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DISPERSION CORRECTIONS FOR ATOMIC SCATTERING FACTORS

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March 1960

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Atomic scattering factors as ordinarily tabulated ($\underline{f}_o$) take account of the spatial distribution of electrons in the atom, but they are calculated with the assumption that the electronic binding energy is so small compared to the energy of the X-ray photon that the scattering power of each electron is like that of a free electron. However, the scattering power of a bound electron may be greater than or less than that of a free electron, and the phase of the scattered wave may be different. These effects may be taken into account by representing the atomic scattering factor $\underline{f}$ as a complex number:

$$\underline{f} = \underline{f}_o + \Delta\underline{f}' + i\,\Delta\underline{f}''$$

where $\Delta\underline{f}'$ and $\Delta\underline{f}''$ are called the real and imaginary dispersion corrections. All of these terms are to be multiplied by the correction factor for thermal motion of the atom.

The dispersion corrections depend on the X-ray wave length λ and the diffraction angle θ. They are less sensitive functions of θ than is $\underline{f}_o$, because the tightly bound electrons responsible for these effects are concentrated in a small volume near the atomic nucleus.

In the following tables are listed values of the dispersion corrections calculated for three wave lengths and various values of $\sin\theta/\lambda$. The values for $\sin\theta/\lambda = 0$ are those published by Dauben and Templeton,[1] modified by inclusion of N-shell electrons where their effects are appreciable. The calculations have also been extended to lighter elements. The corrections for other values of $\sin\theta/\lambda$ are derived by multiplying the contribution of each electron group by its individual $\underline{f}$-factor, or orbital transform. Separate orbital transforms were available for several elements from the calculations of Berghuis, et al.,[2] and others are published by Veenendaal, et al.[3] These data were the basis for graphical interpolation for other elements.

It may be noted that the magnitude of the real correction increases with increasing angle in many cases, because loosely bound electrons give positive contributions while tightly bound electrons give negative contributions, and the transforms for the loosely bound electrons are much more sensitive to angle.

These calculations are based on theoretical approximations for which it is difficult to assess the accuracy, and they involve considerable arbitrariness with regard to the oscillator strengths assigned to the various electron groups. Experimental verification of these corrections is fragmentary. Therefore caution should be exercised in applications where high accuracy is important. Values given in parentheses are especially uncertain because of proximity to absorption edges.

This method of calculation of the angular dependence was suggested to me by Prof. K. Lonsdale. I thank her and Prof. C. H. MacGillavry for sending me the unpublished orbital transforms.

References

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2. J. Berghuis, IJ. M. Haanappel, M. Potters, B. O. Loopstra, C. H. MacGillavry, and A. L. Veenendaal, Acta Cryst. 8, 478 (1955).

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DISPERSION CORRECTIONS FOR ATOMIC SCATTERING FACTORS

Cr K α radiation (λ = 2.291 Å)

Atom		$\Delta f'$		$\Delta f''$		
		$\sin\theta/\lambda$ = 0.0	0.4	$\sin\theta/\lambda$ = 0.0	0.3	0.4
5	B	0.0	0.0	0.0	0.0	0.0
6	C	0.0	0.0	0.1	0.1	0.1
7	N	0.0	0.0	0.1	0.1	0.1
8	O	0.1	0.1	0.2	0.1	0.1
9	F	0.1	0.1	0.2	0.2	0.2
10	Ne	0.1	0.1	0.3	0.3	0.3
11	Na	0.2	0.2	0.4	0.4	0.4
12	Mg	0.2	0.2	0.5	0.5	0.5
13	Al	0.2	0.2	0.6	0.6	0.6
14	Si	0.3	0.3	0.8	0.8	0.8
15	P	0.3	0.3	1.0	0.9	0.9
16	S	0.3	0.3	1.2	1.2	1.2
17	Cl	0.3	0.3	1.5	1.5	1.4
18	A	0.2	0.2	1.8	1.7	1.7
19	K	0.0	0.0	2.2	2.1	2.1
20	Ca	-0.2	-0.2	2.7	2.7	2.6
21	Sc	-0.7	-0.7	3.2	3.1	3.1
22	Ti	-1.7	-1.7	3.8	3.7	3.7
23	V	(-4.4)	(-4.4)	0.6	0.6	0.5
24	Cr	-2.2	-2.2	0.7	0.7	0.6
25	Mn	-1.8	-1.8	0.8	0.8	0.7
26	Fe	-1.6	-1.6	0.9	0.9	0.8
27	Co	-1.4	-1.4	1.0	1.0	0.9
28	Ni	-1.2	-1.2	1.2	1.2	1.1
29	Cu	-1.1	-1.1	1.3	1.3	1.2
30	Zn	-1.0	-1.0	1.5	1.5	1.4
31	Ga	-0.9	-0.9	1.7	1.6	1.6
32	Ge	-0.8	-0.8	1.9	1.8	1.8

