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Complex Equilibria in Unsaturated Vapor over AlBr₃

A. D. Rusin^{*a*} and L. A. Nisel'son^{*b*}

^a Faculty of Chemistry, Moscow State University, Moscow, 119992 Russia ^b VGUP "GIREDMET," Moscow, Russia e-mail: rusin@phys.chem.msu.ru

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Abstract—Unsaturated AlBr₃ vapor pressure was measured over the temperature and pressure ranges 560–845 K and 54–145 torr by the static method using a quartz diaphragm pressure gauge with increased sensitivity (the confidence interval of pressure, including thermal drift of zero pressure gauge point, was 0.3 torr, and that of temperature, 0.3 K). Two equilibrium models were considered, one including AlBr₃ and Al₂Br₆ and the other, AlBr₃, Al₂Br₆, and Al₃Br₉. The molecular constants of all vapor constituents were determined using density functional theory at the B3LYP/6-31G(*d*,*p*) level. The thermodynamic functions of all bromides were calculated in the rigid rotator–harmonic oscillator approximation. The enthalpies of independent equilibria for each model were determined by minimizing the residual sum of the squares of pressure discrepancies. According to the first model, $0.5Al_2Br_6 = AlBr_3$, $\Delta H^{\circ}(298.15) = 13629.1 \pm 9$ cal/mol. According to the second model, $0.5Al_2Br_6 = AlBr_3$, $\Delta H^{\circ}(298.15) = 13638.8 \pm 8$ cal/mol, and $1.5Al_2Br_6 = Al_3Br_9$, $\Delta H^{\circ}(298.15) = -8528 \pm 800$ cal/mol. The second model, for which the variance of pressure differs insignificantly from the experimental variance of pressure, should be given preference.

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INTRODUCTION

Unsaturated AlBr₃ vapor pressure was measured in [1]. In that work and in [2–5], it was found that equilibria $Al_2Hal_6 = 2AlHal_3$ took place in vapors of Group III metal halides. It was, however, shown in [6] that errors in vapor pressures measured in these works could be substantial. In addition, there was a significant temperature gradient along the reaction vessel in [1], which was not duly taken into account. In all the preceding works, the influence of the thermal drift of the zero point of diaphragm pressure gauges on the results of vapor pressure measurements was ignored. In any event, there are no numerical thermal drift data in the literature, except one of the earliest works [7]. It was shown in [8] that the thermal drift of the zero pint of quartz diaphragm pressure gauges was the main source of errors in vapor pressure measurements. A new technique for performing tensimetric experiments and analyzing experimental data with corrections for thermal zero point drift was suggested in [9, 10]. In [10], a model experiment was performed with inert gas pressure measurements over the temperature range 300-1000 K. It was of interest to perform similar measurements for a real object. In this work, unsaturated AlBr₃ vapor pressure was measured.

EXPERIMENTAL

The synthesis of $AlBr_3$ from the elements was performed in a doubly fused quartz reactor. Aluminum was of A 9999 grade. Bromine of ch. (pure) grade with the major component content no less than 99.9% was subjected to additional deep purification by rectification on a high-performance column. The product, AlBr₃, was also subjected to deep purification by rectification on a plate column with slit perforation and overflow pipes. In experiments, the purest middle AlBr₃ fraction was used. A mass spectrometric analysis of purified AlBr₃ transformed into Al₂O₃ showed that the content of impurities most characteristic and difficult to remove (Fe, Ni, Cr, Cu, Ca, Mg, Ti, Ga, Na, K, and other socalled metallic impurities) did not exceed 1-0.1 ppm $(1 \text{ ppm} = 10^{-4} \text{ wt}\%)$. With respect to the impurities specified, AlBr₃ used in experiments was no less than 99.9995% pure. AlBr₃ is one of the most hygroscopic compounds. It is easily hydrolyzed and oxidized (even with air oxygen at comparatively low temperatures). All operations with it were therefore performed taking special precautions. Ampules were opened and filled in special boxes in the atmosphere of dry nitrogen from Dewar flasks with liquid nitrogen.

