Dissociation Energies of the Cu and Ag Monohalides and of Ni Monofluoride

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Gaseous isomolecular equilibria of the type CuX + Ag = Cu + AgX, where X = F, Cl, Br, and I, were studied by effusion-beam mass spectrometry at elevated temperatures, and the differences between the dissociation energies of the CuX and AgX molecular species were determined with relatively high accuracy from thermochemical analysis of the equilibrium data. Analysis of literature data, plus new information on AgBr, yielded accurate values of $D°_0$ in kcal mol^{-1} for CuF (102.0), AgCl (74.4), AgBr (66.4), and AgI (59.7), from which values were derived for AgF (81.5), CuCl (89.6), CuBr (79.2), and CuI (69.4), all ±1 kcal mol^{-1}. The result is a consistent set of dissociation energies for all eight of the Cu and Ag monohalides that will be useful in checking the reliability of quantum chemical calculations for these molecular species containing elements of increasing atomic number. Also, the isomolecular exchange equilibrium between CuF and NiF was studied in a similar fashion, leading to $D°_0(\mathrm{NiF}) = 104.4 \pm 1.4$ kcal mol^{-1}.

Introduction

In the course of earlier thermochemical studies of the Cu−Ag−Cl system,[1] we utilized a molecular beam source in which the desired species were generated by admitting $Cl_2(g)$ to the base of an effusion cell containing Cu and Ag granules. Corresponding studies of the Cu/Ag fluorides, bromides, and iodides were also completed by sequentially changing the reactive gas to SF_6, HBr, and HI, but these secondary studies were never published. In each instance, equilibrium data were obtained for the gaseous reaction

$$\mathrm{CuX} + \mathrm{Ag} = \mathrm{Cu} + \mathrm{AgX} \tag{1}$$

where X = F, Cl, Br, or I, and the reaction enthalpy changes, $\Delta H°$, were derived by thermodynamic analysis. Since the reaction enthalpy change, when corrected to 0 K, is precisely the difference between the dissociation energies, $D°_0$, of CuX and AgX, the analysis yields a consistent and reliable route to evaluating $D°_0$ for one of the diatomic halides when the other is known accurately. Third-law treatment of the equilibrium data is especially reliable here, as the spectroscopic and molecular constants of the CuX and AgX species used in the thermodynamic analysis have been determined accurately from electronic and microwave spectra.[2]

Because there remain some inconsistencies in the literature $D°_0$ values for the Cu and Ag monohalides, it seemed worthwhile to report these additional thermochemical data for the F, Br, and I species. The most recent compilation of $D°_0$ values of interest here is the critical compilation on constants of diatomic molecules by Huber and Herzberg,[2] covering the literature up to 1978. Tabulated values for the species CuBr, CuI, AgBr, and AgI stem from the earlier work of Brewer and Lofgren,[3] with stated uncertainties of ±6 to 9 kcal mol^{-1}, while the remaining uncertainties are on the order of ±3 kcal mol^{-1} or less. Yet, the 1984 compilation of Pankratz[4] on metal halides yields a $D°_0$ for CuF differing by as much as 17 kcal mol^{-1}. The thermochemical values reported here permit the differences between the $D°_0$ values of the Cu and Ag monohalides to be tightened up so that the overall uncertainties for all the species are reduced to about 1 kcal mol^{-1}. Among other applications, these results will provide some useful test cases for evaluating the accuracy of quantum chemical calculations of $D°_0$ values on these heavier, transition metal species, which are currently problematic. We also report a new, more accurate value for $D°_0$(NiF), derived from equilibrium studies of the CuF/NiF analogue of reaction 1.

