NIST-JANAF Thermochemical Tables. III. Diatomic Hydrogen Halide Gases

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The spectroscopic and thermodynamic properties of the four diatomic hydrogen halide molecules—HX(g), where X=F, Cl, Br, and I—have been reviewed. Four revised thermochemical tables result from this critical review. The revisions involved the consideration of new spectroscopic information and the use of a direct summation over states for the generation of the thermochemical tables. Compared to previous calculations, the entropies at 298.15 K are unchanged, but the high temperature values ($T>4000$ K) are significantly different. © *2004 American Institute of Physics.*
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Key words: critical evaluation; hydrogen halides; molecular structure; spectroscopic properties; thermodynamic properties.

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1. Introduction

The thermodynamic and spectroscopic properties of the four hydrogen halide ideal gases have been reassessed for the NIST-JANAF Thermochemical Tables. The data for these gases was last critically evaluated in the 1960's, with the exception of HF(g), which was updated in 1977 based on a study by NBS (now NIST) on the thermochemical tables for numerous fluorides

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Hydrogen halide	Date
HF(g)	June 1977
HCl(g)	September 1964
HBr(g)	September 1965
HI(g)	September 1961

The reassessment is necessary for at least two reasons: (1) the existence of newer and more extensive data, and (2) the use of a more highly sophisticated statistical mechanical approach—a direct summation over the energy levels.

The Extended Bibliography not only contains detailed information on the references for the hydrogen halides, but also references for the deuterium and tritium substituted halides. These references contain information dealing with experimental measurements, theoretical calculations, and previously derived thermochemical tables.

2. Hydrogen Halides

In each of the following subsections for the four hydrogen halide gases, a discussion of the rationale used in determining the recommended spectroscopic and thermodynamic information is presented, followed by thermochemical tables for the temperature range 0 K–6000 K. The style and format is that used in the traditional NIST-JANAF Thermochemical Tables.

2.1. Hydrogen Fluoride

Hydrogen fluoride (HF) Ideal gas $M_r = 20.006\,343$

$\Delta_f H^o(0\ \mathrm{K}) = -273.253 \pm 0.70\ \mathrm{kJ \cdot mol^{-1}}$

$S^o(298.15\ \mathrm{K}) = 173.778 \pm 0.005\ \mathrm{J \cdot K^{-1} \cdot mol^{-1}}$ $\Delta_f H^o(298.15\ \mathrm{K}) = -273.300 \pm 0.70\ \mathrm{kJ \cdot mol^{-1}}$

Molecular constants

Ground electronic state: $X\ ^1\Sigma^+$ Energy: $\varepsilon_X = 0\ \mathrm{cm^{-1}}$ Symmetry number: $\sigma = 1$ Quantum weight: $g_X = 1$

Vibrational and rotational levels ($\mathrm{cm^{-1}}$)

v	$G_v - G_0$	B_v	v	$G_v - G_0$	B_v
0	0	20.559 73	10	32311.79	13.4729
1	3961.422 551	19.787 47	11	34687.32	12.78
2	7750.793 391	19.034 96	12	36903.88	12.0696
3	11372.799 3	18.300 71	13	38955.56	11.328
4	14831.62	17.582 90	14	40833.4	10.5428
5	18130.96	16.8792	15	42525.06	9.6869
6	21273.69	16.1895	16	44013.22	8.7396
7	24262.18	15.5033	17	45274.57	7.6528
8	27097.87	14.8266	18	46277.52	6.344
9	29781.33	14.1497	19	46975.55	4.419

$E = G_v - G_0 + \mathrm{F}$

$F_v = B_v Z - D_v Z^2 + H_v Z^3 - L_v Z^4 + (L_v Z^4)^2/(H_v Z^3 - L_v Z^4)$

$D_v = 2.155\,371 \times 10^{-3} - 6.5822 \times 10^{-5} Y + 2.938 \times 10^{-6} Y^2 + 2.78 \times 10^{-7} Y^3 - 1.05 \times 10^{-7} Y^4 + 5.839\,999 \times 10^{-9} Y^5$

$H_v = 1.659 \times 10^{-7} - 4.664 \times 10^{-9} Y - 1.94 \times 10^{-10} Y^2$

$L_v = 8.228\,201 \times 10^{-12}$ where $Z = J(J+1)$, $Y = v + 1/2$

$r_e = 0.916\,809 \pm 0.000\,001$ Å

2.1.1. Enthalpy of Formation

The enthalpy of formation of hydrogen fluoride, HF, was recommended by CODATA-ICSU.[1] It was calculated from measurements of the enthalpy of formation of liquid HF by Johnson *et al.*[2] ($-303.55 \pm 0.25\ \mathrm{kJ \cdot mol^{-1}}$), and the enthalpy of vaporization of HF by Vanderzee and Rodenburg[3,4] ($30.26 \pm 0.10\ \mathrm{kJ \cdot mol^{-1}}$). Considerably less accurate values of $\Delta_f H^o$(HF,g), in particular because of polymerization of HF vapor, were obtained in earlier papers.[4–8]

The spectroscopic values for the dissociation energy of HF were derived from predissociation by rotation in the $X\ ^1\Sigma^+$ state by Di Lonardo and Douglas[10] ($473\,33 \pm 60\ \mathrm{cm^{-1}}$

$=566.2\pm0.7\ \mathrm{kJ\cdot mol^{-1}}$) and by Johnson and Barrow[11] ($47\,241\pm100\ \mathrm{cm^{-1}}=565.1\pm1.2\ \mathrm{kJ\cdot mol^{-1}}$). Both values are in excellent agreement with the calculated value $D_0=566.5\ \mathrm{kJ\cdot mol^{-1}}$. Zemke *et al.*[12] have constructed hybrid potential curves with proper long-range behavior for the ground states of HF and DF and proposed improved $D_e(D_0)$ values for HF: $D_e=49362\pm5\ \mathrm{cm^{-1}}$ and $D_0=47\,311\ \mathrm{cm^{-1}}$. The photoionization study of HF by Berkowitz *et al.*[9] gave a value for the dissociation energy ($47\,143\pm81\ \mathrm{cm^{-1}}$), but it does not agree with the adopted value within the limits of the error indicated.

The accepted enthalpy of formation of HF(g) also agrees with the value of enthalpy of formation of the F^- ion in the state of standard aqueous solution

$$\Delta_f H^o(F^-,\ \text{sol. } H_2O,\ \text{stand. state},\ 298.15\ \text{K})$$
$$=-335.35\pm0.65\ \ \mathrm{kJ\cdot mol^{-1}},$$

which was recommended by CODATA-ICSU[1] as a result of calculations over a number of thermochemical cycles, based on measurements in numerous studies.[2,5,7,13–19]

2.1.2. Heat Capacity and Entropy

These are calculated by direct summation over vibration–rotation levels of the ground electronic state. The information on vibration–rotation levels of HF in the ground $X\ ^1\Sigma^+$ state was obtained from the rotational analyses of vibration–rotation bands[20–38] and pure rotational spectra[39–52] and the electronic transition,[10,11,61] $B\ ^1\Sigma^+-X\ ^1\Sigma^+$. Based on experimental data, the potential energy curve for the ground state was studied in the literature.[12,53–56] The adopted constants are results of our fit of the best data for $v\leqslant2$ as given by Le Blanc, Walker, and Bernath,[37] for $v=3$ by Susada,[38] for $v=4-6$ by Webb and Rao,[31] and for $7\leqslant v\leqslant19$ by Di Lonardo and Douglas.[10] The rotational constants for $v=0$ in LeBlanc *et al.*[37] were fixed at the values obtained from pure rotational spectrum by Hedderich *et al.*[51]

All the constants given above were included in the procedure described in Gurvich *et al.*[96] (pp. 24–32). The fitting procedure provided the convergence of vibrational levels to its dissociation limit and extrapolation of F_v to the limiting curve of dissociation:

$$A(J)=493\,56.23+1.365\,707\times10^{-3}Z-3.690\,901$$
$$\times10^{-7}Z^2+4.306\,919\times10^{-11}Z^3$$
$$v_{\max}=20,\quad J_{\lim}=68.$$

The procedure gives the last vibrational level of the ground state $v=20$. The last observed vibrational level is $v=19$. The $v=20$ level as the last level was predicted in works dealing with potential curves of the ground state.[56,12]

The electronic spectrum was investigated in many studies.[10,11,57–67] According to the experimental[57–60] and theoretical[68–70] data, the electronic states correlating with the ground state limit are repulsive. The other excited states lie above $80\,000\ \mathrm{cm^{-1}}$ and are not taken into account for the calculation of the thermodynamic functions. There are many theoretical calculations on the ground and Rydberg states of HF.[71–95] These do not contradict experimental data (see Table 1).

