If it happens that the ratios of the crystal gram molecular refractivities are nearly equal to the corresponding ratios of the mean squares of the direction cosines of one of the molecular principal axes, two of the relative molecular refractivity uncertainties, those along the two other molecular principal axes, will be relatively large, *e.g.* if $R_a:R_b:R_c \simeq \alpha_1^2:\beta_1^2:\gamma_1^2$, then, as seen from equation (5), the determinants D_2 and D_3 will be very small, and consequently, from equation (8), $\delta(r_M)/r_M$ and $\delta(r_N)/r_N$ will have rather high values.

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A new analytic approximation to atomic incoherent X-ray scattering intensities.

By VEDENE H. SMITH JR, AJIT J. THAKKAR and DOUGLAS C. CHAPMAN, *Department of Chemistry, Queen's University, Kingston, Ontario K7L 3N6, Canada*

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A new analytic approximation to atomic incoherent X-ray scattering intensities is proposed. Unlike other approximations in the literature, the present function has the correct asymptotic behaviour at both large and small values of s. Fits to the incoherent intensities calculated by Cromer are presented for all atoms from He through Am.

Several analytic approximations to the intensity of the incoherent scattering of X-rays by N-electron atoms are available in the literature (Furukawa, Orton, Hamor & Williams, 1963; Rodriguez & Pings, 1965; Hajdu, 1971, 1972; Palinkas, 1972).

The more accurate approximations are those of Hajdu (1971, 1972) and of Palinkas (1972). Hajdu's function is given by

$$I_{\text{inc}}(s)=[Z-I_{\text{coh}}(s)Z^{-1}]\,[1-M\exp(-Ks) + M\exp(-Ls)] \quad (1)$$

where Z is the atomic number, $s=\lambda^{-1}\sin\theta$, θ is twice the scattering angle, $2\pi/\lambda$ is the propagation constant of the X-ray, and

$$I_{\text{coh}}(s)=[F(s)]^2 \quad (2)$$

is the intensity of the coherent scattering where the form factor, $F(s)$, is approximated by

$$F(s)=\sum_{i=1}^{4} A_i \exp(-B_i s^2)+C\,. \quad (3)$$

Palinkas (1972) uses the following approximation

$$I_{\text{inc}}(s)=Z[1-a(1+bs)^{-c}]. \quad (4)$$

Neither of the above functions has the correct asymptotic behavior either for large or for small values of s. The small-s behaviour of the total scattered intensity is known to be (Benesch & Smith, 1973)

$$I_{\text{tot}}(\mu)=N^2-\mu^2\langle r_{12}^2\rangle/3+O(\mu^4) \quad (5)$$

where $\mu=4\pi s$, and the small-s behaviour of the form factor is known to be (Benesch & Smith, 1973)

$$F(\mu)=N-\mu^2\langle r^2\rangle/6+O(\mu^4). \quad (6)$$

Hence the small-s behaviour of the incoherent scattering function is

$$I_{\text{inc}}(s)=a_2 s^2+a_4 s^4+\ldots \quad (7)$$

where $a_2=16\pi^2(N\langle r^2\rangle-\langle r_{12}^2\rangle)/3$. The large-$s$ behaviour of the incoherent scattering function has been shown (Smith, 1970) to be

$$I_{\text{inc}}(s)=N+b_4 s^{-4}+b_6 s^{-6}+\ldots\,. \quad (8)$$

In this work we propose a new analytic approximation to the incoherent scattering function:

$$I_{\text{inc}}(s)=N[1-(1+as^2+bs^4)\,(1+cs^2+ds^4)^{-2}]. \quad (9)$$

Of course, for neutral atoms $N=Z$. As can be easily verified, equation (9) has the correct asymptotic behaviour for both large and small values of s.

