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Torsion Vapor Pressures and Sublimation Enthalpies of Aluminum Trifluoride and Aluminum Trichloride

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The vapor pressures of solid AlF_3 and $AlCl_3$ were measured by the torsion-effusion method. Their temperature dependences fit the following equations: $\log(p/\mathrm{kPa}) = (11.70 \pm 0.20) - (14\,950 \pm 200)(T/\mathrm{K})$ (from (956 to 1113) K) and $\log(p/\mathrm{kPa}) = (15.50 \pm 0.30) - (6200 \pm 200)(T/\mathrm{K})$ (from (321 to 378) K) for AlF_3 and $AlCl_3$, respectively. Treating the measured vapor pressures by the second- and third-law methods, the average standard enthalpies of the sublimation of 1 mol solid AlF_3 and $AlCl_3$ to $AlF_3(g)$ and $Al_2Cl_6(g)$, $\Delta_{sub}H°$ (298.15 K) = (301 ± 4) $\mathrm{kJ \cdot mol^{-1}}$ and (59 ± 2) $\mathrm{kJ \cdot mol^{-1}}$, respectively, were calculated.

Introduction

The vapor pressure of solid aluminum trifluoride has been measured by several investigators using different techniques and, in particular, at high temperatures by manometric,[1,2] boiling point,[3,4] and transpiration methods[5] and at low temperatures by Knudsen,[6] torsion,[7] transpiration,[8] and mass spectrometric[9−12] methods. The results are not in good agreement. From the temperature dependence of the measured pressure data, the second-law sublimation enthalpy values of this compound were calculated. The results might be influenced, as thoroughly discussed by Krause and Douglas,[5] by the presence of a small amount of dimer in the saturated vapor. As concerns aluminum trichloride, at low temperatures, the vapor above this compound predominantly consists of dimer molecules, as observed mass spectrometrically,[13] whereas at higher temperatures, a small partial dissociation to the monomeric form occurs. Most of the vapor pressure data above solid $AlCl_3$ were measured by a static method using a null manometer[14−18] and boiling points.[19] Some vapor pressure values were also obtained by the Knudsen[20] and transpiration[14,21] methods. Also, for $AlCl_3$, the reported values are not in good agreement. Konings and Booij,[22] from the infrared spectra of the vapor above $AlCl_3$, calculated the thermal functions of $Al_2Cl_6(g)$. The same investigators, using these functions and those reported by JANAF[23] for solid $AlCl_3$, calculated some molar sublimation enthalpy values of this compound by third-law treatment of all vapor pressure data found in the literature. The aim of the present work was to perform new measurements of the total vapor pressures of AlF_3 and $AlCl_3$ using a torsion effusion apparatus and to derive the sublimation enthalpies of these compounds by second- and third-law treatment of the obtained pressure data.

Table 1. Torsion Vapor Pressures and Third-Law Standard Sublimation Enthalpies of AlF_3

