

4.2. X-RAYS

Table 4.2.6.5. Comparison of measurements of $f'(\omega, 0)$ for C, Si and Cu for characteristic wavelengths $AgK\alpha_1$, $MoK\alpha_1$ and $CuK\alpha_1$ with theoretical predictions; the measurements are from the IUCr X-ray Attenuation Project Report (Creagh & Hubbell, 1987, 1990), corrected for the effects of Compton, Laue–Bragg, and small-angle scattering

Sample	Reference	$f'(\omega, 0)$		
		Cu $K\alpha_1$	Mo $K\alpha_1$	Ag $K\alpha_1$
⁶ C	Theory			
	This work	0.0091	0.0016	0.0009
	Cromer & Liberman (1981)	0.0091	0.0016	0.0009
	Wagenfeld (1975)	–	–	–
	Scofield (1973)	0.0093	0.0016	0.0009
	Storm & Israel (1970)	0.0090	0.0016	0.0009
	Experiment IUCr Project	0.0093	0.0016	0.0009
¹⁴ Si	Theory			
	This work	0.330	0.070	0.043
	Cromer & Liberman (1981)	0.330	0.0704	0.0431
	Wagenfeld (1975)	0.330	0.071	0.044
	Scofield (1973)	0.332	0.0702	0.0431
	Storm & Israel (1970)	0.331	0.0698	0.0429
	Experiment IUCr Project	0.332	0.0696	0.0429
²⁹ Cu	Theory			
	This work	0.588	1.265	0.826
	Cromer & Liberman (1981)	0.589	1.265	0.826
	Scofield (1973)	0.586	1.256	0.826
	Experiment IUCr Project	0.588	1.267	0.826

the incident photon beam. Another important feature is the difference of 0.16 electrons between the Kramers–Kronig and the interferometer values. Bonse & Henning (1986) did not add the relativistic correction term to their Kramers–Kronig values. Inclusion of this term would have reduced the quoted values by 0.20, bringing the two data sets into close agreement with one another.

Katoh *et al.* (1985b) have made measurements spanning the K -absorption edge of germanium using the deviation by a prism method, and these data have been shown to be in excellent agreement with the theory on which these tables are based (Creagh, 1993). In contrast, the theoretical approach of Pratt, Kissell & Bergstrom (1994) does not agree so well, especially near to, and at higher photon energies, than the K -edge energy. Also, Chapuis *et al.* (1985) have measured the dispersion corrections for holmium in $[HoNa(edta)] \cdot 8H_2O$ for the characteristic emission lines $CuK\alpha_1$, $CuK\alpha_2$, $CuK\beta$, and $MoK\alpha_1$ using a refinement technique. Their results are in reasonable agreement with the relativistic multipole theory, *e.g.* for $f'(\omega, \Delta)$ at the wavelength of $CuK\alpha_1$ experiment gives $-(16.0 \pm 0.2)$ whereas the relative multipole approach yields -15.0 . For $CuK\alpha_2$, experiment yields $-(13.9 \pm 0.3)$ and theory gives -13.67 . The discrepancy between theory and experiment may well be explained by the oxidation state of the holmium ion, which is in the form Ho^{3+} . The oxidation state of an atom affects both the position of the absorption edge and the magnitude of the

relativistic correction. Both of these will have a large influence on the value of $f'(\omega, \Delta)$ in the neighbourhood of the absorption edge. Another problem that may be of some significance is the natural width of the absorption edge, about 60 eV. What is remarkable is the extent of the agreement between theory and experiment given the nature of the experiment. In these experiments, the intensities of many reflections (usually nearly 1000) are analysed and compared. Such a procedure can be followed only if there is no dependence of $f'(\omega, \Delta)$ on Δ .

It had often been thought that the dispersion corrections should exhibit some functional dependence on scattering angle. Indeed, some texts ascribe to these corrections the same functional dependence on angle of scattering as the form factor. A fundamental dependence was also predicted theoretically on the basis of non-relativistic quantum mechanics (Wagenfeld, 1975). This prediction is not supported by modern approaches using relativistic quantum mechanics [see, for example, Kissel *et al.* (1980)]. Reference to Tables 4.2.6.4 and 4.2.6.6 shows that the agreement between experimental values derived from diffraction experiments and those derived from 'direct' experiments is excellent. They are also in excellent agreement with the recent calculations, using relativistic quantum mechanics, so that it may be inferred that there is indeed no functional dependence of the dispersion corrections on scattering angle. Moreover, Suortti, Hastings & Cox (1985) have recently demonstrated that $f'(\omega, \Delta)$ was independent of Δ in a powder-diffraction experiment using a nickel specimen.