The thermodynamic functions of HF(g) were calculated using the program described in Gurvich *et al.*[96] The uncertainties in the calculated thermodynamic functions for $T<5000$ K are determined mainly by the uncertainty of the fundamental constants. With increasing temperature the uncertainties increase because of the absence of experimental data for vibrational–rotational energy levels with $J>40$ and because of the use of an approximate method for calculating the limiting curve of dissociation. The uncertainties in the values of $S^o(T)$ are estimated to be 0.005, 0.01, 0.02, and $0.15\ \mathrm{J\cdot K^{-1}\cdot mol^{-1}}$ at 298.15, 1000, 3000, and 6000 K, respectively.

The thermodynamic functions of HF(g) have been calculated earlier in numerous studies[96–108] for temperatures not exceeding 6000 K. Despite the difference of the constants and methods of calculations used in the various studies, and because of the large values of vibrational frequency, the rotational constant and the dissociation energy of HF, the results of these calculations coincide satisfactorily with each other and with the present calculation. For example, the calculations given in Gurvich *et al.*[96] were performed by direct summation over the energy levels and in the NIST-JANAF Thermochemical Tables[105] by the method of Meyer and Goeppert-Meyer. The differences between the results of these two studies are negligible at low temperatures and at 6000 K do not exceed 0.9 and $0.4\ \mathrm{J\cdot K^{-1}\cdot mol^{-1}}$ in the values of $C_p^o(T)$ and $S^o(T)$, respectively.

2.1.3. References

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2.2. Hydrogen Chloride

Hydrogen chloride (HCl) Ideal gas $M_r = 36.460\,94$

$\Delta_f H^o(0\ \mathrm{K}) = -92.125 \pm 0.10\ \mathrm{kJ \cdot mol^{-1}}$

$S^o(298.15\ \mathrm{K}) = 186.901 \pm 0.005\ \mathrm{J \cdot K^{-1} \cdot mol^{-1}}$ $\Delta_f H^o(298.15\ \mathrm{K}) = -92.31 \pm 0.10\ \mathrm{kJ \cdot mol^{-1}}$

Molecular constants

Ground electronic state: $X\ ^1\Sigma^+$ Energy: $\varepsilon_X = 0\ \mathrm{cm^{-1}}$ Symmetry number: $\sigma = 1$ Quantum weight: $g_X = 1$

Vibrational and rotational levels ($\mathrm{cm^{-1}}$)

v	$G_v - G_0$	B_v	v	$G_v - G_0$	B_v
0	0	10.43552	10	24193.84	7.394749
1	2885.36	10.13171	11	26026.77	7.062304
2	5666.79	9.830326	12	27741.70	6.714696
3	8345.05	9.530733	13	29332.42	6.344519
4	10920.63	9.232105	14	30790.40	5.945010
5	13393.64	8.933706	15	32104.69	5.503231
6	15763.84	8.633476	16	33260.68	5.008014
7	18030.53	8.333761	17	34238.36	4.416872
8	20192.66	8.026480	18	35015.76	3.937957
9	22247.99	7.714602			

$$E = G_v - G_0 + \mathrm{F}$$

$$F_v = B_v Z - D_v Z^2 + H_v Z^3 - L_v Z^4 + (L_v Z^4)^2/(H_v Z^3 - L_v Z^4)$$

$$D_v = 5.310\,706 \times 10^{-4} - 7.045\,081 \times 10^{-6} Y + 1.609\,801 \times 10^{-7} Y^2 + 3.194\,908 \times 10^{-8} Y^3 - 6.009\,053 \times 10^{-9} Y^4 + 5.388\,955 \times 10^{-10} Y^5$$

$$H_v = 1.694\,805 \times 10^{-8} - 5.405\,885 \times 10^{-10} Y + 3.583\,473 \times 10^{-11} Y^2$$

$$L_v = 5.917\,307 \times 10^{-12} \quad \text{where} \quad Z = J(J+1), \quad Y = v + 1/2$$

$$r_e = 1.274\,561 + 0.000\,001\ \text{Å}$$

2.2.1. Enthalpy of Formation

The enthalpy of formation of hydrogen chloride, HCl, was recommended by CODATA-ICSU[1] and is based on the results of measurements of enthalpy of the reaction of hydrogen with chlorine by Rossini,[2] Roth and Richter,[3] Wartenberg and Hanish,[4] Lacher *et al.*,[5] Faita *et al.*,[6] Cerquetti *et al.*,[7] and King and Armstrong.[8] The value for the dissociation energy,

$$D_0(\mathrm{H^{35}Cl}) = 427.768 \pm 0.010\ \mathrm{kJ \cdot mol^{-1}} = 35\,759 \pm 8\ \mathrm{cm^{-1}},$$

corresponds to the selected value of $\Delta_f H^o(\mathrm{HCl,g})$.

2.2.2. Heat Capacity and Entropy

These are calculated by direct summation over the vibration–rotation levels of the ground electronic state. The information on the vibration–rotation levels of HCl in the ground $X\ ^1\Sigma^+$ state was obtained from the rotational analyses of vibration–rotation bands,[9–43] microwave spectra,[44–54] CARS spectrum,[55] and the electronic transition,[56,57] $B\ ^1\Sigma^+ - X\ ^1\Sigma^+$. The vibration–rotation spectrum of HCl was investigated also in low-temperature matrices.[63–66] The potential energy curve for the ground state derived from experimental data was studied in numerous other works.[38,58–62]

The adopted constants were selected from the following works. The constants for $v \leqslant 3$ were obtained by Le Blanc *et al.*,[41] who included pure rotational data by Rinsland *et al.*[40] in their treatment. $G_0(v)$ for $4 \leqslant v \leqslant 17$ were derived by Coxon and Roychowdhury[57] from the analysis of the $B\ ^1\Sigma^+ - X\ ^1\Sigma^+$ transition ($7 \leqslant v \leqslant 17$) and for $4 \leqslant v \leqslant 7$ were recalculated from data by Coxon and Ogilvie.[38] The rotational constants for $7 \leqslant v \leqslant 17$ were also taken from Coxon and Roychowdhury.[57] The rotational constants for $4 \leqslant v \leqslant 6$ were taken from work by Clayton *et al.*[39] The rotational constants for $v = 1$, obtained by De Natale *et al.*[53] and for $v = 7$ by Reddy[36] agree well with those adopted here.[63–66]

The selected experimental data for $\mathrm{H^{35}Cl}$ were included in the procedure described in Gurvich *et al.*[107] (pp. 24–32). The fitting procedure provided the convergence of the vibrational

levels to the dissociation limit and extrapolation of F_v to the limiting curve of dissociation:

$$A(J) = 37\,240.98 + 6.720\,724 \times 10^{-4} Z - 1.230\,987 \times 10^{-7} Z^2 + 9.750\,313 \times 10^{-12} Z^3$$

$$v_{\max} = 19, \quad J_{\lim} = 81.$$

Simultaneously, constants were recalculated for the ''effective isotopic modification.'' These are presented above. The procedure gives the last vibrational level of the ground state, $v = 19$, and the extrapolated position of the level $v = 18$. The last vibrational level observed in Coxon and Roychowdhury[57] is $v = 17$, and in Jacques and Barrow[56] is $v = 18$.

The electronic spectrum was investigated in numerous studies.[56,57,67–83] According to the experimental[68,70] and theoretical[84–89] data, the electronic states correlating with the ground state limit are repulsive. The stable excited states lie above 75 000 cm^{-1} and are not taken into account for the calculation of the thermodynamic functions. There are numerous theoretical studies[90–106] on the ground and Rydberg states of HCl (see Table 2).