Non-linear least-squares fits, over the range $0\leq s\leq 8{\cdot}0$, of equation (9) to the $I_{\text{inc}}(s)$ values calculated by Cromer & Mann (1967) and Cromer (1969) have been carried out with the algorithm of Fletcher (1971). Table 1 lists values of the parameters a,b,c, and d for all the atoms from He through Am. A measure of the 'goodness-of-fit', ε, is also listed in Table 1 for each atom. It is defined by

$$\varepsilon=100[\sum_{i=1}^{k}\delta_i^2/(k-1)]^{1/2}/N \quad (10)$$

where δ_i are the deviations. ε can be considered to be a standard percent deviation because $N=\lim_{s\to\infty} I_{\text{inc}}(s)$. Table 1 shows that ε does not exceed $\sim 2\%$ for any of the atoms except Li. It should be noted that global optimization is currently impossible (Powell, 1970) and hence the parameters listed in Table 1 cannot be considered as defining anything better than a local minimum. Table 2 shows the typical quality of the fits for atoms of low ($Z=7$), medium ($Z=46$), and high ($Z=88$) atomic numbers.

A perusal of Table 1 shows that the fits worsen with increasing atomic number. For atoms of low and medium atomic number the overall quality of the fits obtained is comparable to the fits of Hajdu (1972) and Palinkas (1972). For atoms of high atomic number the fits are somewhat inferior to those of Palinkas (1972). However equation (9)

Table 1. *Parameters for the analytic approximation, equation (9), to incoherent scattered X-ray intensities; the notation used is*: 1.5566D 01 = 1.5566×10^1.

