P_4O_7. Analysis of the THF-soluble, benzene-insoluble solid showed Ph_3PO and no Ph_3P. The reaction was also attempted in benzene and diethyl ether, and no reaction occurred at room temperature over a several-day period. Similarly, no reaction occurred between P_4O_6 and Me_3NO in THF at room temperature.

(k) Reaction of P_4O_7 with P_4S_{10}. In a typical reaction 0.3 g (1.3 mmol) of P_4O_7 and 0.8 g (1.8 mmol) of P_4S_{10} were added to an NMR tube in a drybox. The tube was placed on a vacuum line, and about 1.0 mL of toluene was transferred to the tube which was then sealed. The tube was inverted, transferring all of the liquid and solid to the sealed end of the tube. The tube was then heated to 125 °C for about 1 h until all of the P_4O_7 had reacted. After all of the P_4O_7 had been consumed, the temperature was increased to 150 °C. The reaction was monitored by ^{31}P NMR spectroscopy every 2 h. Initially after 1 h of heating, the major product was P_4O_7S, with 2 h of additional heating producing $P_4O_7S_2$ with some P_4O_8 and $P_4O_6S_2$. Further oxidation of $P_4O_6S_2$ occurred more readily than P_4O_7S or P_4O_8, as observed by the large quantities of $P_4O_6S_3$ and $P_4O_6S_4$. Extended heating for 30–45 h yielded P_4O_8S, $P_4O_8S_2$, $P_4O_7S_3$, $P_4O_6S_3$, and primarily $P_4O_6S_4$. Some P_4S_3 was also observed.

(l) Reaction of P_4O_7 with P_4Se_{10}. The same procedure was used as in the above reaction of P_4O_7 with P_4S_{10}. The products identified by NMR spectroscopy after 2 h of heating at 145 °C were P_4O_7Se, P_4O_8, and $P_4O_6Se_2$. Due to the extreme sensitivity and the mixture of products, no compound isolation was achieved.

Acknowledgment. Support of this research by the Robert A. Welch Foundation is gratefully acknowledged. D.E.P. also thanks the Graduate School for a fellowship.

Registry No. P_4O_7, 55230-51-8; P_4O_6S, 70983-15-2; P_4O_6Se, 70983-16-3; P_4O_8, 70983-17-4; P_4O_7S, 70983-18-5; P_4O_7Se, 70983-19-6; $P_4O_6S_2$, 70983-20-9; P_4O_6SSe, 70983-21-0; $P_4O_6Se_2$, 70983-22-1; P_4O_8S, 70983-23-2; $P_4O_7S_2$, 70983-24-3; $P_4O_6S_3$, 70983-25-4; $P_4O_6Se_3$, 70983-26-5; $P_4O_8S_2$, 70983-27-6; $P_4O_7S_3$, 70983-28-7; $P_4O_6S_4$, 15780-31-1; P_4O_6, 10248-58-5; P_4S_{10}, 15857-57-5; S_8, 10544-50-0; P_4O_{10}, 16752-60-6; Ph_3P, 603-35-0; P_4Se_{10}, 62493-85-0; Ph_3PO, 791-28-6.