(continued)

Cr K α

Atom		$\Delta f'$		$\Delta f''$		
		sin θ/λ = 0.0	0.4	sin θ/λ = 0.0	0.3	0.4
33	As	-0.7	-0.7	2.2	2.1	2.1
34	Se	-0.7	-0.7	2.4	2.3	2.3
35	Br	-0.6	-0.7	2.7	2.6	2.5
36	Kr	-0.6	-0.7	3.0	2.9	2.8
37	Rb	-0.6	-0.7	3.4	3.3	3.2
38	Sr	-0.6	-0.7	3.8	3.7	3.6
39	Y	-0.6	-0.7	4.2	4.0	3.9
40	Zr	-0.7	-0.8	4.6	4.4	4.3
41	Nb	-0.8	-0.8	5.1	4.9	4.8
42	Mo	-0.9	-0.9	5.6	5.4	5.3
43	Tc	-1.0	-1.1	6.2	6.0	5.9
44	Ru	-1.2	-1.2	6.7	6.5	6.4
45	Rh	-1.3	-1.4	7.3	7.1	6.9
46	Pd	-1.6	-1.7	7.9	7.7	7.5
47	Ag	-1.9	-2.0	8.6	8.4	8.2
48	Cd	-2.2	-2.3	9.2	9.0	8.8
49	In	-2.7	-2.8	9.9	9.7	9.5
50	Sn	-3.2	-3.3	10.7	10.5	10.3
51	Sb	-3.9	-4.0	11.6	11.3	11.1
52	Te	-4.9	-5.0	12.4	12.1	11.9
53	I	(-7.1)	(-7.1)	13.6	13.3	13.1
54	Xe	--	--	11	11	10
55	Cs	(-12)	(-12)	12	12	11
56	Ba	(-11)	(-11)	8	8	8
57	La	(-14)	(-14)	3	3	3
58	Ce	-10	-10	3	3	3
59	Pr	-9	-9	4	3	3
60	Nd	-8	-8	4	4	4
61	Pm	-7	-7	5	4	4
62	Sm	-7	-7	5	5	4

(continued)

Cr K α

Atom	$\Delta f'$		$\Delta f''$		
	$\sin \theta/\lambda = 0.0$	0.4	$\sin \theta/\lambda = 0.0$	0.3	0.4
63 Eu	-6	-6	5	5	5
64 Gd	-6	-6	6	5	5
65 Tb	-6	-6	6	6	6
66 Dy	-5	-6	7	6	6
67 Ho	-5	-5	7	7	7
68 Er	-5	-5	8	7	7
69 Tm	-5	-5	8	8	8
70 Yb	-5	-5	9	8	8
71 Lu	-5	-5	9	9	9
72 Hf	-5	-5	10	10	9
73 Ta	-5	-5	11	10	10
74 W	-5	-5	11	11	10
75 Re	-5	-5	12	12	11
76 Os	-5	-5	13	12	12
77 Ir	-5	-5	14	13	13
78 Pt	-5	-5	15	14	14
79 Au	-5	-5	15	15	14
80 Hg	-5	-5	16	16	15
81 Tl	-5	-5	17	17	16
82 Pb	-6	-6	18	18	17
83 Bi	-6	-6	19	19	18
84 Po	-7	-7	20	20	19
85 At	-8	-8	21	21	20
86 Rn	-9	-9	23	22	22
87 Fr	-10	-10	24	23	23
88 Ra	-11	-11	25	24	24
89 Ac	-12	-12	27	26	26
90 Th	-13	-13	28	27	27
91 Pa	(-15)	(-15)	29	28	28
92 U	(-17)	(-17)	28	27	27

Cu K α radiation (λ = 1.542 Å)