run 2, cell A				run 3, cell A			
T	$-\log(p)$	$-\Delta$fef	$\Delta_{sub}H°$ (298 K)	T	$-\log(p)$	$-\Delta$fef	$\Delta_{sub}H°$ (298 K)
K	kPa	$\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$	$\mathrm{kJ \cdot mol^{-1}}$	K	kPa	$\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$	$\mathrm{kJ \cdot mol^{-1}}$
960	3.88	200.8	301.0	960	3.88	200.8	301.0
974	3.68	200.6	301.4	968	3.68	200.7	299.6
982	3.50	200.5	300.4	977	3.58	200.5	300.4
991	3.38	200.3	300.7	987	3.44	200.4	300.6
1001	3.20	200.2	300.2	998	3.24	200.2	300.1
1014	3.03	200.0	300.5	1010	3.09	200.1	300.6
1026	2.85	199.8	300.4	1023	2.90	199.9	300.6
1040	2.66	199.6	300.5	1036	2.73	199.7	300.7
1053	2.49	199.4	300.6	1048	2.56	199.5	300.6
1066	2.30	199.2	300.3	1059	2.41	199.3	300.7
1078	2.16	199.1	300.6	1070	2.27	199.2	300.6
1089	2.03	198.9	300.7	1083	2.09	199.0	300.4
1100	1.89	198.7	300.5	1097	1.91	198.8	300.3
1112	1.74	198.6	300.5	1109	1.77	198.6	300.3
		average	300.6			average	300.5
run 5, cell A				run 7, cell A			
T	$-\log(p)$	$-\Delta$fef	$\Delta_{sub}H°$ (298 K)	T	$-\log(p)$	$-\Delta$fef	$\Delta_{sub}H°$ (298 K)
K	kPa	$\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$	$\mathrm{kJ \cdot mol^{-1}}$	K	kPa	$\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$	$\mathrm{kJ \cdot mol^{-1}}$
975	3.68	200.6	301.7	956	3.98	200.9	301.6
985	3.44	200.4	300.0	970	3.68	200.6	300.2
994	3.33	200.3	300.6	982	3.50	200.5	300.4
1007	3.14	200.1	300.6	991	3.33	200.3	299.7
1018	2.95	199.9	300.1	1002	3.17	200.2	299.8
1029	2.81	199.8	300.3	1013	3.03	200.0	300.2
1040	2.66	199.6	300.5	1022	2.90	199.9	300.3
1052	2.50	199.4	300.6	1033	2.74	199.7	300.1
1063	2.36	199.3	300.6	1043	2.60	199.6	300.1
1074	2.20	199.1	300.4	1052	2.49	199.4	300.3
1086	2.05	198.9	300.4	1062	2.35	199.3	300.2
1098	1.92	198.8	300.7	1071	2.24	199.2	300.3
1107	1.81	198.6	300.6	1083	2.08	199.0	300.2
		average	300.5	1093	1.97	198.8	300.5
				1104	1.83	198.7	300.3
				1113	1.73	198.5	300.5
						average	300.3

Experimental Section

The AlF_3 and $AlCl_3$ used in the present work had a nominal purity of 99.9 % and 99.985 % respectively, as certified by the suppliers (Aldrich and Alpha Aesar for AlF_3 and $AlCl_3$ respectively). The samples were loaded into the cells in an efficient dry box and transferred into the torsion assembly, which was rapidly evacuated at low operative pressure (~ 10^{-6} kPa). The assembly used is practically the same as that described in our previous work.[24] The samples were heated by a furnace that could also be let down for rapid cooling. The temperatures

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Table 2. Temperature Dependence of Torsion Vapor Pressures of AlF_3 and $AlCl_3$

compound	run	cell	ΔT / K	no. of points	log(p/kPa) = (A − B)/(T/K) A^a	B^a
AlF_3	2	A	960 to 1112	14	11.77 ± 0.09	15 017 ± 94
	3	A	960 to 1109	14	11.63 ± 0.11	14 864 ± 109
	5	A	975 to 1107	13	11.73 ± 0.15	14 968 ± 158
	7	A	956 to 1113	16	11.72 ± 0.13	14 943 ± 130
$AlCl_3$	11	C	323 to 355	12	15.43 ± 0.17	6160 ± 58
	12	B	338 to 378	14	15.55 ± 0.19	6214 ± 68
	15	C	321 to 353	11	15.50 ± 0.41	6195 ± 136
	16	B	339 to 372	12	15.55 ± 0.16	6214 ± 57

[a] The quoted errors are standard deviations.

were measured by a calibrated chromel−alumel thermocouple inserted in a cell similar to the one posted under the torsion cell, with an uncertainty of ± 2 K around the temperatures operative for the sublimation of AlF_3 (~ 1000 K) and of ± 1 K at low temperatures when the vapor pressures of $AlCl_3$ were measured. The pressure measurements in each run were made randomly in both ascending and descending temperature steps even though Tables 1 and 4 report ascending temperatures.

