Composition and Thermochemistry of Silver Bromide Vapor

D. L. Hildenbrand* and K. H. Lau

SRI International, Menlo Park, California 94025

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The mole fractions of AgBr and Ag_3Br_3 in the saturated vapor at 840 K have been evaluated from the vapor mass spectrum, by comparison with the corresponding spectrum of AgCl vapor, where the monomer/trimer ratio is known accurately from vapor molecular weight measurements. Combination of these results with new measurements of the vapor pressure of molten AgBr by the torsion-effusion method in the range 805−936 K yielded the third law enthalpies of vaporization and the standard enthalpies of formation $\Delta_f H°_{298}$(AgBr, g) = 27.8 ± 0.3 kcal mol^{-1} and $\Delta_f H°_{298}(Ag_3Br_3, g) = -19.0 \pm 1$ kcal mol^{-1}. The dissociation energy, $D°_0$(AgBr), is found to be 66.4 ± 0.3 kcal mol^{-1}, or 2.88 ± 0.01 eV, some 3.5−5 kcal mol^{-1} lower than previous literature values. Approximate thermochemical stabilities of the dimer species Ag_2Cl_2 and Ag_2Br_2 have also been evaluated.

Introduction

Although the saturated vapors of the silver halides AgCl, AgBr, and AgI are known from mass spectrometric studies[1−6] to contain primarily monomeric and trimeric species in the molecular effusion pressure regime, only for AgCl[7] and AgI[6] are the vapor compositions known with sufficient accuracy so that the dissociation energies and other thermochemical properties can be evaluated reliably from the vaporization data. In their 1979 compilation of spectroscopic constants of diatomic molecules, Huber and Herzberg[8] list the dissociation energy $D°_0$(AgBr) = 71.5 kcal mol^{-1}, which at least partly stems from Brewer and Lofgren's[9] 1950 analysis of older silver halide vaporization data that led to $D°_0$(AgBr) = 70 ± 9 kcal mol^{-1}. To establish a new and more reliable value for $D°_0$(AgBr), we have determined the total vapor pressure of AgBr accurately by the torsion-effusion method, and again examined the vapor mass spectrum, from which the partial pressures and thermochemical properties of AgBr and Ag_3Br_3 were evaluated.

It is worth noting that trimeric gaseous species have also been observed in the lighter alkali halide vapors, particularly those of Li and Na. However, the dimeric species are significantly more abundant than the trimers in these systems. The Cu and Ag halides behave quite differently with the relatively large trimer abundances, perhaps due to the stronger metallic bonding in these transition elements, as discussed later.

Experimental Section

The total vapor pressure of molten AgBr, melting point 705 K, was measured by the torsion-effusion method, using a high-density graphite cell of the four-chamber, square cross-section variety,[10] with orifice diameters of 0.150 cm. The torsion system is basically an effusion manometer in which the cell with offset orifices is suspended from a Pt−Ni ribbon, and the recoil force associated with vapor effusion induces an angular rotation of the cell. This is a purely mechanical device that yields absolute total pressure in terms of the torsion constant of the ribbon, the observed angular deflection, and the geometrical constants of the cell. Temperature is measured with a Pt, Pt/Rh thermocouple of known calibration; checks with lab standards such as Ag and KCl have shown that measured pressures are accurate to within 5%. Details of the torsion system and the evaluation of results have been described in the literature.[11]

TABLE 1: Total Vapor Pressure of Molten AgBr Determined by Torsion-Effusion Method[a]

T/K	pressure, atm × 10^6	T/K	pressure, atm × 10^6
805.3	0.404	895.8	5.13
825.0	0.722	900.8	5.89
836.6	1.00	905.6	6.92
841.7	1.16	906.0	6.73
851.7	1.55	915.3	8.57
863.9	2.17	921.9	10.1
876.2	3.05	929.5	12.3
884.9	3.86	936.0	14.5
890.1	4.64		

[a] $\log P$ (atm) = (4.79 ± 0.05) − (9023 ± 44)/T.

