\circ$	C_p°	ΔH_f°	ΔF_f°	$\log K_f$
$^\circ K$	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/mole</i>	<i>cal/deg mole</i>	<i>kcal/mole</i>	<i>kcal/mole</i>	
0	0	0	0	0	0	17.77	17.77	-----
250	-37.3406	4.9680	42.3086	1242.0	4.9680	18.015	15.030	-13.1386
273.16	-37.7808	4.9680	42.7488	1357.1	4.9680	18.030	14.752	-11.8029
298.16	-38.2158	4.9680	43.1838	1481.3	4.9680	18.042	14.452	-10.5932
300	-38.2464	4.9680	43.2144	1490.4	4.9680	18.043	14.430	-10.5119
400	-39.6756	4.9680	44.6436	1987.2	4.9680	18.10	13.22	-7.221
500	-40.7842	4.9680	45.7522	2484.0	4.9680	18.15	11.99	-5.241
600	-41.6899	4.9680	46.6579	2980.8	4.9680	18.20	10.76	-3.917
700	-42.4557	4.9680	47.4237	3477.6	4.9680	18.24	9.51	-2.969
800	-43.1191	4.9680	48.0871	3974.4	4.9682	18.29	8.26	-2.257
900	-43.7043	4.9681	48.6724	4471.3	4.9688	18.33	7.00	-1.700
1,000	-44.2277	4.9682	49.1959	4968.2	4.9700	18.38	5.74	-1.255
1,100	-44.7013	4.9685	49.6698	5465.4	4.9726	18.42	4.48	-0.889
1,200	-45.1336	4.9690	50.1026	5962.8	4.9770	18.47	3.21	-.584
1,300	-45.5313	4.9698	50.5011	6460.7	4.9836	18.51	1.93	-.325
1,400	-45.8997	4.9711	50.8708	6959.5	4.9925	18.55	0.66	-.103
1,500	-46.2427	4.9729	51.2156	7459.4	5.0039	18.60	-.62	.090
1,600	-46.5638	4.9753	51.5391	7960.5	5.0178	18.64	-1.90	.260
1,700	-46.8655	4.9783	51.8438	8463.1	5.0340	18.68	-3.19	.410
1,800	-47.1501	4.9818	52.1319	8967.2	5.0521	18.73	-4.48	.544
1,900	-47.4196	4.9860	52.4056	9473.4	5.0718	18.78	-5.77	.663
2,000	-47.6754	4.9908	52.6662	9981.6	5.0928	18.83	-7.06	.771
2,100	-47.9190	4.9962	52.9152	10492.0	5.1147	18.88	-8.36	.870
2,200	-48.1516	5.0021	53.1537	11004.6	5.1371	18.93	-9.66	.959
2,300	-48.3742	5.0085	53.3827	11519.6	5.1597	18.98	-10.96	1.041
2,400	-48.5874	5.0152	53.6026	12036.5	5.1822	19.03	-12.26	1.116
2,500	-48.7923	5.0224	53.8147	12556.0	5.2045	19.09	-13.56	1.185
2,750	-49.2719	5.0414	54.3133	13863.8	5.2571	19.23	-16.84	1.338
3,000	-49.7114	5.0613	54.7727	15183.9	5.3039	19.69	-20.12	1.466
3,250	-50.1173	5.0816	55.1989	16515.2	5.3437	-----	-----	-----
3,500	-50.4946	5.1015	55.5961	17855.2	5.3762	-----	-----	-----
3,750	-50.8473	5.1207	55.9680	19202.6	5.4016	-----	-----	-----
4,000	-51.1783	5.1389	56.3172	20555.6	5.4205	-----	-----	-----
4,250	-51.4904	5.1559	56.6463	21912.6	5.4337	-----	-----	-----
4,500	-51.7855	5.1716	56.9571	23272.2	5.4419	-----	-----	-----
4,750	-52.0655	5.1859	57.2514	24633.0	5.4458	-----	-----	-----
5,000	-52.3319	5.1989	57.5308	25994.5	5.4462	-----	-----	-----

