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NUMERICAL TABLES OF ANOMALOUS SCATTERING FACTORS CALCULATED BY THE CROMER AND LIBERMAN'S METHOD

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Abstract

Anomalous scattering factors f' and f'' have been calculated for the atoms Li through Bi, plus U, using the relativistic treatment described by Cromer and Liberman. The final f' value does not include the Jensen's correction term on the magnetic scattering. The tables are presented with the f' and f'' values (i) at 0.01 Å intervals in the wavelength range from 0.1 to 2.89 Å and (ii) at 0.0001 Å intervals in the neighborhood of the K, L_1, L_2, and L_3 absorption edges.

KEYWORDS: Anomalous scattering factors, Anomalous dispersion, Resonant scattering, Cromer and Liberman's method, Relativistic treatment, Synchrotron radiation.

INTRODUCTION

A broad and continuous spectrum of x-rays, intense enough for diffraction or scattering experiments at arbitrary wavelengths, is now available using synchrotron radiation from storage rings. This characteristic is vital in measuring or utilizing anomalous scattering effects. The anomalous scattering factor accounts for the absorption of x-rays by electrons of finite binding energy in an atom. The anomalous scattering effect is of interest for such applications as absorption and scattering experiments and phase determination of crystal structures, as well as the x-ray dispersion experiment itself. This effect is strongest at absorption edges and only a synchrotron radiation source can provide a powerful flux at wavelengths close to absorption edges. Nevertheless, the effect is not entirely negligible to calculate the scattering amplitude even for frequencies away from the absorption edge. Therefore, it is both necessary and convenient to have tables of anomalous scattering factors which cover the wavelength range of synchrotron radiation utilized.

CALCULATION METHOD

Anomalous scattering effects are taken into account by representing the atomic scattering factor, f, for frequency ω_i as a complex number:

$$f = f_0 + f' + if'' , \tag{1}$$

where f_0, f', and f'' are the frequency-independent Thomson scattering factor, and the real and imaginary parts of the anomalous dispersion, respectively. Then, in the classical theory of dispersion,$^{1),2)}$

$$f' = \sum_K \int_{\omega_K}^{\infty} \frac{\omega^2 (dg/d\omega)_K}{(\omega_i^2 - \omega^2)} d\omega \tag{2}$$

and

$$f'' = \frac{\pi}{2} \omega_i \sum_K (dg/d\omega)_{Ki} , \tag{3}$$

where ω_i = incident frequency, ω_K = frequency of the absorption edge, $dg/d\omega$ = oscillator density, and the summation is over all of the absorption edges and damping is neglected.

When relativistic theory for a free atom is used, similar expressions to those above can be derived. The scattering factor for light by a bound electron is written as

$$\begin{aligned} f = mc^2 \sum_{n^+} & \left\{ \frac{<2|E_2Q_2|n^+><n^+|E_1Q_1|1>}{\varepsilon_1 - \varepsilon_n{}^+ + \hbar\omega_1} + \frac{<2|E_1Q_1|n^+><n^+|E_2Q_2|1>}{\varepsilon_1 - \varepsilon_n{}^+ - \hbar\omega_2} \right\} \\ + mc^2 \sum_{n^-} & \left\{ \frac{<2|E_2Q_2|n^-><n^-|E_1Q_1|1>}{\varepsilon_2 - |\varepsilon_n{}^-| + \hbar\omega_2} + \frac{<2|E_1Q_1|n^-><n^-|E_2Q_2|1>}{\varepsilon_2 - |\varepsilon_n{}^-| - \hbar\omega_1} \right\} , \end{aligned} \tag{4}$$

where 1, 2 and n indicate the initial, final, and intermediate electron states; $E_i = e_i \cdot \alpha$ and $Q_i = \exp(i\mathbf{k}_i \cdot r)$; $\mathbf{e}_i$ and $\mathbf{k}_i$ are the polarization and wave vectors of the incident and scattered light, respectively. The reader is referred to Cromer and Liberman (1970)[3)] for the detailed derivations. Here, equation (1) is redefined as

$$f = f_0 + f^+ - f_0^+ + (f^- - f_0^-), \tag{5}$$

where the factors with the suffix 0 are defined by the equation (4) except that all denominators are replaced by $2mc^2$, and superscripts + and - mean summation over positive and negative energy states, respectively. The frequency-dependent term f^+ can be evaluated through relation to the photoelectric cross section, and f_0^+ and $f^- - f_0^-$ are evaluated from the nonrelativistic approximation using electric dipole contributions. The largest contribution to the anomalous dispersion is the term f^+, which has the form