References and Notes

(1) J. G. Riess and J. R. Van Wazer, *J. Am. Chem. Soc.*, **88**, 2166 (1966).
(2) J. G. Riess and J. R. Van Wazer, *J. Am. Chem. Soc.*, **88**, 2339 (1966).
(3) J. G. Riess and J. R. Van Wazer, *J. Am. Chem. Soc.*, **89**, 851 (1967).
(4) G. Kodama and H. Kondo, *J. Am. Chem. Soc.*, **88**, 2045 (1966).
(5) M. L. Walker and J. L. Mills, *Inorg. Chem.*, **14**, 2438 (1975).
(6) T. E. Thorpe and A. E. Tutton, *J. Chem. Soc.*, **59**, 1023 (1891).
(7) D. Heinz, *Z. Anorg. Allg. Chem.*, **336**, 137 (1965).
(8) D. Heinz, H. Rienitz, and D. Rodeck, *Z. Anorg. Allg. Chem.*, **383**, 12 (1972).
(9) D. E. C. Corbridge, *Top. Phosphorus Chem.*, **3**, 57 (1966).
(10) M. L. Walker and J. L. Mills, *Synth. React. Inorg. Met.-Org. Chem.*, **5**, 29 (1975).
(11) M. L. Walker and J. L. Mills, *Inorg. Chem.*, **16**, 3033 (1977).
(12) J. R. Van Wazer, "Phosphorus and Its Compounds", Interscience, New York, 1958; D. E. C. Corbridge, "The Structural Chemistry of Phosphorus", Elsevier, London, 1974; D. A. Armitage, "Inorganic Rings and Cages", Arnold, New York, 1972.
(13) F. Casabianca, A. A. Pinkerton, and J. G. Riess, *Inorg. Chem.*, **16**, 864 (1977).
(14) E. W. Abel, D. A. Armitage, and R. P. Bush, *J. Chem. Soc.*, 5585 (1964). The structure of this molecule was proposed to consist of a P_4S_6 cage with four exocyclic oxygens. Elemental analysis was the only evidence given for the compound. In light of our studies and those of others (M. L. Walker and A. H. Cowley, unpublished results) who have been unable to repeat the preparation, the proposed structure of $P_4S_6O_4$ is unlikely.
(15) Although ^{77}Se has a nuclear spin of $^1/_2$, it is not present in sufficient concentations (7.58% natural abundance) to normally result in observable coupling.
(16) J. R. Van Wazer and J. H. Letcher, *Top. Phosphorus Chem.*, **5**, 169 (1967).
(17) J. C. Pernert and J. H. Brown, *Chem. Eng. News*, **27**, 2143 (1949).
(18) H. Gerding and H. Van Brederode, *Recl. Trav. Chim. Pays-Bas*, **64**, 183 (1945).
(19) R. G. Cavell, R. D. Leary, and A. J. Tomlinson, *Inorg. Chem.*, **11**, 2573, 2578 (1972).
(20) J. H. Letcher and J. R. Van Wazer, *J. Chem. Phys.*, **44**, 815 (1966).
(21) R. G. Pearson, *J. Am. Chem. Soc.*, **85**, 3533 (1963).
(22) D. F. Shriver, "The Manipulation of Air Sensitive Compounds", McGraw-Hill, New York, 1969.

Contribution from the Department of Chemistry and Molecular Sciences, University of Warwick, Coventry CV4 7AL, Warwickshire, United Kingdom, and the Laboratoire de Chimie Minérale 1, Université des Sciences et Techniques de Lille, 59650 Villeneuve d'Ascq, France

Thermodynamics of the $AlCl_4^-$ Ion by Lattice-Energy Studies

HARRY DONALD BROOKE JENKINS,* KENNETH FRANK PRATT, GAETAN MAIRESSE, PIERRE BARBIER, and JEAN PIERRE WIGNACOURT

Received January 8, 1979

Using the recently obtained crystal structure data for lithium, sodium, potassium, cesium, and ammonium tetrachloroaluminates, we have computed the total lattice energies by using the method of Jenkins and Pratt. $\Delta H_f°(AlCl_4^-(g))$ is estimated to be −1188 kJ mol^{-1}, and the halide ion affinities for the processes $AlCl_3(ss) + Cl^-(g) \rightarrow AlCl_4^-(g)$ are determined, where (ss) represents (c), (l), and (g).

This study concerns the crystal structures and associated thermochemical data of tetrachloroaluminate salts. From a knowledge of the crystal structures of $LiAlCl_4$, $NaAlCl_4$, $KAlCl_4$, $CsAlCl_4$, and NH_4AlCl_4, thermodynamic parameters, "basic" radii, and charge distribution for the $AlCl_4^-$ anion are obtained which confirm in part and extend the results of previous studies. Studies on these systems are of inherent interest because of the importance[1,2] of tetrahalometalate salts as electrolytes,[3] as heat-exchange fluids in nuclear reactors,[4] and as catalysts in organic systems and because of their thermal stability and use as media for the preparation of unusual oxidation states. The study of the effective charges in tetrahalometalate ions has received attention in connection with the estimation of bonding energies in conjunction with the ESCA technique[5] and NQR spectroscopy.[6]

Crystal Structure Data

Table I gives the lattice parameters and structural details concerning the tetrachloroaluminates for the alkali metal salts (except rubidium) and the ammonium salt.