The thermodynamic functions of HCl (g) were calculated using the program described in Gurvich *et al.*[107] The uncertainties in the calculated thermodynamic functions for $T < 4000$ K are determined mainly by the uncertainty of the fundamental constants. With increasing temperature, the uncertainties increase because of the absence of experimental data for energy of the vibrational–rotational levels with $J > 39$ and because of the use of an approximate method for calculating the limiting curve of dissociation. The uncertainties in the values of $S^o(T)$ are estimated to be 0.005, 0.01, 0.02, and 0.15 $J \cdot K^{-1} \cdot mol^{-1}$ at 298.15, 1000, 3000, and 6000 K, respectively.

The thermodynamic functions of HCl(g) were calculated earlier for low temperatures,[108–114,126] and for higher temperatures,[107,115–125] up to 5000 K–6000 K. Despite the use of different methods and some differences in the fundamental and molecular constants, the discrepancies between the results of these calculations and present calculation are small. The best agreement occurs with the calculation of Gurvich *et al.*,[107] with small discrepancies occurring at temperatures above 3000 K due to a more correct account of vibrational levels and constants B_v which lead to different values $v_{\max}$. The discrepancies with the NIST-JANAF Thermochemical Tables,[122] which start at temperature 1000 K and consist of 0.01, 0.25, 0.7 in $C_p^o(T)$ and 0.001, 0.09, 0.5 $J \cdot K^{-1} \cdot mol^{-1}$ in $S^o(T)$ at temperatures 1000, 3000, 6000 K, respectively. These differences are due to the fact that a direct summation technique was not used.[121]

2.2.3. References

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2.3. Hydrogen Bromide

Hydrogen bromide (HBr) | Ideal gas | $M_r = 80.911\,94$

$\Delta_f H^o(0\ \mathrm{K}) = -28.450 \pm 0.16\ \mathrm{kJ \cdot mol^{-1}}$

$S^o(298.15\ \mathrm{K}) = 198.699 \pm 0.005\ \mathrm{J \cdot K^{-1} \cdot mol^{-1}}$

$\Delta_f H^o(298.15\ \mathrm{K}) = -36.29 \pm 0.16\ \mathrm{kJ \cdot mol^{-1}}$

Molecular constants

Ground electronic state: $X\ ^1\Sigma^+$ | Energy: $\varepsilon_X = 0\ \mathrm{cm^{-1}}$ | Symmetry number: $\sigma = 1$; Quantum weight: $g_X = 1$

Vibrational and rotational levels ($\mathrm{cm^{-1}}$)

$$E = G_v - G_0 + \mathrm{F}$$

$$G_v = 2649.301Y - 45.421\,61Y^2 + 6.288\,3844\times10^{-2}Y^3 - 4.777\,815\times10^{-3}Y^4 - 6.296\,399\times10^{-4}Y^5 + 6.939\,238\times10^{-6}Y^6 - 1.082\,333\times10^{-6}Y^7$$

$$F_v = B_vZ - D_vZ^2 + H_vZ^3 - L_vZ^4 + (L_vZ^4)^2/(H_vZ^3 - L_vZ^4)$$

$$B_v = 8.465\,609 - 0.233\,320Y + 7.866\,402\times10^{-4}Y^2 - 7.395\,769\times10^{-5}Y^3 - 5.696\,09\times10^{-6}Y^4$$

$$D_v = 3.461\,416\times10^{-4} - 4.387\,490\times10^{-6}Y + 4.716\,763\times10^{-7}Y^2$$

$$H_v = 8.024\,492\times10^{-9} - 6.59\,472\times10^{-10}Y$$

$$L_v = 5.023\,602\times10^{-13} \quad \text{where} \quad Z = J(J+1), \quad Y = v + 1/2$$

$$r_e = 1.414\,433 \pm 0.000\,001\ \text{Å}$$

2.3.1. Enthalpy of Formation

The enthalpy of formation of hydrogen bromide, HBr, was recommended by CODATA-ICSU[1] and is based on the results of calorimetric measurements of the enthalpy of solution of HBr(g) in water ($\Delta_r H = -85.12 \pm 0.06\ \mathrm{kJ \cdot mol^{-1}}$) by Vanderzee and Nutter,[2] Roth and Bertram,[3,4] and Thompsen.[5] The dissociation energy

$$D_0(\mathrm{HBr}) = 30\,295 \pm 17\ \ \mathrm{cm^{-1}}$$

corresponds to the accepted enthalpy of formation. The bond energy derived by Smith and Adams[6] from the study of the reaction $\mathrm{HBr} + e = \mathrm{Br^-} + \mathrm{H}$ agrees with the thermochemical data.

2.3.2. Heat Capacity and Entropy

These are calculated by direct summation over the vibration–rotation levels of the ground electronic state. The information on the ground $X\ ^1\Sigma^+$ state levels was derived from the rotational analyses of vibration–rotation bands[7–30] and pure rotation spectra.[31–38] Vibration–rotation spectra of HBr were studied also in low temperature matrices.[39–41] The data for $v \leqslant 2$, obtained by Braun and Bernath,[26] the data for $v = 3$, 5, 6, obtained by Nishimiya *et al.*,[30] and the constants for levels $v = 4$ and 7 calculated from the constants given by Bernage and Niay[20] were used in the fit.

The fitting procedure (Gurvich *et al.*[84] pp. 24–32) provided the convergence of vibrational levels to its dissociation limit and extrapolation F_v to the limiting curve of dissociation:

$$A(J) = 31\,615.55 + 5.993\,531\times10^{-4}Z - 1.031\,549\times10^{-7}Z^2 + 7.540\,218\times10^{-12}Z^3$$

$$v_{\max} = 19, \quad J_{\lim} = 83.$$

Simultaneously, the program corrected the constants to the average isotopic species. These are presented above.

The electronic spectrum was investigated in numerous studies.[42–60] According to the experimental[42–47] and theoretical[61–64] data, the electronic states correlating with the ground state limit are repulsive. The stable excited states lie above 66 000 $\mathrm{cm^{-1}}$ and are not taken into account for the calculation of thermodynamic functions. Theoretical studies[65–69,25] deal with the potential energy curve and Born–Oppenheimer breakdown effects in the ground state of hydrogen bromide.

Numerous calculations of the ground state properties[70–83] have been performed using different methods and are in good agreement with available experimental data (see Table 3).

The thermodynamic functions of HBr (g) were calculated using a program described by Gurvich *et al.*[84] The uncertainties in the calculated thermodynamic functions for $T < 3000$ K are determined mainly by the uncertainty of the

fundamental constants. With increasing temperature, the uncertainties increase because of the absence of experimental data for the energy of the vibrational–rotational levels with $v>7$ and because of the use of an approximate method for calculating the limiting curve of dissociation. The uncertainties in the values of $S^o(T)$ are estimated to be 0.005, 0.02, 0.2, and 0.3 $J\cdot K^{-1}\cdot mol^{-1}$ at 298.15, 1000, 3000, and 6000 K, respectively.

The thermodynamic functions of HBr (g) were calculated earlier for the temperature range ($T\leqslant 1600$ K),[85] ($T\leqslant 2000$ K),[86] and ($T\leqslant 6000$ K).[84,87–92] In all these calculations, less accurate values of molecular constants were used than in this work. In these examples the calculations were performed by the method of Gordon and Barnes[85,89,90] and by the method of Meyer and Goeppert-Meyer[87,91] was used. Feber and Herrik[88] and Gurvich *et al.*[84] calculated the thermodynamic functions by direct summation over the energy levels. Despite the difference in the methods of calculation and in the values of the constants, the results of all calculations differ very little from the present calculation. The best agreement with present work occurs with the functions calculated by Feber and Herrik[88] and Gurvich *et al.*[84]

Discrepancies with NIST-JANAF Thermochemical Tables[91] in $C_p^o(T)$, $S^o(T)$, $-(G^o-H^o(T_r))/T$ reach at 6000 K, 0.08, 0.5, and 0.184 $J\cdot K^{-1}\cdot mol^{-1}$, respectively.