4.2.6.3.3.3. Accuracy in the tables of dispersion corrections

Experimentalists must be aware of two potential sources of error in the values of $f'(\omega, 0)$ listed in Table 4.2.6.5. One is computational, arising from the error in calculating the relativistic correction. Stibius-Jensen (1980) has suggested that this error may be as large as $\pm 0.25(E_{tot}/mc^2)$. This means, for example, that the real part of the dispersion correction $f'(\omega, 0)$ for lead at the wavelength of 0.55936 Å is $-(1.168 \pm 0.146)$. The effect of this error is to shift the dispersion curve vertically without distorting its shape. Note, however, that the direction of the shift is either up or down for all atoms: the effect of multipole cancellation and retardation will be in the same direction for all atoms.

The second possible source of error occurs because the position of the absorption edge varies somewhat depending on the oxidation state of the scattering atom. This has the effect of displacing the dispersion curve laterally. Large discrepancies may occur for those regions in which the dispersion corrections are varying rapidly with photon energy, *i.e.* near absorption edges.

It must also be borne in mind that in the neighbourhood of an absorption edge polarization effects may occur. The tables are valid only for average polarization.

4.2.6.3.3.4. Towards a tensor formalism

The question of how best to describe the interaction of X-rays with crystalline materials is quite difficult to answer. In the form factor formalism, the atoms are supposed to scatter as though they are isolated atoms situated at fixed positions in the unit cell. In the vast majority of cases, the polarization on scattering is not detected, and only the scattered intensities are measured. From the scattered intensities, the distribution of the electron density within the unit cell is calculated, and the difference between the form-factor model and that calculated from the intensities is taken as a measure of the nature and location of chemical bonds between atoms in the unit cell.

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Table 4.2.6.6. Comparison of $f'(\omega_A, 0)$ for copper, nickel, zirconium, and niobium for theoretical and experimental data sets; in this table: BR \equiv Bragg reflection; IN \equiv interferometer; KK \equiv Kramers–Kronig; CA = critical angle; and REF = reflectivity; measurements have been made for the K-absorption edges of copper and nickel and near the K-absorption edges of zirconium and niobium; claimed experimental errors are not worse than 5%

Reference	Method	$f'(\omega_A, 0)$			
		Cu	Ni	Nb	Zr
Experiment					
Freund (1975)	BR	−8.2			
Begum, Hart, Lea & Siddons (1986)	IN	−7.84	−7.66		
Bonse & Materlik (1972)	IN		−8.1		
Bonse, Hartmann-Lotsch & Lotsch (1983a)	IN	−8.3			
Hart & Siddons (1981)	IN	−9.3	−9.2	−4.396	−6.670
Kawamura & Fukimachi (1978; cited in Bonse & Hartmann-Lotsch, 1984)	KK		−7.9		
Dreier <i>et al.</i> (1984)	KK	−8.2	−7.8		−7.83
	IN	−8.3	−8.1		
Bonse & Hartmann-Lotsch (1984)	KK	−8.3	−7.7		
Fukamachi <i>et al.</i> (1978; cited in Bonse & Hartmann-Lotsch, 1984)	KK	−8.8			
	CA	−10.0			
Bonse & Henning (1986)	IN			−7.37; −7.73	
	KK			−7.21; −7.62	
Stanglmeier, Lengeler, Weber, Gobel & Schuster (1992)	REF	−8.5	−8.1		
Creagh (1990, 1993)	REF	−8.2	−7.7		−6.8
Theory					
Cromer & Liberman (1981)		−13.50	−9.45	−4.20; −7.39	−6.207
This work		−9.5	−9.40	−4.04; −7.23	−6.056
Averaged values (5 eV) window		−9.0	−7.53	−8.18	−6.04

This is the zeroth-order approximation to a solution, but it is in fact the only way crystal structures are solved *ab initio*.

The existence of chemical bonding imposes additional restrictions on the symmetry of lattices, and, if the associated influence this has on the complexity of energy levels is taken into account, significant changes in the scattering factors may occur in the neighbourhood of the absorption edges of the atoms comprising the crystal structure. The magnitudes of the dispersion corrections are sensitive to the chemical state, particularly oxidation state, and phenomena similar to those observed in the XAFS case (Section 4.2.4) are observed.

The XAFS interaction arising from the presence of neighbouring atoms is proportional to $f''(\omega, 0)$ and therefore is related to $f'(\omega, 0)$ through the Kramers–Kronig integral. It is not surprising that these modulations are observed in diffracted intensities in those X-ray diffraction experiments where the photon energy is scanned through the absorption edge of an atomic species in the crystal lattice. Studies of this type are referred to as diffraction absorption fine structure (DAFS) experiments. A recent review of work performed using counter techniques has been given by Sorenson (1994). Creagh & Cookson (1995) have described the use of imaging-plate techniques to study the structure and site symmetry using the DAFS technique. This technique has the ability to discriminate between different lattice sites in the unit cell occupied by an atomic species. XAFS cannot make this discrimination. The DAFS modulations are small perturbations to the diffracted intensities. They are, however, significantly larger than the tensor effects described in the following paragraphs.