Experimental Section

Chemical species in the Cu−Ag−X system, where X = F, Br, and I, were generated by the sequential admission of gaseous SF_6, HBr, and HI into the base of a graphite effusion cell containing Cu and Ag granules, as in the Ag−Cu−Cl[1] and other gas−solid reaction studies.[5] Reactive gas flow was controlled with a precision leak valve. For studies of the Cu−Ni−F equilibrium, NiF_2 vaporized from a lower chamber reacted with Cu and Ni granules in the graphite cell to yield the Cu−Ni−F product species. The resulting molecular effusion beam entered the ion source of the magnetic sector mass spectrometer described previously,[6,7] where the species were ionized by electron impact, following which the ions were drawn out, mass analyzed, and collected with a particle multiplier. As always, the effusion cell origin of each signal was verified from profiles obtained with the neutral-beam defining slit. Cell temperatures were measured by optical pyrometry, focusing on a blackbody cavity in the lid. Neutral precursors were identified from the masses, isotopic patterns, and threshold appearance energies (AE) of the observed ion signals. All other aspects of the experimental procedure and interpretation of the results are as described in earlier publications.[6,7]

The Cu, Ag, and Ni granules and the NiF_2 were reagent grade materials of nominal 99.99% purity, while the halogenating agents SF_6, HBr, and HI were commercial samples of minimum 99.5% purity obtained from the Matheson Co. and used as received.

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TABLE 1: Threshold Appearance Energies of Ionic Species Observed in Cu−Ag Fluoride, Bromide, and Iodide Effusion Beams

ion species	threshold AE, eV[a]	literature IE, eV	ion species	threshold AE, eV[a]	literature IE, eV
CuF^+	11.0	10.90[8]	CuI^+	9.0	
AgF^+	11.0		AgI^+	9.0	8.80[9]
NiF^+	9.4		Cu^+	7.8	7.73[27]
$CuBr^+$	9.7		Ag^+	7.5	7.58[27]
$AgBr^+$	9.4	9.59[9]	Ni^+	7.5	7.64[27]

[a] All values ±0.3 eV.

Results

The threshold AE values of the Cu and Ag metal and metal monohalide ions observed in these studies of the F, Br, and I analogues of reaction 1 are listed in Table 1. AE values of the metal ions are in good agreement with the known ionization energies (IE) of Cu and Ag, while those of the MX^+ species are several eV higher, as expected for the $^1\Sigma$ ground states of the Cu and Ag monohalides. Our AE values for CuF^+, $AgBr^+$, and AgI^+ are in good agreement with the vertical IE's of CuF,[8] AgBr,[9] and AgI[9] evaluated from photoelectron spectra, providing positive identification of the Cu and Ag monohalides in the molecular effusion beams. All equilibrium data pertinent to the Cu−Ag−Cl system have been reported in the literature.[1]

With the chemical compositions of the neutral effusion beams established, a series of equilibrium measurements was made on each system within the approximate range 1200−1500 K. Parent ions of the Cu−Ag monohalides and the corresponding metal atom species were measured at an ionizing energy of AE + 3 eV in order to minimize ion fragmentation effects. Only for the parent ion AgF^+ was a fragmentation correction required, since separate threshold measurements on AgF vaporized from a Pt cell showed a significant Ag^+ fragment contribution with an AE of 11.0 eV and an intensity higher by a factor of 4 than that of parent AgF^+ at AE + 3 eV. The Cu^+ AE curve also showed a noticeable contribution from CuF fragmentation above about 12 eV, but because of the much larger CuF^+ parent ion signal, this Cu^+/CuF fragment contribution to the total ion yield from CuF was negligible. Otherwise, the derived equilibrium constants, K, were calculated from the parent ion intensity ratios, without further correction. For isomolecular reactions of this type, all factors other than the ionization cross section ratios cancel directly. However, experience has shown that K values derived from such ion current ratios are accurate to within a factor of 1.5. The measured equilibrium data and derived thermochemical results for the gaseous reactions

$$\mathrm{Ag} + \mathrm{CuF} = \mathrm{AgF} + \mathrm{Cu} \qquad (2)$$

$$\mathrm{Ag} + \mathrm{CuBr} = \mathrm{AgBr} + \mathrm{Cu} \qquad (3)$$

$$\text{and } \mathrm{Ag} + \mathrm{CuI} = \mathrm{AgI} + \mathrm{Cu} \qquad (4)$$