All the tetrachloroaluminates crystallize with four molecules per unit cell ($Z = 4$). The structure of $LiAlCl_4$ is given in ref 7. The $NaAlCl_4$ structure of Baenziger[8] has been refined by Scheinert and Weiss[6] and refined also in this laboratory[9] with an improved accuracy. $KAlCl_4$[10] has been determined to have two molecular formulas in the asymmetric unit.

---

* To whom correspondence should be addressed at the University of Warwick.

0020-1669/79/1318-2796$01.00/0

Table I. Structural Parameters for $MAlCl_4$

salt	cell parameters				V, Å^3	space group	coordination	
	a, Å	*b*, Å	*c*, Å	angle, deg			$M^+/AlCl_4^-$	M^+/Cl^a
$LiAlCl_4$	7.007 (3)	6.504 (4)	12.995 (10)	$\beta = 93.32$ (5)	591	$P2_1/c$	4/4	1/6
$NaAlCl_4$	10.322 (3)	9.886 (3)	6.167 (2)	90	629	$P2_12_12_1$	6/6	1/8
$KAlCl_4$	10.481 (9)	7.183 (5)	9.273 (5)	$\alpha = 93.10$ (3)	698	$P2_1$	7/7	1/9
$CsAlCl_4$	11.641 (8)	7.116 (5)	9.373 (7)	90	776	*Pnma*	7/7	1/12
NH_4AlCl_4	11.022 (6)	7.072 (3)	9.257 (5)	90	722	*Pnma*	7/7	1/12

[a] Taking into account the $M^+\cdots Cl$ distances lower than the shortest $M^+\cdots Al$ length.

Table II. Previous Calculations on $AlCl_4^-$ Salts

salt	U_{pot}, kJ mol^{-1}	q_{Cl}	$\Delta H_f°(AlCl_4^-(g))$, kJ mol^{-1}	halide ion affinity, kJ mol^{-1}
$NaAlCl_4$[b]	592.0	−1.0	−1188 ± 28	−364 ± 28
	536.0	−0.2		
	540.6	0.0		
av	556.2	−0.4[a]		
$CsAlCl_4$[b]	491.6	−0.1		
	510.4	−0.2		
	510.9	0.0		
av	504.3	−0.4[a]		
$NaAlCl_4$[c]	555.8	−0.59	−1196	
$CsAlCl_4$[c]	486.4	−0.59		

[a] Average value corresponds to charge $q_{Cl} = -0.4$. [b] Reference 13. [c] Reference 18.