A scheme of the experimental unit is shown in Fig. 1. A reaction vessel with a crescent-shaped quartz manometer was rigidly fixed on a steel bench. A threesection furnace with a 70 mm inside diameter was mounted on a stand and could be moved in the vertical direction. Each furnace section was fed from a separate VRT-3 temperature controller. An equalizing block made of stainless steel with walls 5 mm thick was inserted into the furnace. Temperature was measured by two Pt/Pt–10% Rh thermocouples, mobile and immobile, calibrated against a gas thermometer, which was a



Fig. 1. Scheme of experimental unit: *1*, furnace; *2*, equalizing block; *3*, reaction vessel; *4*, entry for immobile thermocouple; *5*, diaphragm; *6*, chamotte insert; *7*, asbestos cap; *8*, mobile thermocouple; *9*, cylinder with dry argon; *10*, glass–metal junction; *11*, damping volume (5 l); *12*, PMT-2 vacuum gauge; *13*, mercury manometer; *14*, LGN-2 laser; *15*, screen; *16* and *17*, fine adjustment valves; and *18*, vacuum valve.

reaction vessel with a diaphragm of sensitivity 45 mm/torr. The error in temperature measurements was 0.3 K. The position of the mobile thermocouple along the vessel was measured on a millimeter scale. No rubber or silicon pipe connections were used. Compensation pressure was measured with a KM-10 cathetometer and a mercury manometer with tubes with an inside diameter of 18 mm. Movable meniscus illuminators made them clearly seen in the field of vision of KM-10. One manometer arm was evacuated with a fore pump.

Argon preliminarily held for no less than two weeks in a cylinder with granulated KOH at a pressure of 10– 12 atm was used as a compensating gas. The error in compensation pressure measurements was 0.03 torr. Here and throughout, all errors correspond to a 0.95 confidence probability. The total pressure variance was $s^2(p) = 0.0222147$ torr², the confidence interval of pressure was 0.3 torr. The major contribution to the pressure variance was made by the thermal drift of the zero pint of the diaphragm pressure gauge (~89%). The unit was always either evacuated (fore vacuum) or filled with dry argon. The diaphragm rod position was determined using an optical system. Light from a source (an LGN-2 laser) passed through a lens and was reflected from the rod mirror and focused on a screen of a scaled chart paper. The diameter of the light spot on the screen was ~1 mm. In addition, two more light spots were always present on the screen because of laser beam reflection from the outside and inside optical window planes. The coordinates of the rod mirror and one of the spots from the optical window are denoted below by y_1 and y_3 , respectively. The y_3 coordinate characterized the position of the reaction vessel as a whole.

Before measurements, manometer sensitivity and zero point thermal drift were measured. To determine sensitivity, the diaphragm chamber was filled with argon to a pressure of ~ 60 torr. The position of the zero

gauge.

point y_1^0 was fixed. Next, pressure drop Δp ($\pm \sim 2$ torr) was sequentially created between the reaction and compensation volumes and y_1 was measured. The results of 18 y_1^0 Δp and y_1 measurements were processed by the

18 y_1^0 , Δp , and y_1 measurements were processed by the method of least squares according to the equation

$$\Delta y = \alpha \Delta p,$$

where $\Delta y = y_1^0 - y_1$. This gave $\alpha = 20.16 \pm 0.3$ torr. The thermal drift of the zero point was measured in a vacuum. According to [8], corrections (~0.1 torr) were introduced into vapor pressure measurements for zero point shift at pressure *p* with respect to the vacuum. Thermal drift measurements were performed during one month. The thermal drift curve is shown in Fig. 2, where the electromotive force (EMF) of the mobile thermocouple E_1 measured at the center of the diaphragm is plotted on the abscissa axis. On the axis of ordinates, the