2.3.3. References

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2.4. Hydrogen Iodide

Hydrogen iodide (HI) Ideal gas $M_r = 127.9124$

$\Delta_f H^o(0\ \mathrm{K}) = 28.676 \pm 0.10\ \mathrm{kJ \cdot mol^{-1}}$

$S^o(298.15\ \mathrm{K}) = 206.589 \pm 0.005\ \mathrm{J \cdot K^{-1} \cdot mol^{-1}}$ $\Delta_f H^o(298.15\ \mathrm{K}) = 26.50 \pm 0.10\ \mathrm{kJ \cdot mol^{-1}}$

Molecular constants

Ground electronic state: $X\ ^1\Sigma^+$ Energy: $\varepsilon_X = 0\ \mathrm{cm^{-1}}$ Symmetry number: $\sigma = 1$ Quantum weight: $g_X = 1$

Vibrational and rotational levels ($\mathrm{cm^{-1}}$)

$$E = G_v - G_0 + \mathrm{F}$$

$$G_v = 2308.975Y - 39.6112Y^2 - 2.7419\times 10^{-2}Y^3 - 1.6870\times 10^{-2}Y^4 + 3.8732\times 10^{-4}Y^5 - 5.513\times 10^{-6}Y^6 + 2.7143\times 10^{-6}Y^7 - 1.403\,25\times 10^{-7}Y^8$$

$$F_v = B_v Z - D_v Z^2 + H_v Z^3 - L_v Z^4 + (L_v Z^4)^2/(H_v Z^3 - L_v Z^4)$$

$$B_v = 6.511\,628 - 0.170\,372Y^2 - 2.8469\times 10^{-4}Y^4 - 4.0465\times 10^{-5}Y^3 - 8.625\times 10^{-6}Y^4$$

$$D_v = 2.071\,68\times 10^{-4} - 7.868\times 10^{-7}Y + 1.676\times 10^{-7}Y^2 - 2.85\times 10^{-8}Y^3$$

$$H_v = 2.975\times 10^{-9} - 1.87\times 10^{-10}Y$$

$$L_v = 2.143\,053\times 10^{-13} \quad \text{where} \quad Z = J(J+1), Y = v + 1/2$$

$$r_e = 1.609\,083 \pm 0.000\,004\ \text{Å}.$$

2.4.1. Enthalpy of Formation

Enthalpy of formation of hydrogen iodide, HI, was recommended by CODATA-ICSU[1] and is based on the results of measurements of standard enthalpy of solution of HI(g) in water ($-83.283 \pm 0.085\ \mathrm{kJ \cdot mol^{-1}}$) by Vanderzee and Geer.[2] The close but less accurate values of the enthalpy of formation of HI(g) can be obtained from study of the equilibrium of $2\mathrm{HI(g)} = \mathrm{I_2(g)} + \mathrm{H_2(g)}$ by Taylor and Criste,[3] a determination of the degree of decomposition of HI(g) by Rittenberg and Urie,[4] a photocalorimetric study of the equilibrium of the decomposition of HI(g) by Bright and Hagerty,[5] the theoretical calculations of Murphy[6] and calorimetric determination of the enthalpy of the reaction $2\mathrm{HI(g)} + \mathrm{Cl_2} = 2\mathrm{HCl(g)} + \mathrm{I_2(g)}$ by Günther and Wekua.[7] The accepted enthalpy of formation of HI(g) agrees with the values of enthalpy of formation of the $\mathrm{I^-}$ ion in the state of standard aqueous solution

$$\Delta_f H^o(\mathrm{I^-},\ \text{sol. } \mathrm{H_2O},\ \text{stand. state},\ 298.15\ \mathrm{K}) = -56.78 \pm 0.05\ \mathrm{kJ \cdot mol^{-1}}$$

found in the calorimetric investigations by Johnson[8] and adopted by CODATA-ICSU.[1]

The dissociation energy, $D_0(\mathrm{HI}) = 24\,620 \pm 10\ \mathrm{cm^{-1}}$, corresponds to the accepted enthalpy of formation. The results of studies of reaction $\mathrm{HI} + e = \mathrm{I^-} + \mathrm{H}$ by Smith and Adams[9] agree with thermochemical data.

2.4.2. Heat Capacity and Entropy

These are calculated by direct summation over the vibration–rotation levels of the electronic ground state.

The molecular constants of HI in the ground $X\,^1\Sigma^+$ state were obtained from the rotational analyses of vibration–rotation bands[10–26] and microwave spectra.[27–34] The adopted constants are results of our fit of the best data for $v \leqslant 7$ were given by Guelashvili *et al.*[23] and by Katayama *et al.*[26] where parameters for $v=0$ were fixed at the values derived from microwave study by De Lucia *et al.*[32]

The fitting procedure (Gurvich *et al.*,[35] pp. 24–32) provided the convergence of vibrational levels to the dissociation limit and extrapolation of F_v to the limiting curve of dissociation:

$$A(J)=25\,768.81+5.397\,226\times10^{-4}Z-8.808\,481\times10^{-8}Z^2+5.879\,664\times10^{-12}Z^3$$

$$v_{\max}=17, \quad J_{\lim}=86.$$

The electronic spectrum was investigated in numerous studies.[36–46] According to the experimental[36–39,42] and theoretical[47–50] data, the electronic states correlating with the ground state limit are repulsive. The stable excited states lie above 50 000 cm^{-1} and are not taken into account for the calculation of the thermodynamic functions.

Vibration–rotation spectra of HI were also studied in low temperature matrices.[51–56]

Theoretical studies[57–61] deal with the potential energy curve and Born–Oppenheimer breakdown effects in the ground state of hydrogen iodide.

Numerous calculations[62–74] of the ground state properties have been performed using different methods. Some [73,74] are in good agreement with available experimental data.

The thermodynamic functions of HI (g) were calculated using a program described in Gurvich *et al.*[35] The uncertainties in the calculated thermodynamic functions for $T<3000$ K are determined mainly by the uncertainty of the fundamental constants. With increasing temperature, the uncertainties increase because of the absence of experimental data for the energy of the vibrational–rotational levels with $v>7$ and because of the use of an approximate method for calculating the limiting curve of dissociation. The uncertainties in the values of $S^o(T)$ are estimated to be 0.005, 0.02, 0.2, and 0.3 $J\cdot K^{-1}\cdot mol^{-1}$ at 298.15, 1000, 3000, and 6000 K, respectively (see Table 4).

The thermodynamic functions of HI(g) have been calculated earlier.[75–83,35,6] In all these calculations, less accurate values of molecular constants were used than in this work. These calculations were performed by the direct summation over the energy levels,[35,78,79] by the method of Gordon and Barnes,[76] and by the method of Meyer and Goeppert-Meyer.[77] Discrepancies with the calculations of four of these studies[79,78,76,35] do not exceed 0.2 $J\cdot K^{-1}\cdot mol^{-1}$ in the values of $-(G^o-H^o(T_r))/T$ in the whole range of temperatures. Deviations in the values of $S^o(T)$ and especially $C_p^o(T)$ are significantly greater and reach in $C_p^o(T)$ 2.12 $J\cdot K^{-1}\cdot mol^{-1}$ at 6000 K for the fifth study.[77]

2.4.3. References

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3. Conclusions

The structural, spectroscopic, and thermodynamic properties of four hydrogen halide ideal gases have been critically reviewed. The thermal functions have been calculated using a direct summation over the vibrational-rotational states with summation cutoff at the dissociation energy. As extensive experimental data exists for the description of the vibrational–rotational energy levels (and in the vicinity of the dissociation energy), the thermal functions should reflect an extremely reliable set of values.