Atom	Z	a	b	c	d	ε
HE	2	7.2391D-01	-2.1464D-01	9.1019D 00	1.5566D C1	0.01
LI	3	2.6676D 01	6.8817D 00	2.6299D 01	8.8062D-C1	5.1E
BE	4	1.6566D 01	1.1177D 03	4.0948D 01	1.0399D 02	0.2E
B	5	7.2557D 00	2.7281D 02	2.2693D C1	3.4403D C1	C.2E
C	6	4.3253D CC	9.3125D 01	1.4656D 01	1.4628D C1	0.2E
N	7	4.5091D 0C	4.0969D 01	1.1061D 01	7.3225D 00	0.2E
O	8	3.2434D 00	1.9377D 01	8.2735D CC	4.0087D CC	0.2E
F	9	2.7771C 00	1.0031D 01	6.5952D 00	2.3142D C0	0.2E
NE	10	3.1885D C0	5.6531D 00	5.7748D 0C	1.3790D CC	0.32
NA	11	1.6225C 01	4.5169D 01	1.3167D 01	5.4565D CC	1.7E
MG	12	1.1558D 02	3.2270D 03	7.0762D 01	7.7161C 01	1.8E
AL	13	1.0762C 02	2.7409D 03	6.7151D C1	5.9872D C1	1.E7
SI	14	8.0719C 01	1.5C84D 03	5.2054D 01	3.6898C C1	1.3E
P	15	6.5633D 01	7.0348D 02	3.7402D 01	2.0872D 01	1.1E
S	16	4.3655D 01	4.1647C 02	3.0100D 01	1.3430D C1	0.97
CL	17	3.4552C 01	2.5266D 02	2.4481D 01	8.8480D C0	0.61
AR	18	2.7153D C1	1.5C48D 02	1.9697D 01	5.8774D C0	0.69
K	19	3.0545D 01	1.9371C 02	2.1865D 01	6.5615D CC	1.14
CA	20	3.1545D 01	2.8598D 02	2.5950C C1	8.1578C 0C	1.5E
SC	21	3.3212D 01	2.3259D 02	2.3472D C1	6.8604D C0	1.61
TI	22	2.9486D 01	1.8205C 02	2.0962D 01	5.7117D C0	1.64
V	23	2.6193D 01	1.4317C 02	1.8683D 01	4.8164D 00	1.6E
CR	24	1.8525D 01	7.2508D 01	1.3819D 01	3.0415D CC	1.4E
MN	25	2.1252D 01	9.4848D 01	1.5188D 01	3.6204D 00	1.7E
FE	26	1.9276D 01	7.7511D 01	1.3788D 01	3.1076D C0	1.7E
CO	27	1.7616D 01	6.4657D 01	1.2621D 01	2.7056D CC	1.74
NI	28	1.6346D C1	5.5896D 01	1.1687C 01	2.4272D CC	1.74
CU	29	1.2651D 01	3.3E34D 01	9.3436D C0	1.7194C C0	1.53
ZN	30	1.4619C 01	4.5462D 01	1.0338D C1	2.082CD CC	1.74
GA	31	1.7178D 01	6.4552D C1	1.1820D 01	2.5707C 00	1.82
GE	32	1.9343D 01	8.2421C 01	1.3080D C1	2.9211D 00	1.80
AS	33	1.9471D 01	8.4720C 01	1.3126D 01	2.8165C 0C	1.6E
SE	34	2.0355D 01	9.2997D 01	1.3650D 01	2.8488D C0	1.60
BR	35	2.0316C 01	9.2534C C1	1.3623D C1	2.7928D CC	1.EC
KR	36	1.8566C 01	8.0312C 01	1.2812C 01	2.3584C 00	1.3E
RB	37	2.1265D 01	1.0161D 02	1.4209D 01	2.6226D 00	1.54
SR	38	2.4457D C1	1.3593D 02	1.6192D 01	3.0174D CC	1.73
Y	39	2.4539C 01	1.3620D 02	1.6237D 01	2.9014C CC	1.73
ZR	40	2.3652D C1	1.2653D 02	1.5732D C1	2.6710C 00	1.72
NB	41	1.9178D 01	8.1654D 01	1.2952D 01	1.9678D C0	1.6E
MO	42	1.7443D 01	6.7555D 01	1.1867D 01	1.6907C 0C	1.5E
TC	43	1.8256D 01	7.3766C 01	1.2363D C1	1.7500D CC	1.72
RU	44	1.5431D 01	5.1934C 01	1.0601D 01	1.3610D CC	1.5E
RH	45	1.4236D 01	4.3614C 01	9.8385D 0C	1.1954D 00	1.5E
PD	46	1.2128D 01	3.1377D 01	8.4946D 00	9.4341D-C1	1.4E
AG	47	1.1510D 01	3.0295C 01	8.3388D 00	9.0612D-C1	1.5E
CD	48	1.2263D 01	3.2428D 01	8.5514D 00	9.3212D-C1	1.7E
IN	49	1.2853D 01	3.6009D 01	8.9130D 00	9.8156D-C1	1.E3
SN	50	1.3547D 01	4.0031D 01	9.3037D 00	1.0326C 00	1.8E
SB	51	1.3466D 01	3.9657D 01	9.2631D 00	1.0057D C0	1.90
TE	52	1.4450D 01	4.6190C 01	9.8671D 00	1.0869D 00	1.87
I	53	1.4575D 01	4.9456C 01	1.0161D 01	1.1116D 00	1.8E
XE	54	1.4885D 01	4.8883C 01	1.0102D 01	1.0775D CC	1.7E
CS	55	1.6155D 01	5.7696C 01	1.0886D 01	1.1773D C0	1.9C
BA	56	1.3153D 01	7.1158D 01	1.1921D 01	1.3128D 0C	2.04
LA	57	1.8225C 01	7.4363D 01	1.2167D 01	1.3151D CC	2.04
CE	58	1.7550D 01	6.9295D 01	1.1741D 01	1.2501C 00	2.03
PR	59	1.6613D 01	6.1934D 01	1.1071D C1	1.1678D C0	2.04
ND	60	1.6148D 01	5.8598C 01	1.0747C 01	1.1155D 00	2.04
PM	61	1.5741D 01	5.5777D C1	1.0458D 01	1.0774D 00	2.04
SM	62	1.5356D 01	5.3212C 01	1.0182D 01	1.0356D C0	2.0E
EU	63	1.5027D 01	5.1053C 01	9.9393D 00	1.0055D C0	2.0E
GD	64	1.4E68D 01	5.0133D 01	9.8426D 00	9.7728D-01	2.03
TB	65	1.4449C 01	4.7248C 01	9.5464D 00	9.3283D-C1	2.02
DY	66	1.3755D 01	4.3137C 01	9.1027D 00	8.7906C-01	2.02
HO	67	1.3447D 01	4.1645D 01	8.8604D 00	8.4486D-C1	2.01
ER	68	1.3146C 01	3.9287C 01	8.6467D 0C	8.1464D-C1	2.0C
TM	69	1.2882D 01	3.7803D 01	8.4552D 00	7.8869C-01	1.99
YB	70	1.2677D 01	3.6643D 01	8.2568D 0C	7.6627D-01	1.98
LU	71	1.2576D 01	3.6129C 01	8.2264D 00	7.4720D-01	1.97
HF	72	1.2352D 01	3.5077D C1	8.1062D 00	7.2892D-C1	1.9E
TA	73	1.1966D 01	3.2657C 01	7.8420D 00	6.7758D-C1	1.92
W	74	1.1426D 01	2.9720C 01	7.5123D 00	6.2773D-C1	1.87
RE	75	1.0841D 01	2.6666D 01	7.1515D 00	5.7682D-01	1.84
OS	76	1.0453D 01	2.5229D 01	6.9734D 00	5.4767D-C1	1.81
IR	77	1.0265C 01	2.3781D 01	6.7889D 00	5.1853D-01	1.7E
PT	78	9.1444D 00	1.8754D 01	6.1116D 00	4.3980D-01	1.66
AU	79	8.6652D 00	1.6793C 01	5.8176D 00	4.0417D-C1	1.62
HG	80	8.8187D 00	1.7414D C1	5.9035D C0	4.0768D-01	1.70
TL	81	9.0767C 00	1.8476C 01	6.0519D 0C	4.1721D-C1	1.7E
PB	82	9.3622D 00	1.9739C 01	6.2252D CC	4.2863D-01	1.8C
BI	83	9.5574D 00	2.0605D 01	6.3414D 00	4.3371D-01	1.80
PO	84	9.9256D 00	2.2287C 01	6.5624D 00	4.4878D-C1	1.8E
AT	85	1.0267D 01	2.3502C 01	6.7681D 00	4.6167D-C1	1.84
RN	86	1.0425D 01	2.4663D 01	6.8643D 00	4.6342D-C1	1.81
FR	87	1.1077D 01	2.7547C 01	7.2583D 00	4.9341D-C1	1.9C
RA	88	1.1506D 01	3.2420D 01	7.7600D CC	5.3275D-C1	2.00
AC	89	1.2372D 01	3.5070D C1	8.0440D CC	5.5039D-C1	2.01
TH	90	1.2708D 01	3.7029C 01	8.2501D 00	5.6015D-01	2.01
PA	91	1.1521D 01	3.2573C 01	7.7684D 00	5.1436D-C1	2.00
U	92	1.1596C 01	3.0746C 01	7.5550D 0C	4.9185D-C1	2.0C
NP	93	1.1277D 01	2.9055D 01	7.3579C 00	4.7057D-C1	2.01
PU	94	1.0565D 01	2.5479D 01	6.9123D 00	4.3325D-01	2.04
AM	95	1.0243C 01	2.3618C 01	6.7044D 0C	4.1402D-C1	2.C5