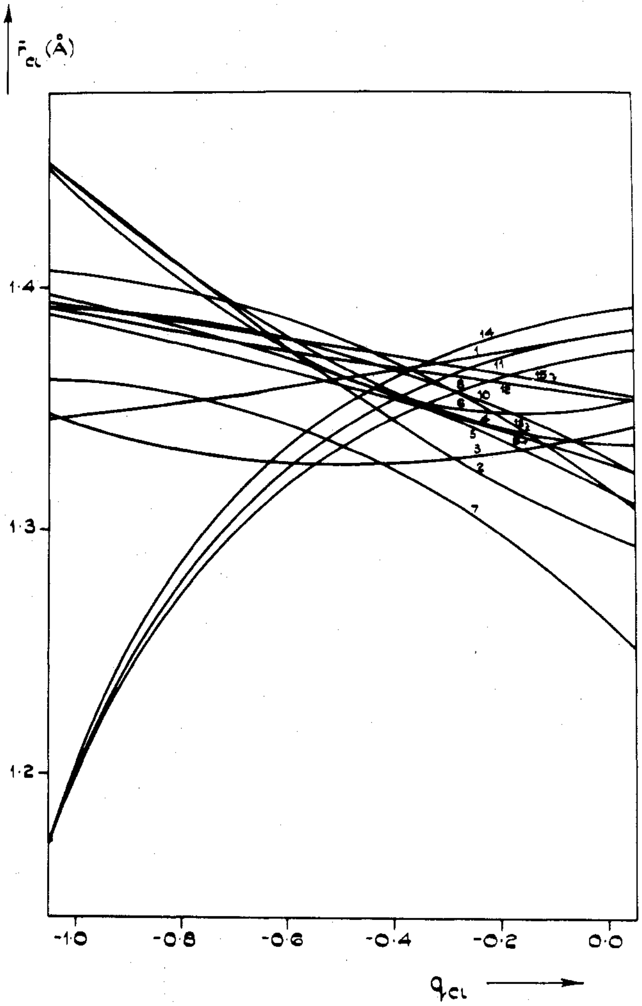

Figure 1. "Basic" radii (Å) of chlorine atoms having charge q_{Cl} in the model of the $AlCl_4^-$ ion plotted as a function of q_{Cl}. Key: 1, Li_a^+; 2, Li_b^+; 3, Li_c^+; 4, Na_a^+; 5, Na_b^+; 6, Na_c^+; 7, K_a^+; 8, K_b^+; 9, K_c^+; 10, Cs_a^+; 11, Cs_b^+; 12, Cs_c^+; 13, $NH_{4_a}^+$; 14, $NH_{4_b}^+$; 15, $NH_{4_c}^+$.

The structure of the cesium salt $CsAlCl_4$ has previously been determined by Gearhart,[11] and the more recent and more accurate structure used here was determined by using counter reflections in these laboratories.[9] NH_4AlCl_4,[12] determined to be isomorphous with the cesium salt and confirmed from X-ray, NMR, and molecular spectroscopy (Raman and infrared) studies to have a freely rotating NH_4^+ ion at room temperature, has the structural features given in Table I.

Previous Literature Calculations

Gearhart[11] and Gearhart, Beck, and Wood[13] have calculated, on the basis of the structures of $NaAlCl_4$[8] and $CsAlCl_4$,[11] the enthalpy of formation of the gaseous $AlCl_4^-$ ion, $\Delta H_f°(AlCl_4^-(g))$, and the halide ion affinity of $AlCl_3$, on the basis of Wood's modifications[14–16] of the Ladd and Lee equation.[17] Their results are summarized in Table II. Jenkins[18] repeated the Gearhart et al.[11,13] calculations retaining the lattice energy as a function of the charge q_{Cl} on the terminal atoms of the $AlCl_4^-$ ion, obtaining the results of Table II.

Theoretical Section

Jenkins and Pratt have recently described what they regard as an improved method for the calculation of the lattice energies of complex salts (in that the method incorporates a minimization procedure within the Huggins and Mayer[19] framework). An account of the theory for cubic salts is given in ref 20 and for noncubic salts in ref 21.

Briefly, the method involves minimization of eq 1 with

$$U_{pot} = U_{elec} - U_R + U_{dd} + U_{qd} \qquad (1)$$

respect to the cell lengths *a*, *b*, and *c*. U_{elec} is the electrostatic energy, and it and its derivatives are calculated as a function of the charge on the chlorine atom of the $AlCl_4^-$ ion, q_{Cl}, by using a recently developed program.[22] U_R, the repulsion energy, is calculated by using the extended Huggins and Mayer[19] approach, in a manner almost identical with that for the ClO_4^- ion, as described in ref 21. Dispersion energies U_{dd} (dipole–dipole) and U_{qd} (dipole–quadrupole) and their derivatives are calculated by extensive summations as outlined in previous work. This approach yields three derivatives of U_{pot} with respect to cell length, each of which gives a relationship between an unknown "basic" radius and the unknown charge on the Cl atoms. We can take the basic radius of the cation from previous work, so assigning $\bar{r}_{Cl}$, the basic radius of the chlorine atom, as a function of q_{Cl}, when a model of four partially charged chlorine atoms is taken to represent the $AlCl_4^-$ ion, in considering the repulsion energy. On the graphs (Figure 2) of lattice energy variation with q_{Cl} we give the curves derived from the "spherical" model of the $AlCl_4$- ion. This model clearly is not a good one for an ion with T_d symmetry, and this is borne out by the poor intersection points obtained (especially Na^+ and K^+). The clear superiority of the four chlorine atom model is brought out in Figure 2. Figure 1 shows the combined radii plots for this model of the $AlCl_4^-$ ion for the three derivatives of the five salts $LiAlCl_4$, $NaAlCl_4$, $KAlCl_4$, $CsAlCl_4$, and NH_4AlCl_4. In the key to Figure 1, Li_c^+ denotes the curves generated by the derivative with respect to *c* for $LiAlCl_4$.