The thermodynamic values are summarized in the following table:

Diatomic halide HX (g)	$S^o(298.15\ K)$ $J\cdot K^{-1}\cdot mol^{-1}$	$\Delta_f H^o(298.15\ K)$ $kJ\cdot mol^{-1}$	$D_0(HX)$ cm^{-1}	$\Delta_{at}H^o(0\ K)$ $kJ\cdot mol^{-1}$
HF (g)	173.778±0.005	−273.300±0.70	47339±80	566.572
HCl (g)	186.901±0.005	−92.31±0.10	35759±8	427.781
HBr (g)	198.699±0.005	−36.29±0.16	30295±17	362.402
HI (g)	206.589±0.005	26.50±0.10	24620±10	254.523

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The work is a continuation of two earlier evaluations:

1. O. Dorofeeva, V. P. Novikov, D. B. Neumann, ''NIST-JANAF Thermochemical Tables. I. Ten Organic Molecules Related to Atmospheric Chemistry,'' J. Phys. Chem. Ref. Data **30**(2), 475–513 (2001).

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The work literature survey for the four hydrogen halides was complete through 1999.

5. Extended Bibliographies

The following bibliography lists articles that were found in the literature pertaining to the molecules discussed above, but including a few sources that were not used in the evaluation, as well as separately listing articles dealing with the deuterium and tritium species.

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TABLE 1. Ideal gas thermochemical properties of hydrogen fluoride, HF(g), at standard state pressure, $p^o = 0.1$ MPa ($T_r = 298.15$ K)

T (K)	C_p^o ($J \cdot K^{-1} \cdot mol^{-1}$)	S^o ($J \cdot K^{-1} \cdot mol^{-1}$)	$-(G^o - H^o(T_r))/T$ ($J \cdot K^{-1} \cdot mol^{-1}$)	$H^o - H^o(T_r)$ ($kJ \cdot mol^{-1}$)	$\Delta_f H^o$ ($kJ \cdot mol^{-1}$)	$\Delta_f G^o$ ($kJ \cdot mol^{-1}$)	$\log K_f^o$
0	0.000	0.000	∞	−8.599	−273.253	−273.253	∞
25	29.901	101.286	419.957	−7.967	−273.249	−273.466	571.362
50	29.227	121.741	266.342	−7.230	−273.292	−273.684	285.908
75	29.150	133.573	220.247	−6.501	−273.369	−273.859	190.728
100	29.133	141.956	199.677	−5.772	−273.379	−274.020	143.130
150	29.126	153.767	182.538	−4.316	−273.325	−274.351	95.535
180	29.127	159.077	178.199	−3.442	−273.292	−274.559	79.673
190	29.128	160.652	177.234	−3.151	−273.284	−274.629	75.499
200	29.128	162.146	176.443	−2.859	−273.278	−274.700	71.743
210	29.129	163.567	175.796	−2.568	−273.273	−274.772	68.344
220	29.130	164.922	175.271	−2.277	−273.270	−274.843	65.254
230	29.131	166.217	174.850	−1.985	−273.268	−274.914	62.433
240	29.132	167.457	174.516	−1.694	−273.269	−274.986	59.848
250	29.132	168.646	174.257	−1.403	−273.270	−275.057	57.469
260	29.133	169.789	174.064	−1.111	−273.274	−275.129	55.273
270	29.134	170.888	173.926	−0.820	−273.279	−275.200	53.239
280	29.135	171.948	173.836	−0.529	−273.285	−275.271	51.351
290	29.136	172.970	173.789	−0.237	−273.292	−275.342	49.593
298.15	29.137	173.778	173.778	0.000	−273.300	−275.400	48.248
300	29.138	173.958	173.778	0.054	−273.302	−275.413	47.952
350	29.143	178.450	174.133	1.511	−273.364	−275.760	41.154
400	29.150	182.342	174.921	2.968	−273.450	−276.097	36.054
450	29.159	185.776	175.940	4.426	−273.556	−276.421	32.085
500	29.173	188.849	177.080	5.884	−273.679	−276.733	28.909
600	29.230	194.172	179.499	8.804	−273.960	−277.319	24.142
700	29.351	198.686	181.925	11.732	−274.276	−277.854	20.733
800	29.550	202.617	184.271	14.677	−274.613	−278.343	18.173
900	29.827	206.113	186.507	17.645	−274.959	−278.789	16.180
1000	30.169	209.273	188.628	20.644	−275.307	−279.195	14.583
1100	30.558	212.166	190.638	23.680	−275.650	−279.567	13.275
1200	30.975	214.843	192.545	26.757	−275.985	−279.909	12.184
1300	31.403	217.339	194.358	29.876	−276.312	−280.223	11.259
1400	31.831	219.682	196.084	33.037	−276.627	−280.511	10.466
1500	32.249	221.892	197.731	36.242	−276.932	−280.778	9.777
1600	32.653	223.986	199.307	39.487	−277.227	−281.025	9.174
1700	33.038	225.978	200.818	42.771	−277.512	−281.254	8.642
1800	33.402	227.876	202.269	46.094	−277.787	−281.466	8.168
1900	33.746	229.692	203.665	49.451	−278.051	−281.663	7.743
2000	34.069	231.431	205.010	52.842	−278.306	−281.846	7.361
2100	34.371	233.101	206.308	56.264	−278.550	−282.018	7.015
2200	34.655	234.706	207.563	59.716	−278.783	−282.177	6.700
2300	34.921	236.253	208.777	63.195	−279.003	−282.326	6.412
2400	35.170	237.744	209.953	66.699	−279.211	−282.466	6.148
2500	35.404	239.185	211.093	70.228	−279.404	−282.597	5.904
2600	35.625	240.577	212.201	73.780	−279.583	−282.721	5.680
2700	35.832	241.926	213.277	77.353	−279.745	−282.839	5.472
2800	36.028	243.233	214.323	80.946	−279.891	−282.950	5.278
2900	36.214	244.500	215.342	84.558	−280.018	−283.058	5.098
3000	36.390	245.731	216.335	88.188	−280.127	−283.161	4.930
3100	36.558	246.927	217.303	91.836	−280.217	−283.261	4.773
3200	36.717	248.090	218.247	95.500	−280.287	−283.358	4.625
3300	36.870	249.222	219.168	99.179	−280.337	−283.452	4.487
3400	37.017	250.325	220.068	102.873	−280.367	−283.547	4.356
3500	37.158	251.400	220.948	106.582	−280.377	−283.640	4.233
3600	37.293	252.449	221.809	110.305	−280.366	−283.733	4.117
3700	37.424	253.473	222.651	114.041	−280.334	−283.826	4.007
3800	37.551	254.472	223.475	117.790	−280.283	−283.923	3.903
3900	37.675	255.449	224.282	121.551	−280.211	−284.017	3.804
4000	37.795	256.405	225.074	125.325	−280.120	−284.117	3.710
4100	37.912	257.339	225.849	129.110	−280.009	−284.218	3.621
4200	38.027	258.254	226.610	132.907	−279.879	−284.322	3.536
4300	38.139	259.151	227.356	136.715	−279.731	−284.431	3.455
4400	38.249	260.029	228.089	140.535	−279.563	−284.542	3.378
4500	38.357	260.889	228.808	144.365	−279.377	−284.655	3.304

TABLE 1. Ideal gas thermochemical properties of hydrogen fluoride, HF(g), at standard state pressure, $p^o = 0.1$ MPa ($T_r = 298.15$ K)–Continued

T (K)	C_p^o ($J \cdot K^{-1} \cdot mol^{-1}$)	S^o ($J \cdot K^{-1} \cdot mol^{-1}$)	$-(G^o - H^o(T_r))/T$ ($J \cdot K^{-1} \cdot mol^{-1}$)	$H^o - H^o(T_r)$ ($kJ \cdot mol^{-1}$)	$\Delta_f H^o$ ($kJ \cdot mol^{-1}$)	$\Delta_f G^o$ ($kJ \cdot mol^{-1}$)	$\log K_f^o$
4600	38.463	261.734	229.515	148.206	−279.174	−284.777	3.234
4700	38.568	262.562	230.209	152.058	−278.953	−284.901	3.166
4800	38.671	263.375	230.892	155.920	−278.715	−285.030	3.102
4900	38.773	264.173	231.563	159.792	−278.460	−285.165	3.040
5000	38.873	264.958	232.223	163.674	−278.188	−285.302	2.980
5100	38.972	265.728	232.872	167.567	−277.901	−285.449	2.924
5200	39.070	266.486	233.511	171.469	−277.596	−285.598	2.869
5300	39.166	267.231	234.141	175.381	−277.276	−285.758	2.816
5400	39.261	267.964	234.760	179.302	−276.940	−285.917	2.766
5500	39.354	268.686	235.371	183.233	−276.588	−286.087	2.717
5600	39.445	269.396	235.972	187.173	−276.222	−286.263	2.670
5700	39.535	270.095	236.564	191.122	−275.839	−286.447	2.625
5800	39.623	270.783	237.148	195.080	−275.441	−286.638	2.581
5900	39.709	271.461	237.724	199.047	−275.028	−286.834	2.539
6000	39.793	272.129	238.292	203.022	−274.601	−287.039	2.499

