A study of the atomic scattering factor for aluminium.* By G. S. PARRY,† *The University of Pittsburgh, Pittsburgh* 13, *Pa., U.S.A.*

During a recent refinement of the structure of aluminium nitride (Jeffrey & Parry, 1955) the atomic scattering factor for aluminium derived by Viervoll & Ögrim (1949), using the James & Brindley (1931) interpolation method, was employed. It has been shown by Cochran (1953) that atomic scattering factors obtained this way may be in error, and it was thought advisable to examine the Viervoll & Ögrim values. The method suggested by Cochran was employed, and it showed that the tabulated values gave an electron count of only 12·18 e. within a radius of 3·14 Å. Even when additional values were interpolated so that the count was made within a radius of 6·28 Å, the result was only 12·48 e. Corresponding calculations for the Pauling & Sherman (1932) scattering factors gave 13·0 e. within 2·5 Å, using the tabulated values, and when interpolated values were also used there was no change either in the electron count or in the shape of the transform in real space. Since Pauling & Sherman factors are derived from normalized wavefunctions, this was taken to indicate that neither the method nor the graphical interpolation processes were responsible for the low count with the Viervoll & Ögrim values, and it was concluded that these are derived from an electron-density distribution in which the 3*p* electrons are too diffuse.

As the James & Brindley interpolation method exaggerates the spread of the 3*p* electrons, and as any correction to the interpolation process would be somewhat arbitrary, an attempt was made instead to derive an extrapolated atomic scattering factor by consideration of some early calculations of James, Brindley & Wood (1929) for Al³⁺, Al²⁺ and Al⁺ based on Hartree electron-density distributions. These functions are tabulated at intervals sin θ/λ = 0·094, but James & Brindley give

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Table 1. *Calculated data of James, Brindley & Wood, together with extrapolated values for neutral aluminium*

sin θ/λ	Al³⁺	Al²⁺	Al⁺	Al f(a)	Al f(b)	Al (mean)
0·0	10·00	11·00	12·00	13·00	13·00	13·00
0·038	9·93	10·87	11·76	12·65	12·60	12·63
0·056	9·88	10·74	11·51	12·28	12·19	12·24
0·075	9·83	10·60	11·27	11·94	11·84	11·89
0·094	9·75	10·41	10·96	11·51	11·39	11·45
0·188	9·02	9·17	9·22	9·27	9·22	9·24
0·282	8·01	7·97	7·93	7·89	7·89	7·89
0·376	6·93	6·92	6·91	6·90	6·90	6·90
0·470	5·82	5·83	5·84	5·85	5·85	5·85
0·564	4·80	4·83	4·85	4·87	4·86	4·87
0·658	3·89	4·01	4·03	4·05	4·04	4·05
0·752	3·33	3·35	3·37	3·39	3·39	3·39
0·940	2·48	2·49	2·50	2·51	2·51	2·51
1·128	1·93	1·93	1·94	1·95	1·94	1·94
1·316	1·61	1·61	1·61	1·61	1·61	1·61
1·504	1·50	1·50	1·50	1·50	1·50	1·50
1·880	1·28	1·28	1·28	1·28	1·28	1·28

electronic scattering factor curves based on the same data at intervals sin θ/λ = 0·1. In deriving extrapolated values both sets of data were considered. The major difficulty in the extrapolation method is that there is a contraction of the 3*p* shell on going from Al²⁺ to Al⁺ and there will probably be a further contraction on passing to Al itself. It is unlikely that this will exceed the contraction that has already taken place, so that, although it is not possible to extrapolate to a definite value for the scattering factor of Al, it is possible to state limits within which the value of the function should lie. These two limits, *f*(a) and *f*(b), are given in the tables that follow, together with a mean value which is taken to represent the extrapolated value of the function.

Table 1 gives the James, Brindley & Wood data for the scattering factors of Al³⁺, Al²⁺ and Al⁺, together with extrapolated values for Al based on this data. Table 2 gives values of the extrapolated factor based on the electronic scattering factor data of James & Brindley.