Mass spectrometric measurements on AgBr saturated vapor were made with the magnetic single-focusing instrument used in other high-temperature studies.[12] The molecular beam generated by vaporization of AgBr from a graphite effusion cell entered the spectrometer ion source, and the resulting ion species were drawn out, accelerated to 4.5 kV, mass analyzed, and then detected by an electron multiplier. After verification of the effusion cell origin of observed ion signals by the response to translation of the neutral beam defining slit, neutral precursors were identified from the ion masses, isotopic spectra, and threshold appearance energies.

The AgBr sample used in the torsion pressure measurements was an optical quality material obtained from Harshaw Chemical, and that used in the mass spectrometric studies was from Alfa Aesar; both samples were stated to be of 99.99% purity. In addition, they were shielded from visible light in storage, and were handled under anhydrous conditions.

Results

Table 1 gives the measured total vapor pressures of the molten AgBr sample in the range 805−936 K, as determined by the torsion-effusion method. Measured pressures were very stable and reproducible and are believed to be equilibrium values because our measured effusion pressures for molten AgCl[7]

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showed no variation when orifice area was varied by a factor of 3, indicating the absence of kinetic effects. Least-squares fitting yielded the vapor pressure relation

$$\log P(\text{total, atm}) = (4.79 \pm 0.05) - (9023 \pm 44)/T \quad (1)$$

where the uncertainties are statistical errors derived from the fitting. In turn, eq 1 leads to $P(\text{total}) = 1.12 \times 10^{-6}$ atm for AgBr saturated vapor at 840 K. The only literature data of which we are aware are three data points in the 1273−1473 K range, dating back to 1929.[13] We will discuss the compatibility of the earlier data with our results in the next section.

When the mass spectrometer effusion cell source was heated near 840 K, the major ions observed were Ag^+ (10.5 eV), $AgBr^+$ (9.3 eV), Ag_2Br^+ (11.0 and 13.5 eV), $Ag_3Br_2^+$ (10.5 eV), and $Ag_3Br_3^+$ (9.8 eV), with the indicated appearance energies (AE), all ± 0.5 eV. The Ag_2Br^+ ion yield curve had a very weak threshold at 11.0 eV, followed by a sharp rise at 13.5. These AEs are in fair agreement with those of Bernauer and Weil,[4] and that of $AgBr^+$ is in good agreement with the IP of 9.23 eV determined by Berkowitz et al.[14] from photoelectron spectra. We interpret these results to indicate that Ag^+ and $AgBr^+$ are associated with the neutral precursor AgBr, whereas the weak first threshold for Ag_2Br^+ is likely fragmentation from Ag_2Br_2; the second, strong threshold of Ag_2Br^+, together with $Ag_3Br_2^+$ and $Ag_3Br_3^+$, stem from the precursor Ag_3Br_3. These assignments are in accord with the corresponding angular distribution measurements of Wagner and Grimley[1] on AgCl saturated vapor.

The minor ions Ag_2^+, $Ag_2Br_2^+$, and $Ag_4Br_3^+$, with intensities lower by at least a factor of 10, were also observed. By analogy with the angular distribution results on AgCl[1], Ag_2^+ is doubtless a fragment of Ag_3Br_3, whereas $Ag_2Br_2^+$ is a parent ion near threshold, and $Ag_4Br_3^+$ a fragment of Ag_4Br_4. As with AgCl,[1] the mass spectrum indicates clearly that AgBr and Ag_3Br_3 are the major species in the saturated vapor, with minor amounts of Ag_2Br_2 and Ag_4Br_4 at a level of a few percent at most.