$$\Delta y^{\bullet} = (y_1^{\bullet} - y_3^{\bullet}) - (y_1^{0} - y_3^{0})$$

values are plotted. Here, y_1^{\cdot} and y_3^{\cdot} are measured at EMF E_1 , and y_1^0 , and y_3^0 are the room-temperature values determined before thermal drift measurements. The furnace was heated to the required temperature, and y_1^{\cdot} , y_3^{\cdot} , and temperature field along the reaction vessel were measured (y_1^0 and y_3^0 are the zero point and optical window coordinates). The temperature gradient along the reaction vessel was 0.5–3 K. Pressure was determined by the equation

$$p_0 = p + [(y_1^{\bullet} - y_3^{\bullet}) - (y_1 - y_3)]/\alpha,$$

where p_0 and p are the pressure in the diaphragm chamber and the compensation pressure, respectively, and y_1 and y_3 are the corresponding coordinates at the compensation pressure. The p_0 pressure differed from p by 0.1–0.3 torr.

After thermal drift measurements, the furnace was lowered, the ampule with $AlBr_3$ was broken, placed into the diaphragm chamber, and carefully sealed off under continuous evacuation. The furnace was raised, and the balancing block was closed with chamotte inserts and an asbestos cap, as is shown in Fig. 1.

The furnace was heated to the required temperature. During heating and subsequent cooling, compensation pressure was maintained using fine adjustment needle valves 16 and 17 (Fig. 1). The compensation pressure differed from the pressure inside the diaphragm chamber by tenths of a torr. Thermal equilibrium in the furnace was established in 1–2 h. Next, the temperature field and pressure were determined. The temperature field was measured during ~30 min at eight points along the vessel. During these ~30 min, the mean temperature changed at a rate of 0.01–0.02 K/min according to immobile thermocouple EMF E_2 readings. During

ing a day, measurements at several temperatures were taken. After this, the vessel was cooled to room temperature, and the absence of residual pressure was checked. Sometimes, the furnace was not switched off during night, which allowed conclusions to be drawn concerning the establishment of thermodynamic equilibrium in vapor and pressure gauge zero point shifts. During heating, the mean temperature under thermal equilibrium conditions decreased, and during cooling, it increased. This was related to the special features of VRT-3 temperature controller operation.

Fig. 2. Zero point thermal drift of a diaphragm pressure

During temperature field measurements, the mean diaphragm chamber temperature changed by 0.02–0.4 K. Because of the high diaphragm pressure gauge sensitivity, we observed how pressure changed in parallel with E_2 . For this reason, for each pressure measured, we calculated the temperature field as described in [10]. It was assumed that the rate of temperature variations at

Table 1. Molecular constants of Al₂Br₆ and Al₃Br₉ in the ground electronic state $\hat{X}^{1}A(p_{x} = 1)$

Molecule	Al ₂ Br ₆	Al ₃ Br ₉
Symmetry	C_{2v}	C_{3v}
Symmetry number σ	2	3
$I_A I_B I_C \times 10^{117},$ g ³ cm ⁶	0.84648208+08	0.86965731+09
ν, cm ⁻¹	$\begin{array}{l} A_1: 505, 408.8, 203.3, \\ 134.2, 100.8, 58.3, \\ 21.7; \\ A_2: 210.5, 111.7, 42.8; \\ B_1: 339.7, 96.9, 70.1; \\ B_2: 495, 366.1, \\ 194.5, 87, 68.7 \end{array}$	$\begin{array}{l} A_1: 515.3, 394, 183.5, \\ 132.2, 92.7, 71.7, 40; \\ A_2: 243.5, 119.6, 43.9 \\ E: 497.3, 371.9, 318.6, \\ 200.5, 107.2, 105.1, \\ 69, 58.1, 48.3, 30.5 \end{array}$