***AlF_3*.** A conventional graphite torsion cell (cell A) with both effusion holes having a nominal diameter of 1.00 mm was used to study AlF_3. The instrument constant of this cell, which is necessary for converting the measured torsion data to pressure values, was determined and checked by vaporizing very pure lead (the vapor pressure of which is well known)[25] before and during the study of the compound. The constant values so obtained were found to be reproducible within about 5 % of its average value. To check the accuracy in the second-law vaporization enthalpy measurement with the torsion arrangement used, the temperature dependence of the torsion angles (α) measured during two vaporization runs of lead (run 1 and 6), were expressed by two linear least-squares log α versus $1/T$ equations. From the slopes of those equations, two second-law vaporization enthalpies, (186 ± 2) $kJ \cdot mol^{-1}$ and (185 ± 3) $kJ \cdot mol^{-1}$, were derived at 1000 K. These values are in excellent agreement with that in the IVTANTHERMO database[25] at this temperature, 184.5 $kJ \cdot mol^{-1}$.

The results of four vaporization runs of AlF_3 are reported in Table 1 and Figure 1. For each run, the temperature dependence of the measured vapor pressures expressed by a log p versus $1/T$ equation, as obtained by least-squares treatment of the data, is reported in Table 2, where the reported errors are standard deviations from the means. By weighting the slopes and intercepts of these equations proportionally to the number of points, the following equation, which is representative of the total vapor pressure above solid AlF_3 in the range temperature (956 to 1113) K, was obtained

$$\log(p/\text{kPa}) = (11.70 \pm 0.20) - (14\,950 \pm 200)(T/\text{K}) \quad (1)$$

where the reported errors were overestimated by also considering the uncertainty in the temperature measurements and the variation in the corresponding slope and intercept values obtained in each run. This equation was compared in Table 3 and Figure 2 with those reported by other investigations.

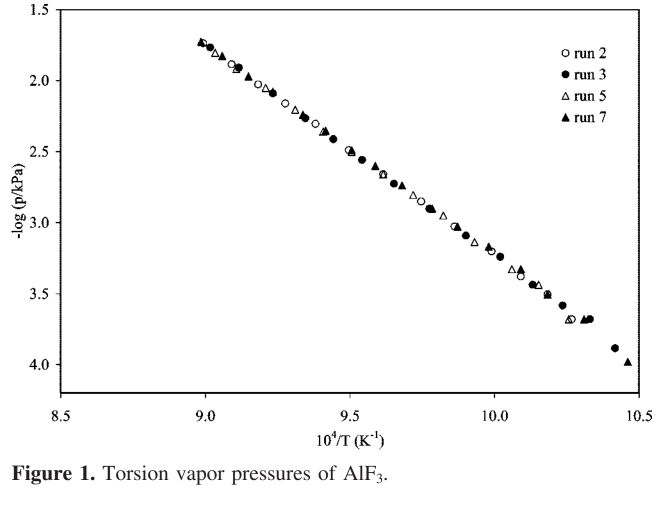

Figure 1. Torsion vapor pressures of AlF_3.