TABLE 2. Ideal gas thermochemical properties for hydrogen chloride, HCl(g), at standard state pressure, $p^o = 0.1$ MPa ($T_r = 298.15$ K)

T (K)	C_p^o ($J \cdot K^{-1} \cdot mol^{-1}$)	S^o ($J \cdot K^{-1} \cdot mol^{-1}$)	$-(G^o - H^o(T_r))/T$ ($J \cdot K^{-1} \cdot mol^{-1}$)	$H^o - H^o(T_r)$ ($kJ \cdot mol^{-1}$)	$\Delta_f H^o$ ($kJ \cdot mol^{-1}$)	$\Delta_f G^o$ ($kJ \cdot mol^{-1}$)	$\log K_f^o$
0	0.000	0.000	∞	−8.640	−92.125	−92.125	∞
25	29.230	114.689	432.926	−7.956	−92.072	−92.391	193.036
50	29.128	134.903	279.443	−7.227	−92.122	−92.706	96.847
75	29.118	146.710	233.363	−6.499	−92.201	−92.978	64.754
100	29.116	155.087	212.797	−5.771	−92.212	−93.234	48.699
150	29.119	166.893	195.661	−4.315	−92.173	−93.753	32.647
180	29.122	172.202	191.322	−3.442	−92.162	−94.071	27.298
190	29.123	173.777	190.357	−3.150	−92.163	−94.176	25.890
200	29.124	175.271	189.566	−2.859	−92.166	−94.282	24.623
210	29.125	176.692	188.919	−2.568	−92.172	−94.388	23.477
220	29.126	178.047	188.395	−2.277	−92.180	−94.493	22.435
230	29.127	179.341	187.973	−1.985	−92.190	−94.598	21.483
240	29.128	180.581	187.639	−1.694	−92.203	−94.703	20.611
250	29.129	181.770	187.381	−1.403	−92.217	−94.807	19.808
260	29.131	182.913	187.187	−1.111	−92.234	−94.910	19.067
270	29.132	184.012	187.050	−0.820	−92.252	−95.012	18.381
280	29.133	185.072	186.960	−0.529	−92.271	−95.114	17.743
290	29.135	186.094	186.913	−0.238	−92.292	−95.216	17.150
298.15	29.136	186.901	186.901	0.000	−92.310	−95.297	16.695
300	29.136	187.081	186.902	0.054	−92.314	−95.316	16.596
350	29.149	191.574	187.257	1.511	−92.441	−95.807	14.298
400	29.175	195.468	188.045	2.969	−92.587	−96.278	12.572
450	29.224	198.906	189.065	4.429	−92.746	−96.730	11.228
500	29.304	201.989	190.206	5.892	−92.911	−97.163	10.150
600	29.576	207.354	192.629	8.835	−93.249	−97.983	8.530
700	29.987	211.942	195.068	11.812	−93.577	−98.746	7.368
800	30.499	215.979	197.435	14.835	−93.880	−99.464	6.494
900	31.062	219.603	199.700	17.913	−94.149	−100.145	5.812
1000	31.638	222.906	201.858	21.048	−94.384	−100.799	5.265
1100	32.200	225.948	203.911	24.240	−94.587	−101.430	4.816
1200	32.732	228.773	205.867	27.487	−94.760	−102.044	4.442
1300	33.227	231.413	207.731	30.785	−94.908	−102.645	4.124
1400	33.682	233.892	209.512	34.131	−95.035	−103.235	3.852
1500	34.097	236.230	211.216	37.521	−95.146	−103.817	3.615
1600	34.476	238.443	212.849	40.950	−95.242	−104.392	3.408
1700	34.820	240.544	214.417	44.415	−95.328	−104.962	3.225
1800	35.135	242.543	215.925	47.913	−95.406	−105.526	3.062
1900	35.421	244.450	217.376	51.441	−95.477	−106.085	2.916
2000	35.684	246.274	218.776	54.996	−95.546	−106.642	2.785
2100	35.926	248.021	220.127	58.577	−95.612	−107.195	2.666
2200	36.149	249.697	221.433	62.181	−95.678	−107.745	2.558
2300	36.356	251.309	222.698	65.806	−95.746	−108.293	2.459
2400	36.548	252.860	223.922	69.451	−95.815	−108.837	2.369
2500	36.729	254.356	225.110	73.115	−95.888	−109.377	2.285
2600	36.898	255.800	226.263	76.797	−95.967	−109.915	2.208
2700	37.058	257.195	227.382	80.495	−96.051	−110.451	2.137
2800	37.210	258.546	228.472	84.208	−96.141	−110.981	2.070
2900	37.355	259.854	229.531	87.937	−96.239	−111.509	2.008
3000	37.494	261.123	230.563	91.679	−96.344	−112.035	1.951
3100	37.627	262.354	231.569	95.435	−96.456	−112.556	1.897
3200	37.756	263.551	232.550	99.204	−96.576	−113.074	1.846
3300	37.881	264.715	233.507	102.986	−96.703	−113.587	1.798
3400	38.002	265.848	234.442	106.780	−96.837	−114.097	1.753
3500	38.120	266.951	235.355	110.587	−96.975	−114.603	1.710
3600	38.236	268.026	236.247	114.404	−97.120	−115.105	1.670
3700	38.348	269.076	237.121	118.234	−97.267	−115.601	1.632
3800	38.459	270.100	237.975	122.074	−97.419	−116.097	1.596
3900	38.567	271.100	238.812	125.925	−97.572	−116.585	1.561
4000	38.672	272.078	239.631	129.787	−97.726	−117.069	1.529
4100	38.776	273.034	240.434	133.660	−97.879	−117.551	1.498
4200	38.877	273.970	241.222	137.543	−98.030	−118.030	1.468
4300	38.975	274.886	241.994	141.435	−98.180	−118.507	1.440
4400	39.070	275.783	242.752	145.337	−98.325	−118.977	1.412
4500	39.163	276.662	243.495	149.249	−98.464	−119.443	1.386

TABLE 2. Ideal gas thermochemical properties for hydrogen chloride, HCl(g), at standard state pressure, $p^o = 0.1$ MPa ($T_r = 298.15$ K)–Continued

T (K)	C_p^o ($J \cdot K^{-1} \cdot mol^{-1}$)	S^o ($J \cdot K^{-1} \cdot mol^{-1}$)	$-(G^o - H^o(T_r))/T$ ($J \cdot K^{-1} \cdot mol^{-1}$)	$H^o - H^o(T_r)$ ($kJ \cdot mol^{-1}$)	$\Delta_f H^o$ ($kJ \cdot mol^{-1}$)	$\Delta_f G^o$ ($kJ \cdot mol^{-1}$)	$\log K_f^o$
4600	39.252	277.524	244.226	153.170	−98.598	−119.908	1.362
4700	39.338	278.369	244.943	157.099	−98.726	−120.370	1.338
4800	39.419	279.198	245.648	161.037	−98.844	−120.830	1.315
4900	39.497	280.011	246.341	164.983	−98.955	−121.288	1.293
5000	39.570	280.810	247.023	168.936	−99.055	−121.740	1.272
5100	39.638	281.594	247.693	172.897	−99.146	−122.194	1.251
5200	39.701	282.365	248.352	176.864	−99.226	−122.644	1.232
5300	39.758	283.121	249.001	180.837	−99.295	−123.096	1.213
5400	39.810	283.865	249.640	184.815	−99.353	−123.543	1.195
5500	39.856	284.596	250.269	188.799	−99.397	−123.990	1.178
5600	39.896	285.315	250.888	192.786	−99.431	−124.438	1.161
5700	39.929	286.021	251.499	196.778	−99.452	−124.885	1.144
5800	39.955	286.716	252.100	200.772	−99.461	−125.330	1.129
5900	39.975	287.399	252.692	204.768	−99.458	−125.776	1.114
6000	39.987	288.071	253.276	208.766	−99.442	−126.224	1.099