Atom		$\Delta f'$		$\Delta f''$		
		$\sin\theta/\lambda$ = 0.0	0.6	$\sin\theta/\lambda$ = 0.0	0.4	0.6
7	N	0.0	0.0	0.0	0.0	0.0
8	O	0.0	0.0	0.1	0.1	0.1
9	F	0.0	0.0	0.1	0.1	0.1
10	Ne	0.1	0.1	0.2	0.1	0.1
11	Na	0.1	0.1	0.2	0.2	0.2
12	Mg	0.1	0.1	0.3	0.2	0.2
13	Al	0.2	0.1	0.3	0.3	0.3
14	Si	0.2	0.2	0.4	0.4	0.4
15	P	0.2	0.2	0.5	0.5	0.5
16	S	0.3	0.3	0.6	0.6	0.6
17	Cl	0.3	0.3	0.7	0.7	0.7
18	A	0.3	0.3	0.9	0.9	0.8
19	K	0.3	0.3	1.1	1.1	1.0
20	Ca	0.3	0.3	1.4	1.4	1.3
21	Sc	0.3	0.3	1.6	1.6	1.5
22	Ti	0.2	0.2	1.9	1.9	1.8
23	V	0.1	0.1	2.3	2.3	2.2
24	Cr	-0.1	-0.1	2.6	2.6	2.5
25	Mn	-0.5	-0.5	3.0	2.9	2.9
26	Fe	-1.1	-1.1	3.4	3.3	3.3
27	Co	-2.2	-2.2	3.9	3.8	3.8
28	Ni	(-3.1)	(-3.1)	0.6	0.6	0.5
29	Cu	-2.1	-2.1	0.7	0.7	0.6
30	Zn	-1.7	-1.7	0.8	0.7	0.7
31	Ga	-1.5	-1.5	0.9	0.8	0.8
32	Ge	-1.3	-1.3	1.1	1.0	0.9
33	As	-1.2	-1.2	1.2	1.1	1.0
34	Se	-1.0	-1.1	1.3	1.2	1.1
35	Br	-0.9	-1.0	1.5	1.4	1.3

(continued)

Cu K α

Atom	$\Delta f'$		$\Delta f''$		
	$\sin \theta/\lambda = 0.0$	0.6	$\sin \theta/\lambda = 0.0$	0.4	0.6
36 Kr	-0.9	-1.0	1.7	1.6	1.5
37 Rb	-0.8	-0.9	1.9	1.8	1.7
38 Sr	-0.7	-0.8	2.1	2.0	1.8
39 Y	-0.7	-0.8	2.3	2.2	2.0
40 Zr	-0.6	-0.7	2.5	2.4	2.2
41 Nb	-0.6	-0.7	2.8	2.6	2.5
42 Mo	-0.5	-0.6	3.0	2.8	2.7
43 Tc	-0.5	-0.6	3.3	3.1	3.0
44 Ru	-0.5	-0.6	3.6	3.4	3.3
45 Rh	-0.5	-0.6	4.0	3.8	3.6
46 Pd	-0.5	-0.6	4.3	4.1	3.9
47 Ag	-0.5	-0.6	4.7	4.5	4.3
48 Cd	-0.6	-0.7	5.0	4.8	4.6
49 In	-0.6	-0.8	5.4	5.2	5.0
50 Sn	-0.7	-0.9	5.8	5.6	5.4
51 Sb	-0.8	-1.0	6.3	6.1	5.8
52 Te	-0.9	-1.1	6.7	6.5	6.2
53 I	-1.1	-1.3	7.2	6.9	6.7
54 Xe	-1.4	-1.6	7.8	7.5	7.2
55 Cs	-1.7	-1.9	8.3	8.0	7.7
56 Ba	-2.1	-2.3	8.9	8.6	8.3
57 La	-2.5	-2.7	9.6	9.2	8.9
58 Ce	-2.9	-3.1	10.3	9.9	9.6
59 Pr	-3.4	-3.6	11.0	10.6	10.2
60 Nd	-4.2	-4.4	11.7	11.3	10.9
61 Pm	-5.1	-5.3	12.4	12.0	11.5
62 Sm	-6.6	-6.7	13.3	12.8	12.4
63 Eu	--	--	11.0	10.6	10.2
64 Gd	(-12)	(-12)	12.0	11.6	11.2
65 Tb	(-11)	(-11)	8	7	7
66 Dy	-10	-10	8	8	8

(continued)

