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**A table of dispersion corrections for X-ray scattering of atoms.** By CAROL H. DAUBEN and DAVID H. TEMPLETON, *Department of Chemistry and Radiation Laboratory, University of California, Berkeley, California, U.S.A.*

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To make more convenient the inclusion of X-ray dispersion effects in intensity calculations we have tabulated values for the real and imaginary corrections for the scattering factors for medium and heavy atoms for Cr, Cu and Mo  $K\alpha$  radiation. The scattering factor  $f$  is a complex number:

$$f = f_0 + \Delta f' + i\Delta f'',$$

where  $f_0$  is the well-known function of  $\sin \theta/\lambda$  (*International Tables*, 1935). The corrections  $\Delta f'$  and  $\Delta f''$  are nearly independent of  $\theta$  because the tightly bound electrons responsible for these effects are concentrated in a small volume near the atomic nucleus.

The values listed in Table 1 were calculated by the

Table 1. *Dispersion corrections*

Atomic number		Cr $K\alpha$ X-rays		Cu $K\alpha$ X-rays		Mo $K\alpha$ X-rays	
		$\Delta f''$	$-\Delta f'$	$\Delta f''$	$-\Delta f'$	$\Delta f''$	$-\Delta f'$
20	Ca	2.7	0.2	1.4	-0.2	0.2	-0.2
21	Sc	3.2	0.7	1.6	-0.2	0.3	-0.2
22	Ti	3.8	1.7	1.9	-0.2	0.4	-0.3
23	V	0.6	4.4*	2.3	-0.2	0.5	-0.3
24	Cr	0.7	2.2	2.6	0.1	0.6	-0.4
25	Mn	0.8	1.8	3.0	0.5	0.8	-0.4
26	Fe	0.9	1.6	3.4	1.1	1.0	-0.4
27	Co	1.0	1.4	3.9	2.2	1.1	-0.4
28	Ni	1.2	1.2	0.6	3.1*	1.2	-0.4
29	Cu	1.3	1.1	0.7	2.1	1.4	-0.4
30	Zn	1.5	1.0	0.8	1.7	1.6	-0.3
31	Ga	1.7	0.9	0.9	1.5	1.7	-0.2
32	Ge	1.9	0.8	1.1	1.3	1.9	-0.2
33	As	2.2	0.7	1.2	1.2	2.2	-0.1
34	Se	2.4	0.7	1.3	1.0	2.4	0.1
35	Br	2.7	0.6	1.5	0.9	2.6	0.3
36	Kr	3.0	0.6	1.7	0.9	2.9	0.6
37	Rb	3.4	0.6	1.9	0.8	3.2	0.9
38	Sr	3.8	0.6	2.1	0.7	3.6	1.4
39	Y	4.2	0.6	2.3	0.7	3.9	2.3
40	Zr	4.6	0.7	2.5	0.6	0.8	2.8
41	Nb	5.1	0.8	2.8	0.6	0.9	2.1
42	Mo	5.6	0.9	3.0	0.5	0.9	1.7
43	Tc	6.2	1.0	3.3	0.5	1.0	1.4
44	Ru	6.7	1.2	3.6	0.5	1.1	1.2
45	Rh	7.3	1.3	4.0	0.5	1.2	1.1
46	Pd	7.9	1.6	4.3	0.5	1.3	1.0
47	Ag	8.6	1.9	4.7	0.5	1.4	0.9
48	Cd	9.2	2.2	5.0	0.6	1.6	0.8
49	In	10	2.7	5.4	0.6	1.7	0.7
50	Sn	11	3.2	5.8	0.7	1.9	0.6
51	Sb	12	4.0	6.3	0.8	2.0	0.6
52	Te	12	5.0	6.7	0.9	2.2	0.5
53	I	14	7.2*	7.2	1.1	2.4	0.5
54	Xe	11	†	7.8	1.4	2.5	0.4
55	Cs	12	12*	8.3	1.7	2.7	0.4
56	Ba	8	11*	8.9	2.1	2.9	0.4
57	La	3	14*	9.6	2.5	3.1	0.3
58	Ce	3	10	10	3.0	3.3	0.3
59	Pr	4	9	11	3.5	3.6	0.3
60	Nd	4	8	12	4.3	3.8	0.3
61	Pm	4	7	12	5.2	4.0	0.3
62	Sm	5	7	13	6.7	4.2	0.3
63	Eu	5	6	11	†	4.5	0.3

Table 1 (cont.)