Figure 2 shows the determination of the lattice potential energies, U_{pot} ($MAlCl_4$) (*k*J mol^{-1}), from their plots against

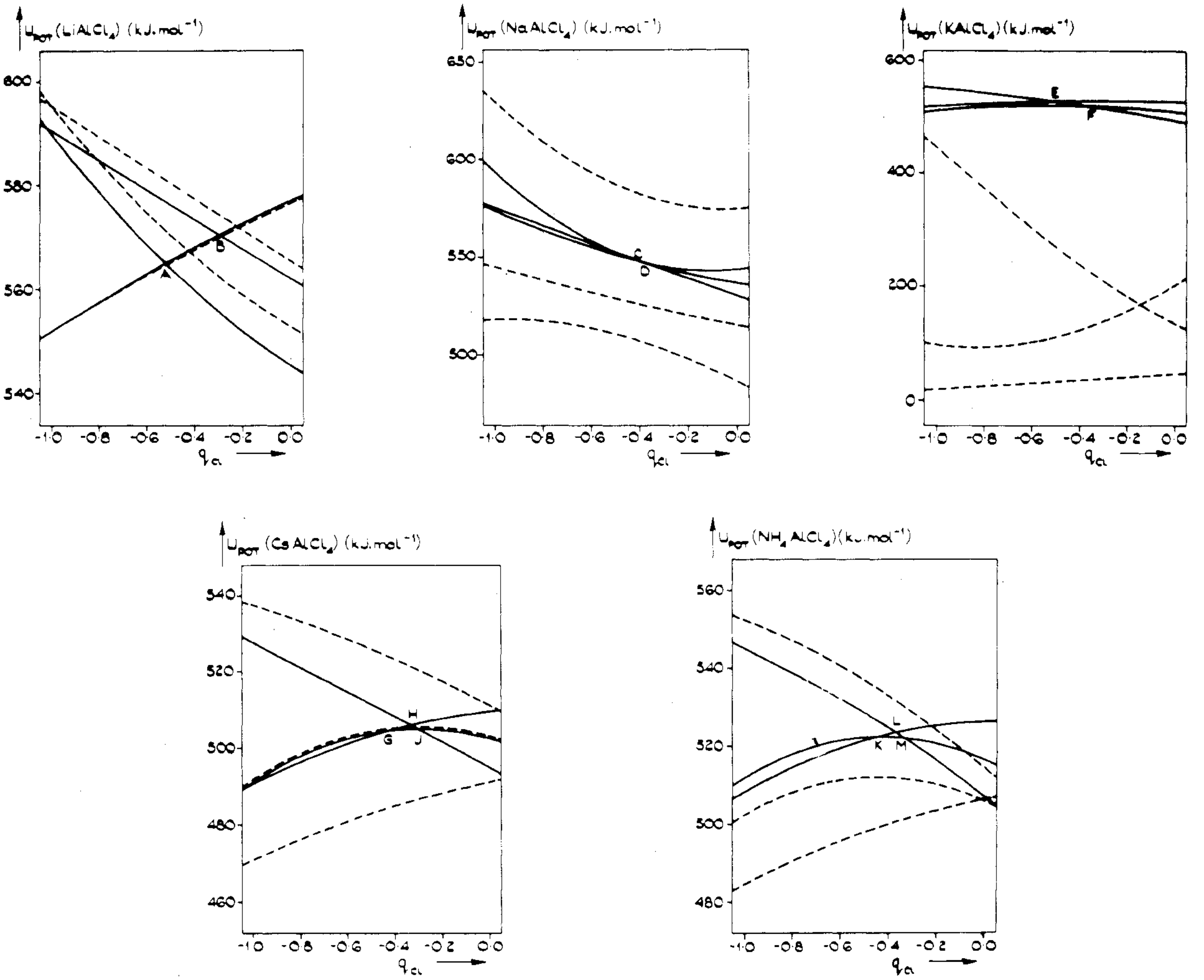

Figure 2. Lattice energies of tetrachloroaluminate salts as a function of q_{Cl} (hashed lines correspond to the spherical $AlCl_4^-$ ion model).