<i>Т</i> , К	р	δρ	<i>Т</i> , К	р	δρ	Т, К	р	δρ
561.87	54.77	0.082	621.06	66.72	-0.049	724.83	102.12	0.086
561.86	54.78	0.089	621.03	66.68	-0.084	724.79	102.09	0.063
561.83	54.75	0.071	620.98	66.69	-0.064	742.75	109.52	0.236
561.79	54.75	0.073	620.91	66.67	-0.063	742.78	109.52	0.216
561.76	54.74	0.068	620.84	66.66	-0.059	742.81	109.53	0.218
561.75	54.74	0.067	620.79	66.64	-0.062	742.86	109.55	0.218
561.75	54.72	0.049	640.61	72.09	0.046	742.90	109.56	0.211
561.75	54.72	0.048	640.65	72.10	0.043	742.93	109.59	0.229
560.66	54.46	-0.033	640.66	72.13	0.064	742.96	109.61	0.241
560.54	54.46	-0.011	640.65	72.11	0.046	742.99	109.63	0.242
560.47	54.41	-0.053	640.64	72.13	0.070	743.12	109.59	0.155
560.35	54.40	-0.046	640.64	72.12	0.065	743.12	109.60	0.165
560.26	54.41	-0.018	640.64	72.11	0.053	743.13	109.63	0.191
560.19	54.42	0.005	640.65	72.09	0.031	743.17	109.64	0.183
560.14	54.40	-0.009	655.64	76.54	-0.043	743.17	109.63	0.177
560.09	54.35	-0.050	655.64	76.51	-0.074	743.13	109.63	0.186
560.04	54.34	-0.049	655.70	76.51	-0.096	743.15	109.64	0.195
560.00	54.37	-0.019	655.72	76.54	-0.071	743.19	109.64	0.169
574.61	56.87	0.001	655.61	76.52	-0.062	758.38	115.32	-0.255
574.60	56.86	-0.003	655.55	76.51	-0.044	758.33	115.25	-0.303
574.61	56.90	0.035	655.38	76.45	-0.057	758.29	115.27	-0.270
574.65	56.91	0.040	675.02	83.13	0.087	758.24	115.24	-0.275
574.70	56.87	-0.011	675.08	83.14	0.074	758.22	115.25	-0.260
574.70	56.89	0.010	675.11	83.14	0.064	758.20	115.25	-0.251
574.70	56.89	0.008	675.14	83.14	0.056	758.19	115.23	-0.271
574.71	56.90	0.014	675.16	83.15	0.054	758.18	115.22	-0.273
574.54	56.85	0.000	675.17	83.15	0.055	779.70	124.09	0.196
574.53	56.82	-0.028	675.16	83.15	0.061	779.76	124.08	0.163
574.52	56.83	-0.024	675.15	83.15	0.061	779.82	124.12	0.178
574.55	56.84	-0.021	690.91	88.76	-0.027	779.85	124.10	0.150
574.57	56.84	-0.018	690.87	88.74	-0.038	779.85	124.09	0.139
574.57	56.83	-0.026	690.85	88.73	-0.038	779.81	124.15	0.211
574.57	56.86	-0.005	690.83	88.73	-0.030	779.70	124.14	0.247
574.55	56.87	0.012	690.80	88.70	-0.048	779.59	124.07	0.220
586.05	58.97	-0.031	690.77	88.66	-0.078	801.75	131.64	-0.346
585.96	59.00	0.015	690.74	88.65	-0.075	801.71	131.60	-0.379
585.92	59.00	0.027	690.71	88.63	-0.080	801.68	131.59	-0.372
585.85	58.98	0.014	724.57	101.81	-0.125	801.65	131.61	-0.348
585.77	59.00	0.060	724.66	101.79	-0.173	801.64	131.59	-0.356
585.70	58.95	0.014	724.69	101.81	-0.174	801.63	131.57	-0.375
585.66	58.96	0.037	724.71	101.84	-0.147	801.61	131.58	-0.356
605.76	63.11	-0.010	724.72	101.87	-0.126	801.60	131.56	-0.374
605.78	63.08	-0.046	724.76	101.86	-0.146	844.66	146.07	0.137
605.82	63.03	-0.104	724.79	101.85	-0.172	844.59	146.06	0.149
605.84	63.11	-0.035	724.82	101.87	-0.163	844.56	146.04	0.140
605.82	63.13	-0.010	725.06	102.20	0.069	844.53	146.07	0.175
605.82	63.07	-0.068	725.03	102.19	0.072	844.49	146.05	0.167
605.82	63.09	-0.050	725.00	102.20	0.090	844.46	146.04	0.169
605.82	63.08	-0.056	724.95	102.15	0.069	844.44	146.02	0.152
621.19	66.72	-0.082	724.91	102.17	0.099	844.42	146.05	0.185
621.11	66.72	-0.067	724.86	102.17				