Cu K α

Atom		$\Delta f'$		$\Delta f''$		
		$\sin\theta/\lambda = 0.0$	0.4	$\sin\theta/\lambda = 0.0$	0.4	0.6
67	Ho	(-13)	(-13)	4	4	3
68	Er	(- 9)	(- 9)	4	4	3
69	Tm	-8	-8	5	4	4
70	Yb	-7	-8	5	4	4
71	Lu	-7	-7	5	5	4
72	Hf	-6	-7	5	5	4
73	Ta	-6	-6	6	5	5
74	W	-6	-6	6	5	5
75	Re	-5	-6	6	6	5
76	Os	-5	-6	7	6	6
77	Ir	-5	-6	7	7	6
78	Pt	-5	-5	8	7	7
79	Au	-5	-5	8	8	7
80	Hg	-5	-5	9	8	8
81	Tl	-4	-5	9	9	8
82	Pb	-4	-5	10	9	9
83	Bi	-4	-5	10	10	9
84	Po	-4	-5	11	10	10
85	At	-4	-5	11	11	10
86	Rn	-4	-5	12	11	11
87	Fr	-4	-5	12	12	11
88	Ra	-4	-5	13	12	12
89	Ac	-4	-5	14	13	12
90	Th	-4	-5	15	14	13
91	Pa	-4	-5	16	15	14
92	U	-4	-5	16	16	15
93	Np	-4	-5	17	16	16
94	Pu	-5	-5	18	17	16
95	Am	-5	-5	19	18	17
96	Cm	-6	-6	20	19	18

Mo K α radiation (λ = 0.7107 Å)

Atom		Δf'			Δf"			
		sin θ/λ = 0.0	0.9	1.3	sin θ/λ = 0.0	0.6	0.9	1.3
10	Ne	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11	Na	0.0	0.0	0.0	0.1	0.1	0.1	0.0
12	mg	0.0	0.0	0.0	0.1	0.1	0.1	0.1
13	Al	0.1	0.1	0.0	0.1	0.1	0.1	0.1
14	Si	0.1	0.1	0.1	0.1	0.1	0.1	0.1
15	P	0.1	0.1	0.1	0.2	0.2	0.1	0.1
16	S	0.1	0.1	0.1	0.2	0.2	0.2	0.1
17	Cl	0.1	0.1	0.1	0.2	0.2	0.2	0.2
18	A	0.1	0.1	0.1	0.3	0.3	0.2	0.2
19	K	0.2	0.2	0.1	0.3	0.3	0.3	0.3
20	Ca	0.2	0.2	0.2	0.4	0.4	0.3	0.3
21	Sc	0.2	0.2	0.2	0.5	0.5	0.4	0.4
22	Ti	0.3	0.2	0.2	0.6	0.6	0.5	0.5
23	V	0.3	0.3	0.2	0.7	0.7	0.6	0.6
24	Cr	0.3	0.3	0.3	0.8	0.8	0.7	0.7
25	Mn	0.4	0.3	0.3	0.9	0.9	0.8	0.7
26	Fe	0.4	0.3	0.3	1.0	0.9	0.9	0.8
27	Co	0.4	0.3	0.3	1.1	1.0	1.0	0.9
28	Ni	0.4	0.3	0.3	1.2	1.1	1.1	1.0
29	Cu	0.3	0.3	0.3	1.4	1.3	1.3	1.2
30	Zn	0.3	0.3	0.2	1.6	1.5	1.5	1.4
31	Ga	0.2	0.2	0.2	1.7	1.6	1.6	1.5
32	Ge	0.2	0.2	0.2	1.9	1.8	1.8	1.7
33	As	0.1	0.1	0.1	2.2	2.1	2.0	1.9
34	Se	-0.1	-0.1	-0.1	2.4	2.3	2.2	2.1
35	Br	-0.3	-0.3	-0.3	2.6	2.5	2.4	2.3
36	Kr	-0.6	-0.6	-0.6	2.9	2.8	2.7	2.6
37	Rb	-0.9	-0.9	-0.9	3.2	3.1	3.0	2.9
38	Sr	-1.4	-1.4	-1.5	3.6	3.5	3.4	3.2

(continued)