TABLE 22. *Thermodynamic properties of I₂ (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> ^o	$H^\circ - H_0^\circ$	<i>C</i> _p ^o	ΔH_f°	ΔF_f°	log <i>K_f</i>
^o K	cal/deg mole	cal/deg mole	cal/deg mole	cal/mole	cal/deg mole	kcal/mole	kcal/mole	
0	0	0	0	0	0	0	0	-----
250	-52.757	7.980	60.737	1995.0	8.74	0	0	0
273.16	-53.467	8.032	61.499	2194.0	8.78	0	0	0
298.16	-54.175	8.109	62.284	2417.8	8.81	0	0	0
300	-54.225	8.114	62.339	2434.2	8.82	0	0	0
400	-56.586	8.301	64.887	3320.4	8.90	0	0	0
500	-58.453	8.426	66.879	4213.0	8.95	0	0	0
600	-59.998	8.516	68.514	5109.6	8.98	0	0	0
700	-61.316	8.584	69.900	6008.8	9.00	0	0	0
800	-62.465	8.638	71.103	6910.4	9.02	0	0	0
900	-63.485	8.682	72.167	7813.8	9.04	0	0	0
1,000	-64.402	8.719	73.121	8719.0	9.06	0	0	0
1,100	-65.234	8.750	73.984	9625.0	9.08	0	0	0
1,200	-65.996	8.778	74.774	10533.6	9.09	0	0	0
1,300	-66.700	8.803	75.503	11443.9	9.11	0	0	0
1,400	-67.354	8.825	76.179	12355.0	9.12	0	0	0
1,500	-67.964	8.845	76.809	13267.5	9.14	0	0	0
1,600	-68.535	8.864	77.399	14182.4	9.15	0	0	0
1,700	-69.074	8.881	77.955	15097.7	9.16	0	0	0
1,800	-69.581	8.897	78.478	16014.6	9.18	0	0	0
1,900	-70.063	8.912	78.975	16932.8	9.19	0	0	0
2,000	-70.520	8.927	79.447	17854.0	9.21	0	0	0
2,100	-70.956	8.940	79.896	18774.0	9.22	0	0	0
2,200	-71.372	8.953	80.325	19696.6	9.23	0	0	0
2,300	-71.770	8.966	80.736	20621.8	9.25	0	0	0
2,400	-72.152	8.978	81.130	21547.2	9.26	0	0	0
2,500	-72.519	8.989	81.508	22472.5	9.27	0	0	0
2,750	-73.377	9.017	82.394	24796.8	9.31	0	0	0
3,000	-74.162	9.041	83.203	27123.0	9.34	0	0	0

TABLE 23. *Thermodynamic properties of IF (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> ^o	$H^\circ - H_0^\circ$	<i>C</i> _p ^o	ΔH_f°	ΔF_f°	log <i>K_f</i>
^o K	cal/deg mole	cal/deg mole	cal/deg mole	cal/mole	cal/deg mole	kcal/mole	kcal/mole	
0	0	0	0	0	0	0	0	-----
250	-47.858	7.177	55.035	1794.2	7.76	-30.080	-30.354	26.5349
273.16	-48.496	7.234	55.730	1976.0	7.88	-30.082	-30.378	24.3047
298.16	-49.133	7.293	56.426	2174.5	8.00	-30.089	-30.405	22.2868
300	-49.177	7.297	56.474	2189.1	8.01	-30.090	-30.407	22.1514
400	-51.308	7.521	58.829	3008.4	8.35	-30.10	-30.51	16.670
500	-53.007	7.710	60.717	3855.0	8.56	-30.10	-30.61	13.381
600	-54.427	7.862	62.289	4717.2	8.69	-30.10	-30.72	11.189
700	-55.648	7.987	63.635	5590.9	8.78	-30.10	-30.82	9.622
800	-56.722	8.090	64.812	6472.0	8.84	-30.10	-30.92	8.448
900	-57.680	8.177	65.857	7359.3	8.89	-30.10	-31.03	7.534
1,000	-58.546	8.250	66.796	8250.0	8.93	-30.11	-31.13	6.803
1,100	-59.335	8.314	67.649	9145.4	8.96	-30.11	-31.23	6.205
1,200	-60.060	8.369	68.429	10042.8	8.99	-30.11	-31.33	5.706
1,300	-60.732	8.418	69.150	10943.4	9.01	-30.11	-31.43	5.284
1,400	-61.358	8.461	69.819	11845.4	9.03	-30.12	-31.53	4.923
1,500	-61.943	8.500	70.443	12750.0	9.05	-30.12	-31.63	4.609