TABLE 3. Ideal gas thermochemical properties for hydrogen bromide, HBr(g), at standard state pressure, p^o=0.1 MPa (T_r=298.15 K)

T (K)	C_p^o (J·K^{-1}·mol^{-1})	S^o (J·K^{-1}·mol^{-1})	$-(G^o-H^o(T_r))/T$ (J·K^{-1}·mol^{-1})	$H^o-H^o(T_r)$ (kJ·mol^{-1})	$\Delta_f H^o$ (kJ·mol^{-1})	$\Delta_f G^o$ (kJ·mol^{-1})	log K_f^o
0	0.000	0.000	∞	−8.648	−28.450	−28.450	∞
25	29.171	126.506	444.717	−7.955	−28.102	−30.463	63.647
50	29.119	146.703	291.241	−7.227	−28.127	−32.845	34.312
75	29.114	158.508	245.162	−6.499	−28.301	−35.166	24.491
100	29.115	166.884	224.595	−5.771	−28.469	−37.429	19.550
150	29.119	178.690	207.458	−4.315	−28.850	−41.830	14.566
180	29.122	183.999	203.120	−3.442	−29.136	−44.399	12.884
190	29.123	185.574	202.155	−3.150	−29.243	−45.244	12.438
200	29.124	187.067	201.364	−2.859	−29.354	−46.085	12.036
210	29.125	188.488	200.717	−2.568	−29.472	−46.917	11.670
220	29.126	189.843	200.192	−2.277	−29.596	−47.745	11.336
230	29.128	191.138	199.770	−1.985	−29.726	−48.567	11.030
240	29.129	192.378	199.437	−1.694	−29.861	−49.383	10.748
250	29.130	193.567	199.178	−1.403	−30.004	−50.195	10.487
260	29.132	194.709	198.985	−1.112	−30.155	−50.999	10.245
270	29.134	195.809	198.847	−0.820	−35.632	−51.716	10.005
280	29.136	196.868	198.757	−0.529	−35.869	−52.307	9.758
290	29.138	197.891	198.710	−0.238	−36.103	−52.890	9.526
298.15	29.141	198.699	198.699	0.000	−36.290	−53.361	9.348
300	29.141	198.879	198.699	0.054	−36.333	−53.466	9.309
350	29.167	203.372	199.054	1.512	−51.925	−55.462	8.277
400	29.220	207.270	199.843	2.971	−52.109	−55.955	7.307
450	29.313	210.717	200.863	4.434	−52.297	−56.424	6.549
500	29.453	213.812	202.006	5.903	−52.484	−56.873	5.941
600	29.872	219.217	204.437	8.868	−52.843	−57.717	5.025
700	30.430	223.862	206.887	11.882	−53.167	−58.503	4.365
800	31.061	227.966	209.270	14.956	−53.446	−59.246	3.868
900	31.708	231.662	211.556	18.095	−53.676	−59.957	3.480
1000	32.333	235.035	213.738	21.297	−53.863	−60.644	3.168
1100	32.916	238.145	215.817	24.560	−54.011	−61.315	2.912
1200	33.451	241.032	217.800	27.879	−54.127	−61.973	2.698
1300	33.934	243.729	219.692	31.249	−54.218	−62.623	2.516
1400	34.370	246.260	221.500	34.664	−54.289	−63.266	2.360
1500	34.761	248.645	223.231	38.121	−54.346	−63.906	2.225
1600	35.113	250.900	224.890	41.615	−54.392	−64.541	2.107
1700	35.431	253.038	226.484	45.143	−54.432	−65.175	2.003
1800	35.719	255.072	228.016	48.700	−54.468	−65.806	1.910
1900	35.981	257.010	229.491	52.285	−54.504	−66.434	1.826
2000	36.221	258.862	230.914	55.896	−54.541	−67.061	1.751
2100	36.442	260.634	232.287	59.529	−54.583	−67.686	1.684
2200	36.646	262.334	233.615	63.184	−54.629	−68.309	1.622
2300	36.836	263.968	234.899	66.858	−54.684	−68.930	1.565
2400	37.015	265.539	236.143	70.550	−54.745	−69.549	1.514
2500	37.183	267.054	237.349	74.260	−54.816	−70.163	1.466
2600	37.342	268.515	238.520	77.987	−54.895	−70.776	1.422
2700	37.494	269.927	239.657	81.729	−54.982	−71.386	1.381
2800	37.640	271.293	240.763	85.485	−55.079	−71.991	1.343
2900	37.780	272.617	241.839	89.257	−55.183	−72.593	1.308
3000	37.916	273.900	242.886	93.041	−55.294	−73.192	1.274
3100	38.047	275.145	243.907	96.840	−55.412	−73.785	1.243
3200	38.174	276.355	244.902	100.651	−55.535	−74.377	1.214
3300	38.298	277.532	245.873	104.474	−55.662	−74.965	1.187
3400	38.418	278.677	246.821	108.310	−55.791	−75.547	1.161
3500	38.535	279.792	247.747	112.158	−55.922	−76.125	1.136
3600	38.648	280.879	248.653	116.017	−56.053	−76.701	1.113
3700	38.758	281.940	249.538	119.888	−56.183	−77.273	1.091
3800	38.863	282.975	250.404	123.769	−56.312	−77.843	1.070
3900	38.965	283.986	251.252	127.660	−56.437	−78.405	1.050
4000	39.061	284.974	252.083	131.561	−56.559	−78.968	1.031
4100	39.152	285.939	252.897	135.472	−56.677	−79.526	1.013
4200	39.238	286.884	253.695	139.392	−56.789	−80.083	0.996
4300	39.317	287.808	254.478	143.320	−56.896	−80.637	0.980
4400	39.390	288.713	255.246	147.255	−56.998	−81.187	0.964
4500	39.456	289.599	255.999	151.197	−57.093	−81.733	0.949

TABLE 3. Ideal gas thermochemical properties for hydrogen bromide, HBr(g), at standard state pressure, $p^o = 0.1$ MPa ($T_r = 298.15$ K)–Continued

T (K)	C_p^o ($J \cdot K^{-1} \cdot mol^{-1}$)	S^o ($J \cdot K^{-1} \cdot mol^{-1}$)	$-(G^o - H^o(T_r))/T$ ($J \cdot K^{-1} \cdot mol^{-1}$)	$H^o - H^o(T_r)$ ($kJ \cdot mol^{-1}$)	$\Delta_f H^o$ ($kJ \cdot mol^{-1}$)	$\Delta_f G^o$ ($kJ \cdot mol^{-1}$)	$\log K_f^o$
4600	39.515	290.466	256.739	155.146	−57.183	−82.282	0.934
4700	39.566	291.317	257.466	159.100	−57.266	−82.827	0.920
4800	39.609	292.150	258.180	163.059	−57.343	−83.370	0.907
4900	39.644	292.967	258.881	167.021	−57.415	−83.913	0.895
5000	39.669	293.769	259.571	170.987	−57.481	−84.451	0.882
5100	39.686	294.554	260.249	174.955	−57.542	−84.990	0.870
5200	39.694	295.325	260.917	178.924	−57.598	−85.528	0.859
5300	39.693	296.081	261.573	182.894	−57.651	−86.064	0.848
5400	39.682	296.823	262.219	186.862	−57.699	−86.600	0.838
5500	39.662	297.551	262.855	190.830	−57.744	−87.136	0.828
5600	39.632	298.265	263.481	194.795	−57.786	−87.668	0.818
5700	39.594	298.966	264.097	198.756	−57.827	−88.202	0.808
5800	39.547	299.655	264.704	202.713	−57.865	−88.737	0.799
5900	39.490	300.330	265.302	206.665	−57.903	−89.266	0.790
6000	39.425	300.993	265.892	210.611	−57.940	−89.799	0.782