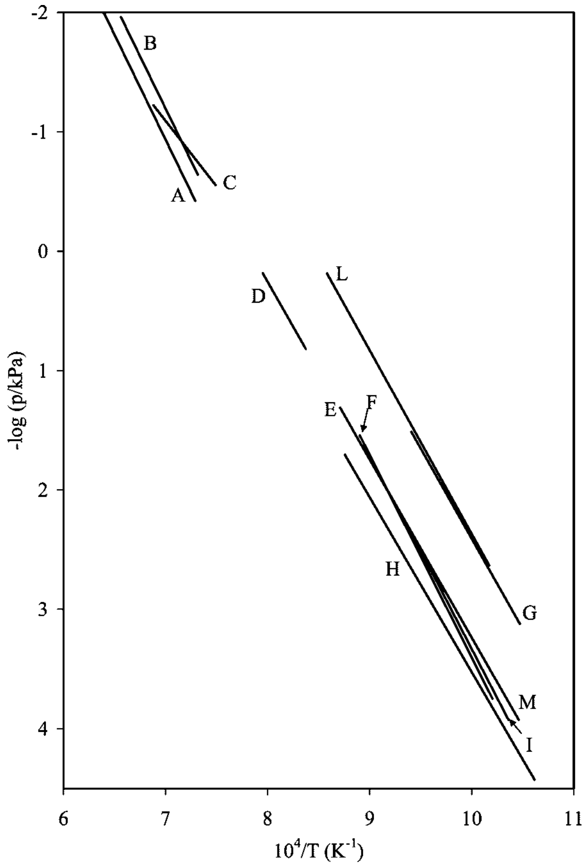

Figure 2. Temperature dependence of the vapor pressures of solid AlF_3: A, ref 1; B, ref 2; C, ref 3; D, ref 5; E, ref 8; F, ref 6; G, ref 7; H, ref 12; I, ref 9; L, ref 11; M, this work. Our data accidently coincide with E, ref 8.

***$AlCl_3$*.** Two conventional graphite torsion cells (B and C) having different diameter effusion holes (0.8 mm and 1.5 mm, respectively) were used. Some calibration runs (10, 13, 14, and 17) were made using benzoic acid[26] as a standard to determine and check the instrument constants. Considering the low operative temperatures and the small increase in these when they were changed, the equilibrium in the cell was ensured at each experimental point by maintaining constant temperature for several minutes until the torsion angle remained decidedly constant. As was also observed by Dunne and Gregory,[20] a white deposit, which was not well identified and not volatile at the operating temperatures, was observed at the end of some experiments around the effusion holes of the cell. This reduced the orifice area of the effusion holes with an obvious gradual decrease in the torsion angles. Moreover, going on the experiment, the gradual decrease can be also due to decreasing pressure caused by hydration, hydrolysis, or both of the sample so that in each run only the first reproducible points were taken into account for the

Table 3. Vapor Pressures and Molar Sublimation Enthalpies of AlF_3 According to Reaction *3*

			ΔT	$\log(p/\text{kPa}) = (A - B)/(T/\text{K})$		$\Delta_{\text{sub}}H^\circ$ (T)	$\Delta_{\text{sub}}H^\circ$ (298 K)/kJ·mol^{-1}	
ref	method	no. of points	K	*A*	*B*	kJ·mol^{-1}	second-law	third-law
1	manometric	9	1370 to 1570	13.22[a]	17 560[a]		377.2 (at 0 K)[b]	311.7 (at 0 K)[b]
2	manometric	9	1367 to 1524	13.47[c]	17 530[c]		371.0 (at 0 K)[b]	307.5 (at 0 K)[b]
3	boiling point	5	1335 to 1453	8.78 ± 0.89[d]	10 988 ± 1240[d]	210 ± 24[d]		
4	boiling point		1400	$\log(p/\text{kPa}) = (18.44 \pm 0.18) - (15\,660 \pm 240)/(T/\text{K}) - 1.948\cdot\log T - 1.34\cdot10^{-4}\cdot T$		272.6 ± 4.6	296.2 ± 6	
5	transpiration	8	1194 to 1257	11.719 ± 0.013[d]	14 969 ± 15[d]	286.5 ± 0.3[d]	286.6 ± 0.4	279.1 ± 2
6	Knudsen	12	980 to 1123	13.56	16 967		335.9 (at 0 K)	307.4 (at 0 K)
7	torsion		955 to 1063	12.714[e]	15 122[e]		302.9	318.2
8	transpiration	23	1027 to 1148	11.733	14 974		300.0 ± 4	
9	mass spectrometric	7	965 to 1065	13.12 ± 0.40[d]	16 453 ± 409[d]	315 ± 8[d]		
10	mass spectrometric		951 to 1077			281.6 ± 12	281.6 ± 12	
11	mass spectrometric	9	983 to 1165	12.987	15 386	294.5	301.7 ± 2 (at 0 K)	
12	mass spectrometric	9	942 to 1142	11.112	14 637 ≤ 308	280.2 ≤ 5.9		
27							256.8 (at 0 K)[b]	310.3 (at 0 K)[b]
this work	torsion	57	956 to 1113	11.70 ± 0.20	14 950 ± 200	286 ± 4	302 ± 5	300.5 ± 1.0

