Short Communications

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Analytic approximation for incoherent scattered X-ray intensities.

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It has been found that the incoherent scattered intensities of various atoms can be accurately approximated by a formula containing three individual parameters and the atomic scattering factor, the latter also being given by one of the known approximative formulae. The parameters and weighted deviations have been calculated for 44 atoms and ions, respectively. Accuracy is demonstrated in detail in the example of the oxygen atom.

Analytic functions previously suggested for approximating incoherent scattered X-ray intensities (Furukawa, Orton, Hamor & Williams, 1963; Rodriguez & Pings, 1965) are of a relatively low degree of accuracy. It was found by the author that the incoherent scattered intensities of various atoms and ions can with high accuracy be approximated

Table 1. *Parameters of the analytic fit for incoherent scattered X-ray intensities*

Atom or ion	Z	M	K	L	ε
He	2	0·00449	4·63354	10·2456	0·0005
Li	3	1·93412	6·43205	9·5329	0·0150
Be	4	1·32466	3·90931	6·4593	0·0293
B	5	0·81997	2·70598	5·8546	0·0229
C	6	0·61876	2·06499	5·7754	0·0267
N	7	0·39484	1·40239	13·5381	0·0286
O	8	0·37033	1·22426	25·4902	0·0189
F	9	0·32925	1·05786	148·8540	0·0400
Ne	10	0·41389	1·18677	24·3301	0·0378
Na	11	0·45524	1·22322	21·7068	0·0349
Mg	12	0·48043	1·20756	15·6220	0·0550
Al	13	0·49920	1·18551	13·6930	0·0418
Si	14	0·50850	1·14764	13·2148	0·0345
P	15	0·51360	1·10729	14·6350	0·0239
S	16	0·51502	1·06379	13·0632	0·0210
Cl	17	0·51320	1·01937	13·3857	0·0165
Ar	18	0·51617	0·99055	15·0641	0·0172
K	19	0·51198	0·94744	15·2652	0·0211
Ca	20	0·50934	0·91720	14·7943	0·0206
Sc	21	0·51921	0·91100	14·2067	0·0326
Ti	22	0·53688	0·91813	13·7543	0·0475
V	23	0·55880	0·93040	12·7813	0·0530
Cr	24	0·59093	0·95408	9·9189	0·0746
Mn	25	0·60736	0·94636	10·7472	0·0555
Fe	26	0·62157	0·94225	9·8927	0·0505
Co	27	0·63943	0·94163	9·1675	0·0468
Ni	28	0·65793	0·93866	8·4868	0·0440
Cu	29	0·69695	0·95915	7·4455	0·0494
Zn	30	0·69910	0·93084	7·3661	0·0444
Ga	31	0·69152	0·89103	7·3405	0·0523
Ge	32	0·67270	0·83800	7·6027	0·0807
As	33	0·64655	0·77760	8·3750	0·1153
Se	34	0·62745	0·72866	8·7680	0·1182
Br	35	0·61014	0·66010	9·4198	0·1582
Li^+	2	0·01972	3·21454	10·0657	0·0056
F^-	10	0·36389	1·22435	31·2425	0·0397
Na^+	10	0·46099	1·15092	15·9754	0·0240
Cl^-	18	0·49797	1·03861	15·2837	0·0077
K^+	18	0·53741	0·95939	13·3178	0·0215
Rb	37	0·55061	0·69379	4·4872	0·3870
I	53	0·64691	0·67347	5·0453	0·5832
I^-	54	0·61306	0·61164	6·2254	0·5067
Cs^+	54	0·64817	0·67375	4·7437	0·6920
Cs	55	0·60466	0·59228	5·8029	0·5528

by an empirical formula containing three individual parameters, and the (coherent) atomic scattering factor:

$$I_{\mathrm{inc}}(s)=\left[Z-\frac{f^2(s)}{Z}\right]\times[1-M(\exp\{-Ks\}-\exp\{-Ls\})] \quad (1)$$

where
Z is the number of electrons in the atom or ion,
$f(s)$ is the coherent atomic scattering factor,
$s=\sin\theta/\lambda$
M, K and L are the individual parameters.

Although the $f(s)$ values might be taken from tables, it is more reasonable to make use of one of the published analytic approximations (Vand, Eiland & Pepinsky, 1957; Forsyth & Wells, 1959; Moore, 1963; Cromer & Waber, 1965; Lee & Pakes, 1969).

Substituting *e.g.* the nine-parameter fit of Cromer & Waber, expression (1) becomes:

$$I_{\mathrm{inc}}(s)=\left[Z-\frac{(\sum_{i=1}^{4}A_i\exp\{-B_is^2\}+C)^2}{Z}\right]\times[1-M(\exp\{-Ks\}-\exp\{-Ls\})] \quad (2)$$

where

A_i, B_i and $C(i=1,4)$ are the parameters given by Cromer & Waber.

This expression is very suitable for entering into a computer. Thus, the coherent, incoherent and total scattered intensities can easily and in a single process be computed for any desired value of s over the entire range. Expression (2) can be completed with the recoil factor which is also a function of s, but is independent of the atomic species.

In Table 1 the values of the individual parameters M, K, L and the standard deviation, ε, between the calculated and tabulated incoherent intensities are given for 44 atoms and ions, respectively. The formula for ε was chosen as

$$\varepsilon=\left(\frac{\sum_{i=1}^{n}s_i\delta_i^2}{\sum_{i=1}^{n}s_i}\right)^{1/2} \quad (3)$$

where the δ_i's are the deviations, $s_i=\sin\theta_i/\lambda$, index i refers to the points in which tabulated incoherent intensities were found.

In the calculations reported here, Cromer & Waber's nine-parameter formula was used for the coherent intensities. Tabulated incoherent intensities of the atoms with atomic numbers from 2 through 35 were taken from the work of Tavard, Nicolas & Rouault (1967), those of the ions Li^+, Na^+,F-, Cl^-, K^+ from *International Tables for X-ray Crystallography* (1962), and those of Rb, I, Cs from Sagel's (1958) *Tabellen zur Röntgenstrukturanalyse.*

The least-squares fit was weighted by s so that the expression $\sum_{i=1}^{n}s_i\delta_i^2$ was to be minimized. This form of weighting was meant to emphasize the upper region of s where the incoherent intensity and particularly its contribution to the total scattered intensity is the greatest.

Formula (2) yields a very good fit as may be seen from Table 2 showing a set of calculated and tabulated intensities for the oxygen atom. (Tabulated data of Milberg & Brailsford, 1958). The accuracy is similar in most other cases.

Table 2. *Comparison of calculated and tabulated incoherent scattered X-ray intensities.*

O atom $Z=8$

s	$Z-f^2/Z$	I_{cal}	I_{tab}
0·0	0·000	0·000	0·000
0·1	1·380	0·968	0·966
0·2	3·897	2·776	2·777
0·3	5·747	4·274	4·275
0·4	6·755	5·222	5·243
0·5	7·250	5·794	5·818
0·6	7·490	6·160	6·170
0·7	7·614	6·417	6·408
0·8	7·683	6·614	6·593
0·9	7·727	6·776	6·750
1·0	7·760	6·915	6·894
1·1	7·787	7·037	7·025
1·2	7·811	7·146	7·148
1·3	7·834	7·243	7·259
1·4	7·855	7·331	7·361

It is evident that any change in the accepted data for either the coherent or the incoherent intensities involves a revision, *i.e.* a recalculation of the parameters M, K and L.

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The computations have been performed on the ICT 1905 computer of the Central Physical Research Institute of the Hungarian Academy of Sciences.

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