Table 2. *The atomic scattering factor for aluminium*

	From individual J.B. electronic f curves			From J.B.W. data, Table 1	From previous determinations		
sin θ/λ	f(a)	f(b)	Mean	f(J.B.W.)	f(J.B.)	f(V.Ö.)	f(P.S.)
0·0	13·00	13·00	13·00	13·00	13·0	13·00	13·00
0·1	11·40	11·26	11·33	11·34	11·0	10·87	11·50
0·2	9·10	8·99	9·05	9·03	8·95	9·03	9·32
0·3	7·61	7·63	7·62	7·66	7·75	7·64	8·11
0·4	6·60	6·61	6·60	6·62	6·6	6·59	7·05
0·5	5·51	5·51	5·51	5·52	5·5	5·45	5·89
0·6	4·53	4·53	4·53	4·53	4·5	4·49	4·72
0·7	3·72	3·72	3·72	3·73	3·7	3·74	3·74
0·8	3·10	3·10	3·10	3·13	3·1	3·10	3·04

J.B.: James & Brindley, 1931.
J.B.W.: James, Brindley & Wood, 1929.
V.Ö.: Viervoll & Ögrim, 1949.
P.S.: Pauling & Sherman, 1932.

For comparison, graphically estimated values of the extrapolated function from Table 1 and of the Viervoll & Ögrim values are given together with the James & Brindley, and Pauling & Sherman values.

The principal difference between the new function and the old occurs at $\sin\theta/\lambda < 0.25$. Within this range the new values, even allowing for the ambiguity in extrapolation, are larger than the earlier results, and the mean values give an electron count of 12·78 e. within a radius of 2·66 Å and 12·91 e. within a radius of 4·1 Å. The Pauling & Sherman values for $\sin\theta/\lambda < 0.7$ are greater than the present results and indicate an even more compact electron-density distribution. Although the results of the present calculation are subject to error as no allowance for exchange was made in the original Hartree calculations, it is considered that these represent the best

scattering function for aluminium so far reported and that they will be useful until more accurate calculations of the Hartree distributions are made.

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Precession camera settings.

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This subject has been discussed recently (King, 1955) without knowledge of my earlier work. The use of King's Fig. 1 to get s values is far more time-consuming than reading from my simple charts (Fisher, 1952, p. 1053), which are similar to Buerger's (1944) Fig. 6, except that they are limited to s values between 25 and 45 mm., the practicable range with standard equipment, and include additional $\bar{\mu}$ values. King's Fig. 1 is misleading in that it extends to values that are practically unobtainable. If, as I suggested, my four charts are put on a single graph (using different colors of ink for different $\bar{\mu}$ values) one can see at a glance the best combination to use for a given situation. Considering the lines on my charts as the central lines of narrow or wider bands, one can decide readily whether a narrow-opening annulus screen is needed in order to isolate a given level, a situation not uncommon when dealing with a crystal having a large unit cell.

Fig. 2 of King is an alignment chart for determining ε, the angular error in orientation. This problem, too, was handled by the writer in much simpler fashion by the use of a graph (Fisher, 1953, p. 400) based on measuring the distance (called $\delta - r$) from O', the center of precession for the film, to c, the center of the circle of precession. Moreover, the resolution of ε into corrected H arc and dial readings was treated, as were equation errors (Fisher, 1952, p. 1047). It should be noted that a rather similar graph appears as Fig. 4 of the *Manual for the Use of the Buerger Precession Camera* by the Charles Supper Company.

If the crystal furnishes reflections which show up reasonably strongly along the central horizontal line of the film (the 'dial axis' of the film), which means that an important reciprocal-lattice line is set parallel to the dial axis, which is very commonly the case, there is possible a very quick way of getting the goniometer head arcs adjusted exactly correctly. This technique is used only after the arcs are adjusted approximately correctly, and

is a modification of Buerger's (1944, p. 26) method. There is no need to go to the trouble of putting cassette dots on the film, as advocated by Evans, Tilden & Adams (1949) and by Barnes, Przybylska & Shore (1951); thus a small scrap piece of film may be used.

This method involves taking four 5–20 min. exposures on the same film; to my knowledge this multiple-exposure method was first used for this purpose by Prof. Fritz Laves; after each exposure the film cassette is raised 2 or 3 mm. The first exposure might be made with the plane of the *large* arc 'horizontal' (parallel to the direct beam, or normal to the film cassette). The second would be with the dial rotated 180°; the third and fourth are with the dial at 90° and 270°. Unless the arcs are in exactly correct adjustment, the ends of the two upper Laue streaks (parallel to the dial axis) will not line up; the ends of the top streak will be a certain distance L to the right (or left) of those of the other streak; a similar situation will hold for the two lower streaks, yielding a distance S (for the case where the plane of the *small* arc is parallel the direct beam). If L and S are measured in millimetres, then $60L/4.26$ equals the number of minutes the large arc must be adjusted, and $60S/4.26$ gives the correction for the small arc, providing $\bar{\mu}$ equals 10°. If $\bar{\mu}$ equals 3°, the denominator is 4·20; both these assume $F = 60$ mm. (see Fisher, 1952, p. 1045; D-values for $\varepsilon = 1°$).

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