$$f^+ = \frac{c\varepsilon_1}{2\pi^2}\int_0^1 \frac{\varepsilon_1^2\sigma(-\varepsilon_1/x) - x^2(\hbar\omega)^2\sigma(\hbar\omega)}{x^2\{x^2(\hbar\omega)^2-\varepsilon_1^2\}}\,dx + \frac{1}{2}\{-(\hbar\omega)\sigma(\hbar\omega)\}\log\frac{|\hbar\omega-\varepsilon_1|}{|\hbar\omega+\varepsilon_1|}, \tag{6}$$

where c = velocity of light, ε_1 = binding energy of the electron, $\sigma(\alpha)$ = photoelectric cross section at energy α, $\hbar\omega$ = energy of the x-ray, ε^+ = energy of a positive energy state,

$$x = -\varepsilon_1/(\varepsilon^+ - \varepsilon_1). \tag{7}$$

With the use of equation (6), it was found that a five-point Gaussian-type numerical integration gave f^+ with a numerical accuracy of about four significant figures.[3)] In the nonrelativistic approximation, the electric dipole term is

$$(-f_0^+ + f^- - f_0^-)_{\mathrm{tot}} = \frac{5}{3}\frac{E_{\mathrm{tot}}}{mc^2}, \tag{8}$$

where E_{tot} is the total energy of the atom. The imaginary part f'' can be expressed directly in terms of the cross section as[1),3)]

$$f'' = \frac{mc\omega\sigma(\hbar\omega)}{4\pi e^2}. \tag{9}$$

The recent improvement of the calculation method by Cromer and Liberman (1981)$^{4)}$ includes a modification of the integration of photoelectric dispersion to modification of the integration of photoelectric dispersion to increase the numerical accuracy for wavelengths near to and on the long-wavelength side of an absorption edge. When the cross section for the incident x-ray is zero, equation (6) is rewritten as

$$f^{+} = \frac{c\varepsilon_1}{2\pi^2}\left\{\int_0^1 \frac{\varepsilon_1\sigma(-\varepsilon_1/x) - x^2\varepsilon_1^2\sigma(\varepsilon_1)}{x^2\{x^2(\hbar\omega)^2-\varepsilon_1^2\}}\,dx + \int_0^1 \frac{x^2\varepsilon_1^2\sigma(\varepsilon_1)}{x^2\{x^2(\hbar\omega)^2-\varepsilon_1^2\}}\,dx\right\}. \qquad (10)$$

Each table listed in this paper was calculated from the photoelectric cross sections by numerical integration using a modified version of the program FPRIME$^{5)}$. The cross sections were calculated from Dirac-Slater wavefunctions based on Brysk and Zerby.$^{6)}$ The cross section data exclude outer orbitals other than those of the ground state. Therefore, the result may not be reasonably accurate for the longer wavelengths, if the outer-most orbital has a significant contribution for such wavelengths. We suggest that this calculation should be valid in the x-ray region with wavelengths shorter than and on the order of Cr $K\alpha$ (λ = 2.3 Å). $^{5)}$

MAGNETIC SCATTERING TERM

In our previous report,$^{7)}$ a frequency-dependent magnetic term, $(-Z/2)(\hbar\omega/mc^2)^2$, by Jensen$^{8)}$ was included for the calculation of f' values. Recently, it was pointed out that this term is canceled out when the calculation up to order of $(\hbar\omega/mc^2)^4$ is performed for the scattering amplitude equation like (4).$^{9)}$ Therefore, the f' values were calculated without the Jensen's correction term on the magnetic scattering. The f' values listed in this and the previous reports are almost identical except for the wavelengths shorter than 0.6 Å. The ω and z (atomic number) dependency of the magnetic term is demonstrated in the following table:

λ (Å)	Si (z = 14)	Fe (z = 26)	Ge (z = 32)	Sn (z = 50)
0.2	-0.103	-0.192	-0.235	-0.368
0.4	-0.026	-0.048	-0.059	-0.092
0.6	-0.012	-0.021	-0.027	-0.041
0.8	-0.006	-0.012	-0.015	-0.023
1.0	-0.004	-0.008	-0.010	-0.014
1.2	-0.003	-0.005	-0.006	-0.010
1.4	-0.002	-0.004	-0.004	-0.007
1.6	-0.002	-0.003	-0.004	-0.005
1.8	-0.001	-0.002	-0.003	-0.005
2.0	-0.001	-0.002	-0.003	-0.004