Mo K α

Atom	Δf'			Δf"			
	sin θ/λ = 0.0	0.9	1.3	sin θ/λ = 0.0	0.6	0.9	1.3
39 Y	-2.3	-2.3	-2.4	3.9	3.8	3.7	3.5
40 Zr	-2.8	-2.8	-2.9	0.8	0.7	0.6	0.5
41 Nb	-2.1	-2.1	-2.2	0.9	0.8	0.6	0.5
42 Mo	-1.7	-1.7	-1.8	0.9	0.8	0.7	0.6
43 Tc	-1.4	-1.5	-1.5	1.0	0.9	0.8	0.6
44 Ru	-1.2	-1.3	-1.3	1.1	1.0	0.8	0.7
45 Rh	-1.1	-1.2	-1.3	1.2	1.1	0.9	0.8
46 Pd	-1.0	-1.1	-1.2	1.3	1.2	1.0	0.8
47 Ag	-0.9	-1.0	-1.1	1.4	1.3	1.1	0.9
48 Cd	-0.8	-0.9	-1.0	1.6	1.4	1.3	1.1
49 In	-0.7	-0.8	-0.9	1.7	1.5	1.4	1.2
50 Sn	-0.6	-0.8	-0.9	1.9	1.7	1.5	1.3
51 Sb	-0.6	-0.8	-0.9	2.0	1.8	1.6	1.4
52 Te	-0.5	-0.7	-0.8	2.2	2.0	1.8	1.5
53 I	-0.5	-0.7	-0.8	2.4	2.2	1.9	1.7
54 Xe	-0.4	-0.6	-0.8	2.5	2.3	2.1	1.8
55 Cs	-0.4	-0.6	-0.8	2.7	2.5	2.3	2.0
56 Ba	-0.4	-0.6	-0.8	3.0	2.8	2.5	2.2
57 La	-0.3	-0.5	-0.7	3.2	2.9	2.7	2.4
58 Ce	-0.3	-0.5	-0.7	3.4	3.1	2.9	2.6
59 Pr	-0.3	-0.5	-0.7	3.7	3.4	3.1	2.8
60 Nd	-0.3	-0.5	-0.7	3.9	3.6	3.3	3.0
61 Pm	-0.3	-0.5	-0.7	4.1	3.8	3.5	3.2
62 Sm	-0.3	-0.5	-0.7	4.3	4.0	3.7	3.4
63 Eu	-0.3	-0.5	-0.7	4.6	4.3	3.9	3.6
64 Gd	-0.3	-0.6	-0.7	4.8	4.5	4.1	3.8
65 Tb	-0.4	-0.6	-0.8	5.1	4.7	4.3	4.0
66 Dy	-0.4	-0.7	-0.8	5.4	5.0	4.7	4.3
67 Ho	-0.4	-0.7	-0.8	5.7	5.3	5.0	4.6
68 Er	-0.4	-0.7	-0.8	6.0	5.6	5.3	4.8

(continued)

Mo K α

Atom		$\Delta f'$			$\Delta f''$			
		sin θ/λ = 0.0	0.9	1.3	sin θ/λ = 0.0	0.6	0.9	1.3
69	Tm	-0.4	-0.8	-0.8	6.3	5.9	5.6	5.1
70	Yb	-0.5	-0.8	-0.9	6.7	6.3	5.9	5.4
71	Lu	-0.6	-0.9	-1.0	7.0	6.6	6.1	5.6
72	Hf	-0.7	-1.0	-1.1	7.3	6.9	6.4	5.9
73	Ta	-0.8	-1.1	-1.2	7.6	7.2	6.7	6.2
74	W	-1.0	-1.3	-1.4	8.0	7.6	7.1	6.5
75	Re	-1.2	-1.5	-1.6	8.3	8.0	7.5	6.9
76	Os	-1.4	-1.7	-1.8	8.8	8.4	7.9	7.3
77	Ir	-1.7	-2.0	-2.1	9.2	8.8	8.3	7.7
78	Pt	-1.9	-2.2	-2.3	9.6	9.1	8.7	8.1
79	Au	-2.2	-2.5	-2.6	10.1	9.6	9.2	8.5
80	Hg	-2.6	-2.9	-3.0	10.6	10.1	9.7	9.0
81	Tl	-3.2	-3.5	-3.6	11.2	10.7	10.2	9.5
82	Pb	-3.8	-4.1	-4.2	11.7	11.2	10.7	9.9
83	Bi	-4.5	-4.8	-4.9	11.2	11.7	11.1	10.3
84	Po	-5.3	-5.5	-5.6	12.8	12.3	11.7	10.8
85	At	--	--	--	10	10	9	9
86	Rn	(-8)	(-8)	(-8)	11	11	10	9
87	Fr	(-8)	(-8)	(-8)	8	7	7	6
88	Ra	-7	-7	-7	8	7	7	6
89	Ac	-6	-7	-7	8	8	8	7
90	Th	-6	-7	-7	9	8	7	7
91	Pa	-7	-7	-7	9	8	8	7
92	U	(-8)	(-8)	(-8)	9	9	8	7
93	Np	--	--	--	6	5	5	4
94	Pu	--	--	--	6	5	5	4
95	Am	--	--	--	6	5	5	4
96	Cm	--	--	--	6	6	5	4