[a] We evaluated by the date reported in Figure 1 in Witt's work.[7] [b] Calculated and reported in Evseev's work.[6] [c] Calculated by Evseev[6] from the data reported in Table 8 of Ruff's work. [d] We evaluated from the experimental points reported in the original work; the associate errors are standard deviations. [e] Equation reported in ref 7 is representative of the data reported in the work[7] and those reported in Ruff and Le Boucher's previous work.[2]

Table 4. Torsion Vapor Pressures and Third-Law Standard Enthalpy Values Associated with the Sublimation of $AlCl_3$ according to Reaction *4*

run 11, cell C				run 12, cell B			
T	$-\log(p)$	$-\Delta$fef	$\Delta_{\text{sub}}H^\circ$ (298 K)	T	$-\log(p)$	$-\Delta$fef	$\Delta_{\text{sub}}H^\circ$ (298 K)
K	kPa	J·mol^{-1}·K^{-1}	kJ·mol^{-1}	K	kPa	J·mol^{-1}·K^{-1}	kJ·mol^{-1}
323	3.63	127.5	58.6	338	2.79	127.5	58.6
329	3.28	127.5	58.6	340	2.73	127.5	58.8
334	3.05	127.5	58.8	343	2.53	127.5	58.6
340	2.68	127.5	58.6	346	2.40	127.5	58.7
344	2.47	127.5	58.6	348	2.32	127.5	58.8
346	2.40	127.5	58.7	351	2.17	127.5	58.8
347	2.31	127.5	58.6	353	2.08	127.5	58.8
349	2.20	127.5	58.6	356	1.93	127.5	58.8
350	2.17	127.5	58.6	358	1.84	127.5	58.8
352	2.08	127.5	58.6	363	1.58	127.5	58.7
354	1.97	127.5	58.6	368.5	1.31	127.5	58.7
355	1.92	127.5	58.6	373	1.07	127.5	58.6
		average	58.6	376.5	0.93	127.5	58.6
				378	0.89	127.5	58.7
						average	58.7

run 15, cell C				run 16, cell B			
T	$-\log(p)$	$-\Delta$fef	$\Delta_{\text{sub}}H^\circ$ (298 K)	T	$-\log(p)$	$-\Delta$fef	$\Delta_{\text{sub}}H^\circ$ (298 K)
K	kPa	J·mol^{-1}·K^{-1}	kJ·mol^{-1}	K	kPa	J·mol^{-1}·K^{-1}	kJ·mol^{-1}
321	3.77	127.5	58.7	339	2.80	127.5	58.8
327	3.42	127.5	58.7	340	2.73	127.5	58.8
329	3.29	127.5	58.6	345	2.43	127.5	58.6
330	3.26	127.5	58.7	347	2.37	127.5	58.8
333	3.17	127.5	58.9	351	2.19	127.5	58.8
336	2.99	127.5	58.9	354	2.04	127.5	58.8
339	2.79	127.5	58.8	355	1.93	127.5	58.6
342	2.61	127.5	58.7	358	1.80	127.5	58.7
345	2.44	127.5	58.7	362	1.62	127.5	58.7
348	2.27	127.5	58.6	366	1.43	127.5	58.7
353	2.05	127.5	58.6	369	1.29	127.5	58.7
		average	58.7	372	1.16	127.5	58.7
						average	58.7