At a cell temperature of 840 K and an ionizing energy (IE) of 20 eV, the relative intensities of the major peaks, normalized to $AgBr^+$ and corrected for isotopic distribution, were as follows: Ag^+ (2.8); $AgBr^+$ (100.0); Ag_2Br^+ (55.4); $Ag_3Br_2^+$ (169.5); and $Ag_3Br_3^+$ (104.0). The ratio of the sums of the ions from Ag_3Br_3 to those from AgBr, (I^+_T/I^+_M), = 3.20 under these conditions, where M and T refer to monomer and trimer. The quantity we are seeking, the ratio of partial pressures of monomer and trimer, P_M/P_T, at a given temperature is related to the ion ratio by the relation

$$P_M/P_T = (I^+_M/I^+_T)(\sigma_T/\sigma_M) \quad (2)$$

which derives from the fundamental equation relating pressure of a specific neutral to ion intensity

$$P = kI^+T/\sigma \quad (3)$$

where k is an instrument sensitivity constant, I^+ is the total ion intensity from that neutral, T is the effusion cell temperature, and σ is the cross section for ionization by electron impact. If the ionization cross section ratio σ_T/σ_M is known or can be estimated reliably, then the monomer/trimer pressure ratio P_M/P_T and the binary vapor composition can be evaluated, and the desired thermochemical properties of AgBr and Ag_3Br_3 can be derived.

In the course of earlier studies of the composition and thermochemistry of AgCl vapor, we determined P_M/P_T from vapor molecular data determined by the torsion/mass loss method[7] and also obtained AgCl vapor mass spectra identical to those described above for the AgBr system. Although our AgCl mass spectra were never published, they can be presented here and used in estimating the desired σ_T/σ_M cross section ratio for AgBr vapor, because the AgCl and AgBr vapor systems are entirely analogous, differing only in the ratio P_M/P_T. Table 2 shows two separate determinations at several temperatures of the relative intensities of the five major ions in the AgCl mass spectrum, where Ag^+ and $AgCl^+$ are products of the AgCl monomer precursor, and Ag_2Cl^+, $Ag_3Cl_2^+$, and $Ag_3Cl_3^+$ are from the Ag_3Cl_3 trimer, just as with the AgBr system. All measurements were made at an IE of 20 eV, and the intensities are corrected for isotopic distribution. Also shown are values of the ratio (I^+_T/I^+_M) calculated from these intensities, and the pressure ratio P_M/P_T evaluated from the vapor molecular weight determinations.[7] And, finally, the ionization cross section ratio σ_T/σ_M, evaluated from eq 2 in the form

$$(\sigma_T/\sigma_M) = (I^+_T/I^+_M)(P_M/P_T) \quad (4)$$

is shown in the last column. These six determinations over the range 800−900 K are in good accord, indicating that $\sigma(Ag_3Cl_3)/\sigma(AgCl) \sim 3$, a reasonable value at the relatively low IE of 20 eV. Subsequent measurements on AgCl at 886 K and an IE of 50 eV gave a corresponding σ_T/σ_M ratio of 1.3, showing the ratio to be strongly dependent on ionizing energy.

TABLE 2: Relative Intensities[a] of Ions in Mass Spectrum of AgCl Vapor at Several Temperatures and Evaluation of Trimer/Monomer Ionization Cross Section Ratio (Ionizing Energy = 20 eV)

T/K	Ag^+	$AgCl^+$	Ag_2Cl^+	$Ag_3Cl_2^+$	$Ag_3Cl_3^+$	I^+_T/I^+_M	P_M/P_T	σ_T/σ_M
Run 1								
845	8.7	85.7	20.2	75.6	35.8	1.39	2.15	3.0
892	30.1	300.0	56.2	210.0	80.4	1.05	2.78	2.9
904	42.4	448.0	69.7	285.0	104.3	0.937	2.94	2.8
Run 2								
803	1.97	30.0	6.52	29.4	17.9	1.69	1.70	2.9
850	9.07	137.5	21.6	106.4	59.9	1.28	2.20	2.8
883	24.9	358.0	54.0	226.8	107.3	1.01	2.65	2.7

[a] Intensities in arbitrary units.

