Lawrence Berkeley National Laboratory

Recent Work

Title

A TABLE OF DISPERSION CORRECTIONS FOR X-RAY SCATTERING OF ATOMS

Permalink

<https://escholarship.org/uc/item/8j83x8dj>

Authors

Dauben, Carol H.
Templeton, David H.

Publication Date

1955-06-02

UNIVERSITY OF
CALIFORNIA

*Radiation
Laboratory*

A TABLE OF DISPERSION CORRECTIONS
FOR X-RAY SCATTERING OF ATOMS

TWO-WEEK LOAN COPY

*This is a Library Circulating Copy
which may be borrowed for two weeks.
For a personal retention copy, call
Tech. Info. Division, Ext. 5545*

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

UNIVERSITY OF CALIFORNIA

Radiation Laboratory

Berkeley, California

Contract No. W-7405-eng-48

A TABLE OF DISPERSION CORRECTIONS FOR X-RAY
SCATTERING OF ATOMS

Carol H. Dauben and David H. Templeton

June 2, 1955

A TABLE OF DISPERSION CORRECTIONS FOR X-RAY
SCATTERING OF ATOMS

Carol H. Dauben and David H. Templeton

Department of Chemistry and Radiation Laboratory
University of California, Berkeley, California

June 2, 1955

ABSTRACT

Values are tabulated for the real and imaginary dispersion corrections for the x-ray scattering factors for elements 20 to 96 for K_{α} radiation of chromium, copper, and molybdenum.

A TABLE OF DISPERSION CORRECTIONS FOR X-RAY
SCATTERING OF ATOMS

Carol H. Dauben and David H. Templeton

Department of Chemistry and Radiation Laboratory
University of California, Berkeley, California

June 2, 1955

The atomic scattering factor $\underline{f}$ for x-rays is a complex number:

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

where f_0 is a real function of $\sin \theta/\lambda$ which has been tabulated for many atoms.¹ The dispersion corrections $\Delta f'$ and $\Delta f''$ are functions of λ and vanish for wave lengths which are very small compared with the K absorption edge of the atom. These corrections are nearly independent of θ because the tightly-bound electrons responsible for these effects are concentrated in a small volume close to the atomic nucleus.

For convenience in using these corrections, we have tabulated values for elements 20 to 96 for three wave lengths frequently used in crystal analysis, the K_{α} lines of chromium (λ 2.2909 Å), copper (λ 1.5418 Å), and molybdenum (λ 0.7107 Å). These values were calculated by the methods of Parratt and Hempstead² for the contributions of K, L, and M electrons. The absorption edges were obtained from the tables of Cauchois and Hulubei³ or by Moseley interpolation or

extrapolation. The oscillator strengths were estimated in a highly arbitrary way from data from several sources.⁴⁻¹⁰ The uncertainty in these values is the chief source of error in our results. The exponents p have been chosen according to the example given for tungsten by Parratt and Hempstead.² Damping effects have been neglected.

The corrections are listed in Table I. Those for Cu K_{α} radiation are plotted in Figures 1 and 2.

TABLE I

Dispersion Corrections

Atomic Number		Cr K _α X-Rays		Cu K _α X-Rays		Mo K _α X-Rays	
		Δf''	-Δf'	Δf''	-Δf'	Δf''	-Δf'
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

Atomic Number		Cr K _α X-Rays		Cu K _α X-Rays		Mo K _α X-Rays	
		$\Delta f''$	$-\Delta f'$	$\Delta f''$	$-\Delta f'$	$\Delta f''$	$-\Delta f'$
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
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	8	5	4	8	6.4	0.6
71	Lu	9	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

Atomic Number		Cr K _α X-Rays		Cu K _α X-Rays		Mo K _α X-Rays	
		$\Delta f''$	$-\Delta f'$	$\Delta f''$	$-\Delta f'$	$\Delta f''$	$-\Delta f'$
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.

REFERENCES

1. "Internationale Tabellen zur Bestimmung von Kristallstrukturen," Vol. II, Edwards Brothers, Ann Arbor, Michigan (1944).
2. L. G. Parratt and C. F. Hempstead, Phys. Rev. 94, 1593 (1954).
3. Y. Cauchois and H. Hulubei, "Tables de constantes et données numériques, I. Constantes sélectionnées longueurs d'onde des émissions x et des discontinuités d'absorption x," Hermann and Cie, Paris (1947).
4. H. Hönl, Z. Physik 48, 469 (1928); Ann. Physik 18, 654 (1933).
5. E. J. Williams, Proc. Roy. Soc. (London) 143A, 358 (1933).
6. J. A. Wheeler and J. A. Beardeu, Phys. Rev. 46, 755 (1934).
7. M. Wolf, Ann. Physik 16, 973 (1933).
8. F. K. Richtmeyer, Phys. Rev. 27, 1 (1926).
9. B. Walter, Fortschritte a. d. Geb. der Röntgen 35, 929, 1308 (1927), as given by A. H. Compton and S. K. Allison, "X-Rays in Theory and Experiment," D. Van Nostrand Company, New York (1935) 545.
10. H. Eisenlohr and G. J. J. Müller, Z. Physik 136, 511 (1954).

Fig. 1. Real correction to f_0 for copper K_α x-rays.

MU-9754

Fig. 2. Imaginary correction to f_0 for copper K_{α} x-rays.