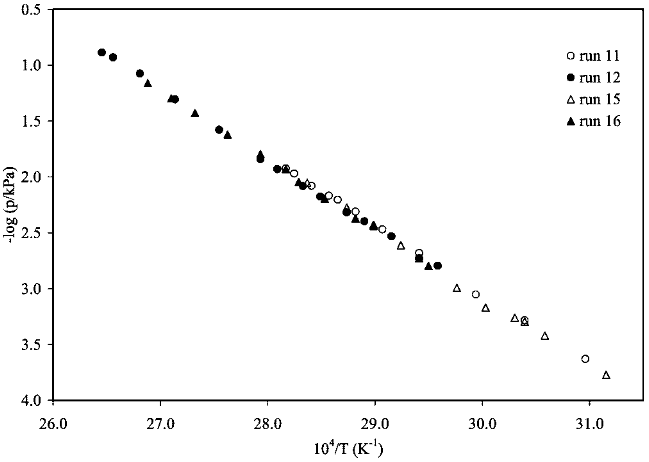

Figure 3. Torsion vapor pressure of $AlCl_3$.

thermodynamic analysis. The experiments were stopped and the values of the pressure were rejected as soon as a decrease from the points that were initially obtained became apparent. These vapor pressures are reported in Table 4 and Figure 3. The temperature dependence of the obtained pressures linearized by least-squares treatment of the data is expressed for each run by a log *p* versus $1/T$ equation with errors listed as standard deviations from the means. These equations are reported in Table 2. Apparently, no dependence on the effusion holes area was observed. As usual, by weighting the slopes and intercepts of these equations proportionally to the number of experimental points, the following equation, which is representative of the vapor pressure of $AlCl_3$ in the temperature range (321 to 378) K, was selected

$$\log(p/\text{kPa}) = (15.50 \pm 0.30) - (6200 \pm 200)(T/\text{K}) \quad (2)$$

where the reported errors were overestimated, considering the small temperature range covered in each run. This equation is reported in Table 5 and Figure 4 for comparison with those measured above the solid phase by other investigators.

Discussion

From the slopes of the selected equations of temperature dependence of the vapor pressures of AlF_3 and $AlCl_3$, the second-law sublimation enthalpies of these compounds were calculated at the middle points of the covered temperature ranges. As concerns AlF_3, considering that (i) Porter and Zeller[9] reported that the dimer contribution is nearly 2 % of the total pressure at 1000 K, (ii) Buechler et al.[10] found that at the same temperature the contribution is at most a few percent of the total pressure, and (iii) Krause and Douglas[5] from a critical analysis of our results found "the mole percent of dimer in the saturated vapor to be (4.6 ± 1.4) at 1225 K", whereas (iv) Kulczycki et al.[12] did not find ions originating from the ionization of dimer molecules at 1000 K, we are persuaded that in the temperature ranges covered in our experiments the dimer contribution is negligible and the sublimation of AlF_3 occurs according to the congruent reaction

Table 5. Vapor Pressures and Sublimation Enthalpies of $AlCl_3$ according to Reaction *4*