Ag_3Cl_3 and Ag_3Br_3 are expected to have the same cyclic structure[15] as that of Cu_3Cl_3, and it is reasonable to assume that $\sigma(Ag_3Br_3)/\sigma(AgBr)$ is also close to 3 at an IE of 20 eV. From the (I^+_T/I^+_M) value of 3.20 found for the AgBr system at 840 K and with $\sigma_T/\sigma_M \sim 3$, then $P_M/P_T \sim 1$. With $P(\text{total, AgBr}) = 1.12 \times 10^{-6}$ atm from eq 1, then both AgBr and Ag_3Br_3 have approximately equal partial pressures of 5.6×10^{-7} atm in the saturated vapor at 840 K. From thermodynamic functions calculated with accurate molecular constants for AgBr and estimated constants for Ag_3Br_3, together with tabulated values for AgBr(c,l), all described in the Appendix, we calculate the change in Gibbs energy function, where gef $= -(G^\circ - H^\circ_{298})/T$, to be Δgef = 33.00 cal/deg mol with a standard state pressure of 1 atm for

$$\text{AgBr(cr,l)} = \text{AgBr(g)} \quad (5)$$

and Δgef = 34.46 cal/deg mol for

$$3\text{AgBr(cr,l)} = Ag_3Br_3\text{(g)} \quad (6)$$

at 840 K, leading to the third law enthalpies of sublimation $\Delta H^\circ_{298}(5) = 51.8 \pm 0.3$ kcal mol^{-1}, and $\Delta H^\circ_{298}(6) = 53.0 \pm 1$ kcal mol^{-1}. Combining these values with the standard enthalpy of formation, $\Delta_f H^\circ_{298}$(AgBr, c) = −24.0 kcal mol^{-1} and auxiliary data noted in the Appendix, we derive $\Delta_f H°_{298}$(AgBr, g) = 27.8 ± 0.3 kcal mol^{-1}, and $\Delta_f H°_{298}$(Ag_3Br_3, g) = −19.0 ± 1 kcal mol^{-1}. Uncertainties are based on a potential error of 20% in the species partial pressures, and of 1 cal K^{-1} mol^{-1} in the Gibbs energy function of Ag_3Br_3. These values lead to the dissociation energies $D°_{298}$(AgBr) = 67.0 ± 0.3 kcal mol^{-1}, $D°_0$(AgBr) = 66.4 ± 0.3 kcal mol^{-1}, and $D°_{298}$(Ag_3Br_3) = 303.4 ± 1 kcal mol^{-1}. For the trimer dissociation process

$$Ag_3Br_3(g) = 3AgBr(g) \qquad (7)$$

$\Delta H°_{298}(7)$ = 102.4 kcal mol^{-1}, virtually identical to the value 102.6 kcal mol^{-1} found for the corresponding dissociation of Ag_3Cl_3.[7] Although quantum chemical methods provide a growing source of reliable thermochemical data for elements up to an atomic number of about 20, there remain difficulties in obtaining comparable accuracy in calculations involving elements of higher atomic number, particularly the transition elements. These new data for AgBr and Ag_3Br_3 will be useful for checking the theoretical procedures best suited for yielding reliable bond dissociation energies and enthalpies of formation for the heavier metal halides.

Discussion

It is interesting to note that our AgBr mass spectum at 840 K, presented in the previous section, bears little resemblance to the spectrum reported by Bernauer and Weil.[5] Whereas our spectrum shows the AgBr$^+$, $Ag_3Br_2{}^+$, and $Ag_3Br_3{}^+$ ions to be roughly comparable in magnitude, their 900 K spectrum at 21 eV IE shows the two trimer ions to be about a factor of 10 smaller than AgBr$^+$. The temperature difference has only a very minor effect, so we conclude that the magnetic mass analyzer of Bernauer and Weil[5] exhibits a high degree of mass discrimination, a not unusual characteristic of some magnetic instruments. As normally operated, our instrument is relatively free of mass discrimination, as shown by checks against isotopic spectra covering a wide mass range.