are shown in Tables 2−4, which also show the relative intensities of the four parent ion signals at one representative temperature; the fragment contribution is included for AgF^+. A few check measurements on several of the reactions showed that, at constant temperature, the derived equilibrium constants, K, were independent of halogenating gas flow rate and significant changes in species partial pressures, indicating the attainment of chemical equilibrium. For example, with reaction 3 at 1318 K, a flow-rate-induced factor of 4 change in the CuBr signal and factor of 2.6 change in the AgBr signal yielded K values agreeing to within 7%, and for reaction 4 at 1259 K, a factor of 12 change in the CuI signal and factor of 8 change in AgI signal gave K values agreeing to within 14%, so that in each case changes in gas composition had no significant effect on the derived equilibrium data.

TABLE 2: Equilibrium Data and Derived Third-Law Enthalpies for the Gaseous Reaction CuF + Ag = Cu + AgF[a]

T/K	$K \times 10^4$	ΔH°_{298} kcal mol^{-1}	T/K	$K \times 10^4$	ΔH°_{298} kcal mol^{-1}
1217	2.89	20.6	1302	4.68	20.8
1217	3.01	20.5	1302	4.59	20.8
1235	3.33	20.5	1307	5.52	20.4
1235	3.21	20.6	1307	5.30	20.5
1247	3.74	20.4	1329	5.75	20.6
1247	3.61	20.5	1335	5.79	20.7
1266	4.24	20.4	1335	5.35	20.9
1266	4.23	20.4	1352	6.06	20.9
1277	4.77	20.3	1352	6.15	20.8
1277	4.59	20.4	1366	6.78	20.8
				av	20.6 ± 0.2
				2nd law	17.5

[a] $\log K = -(0.37 \pm 0.14) - (3825.89 \pm 0.18)/T$. At 1307 K, the parent ion signals were in the ratio $Cu^+/CuF^+/Ag^+/AgF^+ = 1.46/171.4/96.7/6.27$.

TABLE 3: Equilibrium Data and Derived Third-Law Enthalpies for the Gaseous Reaction CuBr + Ag = Cu + AgBr[a]

T/K	$K \times 10^3$	ΔH°_{298} kcal mol^{-1}	T/K	$K \times 10^3$	ΔH°_{298} kcal mol^{-1}
1232	8.03	12.6	1375	12.2	12.9
1232	7.53	12.7	1375	12.7	12.8
1233	7.92	12.6	1375	12.6	12.8
1243	7.84	12.7	1411	13.4	12.9
1243	7.96	12.7	1411	13.5	12.9
1278	9.21	12.7	1456	14.9	13.0
1318	9.65	12.9	1456	15.3	13.0
1318	10.4	12.8	1456	15.1	13.0
1362	11.6	12.9			
				av	12.8 ± 0.1
				2nd law	10.7

[a] $\log K = -(0.20 \pm 0.04) - (2345.78 \pm 0.59)/T$. At 1375 K, the parent ion signals were in the ratio $Cu^+/CuBr^+/Ag^+/AgBr^+ = 18.1/317.1/18.7/3.98$.

TABLE 4: Equilibrium Data and Derived Third-Law Enthalpies for the Gaseous Reaction CuI + Ag = Cu + AgI[a]

T/K	$K \times 10^2$	ΔH°_{298} kcal mol^{-1}	T/K	$K \times 10^2$	ΔH°_{298} kcal mol^{-1}
1259	2.89	9.5	1368	3.30	9.9
1259	2.53	9.8	1368	3.66	9.7
1292	2.66	9.9	1435	3.63	10.2
				av	9.8 ± 0.2
				2nd law	7.1

[a] $\log K = -(0.35 \pm 0.23) - (1545.73 \pm 0.31)/T$. At 1368 K, the parent ion signals were in the ratio $Cu^+/CuI^+/Ag^+/AgI^+ = 13.0/73.4/2.93/0.54$.