			ΔT		$\log(p/\text{kPa}) = (A - B)/(T/\text{K})$		$\Delta_{\text{sub}}H°$ (T)	$\Delta_{\text{sub}}H°$ (298 K)/kJ·mol^{-1}	
ref	method	no. of points	K	phase	A	B	kJ·mol^{-1}	second law	third law
reported in ref 22			441 to 486	sol to liq					113.9 ± 0.3[a]
reported in ref 22			342 to 454	sol					112.5 ± 0.3[a]
reported in ref 22			389 to 476	sol to liq					113.0 ± 0.2[a]
14	null manometric	14	395 to 450	sol	15.18[b]	5967[b]	57.1[b]	58.9[d]	
14	transpiration	9	393 to 428	sol	15.05[b]	5912[b]	56.6[b]	58.2[d]	
15	null manometric		420 to 466	sol	15.24	6000	57.4	59.5[d]	
15	null manometric		466 to 482	liq	6.80	2130	20.4	58.7[d]	
16	null manometric	35	467 to 625	liq	6.34	1835	17.6	58.6[d]	
17	static	48	387 to 466	sol	15.01	5900	56.5	58.3[d]	
17	static	80	466 to 529	liq	6.56	1956	18.7	57.9[d]	
18	null manometric		390 to 455	sol	14.95[c]	5960[c]	57.05	58.8[d]	
19	boiling point	21	471 to 506	liq	6.743	2046	19.6	58.5[d]	
20	Knudsen	12	294 to 322	sol	16.90	6536	62.6	62.7[d]	
21	transpiration	38	377 to 440	sol	12.14[e]	4533[e]	43	44.5[d]	
this work	torsion	49	321 to 378	sol	15.50 ± 0.30	6200 ± 200	59.3 ± 2.0	59.9 ± 2.0	58.7 ± 1.0

[a] Values calculated by Konings and Booij[22] employing previous vapor pressure data reported in their work as references 23, 24, and 26, which were not available to us (ref 23: Friedel, C.; Crafts, J. M. *Comptes Rendus, (Paris)* **1888**, *106*, 1764; ref 24: Maier, C. G. *U. S., Bur. Mines Tech. Paper 360*, **1929**; ref 26: Treadwell, W. D.; Terebesi, L. *Helv. Chim. Acta* **1932**, *15*, 1053). [b] We evaluated from the experimental data reported in the work.[14] [c] We evaluated from the log *p* versus 1/*T* line drawn in Figure 4 of the work.[18] [d] Calculated by using the enthalpic increments reported in the IVTANTHERMO database.[25] [e] We calculated from the data reported in Figure 2 of the original work.[21]

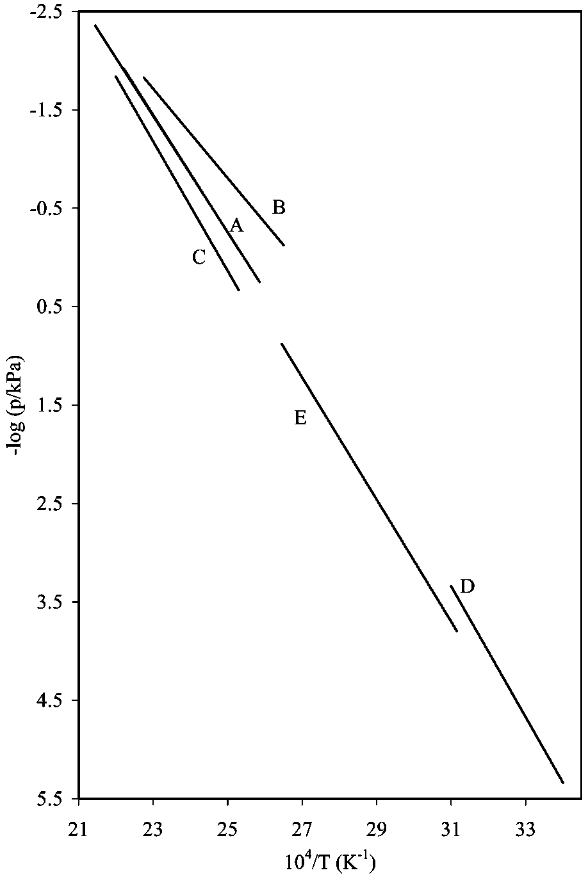

Figure 4. Temperature dependence of the vapor pressure of solid $AlCl_3$: A, representative of equation reported in refs 14, 15, and 17; B, ref 21; C, ref 18; D, ref 20; E, this work.

$$AlF_3(s) \rightarrow AlF_3(g) \qquad (3)$$

On the contrary, as observed mass spectrometrically,[13] in our temperature ranges, $AlCl_3$ sublimes according the reaction

$$AlCl_3(s) \rightarrow 1/2\ Al_2Cl_6(g) \qquad (4)$$

On this basis, the total vapor pressures measured above solid AlF_3 and $AlCl_3$ were considered to be practically equal to $AlF_3(g)$ and $Al_2Cl_6(g)$ pressure, respectively.