COMMENTS ON TABLES

The anomalous scattering factors f' and f'' are given in Table I as a function of wavelengths in Å (10^{-10} m) where calculations can cover the wavelength range commonly used in crystallography with the synchrotron radiation source. The ångström unit can be changed into *k*eV unit by using,

$$1\text{Å} = 12.397639\ k\text{eV}. \qquad (11)$$

Table I-a gives the f' and f'' values for elements with z = 3 to 83 plus z = 92 in the wavelength-range from 0.1 to 2.89 (Å) in intervals of 0.01 Å, which are such that linear interpolation is reasonably accurate in the general case. The f' values for wavelengths shorter than 0.15 Å are omitted for elements larger than z = 79. Table I-b also gives the f' and f'' values for wavelengths near the K, L_1, L_2, or L_3 absorption edge. The 280 points of anomalous scattering factors for the elements z = 12 to 78 and z = 47 to 83 are given in intervals of 0.0001 Å near the K and L absorption edges, respectively. The wavelength values for the respective absorption edges are taken from Bearden's tables in the *International Tables for X-ray Crystallography*, vol. IV.10) For convenience, all tables are arranged in order of atomic number. Appendix 1, given on page 135, may be useful as an index.

Acknowledgement

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Appendix 1. Index for anomalous scattering factor tables. Each number shows the page relevant to the element looked up. The atomic number is given in parentheses.

Element	Table I-a	Table I-b	Element	Table I-a	Table I-b			
		K			K	L_1	L_2	L_3
Li (3)	5		Ru (44)	25	62			
Be (4)	5		Rh (45)	26	62			
B (5)	6		Pd (46)	26	63			
C (6)	6		Ag (47)	27	63	79	98	116
N (7)	7		Cd (48)	27	64	80	98	117
O (8)	7		In (49)	28	64	80	99	117
F (9)	8		Sn (50)	28	65	81	99	118
Ne (10)	8		Sb (51)	29	65	81	100	118
Na (11)	9		Te (52)	29	66	82	100	119
Mg (12)	9	46	I (53)	30	66	82	101	119
Ar (13)	10	46	Xe (54)	30	67	83	101	120
Si (14)	10	47	Cs (55)	31	67	83	102	120
P (15)	11	47	Ba (56)	31	68	84	102	121
S (16)	11	48	La (57)	32	68	84	103	121
Cl (17)	12	48	Ce (58)	32	69	85	103	122
Ar (18)	12	49	Pr (59)	33	69	85	104	122
K (19)	13	49	Nd (60)	33	70	86	104	123
Ca (20)	13	50	Pm (61)	34	70	86	105	123
Sc (21)	14	50	Sm (62)	34	71	87	105	124
Ti (22)	14	51	Eu (63)	35	71	87	106	124
V (23)	15	51	Gd (64)	35	72	88	106	125
Cr (24)	15	52	Tb (65)	36	72	88	107	125
Mn (25)	16	52	Dy (66)	36	73	89	107	126
Fe (26)	16	53	Ho (67)	37	73	89	108	126
Co (27)	17	53	Er (68)	37	74	90	108	127
Ni (28)	17	54	Tm (69)	38	74	90	109	127
Cu (29)	18	54	Yb (70)	38	75	91	109	128
Zn (30)	18	55	Lu (71)	39	75	91	110	128
Ga (31)	19	55	Hf (72)	39	76	92	110	129
Ge (32)	19	56	Ta (73)	40	76	92	111	129
As (33)	20	56	W (74)	40	77	93	111	130
Se (34)	20	57	Re (75)	41	77	93	112	130
Br (35)	21	57	Os (76)	41	78	94	112	131
Kr (36)	21	58	Ir (77)	42	78	94	113	131
Rb (37)	22	58	Pt (78)	42	79	95	113	132
Sr (38)	22	59	Au (79)	43		95	114	132
Y (39)	23	59	Hg (80)	43		96	114	133
Zr (40)	23	60	Tr (81)	44		96	115	133
Nb (41)	24	60	Pb (82)	44		97	115	134
Mo (42)	24	61	Bi (83)	45		97	116	134
Tc (43)	25	61	U (92)	45				

Appendix 2. Calculated anomalous scattering factors of La near the *K* and *L* absorption edges.