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NOTE

A COMPACT REPRESENTATION FOR ATOMIC SCATTERING FACTORS

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THE ADVENT of small, relatively inexpensive desk top computers now allows the in-lab performance of many calculations which formerly required the use of remote facilities. The comparatively few registers available in these machines, however, necessitates efficient memory use. This note presents an analytical representation for atomic scattering factors which is accurate yet modest in its storage requirements.

Of the representations presently in the literature, the two Gaussian plus constant equation

$$f(\mu) = A\,e^{-a\mu^2} + B\,e^{-b\mu^2} + C$$

proposed by Vand *et al.* (1957) appears to be the most efficient in terms of accuracy versus number of stored constants per scattering factor. Forsyth and Wells (1959) and Moore (1964) have published tables of optimum constants for many atomic types. The better than 0·5 per cent accuracy generally obtained over the CuKα range leaves little to be desired in view of both experimental limitations in intensity measurement and the theoretical approximations made in calculating form factors.

Several disadvantages of the above Gaussian form are evident. First, two exponential functions must be evaluated for each scattering factor. Whilst most desk top computers have hard-wired exponential subroutines, execution times can none the less be considerable if many factors are to be calculated. Second and more serious, the representation is nonlinear. If average scattering factors are required, then either each contributing factor must be calculated separately and then averaged, or a prior least sum of squares fit must be made on the averaged numerical data for the form factors. Finally, the least sum of squares procedure involved in determining the constants is nonlinear and, hence, by necessity somewhat complex.

A representation of comparable accuracy which avoids these drawbacks is

$$f(\mu) = \sum_{n=0}^{4} a_n X^n, \qquad (1)$$

where $X = 1/(1 + 2\mu^2)$

and $\mu = 1/d = 2 \sin \theta/\lambda.$

While storage requirements per atom type are no greater than those for the Gaussian equation, the advantages of the polynomial form are obtained.

Evaluation of polynomials is generally quite rapid compared to other functional forms because only additions and multiplications are performed. For the most efficient programming, equation (1) may be written $f(\mu) = a_0 + X\{a_1 + X[a_2 + X(a_3 + Xa_4)]\}$. The time required for the calculation of $X(\mu)$ will usually be negligible since, most often, many scattering factors will be evaluated for each value of μ.

Examination of various simple expressions for $X(\mu)$ in equation (1) suggests that the Lorentzian form used here gives the greatest accuracy. The width factor 2 in the denominator is a compromise value which results in good curve fits for almost all atomic species.

Because $X(\mu)$ is independent of specific atomic types, the a_n coefficients for average scattering factors are obtained simply by averaging the appropriate coefficients of the atoms involved. Thus, in cases of isomorphous substitution or partial charge transfer, constants for all of the species which contribute need not be stored. An additional advantage of this coefficient linearity is that widely available linear least sum of squares procedures can be used for fitting the scattering factor data.

Table 1 presents coefficients for atomic types of use in layer silicate chemistry. The selection of ionic charges reflects to some extent the author's preference for assuming 50 per cent ionic bonds in silicate frameworks. Numerical data for the scattering factors were taken at μ increments of 0·2 over the range 0 to 1·4 Å^{-1} from Table 3. 3.1 A of Lonsdale (1968). These values were all calculated from self-consistent or variational wave functions. In cases where the desired state of ionization was not given, linear interpolation between the two nearest ionization states was employed.

The coefficients in Table 1 are those which minimize the sum of the squares of the percentage deviation at each data point. No weighting scheme was applied. This sort of optimization was accomplished by dividing each side of equation (1) by $f(\mu)$ before applying the linear least sum of squares technique. The resultant root mean square deviation is noted beneath each set of coefficients. Only in the rather unimportant case of neutral Li does this figure exceed 0·5 per cent. For comparison the r.m.s. deviation for the Gaussian representation optimized in the same sense is also noted in parentheses.

The last two species given in Table 1 are H_2O and NH_4^+. The numerical data for these molecules were calculated assuming 50 per cent ionic bonds and a spherical distribution of H atoms about the central O and N atoms, respectively. Though equation (1) was not derived with the idea of representing the form factors for randomly oriented simple molecules, the root mean square errors for these two cases are seen to be quite small.

Baroid Division, NL Industries,
P.O. Box 1675,
Houston, Texas 77001,
U.S.A.