In the case where the excited state lacks high symmetry and is oriented by crystal bonding, the scattering can no longer be

Table 4.2.6.7. List of wavelengths, energies, and linewidths used in compiling the table of dispersion corrections (a) Agarwal (1979); (b) Deutsch & Hart (1982)

Radiation	Wavelength (Å)	Energy (keV)	Linewidth (eV)
⁷⁹ Au $K\alpha_1$	0.180195	68.803	46 (a)
⁷⁴ W $K\alpha_1$	0.209010	59.318	43 (a)
⁷³ Ta $K\alpha_1$	0.215947	57.412	42 (a)
⁴⁷ Ag $K\alpha_1$	0.559360	22.165	7 (a)
⁴² Mo $K\alpha_1$	0.709260	17.480	4 (a)
²⁹ Cu $K\alpha_1$	1.540520	8.04792	2.61 (b)
²⁷ Co $K\alpha_1$	1.788965	6.9302	1.8
²⁶ Fe $K\alpha_1$	1.93597	6.4040	1.6
²⁴ Cr $K\alpha_1$	2.289620	5.4149	1.5
²² Ti $K\alpha_1$	2.748510	4.5108	1.4

described by a scalar scattering factor but must be described by a symmetric second-rank tensor. The consequences of this have been described by Templeton (1994). It follows therefore that material media can be optically active in the X-ray region. Hart (1994) has used his unique polarizing X-ray optical devices to study, for example, Faraday rotation in such materials as iron, in the region of the iron K -absorption edge, and cobalt(III) bromide monohydrate in the region of the cobalt K -absorption edge.

The theory of anisotropy in anomalous scattering has been treated extensively by Kirfel (1994), and Morgenroth, Kirfel

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Table 4.2.6.8. *Dispersion corrections for forward scattering*