The derived thermochemical results for all four Cu−Ag−X systems, including the previously published[1] values for the Cu−Ag−Cl system, are summarized in Table 7. Thermal functions used in the second- and third-law analyses were taken from sources described in the Appendix; the changes in Gibbs energy function, Δgef, where gef $= -(G^\circ - H^\circ_{298})/T$, are summarized for the reactions studied in Table 6. Derived second-law (II) enthalpies with estimated uncertainties of ±3 kcal mol^{-1} are in reasonably good agreement with the third-law (III) values, which are preferred, and are assigned overall uncertainties of ±1 kcal mol^{-1}.

TABLE 5: Equilibrium Data and Derived Third-Law Enthalpies for the Gaseous Reaction Cu + NiF = CuF + Ni[a]

T/K	K	ΔH°_{298} kcal mol^{-1}	T/K	K	ΔH°_{298} kcal mol^{-1}
1463	0.450	2.3	1543	0.502	2.1
1463	0.437	2.4	1578	0.502	2.2
1478	0.433	2.4	1610	0.523	2.1
1478	0.445	2.4	1613	0.539	2.0
1503	0.459	2.3	1655	0.541	2.0
1503	0.469	2.3	1655	0.543	2.0
1517	0.478	2.2	1664	0.540	2.0
1517	0.471	2.3	1664	0.556	1.9
1543	0.480	2.2			
				av	2.2 ± 0.3
				2nd law	5.4

[a] $\log K = (0.45 \pm 0.04) - (1184.59 \pm 0.06)/T$. At 1610 K, the parent ion signals were in the ratio $Cu^+/CuF^+/Ni^+/NiF^+ = 17.0/2.67/10.9/3.27$.

TABLE 6: Gibbs Energy Functions Used in Analysis of Equilibrium Data

	$-\Delta(G^\circ - H^\circ_{298})/T$, cal deg^{-1} mol^{-1}		
reaction	1200 K	1400 K	1600 K
2	0.71	0.72	0.73
3	0.60	0.60	0.60
4	0.49	0.49	0.49
5	0.08	0.02	0.01

TABLE 7: Cu−Ag−X Gaseous Reaction Data

	ΔH°_{298}(III) kcal mol^{-1}	ΔH°_{298}(II) kcal mol^{-1}	T/K	av T
CuF + Ag = Cu + AgF	20.6	17.5	1216−1366	1288
CuCl + Ag = Cu + AgCl	15.2	12.8, 15.2	1218−1424	1312
CuBr + Ag = Cu + AgBr	12.8	10.7	1232−1456	1340
CuI + Ag = Cu + AgI	9.8	7.2	1259−1435	1330

TABLE 8: Dissociation Energies and Enthalpies of Formation (kcal mol^{-1}) of Cu and Ag Monohalides and Ni Monofluoride

	D°_0				
molecule	ref 3	ref 2	this work	D°_{298}	$\Delta_f H^\circ_{298}$
CuF		101.9	102.0 ± 1	102.9	−3.0
CuCl	88.1 ± 6	90.6	89.6	90.3	19.5
CuBr	79.1 ± 6	79.1	79.2	79.8	27.7
CuI	<75.4	<75.4	69.4	70.0	36.3
AgF		83.9	81.5	82.3	4.8
AgCl	76.3 ± 5	74.2	74.4	75.1	22.0
AgBr	70.3 ± 9	71.5	66.4	67.0	27.8
AgI	61.3 ± 9	60.0	59.7	60.2	33.4
NiF			104.4	105.1	16.2

Reference Dissociation Energies. For each Cu/Ag halide pair, one accurately established D°_0 value was chosen as a reference, from which the other metal monohalide D°_0 was evaluated from the derived third-law enthalpies listed in Table 7. All selected values were determined from thermochemical studies, using third-law analysis.