Table III. Thermodynamic Data for Tetrachloroaluminate Salts (kJ mol^{-1})

M^+	$\Delta H_f°(M^+(g))$	$\Delta H_f°(MAlCl_4(c))$
Li^+	687.2	-1126^e
Na^+	609.8	$-1142,^{b,c}$ -1140^a $-1144,^e$ -1148^f
K^+	514.2	$-1197,^{b,c}$ -1194^g -1192^f
Cs^+	452.3	-1222^a
NH_4^+	630.2^d	$-1076,^c$ -1089^h

[a] Reference 13. [b] Reference 24. [c] Reference 25. [d] Reference 28. [e] Reference 29. [f] Reference 30. [g] Reference 31. [h] Reference 32.

q_{Cl}. If the lattice energies determined above, as functions of charge, are combined with the thermodynamic data in Table III by using the Born–Fajans–Haber[23] cycle

$$\begin{tikzcd}
MAlCl_4(c) \arrow[r, "U_{pot}(MAlCl_4) + nRT"] & M^+(g) + AlCl_4^-(g) \\
M(c) + Al(c) + 2Cl_2(g) \arrow[u, "\Delta H_f°(MAlCl_4(c))"] \arrow[ur, "\Delta H_f°(M^+(g)) + \Delta H_f°(AlCl_4^-(g))"'] &
\end{tikzcd}$$

we can estimate values for $\Delta H_f°(AlCl_4^-(g))$ by using the appropriate lattice energies in eq 1

$$\Delta H_f°(AlCl_4^-(g)) = U_{pot}(MAlCl_4) + nRT - \Delta H_f°(M^+(g)) + \Delta H_f°(MAlCl_4(c)) \quad (2)$$

where n is $^1/_2$ for M = Li, Na, K, and Cs and n = 2 for NH_4.

Table IV. Calculated Results[a]

salt	U_{pot}(MAlCl$_4$),[c] kJ mol^{-1}	q_{Cl} intersecn[c]	ref pt[b]	$\Delta H_f°$(AlCl$_4^-$(g)), kJ mol^{-1}
$LiAlCl_4$	564 } 567	−0.51 } −0.40	A	−1245
	570	−0.29	B	
$NaAlCl_4$	547 } 546	−0.40 } −0.37	C	−1203
	545	−0.35	D	
$KAlCl_4$	523 } 519	−0.49 } −0.42	E	−1187
	514	−0.35	F	
$CsAlCl_4$	505 } 505	−0.40 } −0.34	G	−1168
	506	−0.33	H	
	505	−0.30	J	
NH_4AlCl_4	522 } 522	−0.44 } −0.38	K	−1193
	523	−0.37	L	
	522	−0.34	M	

[a] NB: only chemically realistic intercepts are included. [b] See Figure 2. [c] Average values are given on the right-hand side of the braces.

The appropriate plot of $\Delta H_f°(AlCl_4^-(g))$ vs. q_{Cl} is given in Figure 3.

Results

Table IV gives a compilation of the assigned lattice energies, charges (q_{Cl}), and $\Delta H_f°(AlCl_4^-(g))$ values derived from Figures 2 and 3. From Figure 3 it is seen that the curves for $LiAlCl_4$ (1, 2, and 3) lie well below those of the other salts; accordingly, we exclude these curves for the purpose of assigning $\Delta H_f°(AlCl_4^-(g))$ = −1188 ± 15 kJ mol^{-1} at a charge distribution corresponding to q_{Cl} = −0.38 ± 0.07.