is the only one that has the correct asymptotic behaviour at large and small values of s. Hence the present fits should be especially useful in studies of electron scattering where accuracy of the fits for $s \leq 0{\cdot}1$ is rather important.

Table 2. *Comparison of incoherent scattered X-ray intensities computed by Cromer, I_e, with those predicted by equation (9), I_f*

	$Z=7$		$Z=46$		$Z=88$	
s	I_e	I_f	I_e	I_f	I_e	I_f
0·000	0·000	0·000	0·000	0·000	0·000	0·000
0·005	0·003	0·003	0·010	0·006	0·036	0·008
0·010	0·013	0·012	0·039	0·022	0·144	0·032
0·050	0·310	0·296	0·923	0·548	2·520	0·780
0·100	1·080	1·054	3·103	2·068	5·696	2·958
0·150	2·003	1·994	5·536	4·251	8·858	6·122
0·200	2·858	2·876	7·725	6·747	11·964	9·789
0·300	4·097	4·120	11·441	11·646	17·672	17·152
0·400	4·792	4·783	14·824	15·685	22·270	23·378
0·500	5·182	5·160	17·943	18·786	26·283	28·247
0·600	5·437	5·422	20·653	21·173	30·139	32·040
0·700	5·635	5·635	22·904	23·071	33·790	35·080
0·800	5·809	5·821	24·756	24·645	37·136	37·617
0·900	5·968	5·988	26·316	26·002	40·121	39·823
1·000	6·113	6·134	27·677	27·211	42·744	41·811
1·500	6·630	6·614	32·888	32·104	52·502	50·271
2·000	6·860	6·821	36·349	35·881	59·860	57·658
3·000	6·979	6·951	40·389	40·848	69·885	69·484
4·000	6·996	6·982	42·529	43·357	75·363	77·077
5·000	6·999	6·992	43·658	44·579	78·664	81·509
8·000	7·000	6·999	45·019	45·694	83·881	86·363

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