CuF. Published equilibrium data[10] for the gaseous reaction Cu + MgF = CuF + Mg yielding $\Delta H^\circ_{298} = 7.1$ kcal mol^{-1} were combined with the established[2,11,12] value D°_{298}(MgF) =110.0 ± 1 kcal mol^{-1} to yield D°_{298}(CuF) = 102.9 ± 1 kcal mol^{-1} and D°_0(CuF) = 102.0 kcal mol^{-1}.

AgCl. Effusion vaporization studies[1] by the torsion-mass loss method yielded the sublimation enthalpy of AgCl monomer, leading to the standard enthalpy of formation, which corresponds to D°_{298}(AgCl) = 75.1 ± 0.4 kcal mol^{-1} and D°_0(AgCl) = 74.4 kcal mol^{-1}.

AgBr. Effusion−torsion vaporization studies and mass spectrometric analysis of AgBr-saturated vapor[13] led to thermochemical characterization of AgBr monomer and D°_{298}(AgBr) = 67.0 ± 0.3 kcal mol^{-1} with D°_0(AgBr) = 66.4 kcal mol^{-1}.

AgI. Mass spectrometric analysis was used to determine the composition and partial pressures in AgI-saturated vapor,[14] from which the monomer thermochemical properties D°_{298}(AgI) = 60.2 ± 1 kcal mol^{-1} and D°_0(AgI) = 59.7 kcal mol^{-1} were derived.

When the reaction enthalpies in Table 7 are combined with the reference D°_{298} values described above, the new and more accurate dissociation energies of AgF, CuCl, CuBr, and CuI are derived. In Table 8, all of the recommended D°_0 values from this work are summarized and compared with the earlier selected values from ref 2 and 3; also listed are the standard enthalpies of formation, $\Delta_f H^\circ_{298}$, of the eight CuX/AgX species determined from the studies reported here. Note that all of the selected values presented here are based on new experimental determinations and are completely independent of those reported in ref 3. Of the selected D°_0 values in ref 2, only those for CuF, CuCl, and AgCl are based partially on results obtained in our research group.[10,1,15]

In similar fashion, the gaseous reaction equilibrium

$$Cu + NiF = CuF + Ni \tag{5}$$

was studied over the range 1463−1664 K, with the results shown Table 5. We are not aware of any literature values for IE(NiF), but our observed value of 9.4 eV in Table 1 appears reasonable in view of the $^2\Pi$ multiplet ground state of NiF, compared to the higher value of 11.0 eV for neighboring CuF, with its $^1\Sigma$ closed-shell ground state. The derived third-law enthalpy change $\Delta H^\circ_{298}(5) = 2.2$ kcal mol^{-1}, with an overall uncertainty of ±1 kcal mol^{-1}, leads to the result D°_{298}(NiF) = 105.1 ± 1.4 kcal mol^{-1} and D°_0(NiF) = 104.4 kcal mol^{-1}, when combined with our selected value for D°_{298}(CuF). In turn, this value leads to the enthalpy of formation $\Delta_f H^\circ_{298}$(NiF, g) = 16.2 kcal mol^{-1}.

Discussion

Clearly, our new results validate the experimental equilibrium studies of Brewer and Lofgren[3] on CuCl and CuBr, while significantly decreasing the uncertainties in D°_0; their estimates for AgCl, AgBr, and AgI, based on literature vaporization data, are also seen to be in accord, within the large uncertainties. Although our new[13] value for AgBr is 4−5 kcal mol^{-1} lower than the older estimates,[2,3] it does provide, through reaction 3, strong support for the earlier equilibrium data[3] on CuBr and is therefore considered to be established as D°_0(AgBr) = 66.4 ± 1 kcal mol^{-1}.