TABLE 4. Ideal gas thermochemical properties of hydrogen iodide, HI(g), at standard state pressure, $p^o = 0.1$ MPa ($T_r = 298.15$ K)

T (K)	C_p^o ($J \cdot K^{-1} \cdot mol^{-1}$)	S^o ($J \cdot K^{-1} \cdot mol^{-1}$)	$-(G^o - H^o(T_r))/T$ ($J \cdot K^{-1} \cdot mol^{-1}$)	$H^o - H^o(T_r)$ ($kJ \cdot mol^{-1}$)	$\Delta_f H^o$ ($kJ \cdot mol^{-1}$)	$\Delta_f G^o$ ($kJ \cdot mol^{-1}$)	$\log K_f^o$
0	0.000	0.000	∞	−8.656	28.676	28.676	∞
25	29.139	134.408	452.616	−7.955	29.007	26.489	−55.345
50	29.114	154.594	299.137	−7.227	28.947	23.966	−25.036
75	29.112	166.398	253.056	−6.499	28.737	21.520	−14.988
100	29.114	174.773	232.488	−5.772	28.537	19.145	−10.000
150	29.119	186.578	215.350	−4.316	28.119	14.537	−5.062
180	29.122	191.887	211.011	−3.442	27.838	11.848	−3.438
190	29.123	193.462	210.046	−3.151	27.738	10.962	−3.014
200	29.124	194.956	209.254	−2.860	27.636	10.081	−2.633
210	29.126	196.377	208.608	−2.568	27.530	9.207	−2.290
220	29.127	197.732	208.083	−2.277	27.422	8.336	−1.979
230	29.129	199.027	207.661	−1.986	27.311	7.471	−1.697
240	29.131	200.266	207.327	−1.695	27.196	6.611	−1.439
250	29.134	201.456	207.069	−1.403	27.080	5.756	−1.203
260	29.137	202.598	206.875	−1.112	26.963	4.905	−0.985
270	29.141	203.698	206.737	−0.820	26.845	4.060	−0.785
280	29.145	204.758	206.648	−0.529	26.724	3.217	−0.600
290	29.151	205.781	206.600	−0.238	26.602	2.380	−0.429
298.15	29.156	206.589	206.589	0.000	26.500	1.701	−0.298
300	29.158	206.769	206.589	0.054	26.477	1.547	−0.269
350	29.217	211.268	206.945	1.513	25.805	−2.557	0.382
400	29.329	215.176	207.735	2.977	17.127	−6.287	0.821
450	29.503	218.640	208.757	4.447	15.851	−9.137	1.061
500	29.737	221.760	209.904	5.928	−5.481	−9.946	1.039
600	30.351	227.233	212.348	8.931	−5.820	−10.807	0.941
700	31.070	231.965	214.820	12.001	−6.102	−11.615	0.867
800	31.808	236.162	217.230	15.145	−6.324	−12.387	0.809
900	32.512	239.950	219.548	18.362	−6.490	−13.135	0.762
1000	33.157	243.409	221.763	21.646	−6.608	−13.866	0.724
1100	33.736	246.597	223.878	24.991	−6.691	−14.587	0.693
1200	34.250	249.555	225.896	28.391	−6.746	−15.303	0.666
1300	34.705	252.315	227.823	31.839	−6.786	−16.014	0.643
1400	35.108	254.902	229.666	35.330	−6.820	−16.722	0.624
1500	35.466	257.336	231.430	38.859	−6.859	−17.428	0.607
1600	35.786	259.636	233.122	42.422	−6.910	−18.132	0.592
1700	36.074	261.814	234.746	46.015	−6.982	−18.831	0.579
1800	36.335	263.884	236.308	49.636	−7.078	−19.526	0.567
1900	36.574	265.854	237.812	53.282	−7.204	−20.214	0.556
2000	36.794	267.736	239.261	56.950	−7.361	−20.894	0.546
2100	36.998	269.536	240.660	60.640	−7.548	−21.567	0.536
2200	37.189	271.262	242.012	64.349	−7.763	−22.229	0.528
2300	37.369	272.919	243.320	68.077	−8.004	−22.883	0.520
2400	37.540	274.513	244.587	71.823	−8.264	−23.523	0.512
2500	37.703	276.049	245.815	75.585	−8.539	−24.153	0.505
2600	37.859	277.531	247.006	79.363	−8.822	−24.771	0.498
2700	38.008	278.962	248.164	83.156	−9.109	−25.380	0.491
2800	38.152	280.347	249.288	86.965	−9.394	−25.977	0.485
2900	38.290	281.689	250.383	90.787	−9.671	−26.565	0.478
3000	38.423	282.989	251.448	94.622	−9.936	−27.143	0.473
3100	38.549	284.251	252.486	98.471	−10.183	−27.712	0.467
3200	38.668	285.477	253.498	102.332	−10.412	−28.274	0.462
3300	38.780	286.668	254.485	106.204	−10.618	−28.829	0.456
3400	38.885	287.827	255.449	110.088	−10.799	−29.378	0.451
3500	38.981	288.956	256.390	113.981	−10.954	−29.921	0.447
3600	39.068	290.055	257.310	117.884	−11.083	−30.463	0.442
3700	39.145	291.127	258.209	121.794	−11.185	−30.998	0.438
3800	39.211	292.172	259.090	125.712	−11.260	−31.533	0.433
3900	39.266	293.191	259.951	129.636	−11.308	−32.066	0.429
4000	39.310	294.186	260.794	133.565	−11.332	−32.596	0.426
4100	39.341	295.157	261.621	137.498	−11.332	−33.130	0.422
4200	39.360	296.105	262.430	141.433	−11.309	−33.661	0.419
4300	39.366	297.031	263.225	145.369	−11.265	−34.196	0.415
4400	39.360	297.936	264.003	149.306	−11.202	−34.729	0.412
4500	39.340	298.821	264.767	153.241	−11.122	−35.262	0.409

TABLE 4. Ideal gas thermochemical properties of hydrogen iodide, HI(g), at standard state pressure, p^o=0.1 MPa (T_r=298.15 K)–Continued

T (K)	C_p^o ($J \cdot K^{-1} \cdot mol^{-1}$)	S^o ($J \cdot K^{-1} \cdot mol^{-1}$)	$-(G^o-H^o(T_r))/T$ ($J \cdot K^{-1} \cdot mol^{-1}$)	$H^o-H^o(T_r)$ ($kJ \cdot mol^{-1}$)	$\Delta_f H^o$ ($kJ \cdot mol^{-1}$)	$\Delta_f G^o$ ($kJ \cdot mol^{-1}$)	$\log K_f^o$
4600	39.307	299.685	265.517	157.173	−11.026	−35.801	0.407
4700	39.262	300.530	266.253	161.102	−10.918	−36.341	0.404
4800	39.203	301.356	266.975	165.025	−10.797	−36.883	0.401
4900	39.133	302.163	267.685	168.942	−10.666	−37.430	0.399
5000	39.051	302.953	268.383	172.852	−10.528	−37.973	0.397
5100	38.957	303.725	269.068	176.752	−10.385	−38.526	0.395
5200	38.852	304.481	269.742	180.642	−10.236	−39.078	0.393
5300	38.736	305.220	270.404	184.522	−10.085	−39.637	0.391
5400	38.610	305.943	271.056	188.389	−9.932	−40.193	0.389
5500	38.475	306.650	271.697	192.244	−9.779	−40.755	0.387
5600	38.331	307.342	272.327	196.084	−9.628	−41.319	0.385
5700	38.179	308.019	272.947	199.910	−9.479	−41.888	0.384
5800	38.019	308.682	273.558	203.719	−9.335	−42.460	0.382
5900	37.852	309.330	274.159	207.513	−9.194	−43.029	0.381
6000	37.678	309.965	274.750	211.289	−9.059	−43.607	0.380