Using the transport method, Jellinek and Rudat[13] reported three vapor pressure points for AgBr at 1273, 1373, and 1473 K, with values of 0.0114, 0.0343, and 0.101 atm, respectively, with no uncertainties given. In contrast, our newly derived thermochemical data for gaseous AgBr and Ag_3Br_3 plus the AgBr(c,l) data noted in the Appendix yield calculated total pressures of 0.0060, 0.020, and 0.057 atm at the same temperatures and are lower than the reported values[13] by a factor of 1.8. The AgBr monomer makes up close to 90% of the total pressure in this range. In any event, the new torsion−pressure data presented here are considered to be accurate within 5%, and our analysis is believed to yield substantially more reliable thermochemical data for the Ag−Br gaseous species.

Barrow[16] has pointed out that the potential curves of the B 0^+ excited states of AgCl, AgBr, and AgI have significant maxima lying well above the actual dissociation limits of these species, thereby giving erroneous results when excited-state vibrational extrapolations are used to evaluate the ground-state $D°_0$ values. These maxima arise from avoided crossings between potential curves of upper states that are bound and repulsive in zero approximation. Our new value $D°_0$(AgBr) = 66.4 ± 0.3 kcal mol^{-1} indicates a maximum of 17.5 kcal mol^{-1} in the B 0^+ state of AgBr, 7 kcal mol^{-1} higher than the earlier estimate of Barrow,[17] based on a less accurate thermochemical value of $D°_0$(AgBr). The earlier $D°_0$(AgBr) values of Brewer and Lofgren[9] (70 ± 9 kcal mol^{-1}), and Huber and Herzberg[8] (71.5 kcal mol^{-1}) are seen to be too large by 3.6 and 5.1 kcal mol^{-1}, respectively.

Although we evaluated the monomer/trimer composition of AgBr saturated vapor experimentally at only one temperature, 840 K, the derived thermochemical data for gaseous AgBr and Ag_3Br_3, plus auxiliary data for AgBr(c,l) and other Ag and Br species, can be used to calculate the composition at other temperatures. The resulting mol percentages of AgBr monomer at several temperatures are as follows: 800 K, 44%; 1000 K, 69%; 1200 K, 83%; 1400 K, 90%. As expected, and as observed with AgCl saturated vapor,[7] the fraction of monomer increases rapidly with temperature. At 1400 K, where the calculated total pressure reaches 0.29 atm, the vapor is 90% monomer. It was not possible within the available funds to check the vapor composition at higher temperatures, but we feel that the thermochemical calculations give a reasonably accurate representation.

Wong and Schomaker[15] did an electron diffraction study of Cu_3Cl_3 vapor and found the results to be compatible with a cyclic six-membered ring structure in which "the copper atoms form a small triangle and the chlorine atoms a large triangle, each chlorine atom being bonded to two copper atoms and each copper atom being bonded to two chlorine atoms and also the two other copper atoms." It is assumed that this unique structure holds also for the silver halide trimers of the neighboring Ag-family, as seems reasonable. Considering this structure, it is likely that the relatively high stability of the Cu and Ag trimeric halides, relative to those of the alkali halides, results from the stronger, hybridized *s*−*p*−*d* Cu−Cu and Ag−Ag bonding in these systems. This point is illustrated by the $D°_0$ values of 47 and 38 kcal mol^{-1} for gaseous Cu_2 and Ag_2, compared to 24 and 17 kcal mol^{-1} for Li_2 and Na_2.[8]

The rotational and vibrational constants of Cu_3Cl_3 have been evaluated, and the resulting thermodynamic functions were found to be in excellent agreement with the measured equilibrium data involving Cu_3Cl_3.[17] We have used the molecular constants of Cu_3Cl_3 as a guide in estimating those of Ag_3Cl_3 [7] and Ag_3Br_3, as noted in the Appendix. Therefore, we feel that the thermochemical properties of Ag_3Br_3 reported here are reasonably accurate and that the combined results give a good account of the properties of AgBr equilibrium vapor.