Huber and Herzberg[2] refer to the thermochemical determination of D°_0(AgF) = 83.9 kcal mol^{-1} by Zmbov and Margrave from mass spectrometric studies of the vaporization of molten AgF in the range 854−1024 K. A second-law slope measurement of the enthalpy of vaporization, combined with an updated enthalpy of formation of AgF(s), yields D°_0(AgF) = 84.3 ± 4 kcal mol^{-1}; the lack of entropy and heat capacity data for AgF(s,l) precludes a more-accurate third-law evaluation of the vaporization data. They[2] also refer to a predissociation $D^\circ_0 <$ 85.3 kcal mol^{-1}, but Barrow[16] indicates this is “not an independent estimate” of D°_0, though “not inconsistent” with the thermochemical value. The new result reported here tightens the uncertainty limit on D°_0(AgF) to about ±1 kcal mol^{-1}. In addition, Guido et al.[17] reported D°_0(CuCl) = 90.6 ± 1.1 kcal

TABLE 9: Molecular Constants Used in Calculation of Thermal Functions

species	$I \times 10^{39}$ g cm^2	ω, cm^{-1}	T_o, cm^{-1}	g
CuF	7.38	615	0	1
CuCl	15.9	412	0	1
CuBr	27.4	313	0	1
CuI	38.2	263	0	1
AgF	10.5	508	0	1
AgCl	22.8	341	0	1
AgBr	44.2	246	0	1
AgI	62.4	206	0	1
NiF	7.21	637	0	4
			251	2
			565	4
			830	4
			1574	2
			2224	4

mol^{-1}, in accord with the value of 89.6 selected here and reported previously.[1] And from the study of chemiluminescent reactions of excited Cu atoms with ClF, Sadeghi et al.[18] derived the value $D°_0$(CuF) = 98.1 kcal mol^{-1}, in fair agreement with the value 102.0 reported here. Aside from the studies noted here, we are not aware of any other experimental determinations of $D°_0$ for the eight CuX/AgX monohalides under discussion. The new dissociation energies and enthalpies of formation of the eight Cu and Ag monohalides reported here provide an internally consistent set of thermochemical values that may be useful as secondary standards.

$D°_0$(NiF) values of 105.9 ± 1.2,[19] 102.8 ± 2.5,[12] and 96.1 [20] kcal mol^{-1} have been reported. The first[19] is an experimental value based on Ni−NiF−NiF$_2$ gaseous equilibria and is in accord with our new value of 104.4 kcal mol^{-1}. But the origin of the second, compilation[12] value is not clear, while the third[20] is stated to be an estimate and is clearly too low by 8 kcal mol^{-1} or so. The IVTANTHERMO database[12] lists $D°_0$ values for other first row transition metal monofluorides as follows: CrF (105.2 kcal mol^{-1}), MnF (107.1 kcal mol^{-1}), FeF (112.3 kcal mol^{-1}), and CoF (106.6 kcal mol^{-1}), with estimated accuracies of 3−10 kcal mol^{-1}. It seems reasonable that in this Cr to Ni series, the relative constancy of the M−F bond strength indicates that only the metal 4s orbitals are involved in bonding with the F atom, while the sequentially added inner 3d electrons are essentially nonbonding. It is interesting that ScF and TiF, at the beginning of the 3d transition series, have $D°_0$ values of 142[21] and 140[2,11,12] kcal mol^{-1}, suggesting stronger, hybridized s−d bonds in these two monofluorides.

Appendix

The spectroscopic and molecular constants of the eight Cu and Ag diatomic halides used in calculating thermal functions for analysis of the equilibrium data were taken from the compilation of Huber and Herzberg.[2] In contrast to the relatively simple electronic spectra of these Cu−Ag−X monohalides, the spectra of NiF are complex and difficult to interpret, with a number of thermodynamically important low-lying electronic states. We have taken the vibrational and rotational constants and the energies and configurations of the electronic states of NiF from a series of papers by Dufour, Pinchemel, and coworkers;[22−25] the microwave data of Tanimoto et al.[26] yield a rotational constant of the NiF ground state in close agreement. The pertinent values used in calculation of the thermal functions of these species are summarized in Table 9, in terms of the moment of inertia, I; the vibrational frequency, ω; and the energy, T_o, and degeneracy, g, of the electronic state.

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