Table 2. Temperature and vapor pressure (p, torr) measurements

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Equilibrium model	$\Delta H_2(298.15)$, cal/mol	$\Delta H_3(298.15)$, cal/mol	s^2 , torr ²	β, torr/K
1	13629.1±9	-	0.0272382	0.1837
2	13638.8 ± 8	-8528.5	0.0194113	0.18408
1	13740.9 ± 100	-	3.531755	0.1886
1	13658.8 ± 80	-	6.082971	_
2	13638.4	-10143	3.878664	-

Table 3. Vapor pressure optimizations in terms of various equilibrium models

all vessel points equaled that where the immobile thermocouple was fixed. This assumption was justified because the main vessel volume was in the zone of the main furnace section, whereas the remaining volume (diaphragm) was $\sim 2\%$, and the temperature gradient was very small. A method for taking into account the temperature gradient in a vessel in the presence of complex equilibria in the system was suggested in [11]. Calculations performed in this work showed that, because of the low temperature gradient, the mean temperature of the vessel could be calculated on the assumption of equal vapor densities over the whole vessel. Temperature field and pressure measurements were performed at 19 temperatures (ten during heating and nine during cooling) in four days. At two temperatures, seven pressure measurements were made, at one temperature, 10 measurements, and, at other temperatures, eight pressure measurements at each temperature.

RESULTS AND DISCUSSION

Two equilibrium models were considered: model 1

$$0.5 \text{AlBr}_6 = \text{AlBr}_3 + \Delta H_2(298.15),$$

model 2

$$\begin{split} &1.5 \mathrm{Al}_2 \mathrm{Br}_6 = \mathrm{Al}_3 \mathrm{Br}_9 + \Delta H_3(298.15), \\ &0.5 \mathrm{AlBr}_6 = \mathrm{AlBr}_3 + \Delta H_2(298.15). \end{split}$$

The parameters to be determined were ΔH_2 for model 1 and ΔH_2 and ΔH_3 for model 2. In addition, one more variable in both models was the $\beta = n_{AIBr_3}R/V$ value, the vapor density in the diaphragm chamber on the assumption that sample vapors consisted of AIBr₃. The β value was calculated from the sample weight (0.04771 g) and the diaphragm chamber volume (59.6 ml), $\beta = 0.1872$ torr/K. The error in β was determined by the accuracy of diaphragm chamber volume measurements, which was estimated at 0.1–0.2 ml. The real β value was, however, smaller. After the ampule with the sample was opened, an uncontrolled amount of the substance was removed during subsequent evacuation.

The thermodynamic functions of the dimer and monomer were reported in [12]. The functions of the dimer were calculated in [12] for a planar structure of D_{2h} symmetry. According to density functional theory calculations (B3LYP/6-31G(d,p), Gaussian 03 package [13]), the D_{2h} structure is a transition state, and a nonplanar configuration of C_{2v} symmetry corresponds to the potential energy minimum. This method was used for preliminary calculations of the molecular constants and thermodynamic functions of AlBr₃, which were in close agreement with the functions calculated using the molecular constants from [12]. The molecular constants of aluminum bromides are listed in Table 1. These constants were used in thermodynamic function calculations in the harmonic oscillator–rigid rotator approximation. The theoretical vibrational frequencies were scaled with a factor of 0.9611 [13].