In one final point, we can use the ion intensity data to estimate that the gaseous dimers Ag_2Cl_2 and Ag_2Br_2 are each present at mol fractions of about 0.01 in the AgCl and AgBr saturated vapors at 900 and 840 K, respectively. From the observation that Δgef is close to −30 cal deg^{-1} mol^{-1} for the gaseous dimerization reaction $2MX = M_2X_2$ in the KCl, KBr, and CsCl systems at the temperatures of interest, we estimate gef values for both Ag_2Cl_2 and Ag_2Br_2 and use this information with the vapor composition data to estimate the enthalpies of the sublimation processes $2AgX(s,l) = Ag_2X_2(g)$ involving AgCl and AgBr. In turn, these sublimation enthalpies are combined with the established $\Delta_f H°_{298}$ values of AgCl(s,l) and AgBr(s,l) to estimate the upper limiting values $\Delta_f H°_{298}(Ag_2Cl_2) \geq 2$ kcal mol^{-1} and $\Delta_f H°_{298}(Ag_2Br_2) \geq 13$ kcal mol^{-1}, which characterize the approximate thermodynamic stabilities of these species.

Appendix

The auxiliary thermochemical data used in the analysis of the experimental results were taken from sources described here. A summary of the molecular constants used in calculating thermal functions of AgBr and Ag_3Br_3 is given in Table 3, in terms of the moments of inertia, I; the rotational symmetry number, σ; the fundamental vibrational frequency, ω; the degeneracy, *g*, and the energy, ϵ, of the electronic state.

Ag(g), Br(g). All data were taken from the IVTANTHERMO Database.[18]

TABLE 3: Molecular Constants of Ag−Br Species

species	I	σ	g_0	ω, cm^{-1}
AgBr	43.6×10^{-39} g cm^2	1	1	246
Ag_3Br_3	39.8×10^{-111} g^3 cm^6	6	1	65, 90, 150, 125, 225(2), 190(2), 40(2), 50(2)

TABLE 4: Calculated Gibbs Energy Functions of Gaseous AgBr and Ag_3Br_3[a]

	$-(G° - H°_{298})/T$, cal deg^{-1} mol^{-1}			$-(G° - H°_{298})/T$, cal deg^{-1} mol^{-1}	
T/K	AgBr(g)	Ag_3Br_3(g)	T/K	AgBr(g)	Ag_3Br_3(g)
298.15	61.40	117.74	1200	67.06	137.88
300	61.40	117.74	1300	67.61	139.80
400	61.74	118.96	1400	68.12	141.62
500	62.39	121.28	1500	68.61	143.36
600	63.12	123.87	1600	69.07	145.00
700	63.86	126.48	1700	69.51	146.58
800	64.57	129.01	1800	69.94	148.08
900	65.25	131.41	1900	70.34	149.51
1000	65.89	133.69	2000	70.73	150.89
1100	66.49	135.84			

[a] Standard state pressure $p° = 1$ atm.

AgBr(cr,l). All data are from Pankratz,[19] which involve more recent high-temperature enthalpy measurements.[20]

AgBr(g), Ag_3Br_3(g). The molecular constants of AgBr(g) were taken from the compilation of Huber and Herzberg.[8] For Ag_3Br_3, the Cu_3Cl_3 cyclic structure and geometry[15] were adopted, with an estimated Ag−Br distance of 252 pm based on comparison with the known distances in CuCl and Cu_3Cl_3; vibrational frequencies were estimated by analogy with the assignment for Cu_3Cl_3 given in the JANAF Tables.[17] These adopted molecular constants were used to calculate thermal functions for both species, utilized in third law analysis of the equilibrium data. Values of the calculated Gibbs energy function, $-(G° - H°_{298})/T$, for gaseous AgBr and Ag_3Br_3 from 298 to 2000 K are listed in Table 4.

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