TABLE 24. *Thermodynamic properties of IF₅ (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> ^o	$H^\circ - H_0^\circ$	<i>C</i> _p ^o	ΔH_f°	ΔF_f°	log <i>K_f</i>
^o K	cal/deg mole	cal/deg mole	cal/deg mole	cal/mole	cal/deg mole	kcal/mole	kcal/mole	
0	0	0	0	0	0	-200.68	-200.68	-----
250	-60.74	13.89	74.63	3472	21.65	-202.59	-184.19	161.017
273.16	-61.95	14.59	76.54	3985	22.65	-202.59	-182.47	145.987
298.16	-63.32	15.31	78.63	4565	23.70	-202.6	-180.6	132.41
300	-63.41	15.37	78.78	4611	23.77	-202.59	-180.51	131.498
400	-68.19	17.85	86.04	7140	26.57	-202.43	-173.17	94.613
500	-72.38	19.77	92.15	9885	28.19	-202.15	-165.88	72.505
600	-76.13	21.26	97.39	12756	29.18	-201.80	-158.66	57.792
700	-79.50	22.44	101.94	15708	29.82	-201.41	-151.50	47.301
800	-82.56	23.39	105.95	18712	30.26	-201.02	-144.40	39.447
900	-85.36	24.17	109.53	21753	30.57	-200.61	-137.34	33.351
1,000	-87.94	24.83	112.77	24830	30.79	-200.19	-130.33	28.483
1,100	-90.33	25.38	115.71	27918	30.96	-199.78	-123.36	24.510
1,200	-92.56	25.85	118.41	31020	31.09	-199.36	-116.44	21.206
1,300	-94.64	26.25	120.89	34125	31.19	-198.95	-109.54	18.415
1,400	-96.60	26.61	123.21	37254	31.27	-198.53	-102.67	16.028
1,500	-98.45	26.92	125.37	40380	31.34	-198.12	-95.84	13.964

TABLE 25. *Thermodynamic properties of IF₇ (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> [°]	<i>H</i> [°] - <i>H</i> ₀ [°]	<i>C</i> _p [°]	ΔH_f°	ΔF_f°	log <i>K_f</i>
^{°K}	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/mole</i>	<i>cal/deg mole</i>	<i>kcal/mole</i>	<i>kcal/mole</i>	-----
0	0	0	0	0	0	-228.69	-228.69	-----
250	-61.14	16.40	77.54	4100	29.1	-231.73	-202.27	176.820
273.16	-62.64	17.55	80.19	4794	30.8	-231.72	-199.53	159.641
298.16	-64.23	18.96	82.73	5585	32.3	-231.7	-196.6	144.10
300	-64.34	18.81	83.15	5643	32.4	-231.70	-196.37	143.056
400	-70.32	22.77	93.09	9108	36.5	-231.37	-184.64	100.881
500	-75.74	25.77	101.51	12885	38.8	-230.85	-173.02	75.625
600	-80.66	28.07	108.73	16842	40.2	-230.25	-161.51	58.830
700	-85.12	29.87	114.99	20909	41.1	-229.61	-150.10	46.862
800	-89.21	31.31	120.52	25048	41.7	-228.94	-138.79	37.915
900	-92.96	32.48	125.44	29232	42.1	-228.26	-127.55	30.974
1,000	-96.44	33.46	129.90	33460	42.4	-227.56	-116.41	25.440