For each equilibrium model, the optimum β and ΔH_2 (model 1) and β , ΔH_2 , and ΔH_3 (model 2) values were calculated by the method suggested in [14], that is, by the minimization of the residual sum of the squares of pressure discrepancies $\sum_{i=1,m} (p_i - p_i^*)^2$, where p_i denotes the experimental pressures and p_i^* , the vapor pressures calculated according to the model used; m = 152.

The experimental vapor pressures and vapor pressures calculated for both models are listed in Table 2. The table contains mean temperatures (K), experimental pressures (p_{expt}), and the differences $\delta p = p_{expt} - p^*$, where p^* is the pressure calculated according to model 2. At the beginning and at the end of each experiment, vapor pressures were measured at approximately equal temperatures. The δp values allow us to draw conclusions about the reproducibility of vapor pressure measurements. Table 3 contains the results of vapor pressure optimization according to different equilibrium models. The fourth column of the table contains the sample variances of vapor pressures s^2 (torr²), and the last column, the optimum β values (torr/K).

A comparison of the Fisher test values for the models (the first and second rows in Table 3) shows that the difference between models 1 and 2 is significant, although the concentration of the trimers was only 1.2%. This was related to fairly high accuracy of vapor pressure measurements. For model 1, the error in ΔH_2 is specified for a 0.95 confidence probability. For model 2, the confidence region for ΔH_2 and ΔH_3 was constructed (Fig. 3). The response surface in the ΔH_2 , ΔH_3 coordinates was a narrow slit with steep slopes. The



Fig. 3. Confidence region of the enthalpies of equilibria (1) and (2).

boundaries of the confidence region were used as errors in the enthalpies. For ΔH_2 , these boundaries are identical (they are listed in Table 3), whereas, for ΔH_3 , the upper boundary is ~1700 cal/mol, and the lower boundary is 640 cal/mol. The β values found for both models are in agreement with the experimental β value, considering errors in reaction vessel volume values and possible AlBr₃ weight loss before measurements.

We already mentioned that due attention to the zero point thermal drift was not paid in the literature. It would be interesting to learn to what extent the neglect of thermal drift influences the results of vapor pressure optimization. For comparison, we also performed calculations using pressure values obtained without thermal drift corrections. The results are listed in the third row of Table 3 (model 1). Vapor pressure measurements without thermal drift corrections give sharply incorrect results. At low temperatures, pressures are underestimated by ~ 2.5 torr, and, at high temperatures, they are exaggerated by ~3.5 torr. The confidence interval for ΔH_2 increases by an order of magnitude, and the pressure variance, by two orders of magnitude. Calculations by model 2 could not be performed because of the divergence of iterative minimization of the residual sum of the squares of pressure discrepancies.

Similar results can be expected for other vapor pressure measurements burdened with systematic errors related to the thermal drift of the pressure gauge zero point. We therefore recalculated the results obtained for AlBr₃ vapor pressures [1] using the thermodynamic functions calculated in this work. The results are listed in the last two rows of Table 3. For model 2, we constructed a confidence region (Fig. 4) not closed from the side of large ΔH_3 values. The boundary pressure variance value for a 0.95 confidence probability was 12.33 torr², and, at $\Delta H_3 = -5000$ cal/mol, the minimum



Fig. 4. Confidence region of ΔH_2 and ΔH_3 according to calculations based on the experimental data from [1].

pressure variance value (the bottom of the ravine) was 6.67 torr². The lower ΔH_3 limit was -11510 cal/mol.

For all models and also without taking zero point thermal drift into account, close enthalpies of predominant equilibrium (1) were obtained. It follows that, even under the conditions of an insufficiently high accuracy of pressure and temperature measurements, reasonable enthalpy values can be obtained for the predominant equilibrium. An increase in the accuracy of pressure and temperature measurements allows equilibria with the participation of products present in comparatively small concentrations to be revealed and their thermodynamic characteristics determined. The statistical method cannot by itself unambiguously identify the presence of certain products in vapor, but, in combination with other methods, for instance, spectroscopic, such information can be obtained.

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