A. C. WRIGHT

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Table 1. Coefficients for polynomial representation of atomic scattering factors over the Cu Kα range

$$f(\mu) = \sum_{n=0}^{4} a_n \left(\frac{1}{1 + 2\mu^2}\right)^n$$

where $\mu = 1/d$
$= 2 \sin \theta/\lambda$
$0 \leqslant \mu \leqslant 1{\cdot}4$

Format: Species
a_0
a_1
a_2
a_3
a_4
r.m.s. % dev.

H	Li	Li^{1+}	C	N	O
0·0019	0·4931	−0·1923	0·9155	1·2372	1·3641
−0·0321	−2·3194	5·0544	3·5601	0·8913	−0·6136
0·6853	22·2812	−5·1412	−7·4819	2·3177	13·0097
−0·0402	−38·4310	3·0646	12·3140	4·9228	−7·9226
0·3855	20·8983	−0·7857	−3·3153	−2·3755	2·1625
0·28 (0·72)	2·09 (0·19)	0·01 (0·02)	0·16 (0·43)	0·14 (0·26)	0·01 (0·13)
O^{-1}	F	$F^{\frac{1}{2}}$	Na^{+1}	Mg	Mg^{+1}
1·4415	1·1868	1·1551	0·3425	0·8864	0·5195
−1·3709	0·9556	1·5348	11·2534	8·2975	12·3332
15·7765	16·7966	13·9883	5·7734	28·5757	12·5493
−13·7247	−15·0431	−10·1826	−12·9302	−60·3172	−33·9868
6·8675	5·1089	3·0074	5·5675	34·5193	19·5710
0·11 (0·43)	0·06 (0·11)	0·04 (0·10)	0·10 (0·01)	0·32 (0·26)	0·15 (0·24)
Mg^{2+}	Al	Al^{1+}	$Al^{1\frac{1}{2}+}$	Al^{3+}	Si
0·1323	0·3258	−0·5045	−0·5238	−0·3131	−0·0913
16·5772	18·4201	27·2299	27·5813	25·3885	28·9298
−4·2000	1·3058	−30·8128	−32·9244	−26·9193	−34·3872
−6·6534	−33·8581	14·0260	18·9622	15·5482	10·7302
4·1498	26·7635	2·0614	−1·5941	−3·7026	8·7947
0·10 (0·09)	0·31 (0·26)	0·07 (0·10)	0·06 (0·09)	0·02 (0·02)	0·16 (0·24)
Si^{2+}	S	Cl	Cl^{1-}	K^{1+}	Ca^{2+}
−0·3639	0·0411	1·0643	0·7918	4·0544	4·8314
31·7591	42·5904	38·6841	41·6939	15·0697	8·4222
−46·1761	−95·7124	−92·4487	−102·8544	−21·1472	4·3226
33·3949	105·0704	111·2719	123·6521	36·3321	5·4041
−6·6261	−36·0084	−41·6018	−45·3147	−16·3314	−4·9955
0·11 (0·16)	0·13 (0·05)	0·24 (0·08)	0·19 (0·05)	0·20 (0·12)	0·15 (0·06)
Fe	Fe^{1+}	$Fe^{1\frac{1}{2}+}$	Fe^{2+}	Fe^{3+}	Co^{2+}
5·0414	4·3654	4·3269	4·2882	4·1364	3·8015
8·7560	16·8417	17·0051	17·1713	18·3396	23·2907
56·1932	21·5976	22·1010	22·5941	21·3104	12·7656
−88·9328	−30·3643	−31·8237	−33·2686	−34·9806	−25·6621
44·9092	12·5703	12·9020	13·2267	14·2093	10·8158
0·13 (0·34)	0·05 (0·10)	0·06 (0·06)	0·08 (0·03)	0·09 (0·02)	0·07 (0·03)
Ni^{2+}	Cu^{2+}	Zn^{2+}	Ag^{1+}	H_2O	NH_4^{1+}
3·4259	3·0954	2·5852	12·1283	1·3016	1·1459
28·7853	34·3556	42·1051	37·2881	− 0·1171	1·1960
4·6344	−3·8047	−18·6430	−6·3957	12·8091	5·6484
−20·0090	−14·2827	−1·4526	5·8858	−13·1096	−10·7080
9·1742	7·6488	3·4142	−2·9179	9·1072	12·6924
0·07 (0·03)	0·08 (0·01)	0·05 (0·03)	0·04 (0·07)	0·07 (0·49)	0·19 (0·72)

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