TABLE 26. *Thermodynamic properties of ICl (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> [°]	<i>H</i> [°] - <i>H</i> ₀ [°]	<i>C</i> _p [°]	ΔH_f°	ΔF_f°	log <i>K_f</i>
^{°K}	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/mole</i>	<i>cal/deg mole</i>	<i>kcal/mole</i>	<i>kcal/mole</i>	-----
0	0	0	0	0	0	-3.33	-3.33	-----
250	-48.598	7.513	56.111	1878.2	8.33	-3.35	-3.30	2.885
273.16	-50.819	7.586	58.405	2072.2	8.42	-3.351	-3.723	2.9790
298.16	-51.486	7.660	59.146	2283.9	8.50	-3.352	-3.757	2.7539
300	-51.534	7.665	59.199	2299.5	8.50	-3.352	-3.760	2.7388
400	-53.773	7.902	61.675	3160.8	8.70	-3.35	-3.90	2.129
500	-55.555	8.073	63.628	4036.5	8.81	-3.35	-4.03	1.763
600	-57.039	8.201	65.240	4920.6	8.87	-3.34	-4.17	1.519
700	-58.311	8.301	66.612	5810.7	8.92	-3.34	-4.31	1.345
800	-59.425	8.380	67.805	6704.0	8.95	-3.34	-4.45	1.215
900	-60.416	8.445	68.861	7600.5	8.98	-3.34	-4.58	1.113
1,000	-61.309	8.499	69.808	8499.0	9.00	-3.34	-4.72	1.032
1,100	-62.121	8.546	70.667	9400.6	9.02	-3.35	-4.86	0.966
1,200	-62.866	8.586	71.452	10303.2	9.04	-3.35	-5.00	.910
1,300	-63.555	8.621	72.176	11207.3	9.05	-3.35	-5.14	.863
1,400	-64.195	8.652	72.847	12112.8	9.06	-3.35	-5.27	.823
1,500	-64.793	8.680	73.473	13020.0	9.08	-3.35	-5.41	.788

TABLE 27. *Thermodynamic properties of IBr (g)*

<i>T</i>	$(F^\circ - H_0^\circ)/T$	$(H^\circ - H_0^\circ)/T$	<i>S</i> [°]	<i>H</i> [°] - <i>H</i> ₀ [°]	<i>C</i> _p [°]	ΔH_f°	ΔF_f°	log <i>K_f</i>
^{°K}	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/deg mole</i>	<i>cal/mole</i>	<i>cal/deg mole</i>	<i>kcal/mole</i>	<i>kcal/mole</i>	-----
0	0	0	0	0	0	-1.42	-1.42	-----
250	-52.501	7.805	60.306	1951.2	8.62	-1.42	-1.76	1.538
273.16	-53.196	7.877	61.073	2151.7	8.68	-1.420	-1.796	1.4369
298.16	-53.889	7.946	61.835	2369.2	8.72	-1.422	-1.830	1.3417
300	-53.938	7.951	61.889	2385.3	8.72	-1.422	-1.833	1.3351
400	-56.256	8.161	64.417	3264.4	8.84	-1.42	-1.97	1.076
500	-58.093	8.304	66.397	4152.0	8.90	-1.42	-2.11	0.921
600	-59.617	8.407	68.024	5044.2	8.94	-1.42	-2.24	.818
700	-60.918	8.486	69.404	5940.2	8.97	-1.42	-2.38	.743
800	-62.056	8.548	70.604	6838.4	8.99	-1.42	-2.52	.688
900	-63.066	8.599	71.665	7739.1	9.01	-1.42	-2.66	.644
1,000	-63.974	8.641	72.615	8641.0	9.03	-1.42	-2.79	.610
1,100	-64.799	8.677	73.476	9544.7	9.05	-1.42	-2.93	.582
1,200	-65.556	8.708	74.264	10449.6	9.06	-1.42	-3.07	.559
1,300	-66.254	8.736	74.990	11356.8	9.07	-1.42	-3.20	.538
1,400	-66.902	8.761	75.663	12265.4	9.09	-1.42	-3.34	.521
1,500	-67.507	8.783	76.290	13174.5	9.10	-1.43	-3.48	.507

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