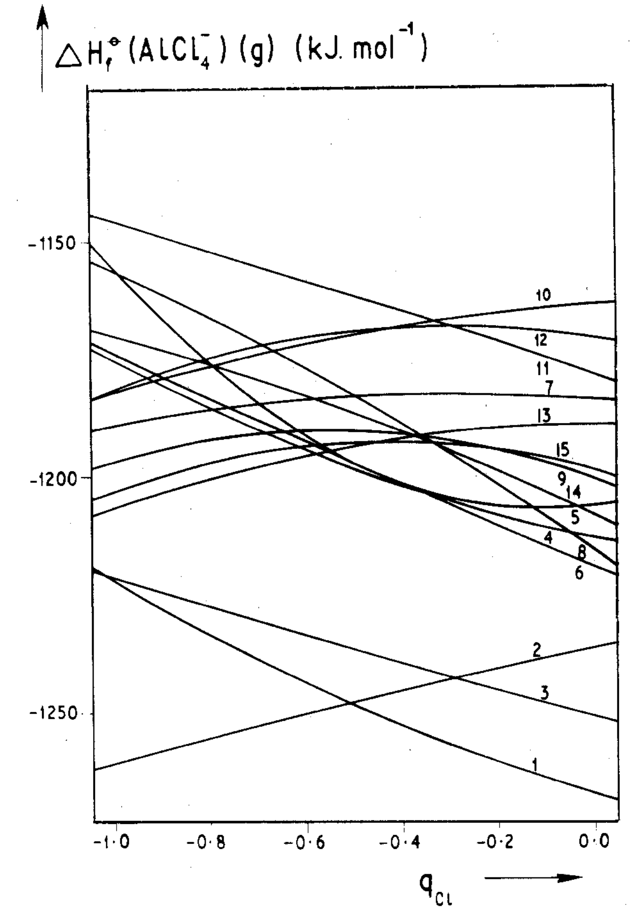

Figure 3. Plot of $\Delta H_f^\circ(AlCl_4^-(g))$ vs. q_{Cl} for the tetrachloroaluminates. Key: 1, Li_a^+; 2, Li_b^+; 3, Li_c^+; 4, Na_a^+; 5, Na_b^+; 6, Na_c^+; 7, K_a^+; 8, K_b^+; 9, K_c^+; 10, Cs_a^+; 11, Cs_b^+; 12, Cs_c^+; 13, $NH_{4_a}^+$; 14, $NH_{4_b}^+$; 15, $NH_{4_c}^+$.

With $\Delta H_f^\circ(Cl^-(g)) = -246$ kJ mol^{-1},[26] $\Delta H_f^\circ(AlCl_3(c)) = -706$ kJ mol^{-1},[24] $\Delta H_f^\circ(AlCl_3(l)) = -675$ kJ mol^{-1},[24] and $\Delta H_f^\circ(AlCl_3(g)) = -585$ kJ mol^{-1},[24] the chloride ion affinities corresponding to the processes

$$Cl^-(g) + AlCl_3(ss) \xrightarrow{\overline{\Delta H}_{Cl(ss)}} AlCl_4^-(g)$$

are $\overline{\Delta H}_{Cl(c)} = -236$ kJ mol^{-1}, $\overline{\Delta H}_{Cl(l)} = -267$ kJ mol^{-1}, and $\overline{\Delta H}_{Cl(g)} = -257$ kJ mol^{-1}.

Discussion

The comparison of $\Delta H_f^\circ(AlCl_4^-(g))$ and $\overline{\Delta H}_{Cl(g)}$ values from this and earlier studies is very satisfactory; so too are the lattice energies of the $NaAlCl_4$ and $CsAlCl_4$ previously computed. The improved crystal structure data and the internal consistency of the calculation, as shown by the curves generated from the various derivatives, enable us to place more confidence in the lattice energy values than previously. The enthalpy of formation data for the complex salts are independently determined for three of the salts (sodium, potassium, and ammonium). There are, of course, inherent difficulties in measuring such quantities by virtue of the hygroscopic nature of the salts, and it is to such factors that we attribute the disappointing spread of the curves in Figure 3.

Table V. Radii for $AlCl_4^-$ Ion

salt	thermochemical radii, Å *a*	*b*	*c*	*d*	"basic" radius, Å
$LiAlCl_4$				3.46	2.3
$NaAlCl_4$	3.94	3.17	3.14	3.10	2.5
$KAlCl_4$				2.97	2.4
$CsAlCl_4$	3.95	2.95	3.14	2.94	2.5
NH_4AlCl_4				2.89	2.5

[a] Radii derived by taking M–X bond distance $r_{M^+} + r_{Cl^-}$.[14] [b] Radii necessary to give Gearhart, Beck, and Wood's lattice energies.[14] [c] Radii taken from Beck[28] and estimated from heat of solution.[14] [d] Thermochemical radii calculated from this study.

Table V gives the thermochemical radii given by Gearhart, Beck, and Wood[13] and the "basic" radius for the $AlCl_4^-$ ion as estimated in this study. One is bound to comment on the consistency of the basic radius of the $AlCl_4^-$ ion as compared with the thermochemical radius.

This paper is the first we have produced to show the wealth of information that our new approach derives from crystal structure data for noncubic systems as compared to the other older approach represented by ref 18.

Acknowledgment. H.D.B.J. thanks G. Mairesse and his wife for their kind hospitality during a visit to the Université de Lille and Professor Heubel and Professor Thomas of the School of Chemistry for their provision of funds in order to enable us to collaborate on this paper. K.F.P. acknowledges the receipt of an SRC Research Studentship.