Atomic number		Cr $K\alpha$ X-rays		Cu $K\alpha$ X-rays		Mo $K\alpha$ X-rays	
		$\Delta f''$	$-\Delta f'$	$\Delta f''$	$-\Delta f'$	$\Delta f''$	$-\Delta f'$
64	Gd	5	6	12	12*	4.7	0.3
65	Tb	6	6	8	11*	5.0	0.4
66	Dy	6	6	8	10	5.2	0.4
67	Ho	7	6	4	13*	5.5	0.4
68	Er	7	5	4	9*	5.8	0.5
69	Tm	8	5	4	8	6.2	0.5
70	Yb	9	5	4	8	6.4	0.6
71	Lu	8	5	5	7	6.8	0.7
72	Hf	9	5	5	7	7.1	0.8
73	Ta	10	5	5	6	7.4	0.9
74	W	11	5	6	6	7.8	1.1
75	Re	11	5	6	6	8.1	1.3
76	Os	12	5	6	6	8.5	1.5
77	Ir	13	5	7	5	8.9	1.8
78	Pt	13	5	7	5	9.3	2.0
79	Au	14	6	8	5	9.8	2.4
80	Hg	15	6	8	5	10	2.8
81	Tl	16	6	8	5	11	3.4
82	Pb	16	7	9	5	11	4.0
83	Bi	17	7	9	5	12	4.8
84	Po	18	8	10	5	12	5.6
85	At	20	9	10	5	10	†
86	Rn	20	9	11	5	10	8*
87	Fr	21	10	11	5	7	8*
88	Ra	23	11	12	5	7	7
89	Ac	24	13	12	5	8	7
90	Th	25	15	13	5	8	7
91	Pa	26	17*	14	5	8	7
92	U	19	19*	15	5	8	8*
93	Np	†	†	15	5	5	†
94	Pu	†	†	16	5	5	†
95	Am	†	†	17	6	5	†
96	Cm	†	†	18	6	5	†

\* These values are especially uncertain because of proximity to absorption edges.

† Not calculated.

methods of Parratt & Hempstead (1954) for the contributions of the  $K$ ,  $L$  and  $M$  electrons. The absorption edges were obtained from the tables of Cauchois & Hulubei (1947) or by Moseley interpolation or extrapolation. The oscillator strengths were estimated by fitting smooth curves to the available data plotted as a function of atomic number. We included in the plots all the data summarized by Compton & Allison (1935) as well as those of Eisenlohr & Müller (1954). The uncertainty in these values is the most obvious source of error in our results. The exponents  $p$  have been chosen according to the example given for tungsten by Parratt & Hempstead (1954). Damping effects have been neglected.

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**X-ray dispersion effects in crystal-structure determinations.** By DAVID H. TEMPLETON, *Radiation Laboratory and Department of Chemistry, University of California, Berkeley, California, U.S.A.*

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Much attention is now devoted toward obtaining more accurate diffraction data and more precise structures of crystals. It seems appropriate to call attention to effects, which have frequently been neglected, caused by the tight bonding of the inner electrons in medium and heavy elements.

The atomic scattering factor  $f$  is a complex function:

$$f = f_0 + \Delta f' + i\Delta f'', \quad (1)$$

where  $f_0$  is a real function of  $\sin \theta/\lambda$  which has been tabulated for many atoms (*International Tables*, 1935). The real and imaginary dispersion corrections  $\Delta f'$  and  $\Delta f''$  are nearly independent of  $\theta$  but are functions of  $\lambda$ . Recent independent calculations by Eisenlohr & Müller (1954) and Parratt & Hempstead (1954) have shown that for the wavelengths used in diffraction these corrections are not negligible for most elements because of contributions from  $K$ ,  $L$ , and in some cases,  $M$  electrons. The effects are not limited to regions 'very near' to absorption edges, although that is where they are greatest. A table of  $\Delta f'$  and  $\Delta f''$  for Cr, Cu and Mo  $K\alpha$  radiation has been prepared by Dauben & Templeton (1955).

For centrosymmetric crystals the structure factor is

$$F = \Sigma Q (f_0 + \Delta f') \cos 2\pi(hx + ky + lz) + i \Sigma Q \Delta f'' \cos 2\pi(hx + ky + lz) \quad (2)$$

$$= F_r + iF_i; \quad (3)$$

$Q$  is a temperature factor. The magnitude of  $F$ , which is to be compared with the experimental value, is

$$|F| = \sqrt{(F_r^2 + F_i^2)}. \quad (4)$$

When the corrections are neglected, the large structure factors are brought more or less into agreement with the observed ones by adjustment of the normalization factor and by use of incorrect temperature factors. Then the small structure factors are of two kinds. If the contribution of each kind of atom separately is small, the agreement is good. If the contributions of two kinds of atoms are large and of opposite sign, substantial errors result. For the real correction the errors may be positive or negative. For the imaginary correction the error always tends to make the correct amplitude larger than the one in which  $\Delta f''$  is omitted. The use of individual incorrect temperature factors can diminish the discrepancy caused

by neglect of  $\Delta f'$ , but it cannot absorb the effect of  $\Delta f''$ .

The observed structure factors are not the correct coefficients for the electron-density function. The correct coefficients can be approximated, for example, by

$$F'_0 = F'_c |F_0| \div |F_c|, \quad (5)$$

where  $F'_c$  is a structure factor calculated for the trial structure with  $f_0$  in place of  $f$ .

Fortunately, for centric crystals most of the reflections are not much affected by these corrections. Atomic positions derived from all the data probably are not in great error, but the electron-density function and the temperature factors may have systematic errors. The criterion of large opposite contributions from two kinds of atoms is the signal that care must be taken.

For noncentrosymmetric crystals equation (2) has four terms, and  $F(hkl)$  and  $F(\bar{h}\bar{k}\bar{l})$  have different magnitudes and nonconjugate phases. Some examples have been discussed by Bijvoet, Peerdeman & van Bommel (1951) and by Bijvoet (1952). Equation (5) can be used in this case also, with  $F'$  a complex number. Because of experimental errors, the magnitudes of  $F'_0(hkl)$  and  $F'_0(\bar{h}\bar{k}\bar{l})$  may be different, and the average value should be taken for each.

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