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A scattering curve for a spherically symmetrical ammonium ion.

By M. F. Davis,* *H. H. Wills Physics Laboratory, University of Bristol, Bristol, England* and A. Whitaker, *Department of Crystallography, Birkbeck College, University of London, England*

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Webb (1965) published figures for the scattering curve for a spherically symmetrical ammonium ion, *i.e.* where the ion is in a state of random rotation. These figures indicated that the scattering factor for ammonium was less than that for nitrogen if $\sin\theta/\lambda$ is greater than 0·10 and this was thought to be unlikely. In addition the figures he obtained appear to be from the electron density distribution curve calculated by Banyard & March (1961). No detailed figures are given of this curve and, as the one printed is too small to obtain accurate measurements from, it was decided to recalculate the electron density distribution curve from the original self-consistent wave functions of Bernal & Massey (1954) before recalculating the scattering factor. The procedure was also repeated with the analytical wave functions of Bernal (1953).

The scattering factor was obtained from the radial distribution curve by use of the formula

$$f=\int_0^\infty 4\pi r^2\varrho(r)\frac{\sin\mu r}{\mu r}\,\mathrm{d}r \qquad \text{(James, 1948)}$$

where $\mu=4\pi\sin\theta/\lambda$ and $\varrho(r)$ is the electron density at a distance r. This integral was evaluated by repeated use of the Newton–Cotes seven point formula.

The figures obtained for the ammonium scattering factors are given in Table 1 together with those obtained by Webb (1965) and those for nitrogen (Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal, 1955; *International Tables for X-ray Crystallography*, 1962). The curves are compared directly in Fig. 1 out to values of $\sin\theta/\lambda$ of 0·75. Comparison of the present scattering curves with that for nitrogen shows that the scattering factors differ widely for small values of $\sin\theta/\lambda$ but hardly at all for the larger

Table 1. *Scattering factors for ammonium and nitrogen*

$\sin\theta/\lambda$	Bernal (1953) These results	Bernal & Massey (1954) These results	Bernal & Massey (1954) Webb (1965)	Nitrogen *International Tables* (1962)
0	9·998	10·001	10	7·000
0·05	9·613	9·531	7·9	6·781
0·1	8·577	8·309	5·6	6·203
0·15	7·172	6·757	3·6	5·420
0·2	5·713	5·275	2·5	4·600
0·25	4·426	4·079	1·8	3·856
0·3	3·415	3·215	1·3	3·241
0·35	2·689	2·637	—	2·760
0·4	2·202	2·265	1·0	2·397
0·45	1·893	2·029	—	—
0·5	1·706	1·875	0·9	1·944
0·55	1·595	1·768	—	—
0·6	1·530	1·687	0·7	1·698
0·65	1·488	1·620		—
0·7	1·458	1·561		1·550
0·75	1·431	1·507		—
0·8	1·404	1·457		1·444
0·85	1·374	1·408		—
0·9	1·342	1·361		1·350
0·95	1·306	1·315		—
1·00	1·267	1·269		1·263
1·05	1·226	1·224		—
1·1	1·184	1·179		1·175
1·15	1·141	1·133		—
1·2	1·097	1·089		1·083
1·25	1·053	1·044		—
1·3	1·010	1·001		1·005
1·35	0·967	0·958		
1·4	0·925	0·917		
1·45	0·884	0·876		
1·5	0·844	0·837		
1·55	0·805	0·799		
1·6	0·768	0·763		
1·65	0·732	0·728		
1·7	0·697	0·694		
1·75	0·664	0·661		
1·8	0·632	0·630		
1·85	0·602	0·600		
1·9	0·573	0·572		

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* Present address; Ministry of Aviation, S.R.D.E., Christchurch, Hants, England.

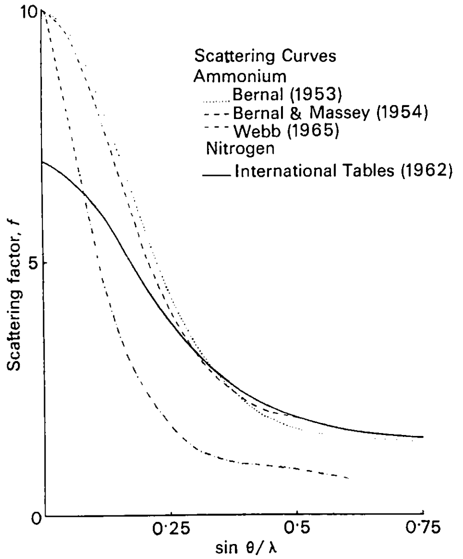

Fig. 1. Scattering curves for ammonium and nitrogen.

values of sin θ/λ. This would be expected; electrons further away from the central nucleus seem to have little effect on the scattering factor at high values of sin θ/λ. This may be easily seen by reference to the atomic scattering factors in *International Tables* (1962), where atomic scattering factors for neutral and ionized atoms differ little at larger values of sin θ/λ. The errors in the present scattering factors are unknown but the calculation for sin $\theta/\lambda=0$ gives 9·998 and 10·001 for the values from the wave functions of Bernal (1953) and Bernal & Massey (1954) respectively compared with the correct value of 10·000, so the errors are probably in the third decimal place. This, of course, assumes that the N–H distances of 0·97 Å for which the wavefunctions were calculated is correct. The effect of a different N–H distance on the wavefunctions and hence on the scattering factors is not known.

Webb's (1965) figures were thought to be due to taking the abscissae of Banyard & March's (1961) curve to be in Å whereas they are in atomic units. However, a check calculation based on this gave moderate agreement at low values of sin θ/λ but very poor agreement at larger values of sin θ/λ. So this assumption cannot be entirely correct.

The scattering curves for ammonium found in the present investigation are very similar although there are differences of up to 10% in individual values. These differences are hardly likely to be important for most work but may cause errors in high accuracy work.

According to Banyard & March (1961) a comparison of the electron distribution curve for ammonium with that for methane suggests that the figures of Bernal & Massey (1954) are the more accurate and for this reason the scattering curve for ammonium taken from their figures is probably the best.

The scattering factor for ammonium has been determined experimentally from intensity measurements on ammonium chloride (Wyckoff & Armstrong, 1930). However, subsequently it has been shown, from infrared spectroscopy (Wagner & Hornig, 1950), neutron diffraction (Levy & Peterson, 1952) and electron diffraction (Vainshtein, 1964) that in the room temperature form of ammonium chloride, phase II, the ammonium is not rotating. It is at random in two orientations. Thus these calculated values cannot be compared with the experimental.

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Chain structure of the orthorhombic modification of dicyclopentadienyl-lead containing bridging π-cyclopentadienyl rings.

By C. Panattoni, G. Bombieri and U. Croatto, *Centri Nazionali di Strutturistica Roentgenografica e Chimica delle Radiazioni e dei Radioelementi, Sezioni di Padova, Padova, Italy*

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Introduction

The structure of $Pb(C_5H_5)_2$ has aroused considerable interest. On the basis of infrared, nuclear magnetic resonance, ultraviolet spectra and dipole moment measurements Dave, Evans & Wilkinson (1959) concluded that the evidence supported the hypothesis of an angular sandwich structure. Previously, Fischer & Grubert (1956) suggested an angular 'σ-bonded structure' in accordance with their dipole moment measurements.