A. AlF_3. From the slope of the eq 1, the second-law sublimation of AlF_3, $\Delta_{\text{sub}}H°$ (1035 K) = (286 ± 4) kJ·mol^{-1}, was calculated. This value agrees well with those obtained mass spectrometrically ($\Delta_{\text{sub}}H°$ (1000 K) = (282 ± 13) kJ·mol^{-1}[10] and $\Delta_{\text{sub}}H°$ (1042 K) = (280 ± 6) kJ·mol^{-1}[12]) and that obtained by a transpiration method[5] ($\Delta_{\text{sub}}H°$ (1225 K) = (286.5 ± 0.5) kJ). By using the enthalpic increments for the solid and gaseous phases reported in the IVTANTHERMO database,[25] the sublimation enthalpy value was reported at 298.15 K, $\Delta_{\text{sub}}H°$ (298.15 K) = (302 ± 5) kJ·mol^{-1}, where the error was increased for the uncertainties in the enthalpic increment values. The standard sublimation enthalpy of AlF_3 was also calculated by third-law treatment of each measured vapor pressure. The free-energy functions, $G°(T) - H°(298.15\ \text{K})/T$, that are necessary for these calculations were taken from the same source as the enthalpic increments.[25] In Table 1 the obtained results at each temperature are reported. It is interesting that in each run no evident temperature trend was observed, their average values are in excellent internal agreement, and the selected third-law value, (300.5 ± 1.0) kJ·mol^{-1} agrees with that obtained by the second law. On this basis, giving an equal weight to the second- and third-law results, we propose as a standard sublimation enthalpy of AlF_3 the value 301 kJ·mol^{-1} with an estimated uncertainty not exceeding 4 kJ·mol^{-1}.

B. $AlCl_3$. As concerns $AlCl_3$, from the slope of eq 2, the second-law enthalpy associated with the sublimation of this compound according to reaction 4 was calculated, $\Delta_{\text{sub}}H°$ (350 K) = (59.3 ± 2.0) kJ·mol^{-1}, where the associated error was estimated. Apart from a Knudsen value[20] ($\Delta_{\text{sub}}H°$ (308 K) = 62.6 kJ·mol^{-1}), our value is slightly higher than others found in the literature[14,15,17,18,21] (Table 5), although these were obtained at slightly higher middle temperatures. The value was corrected to 298.15 K by the enthalpic increments reported in the IVTANTHERMO database,[25] $\Delta_{\text{sub}}H°$ (298.15 K) = (59.9 ± 2.0) kJ·mol^{-1}. At each vapor pressure value, a standard third-law enthalpy associated with sublimation reaction 4 was calculated using the free-energy functions for $AlCl_3(s)$ and $Al_2Cl_6(g)$ reported in the IVTANTHERMO database.[25] The enthalpic values so calculated are reported in Table 4. Also, for this compound, no evident temperature trend was observed, and all of the enthalpy values are in excellent internal agreement. Their average value, $\Delta_{\text{sub}}H°$ (298.15 K) = (58.7 ± 1.0) kJ·mol^{-1}, agrees with the second-law value. On this basis, we propose as the standard enthalpy associated with the sublimation of solid $AlCl_3$ according to reaction 4 the value of 59 $kJ \cdot mol^{-1}$ with an estimated error that does not exceed 2 $kJ \cdot mol^{-1}$.

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