Registry No. $LiAlCl_4$, 14024-11-4; $NaAlCl_4$, 7784-16-9; $KAlCl_4$, 13821-13-1; $CsAlCl_4$, 17992-03-9; NH_4AlCl_4, 7784-14-7.

References and Notes

(1) C. R. Boston, *Adv. Molten Salt Chem.*, **1**, 129 (1971).
(2) H. L. Jones and R. A. Osteryoung, *Adv. Molten Salt Chem.*, **3**, 121 (1975).
(3) GTE Laboratoires Inc., *Chem. Abstr.*, **84**, Patents P20259d, P92669k, P92676k (1976).
(4) M. Taube, M. Mielcarski, A. Kowalen, and S. Porturaj-Gutniak, *Nukleonika*, **10**, 639 (1965).
(5) B. Folkesson and R. Larsson, *Chem. Scr.*, **10**, 105 (1976).
(6) W. Scheinert and A. Weiss, *Z. Naturforsch., A*, **31**, 1354 (1976).
(7) G. Mairesse, P. Barbier, and J. P. Wignacourt, University of Lille, to be submitted for publication.
(8) N. C. Baenzinger, *Acta Crystallogr.*, **4**, 216 (1951).
(9) G. Mairesse, P. Barbier, and J. P. Wignacourt, University of Lille, to be submitted for publication.
(10) G. Mairesse, P. Barbier, and J. P. Wignacourt, *Acta Crystallogr., Sect. B*, **34**, 1328 (1978).
(11) R. C. Gearhart Jr., Doctoral Dissertation, University of Delaware, Newark, DE, June, 1972.
(12) G. Mairesse, P. Barbier, J. P. Wignacourt, A. Rubbens, and F. Wallart, *Can. J. Chem.*, **56**, 764 (1978).
(13) R. C. Gearhart Jr., J. D. Beck, and R. H. Wood, *Inorg. Chem.*, **14**, 2314 (1975).
(14) R. H. Wood, *J. Chem. Phys.*, **32**, 1690 (1960).
(15) R. H. Wood, *J. Chem. Phys.*, **37**, 598 (1962).
(16) R. H. Wood and L. A. D'Orazio, *J. Phys. Chem.*, **69**, 2558 (1965).
(17) M. F. C. Ladd and W. H. Lee, *J. Inorg. Nucl. Chem.*, **11**, 264 (1959).
(18) H. D. B. Jenkins, *Inorg. Chem.*, **15**, 241 (1976).
(19) M. L. Huggins and J. E. Mayer, *J. Chem. Phys.*, **1**, 643 (1933).
(20) H. D. B. Jenkins and K. F. Pratt, *Proc. R. Soc. London, Ser. A*, **356**, 115 (1977).
(21) H. D. B. Jenkins and K. F. Pratt, *J. Chem. Soc., Faraday Trans. 2*, **74**, 968 (1978).
(22) H. D. B. Jenkins and K. F. Pratt, *Comput. Phys. Commun.*, **5**, 341 (1978).
(23) D. F. C. Morris and E. J. Short, *Nature (London)*, **224**, 950 (1969).
(24) D. H. Stull and H. H. Prophet, Eds., *Nat. Stand. Ref. Data Ser., Nat. Bur. Stand.*, **No. 37** (1971).
(25) E. Baud, *Ann. Chim. Phys.*, **1**, 8 (1904).
(26) J. B. Pedley, "Computer Analysis of Thermochemical Data", University of Sussex, Brighton, UK, 1974.
(27) J. D. Beck, Doctoral Thesis, University of Delaware, Newark, DE, 1969.
(28) H. D. B. Jenkins and D. F. C. Morris, *Mol. Phys.*, **32**, 231 (1976).
(29) V. A. Plotnikov and S. I. Yakubson, *Zh. Fiz. Khim.*, **12**, 111 (1938).
(30) R. A. Sandler, E. I. Yaskelyainen, and I. V. Vasilkova, *Russ. J. Phys. Chem. (Engl. Transl.)*, **46**, 1687 (1972).
(31) K. N. Semenenko, V. N. Sirov, and N. S. Kedrova, *Russ. J. Inorg. Chem. (Engl. Transl.)*, **14**, 481 (1969).
(32) W. C. Laughlin, *Diss. Abstr. Int. B.*, **35**, 3858 (1975).