Wavelength (Å)	2.748510	2.289620	1.935970	1.788965	1.540520	0.709260	0.559360	0.215947	0.209010	0.180195
Li	f' =	0.0035	0.0023	0.0015	0.0013	0.0008	-0.0003	-0.0004	-0.0006	-0.0006
	f'' =	0.0013	0.0008	0.0006	0.0005	0.0003	0.0001	0.0000	0.0000	0.0000
Be	f' =	0.0117	0.0083	0.0060	0.0052	0.0038	0.0005	0.0001	-0.0005	-0.0005
	f'' =	0.0050	0.0033	0.0023	0.0019	0.0014	0.0002	0.0001	0.0000	0.0000
B	f' =	0.0263	0.0190	0.0140	0.0121	0.0090	0.0013	0.0004	-0.0009	-0.0009
	f'' =	0.0139	0.0094	0.0065	0.0055	0.0039	0.0007	0.0004	0.0000	0.0000
C	f' =	0.0490	0.0364	0.0273	0.0237	0.0181	0.0033	0.0015	-0.0012	-0.0013
	f'' =	0.0313	0.0213	0.0148	0.0125	0.0091	0.0016	0.0009	0.0001	0.0001
N	f' =	0.0807	0.0606	0.0461	0.0403	0.0311	0.0061	0.0030	-0.0020	-0.0020
	f'' =	0.0606	0.0416	0.0293	0.0248	0.0180	0.0033	0.0019	0.0002	0.0002
O	f' =	0.1213	0.0928	0.0716	0.0630	0.0492	0.0106	0.0056	-0.0025	-0.0026
	f'' =	0.1057	0.0731	0.0518	0.0440	0.0322	0.0060	0.0036	0.0004	0.0004
F	f' =	0.1700	0.1324	0.1037	0.0920	0.0727	0.0171	0.0096	-0.0027	-0.0028
	f'' =	0.1710	0.1192	0.0851	0.0725	0.0534	0.0103	0.0061	0.0007	0.0007
Ne	f' =	0.2257	0.1793	0.1426	0.1273	0.1019	0.0259	0.0152	-0.0025	-0.0028
	f'' =	0.2621	0.1837	0.1318	0.1126	0.0833	0.0164	0.0098	0.0012	0.0011
Na	f' =	0.2801	0.2295	0.1857	0.1670	0.1353	0.0362	0.0218	-0.0028	-0.0031
	f'' =	0.3829	0.2699	0.1957	0.1667	0.1239	0.0249	0.0150	0.0019	0.0017
Mg	f' =	0.3299	0.2778	0.2309	0.2094	0.1719	0.0486	0.0298	-0.0030	-0.0034
	f'' =	0.5365	0.3812	0.2765	0.2373	0.1771	0.0363	0.0220	0.0028	0.0026
Al	f' =	0.3760	0.3260	0.2774	0.2551	0.2130	0.0645	0.0406	-0.0020	-0.0026
	f'' =	0.7287	0.5212	0.3807	0.3276	0.2455	0.0514	0.0313	0.0040	0.0037
Si	f' =	0.3921	0.3647	0.3209	0.2979	0.2541	0.0817	0.0522	-0.0017	-0.0025
	f'' =	0.9619	0.6921	0.5081	0.4384	0.3302	0.0704	0.0431	0.0056	0.0052
P	f' =	0.3821	0.3898	0.3592	0.3388	0.2955	0.1023	0.0667	-0.0002	-0.0012
	f'' =	1.2423	0.8984	0.6628	0.5731	0.4335	0.0942	0.0580	0.0077	0.0071
S	f' =	0.3167	0.3899	0.3848	0.3706	0.3331	0.1246	0.0826	0.0015	0.0003
	f'' =	1.5665	1.1410	0.8457	0.7329	0.5567	0.1234	0.0763	0.0103	0.0096
Cl	f' =	0.1832	0.3508	0.3920	0.3892	0.3639	0.1484	0.0998	0.0032	0.0017
	f'' =	1.9384	1.4222	1.0596	0.9202	0.7018	0.1585	0.0984	0.0134	0.0125
Ar	f' =	-0.0656	0.2609	0.3696	0.3880	0.3843	0.1743	0.1191	0.0059	0.0041
	f'' =	2.3670	1.7458	1.3087	1.1388	0.8717	0.2003	0.1249	0.0174	0.0162
K	f' =	-0.5083	0.0914	0.3068	0.3532	0.3868	0.2009	0.1399	0.0089	0.0067
	f'' =	2.8437	2.1089	1.5888	1.3865	1.0657	0.2494	0.1562	0.0219	0.0204
Ca	f' =	-1.3666	-0.1987	0.1867	0.2782	0.3641	0.2262	0.1611	0.0122	0.0097
	f'' =	3.3694	2.5138	1.9032	0.6648	1.2855	0.3064	0.1926	0.0273	0.0255
Sc	f' =	-5.4265	-0.6935	-0.0120	0.1474	0.3119	0.2519	0.1829	0.0159	0.0130
	f'' =	4.0017	2.9646	2.2557	1.9774	1.5331	0.3716	0.2348	0.0338	0.0315
Ti	f' =	-2.2250	-1.6394	-0.3318	-0.0617	0.2191	0.2776	0.2060	0.0212	0.0179
	f'' =	0.5264	3.4538	2.6425	2.3213	1.8069	0.4457	0.2830	0.0414	0.0387
V	f' =	-1.6269	-4.4818	-0.8645	-0.3871	0.0687	0.3005	0.2276	0.0259	0.0221
	f'' =	0.6340	0.4575	3.0644	2.6994	2.1097	0.5294	0.3376	0.0500	0.0468
Cr	f' =	-1.2999	-2.1308	-1.9210	-0.9524	-0.1635	0.3209	0.2496	0.0314	0.0272
	f'' =	0.7569	0.5468	3.5251	3.1130	2.4439	0.6236	0.3992	0.0599	0.0561
Mn	f' =	-1.0732	-1.5980	-3.5716	-2.0793	-0.5299	0.3368	0.2704	0.0377	0.0330
	f'' =	0.8956	0.6479	0.4798	3.5546	2.8052	0.7283	0.4681	0.0712	0.0666
Fe	f' =	-0.8901	-1.2935	-2.0554	-3.3307	-1.1336	0.3463	0.2886	0.0438	0.0386
	f'' =	1.0521	0.7620	0.5649	0.4901	3.1974	0.8444	0.5448	0.0840	0.0787
Co	f' =	-0.7307	-1.0738	-1.5743	-2.0230	-2.3653	0.3494	0.3050	0.0512	0.0454
	f'' =	1.2272	0.8897	0.6602	0.5731	3.6143	0.9721	0.6296	0.0984	0.0921
Ni	f' =	-0.5921	-0.9005	-1.2894	-1.5664	-3.0029	0.3393	0.3147	0.0563	0.0500
	f'' =	1.4240	1.0331	0.7671	0.6662	0.5091	1.1124	0.7232	0.1146	0.1074
Cu	f' =	-0.4430	-0.7338	-1.0699	-1.2789	-1.9646	0.3201	0.3240	0.0647	0.0579
	f'' =	1.6427	1.1930	0.8864	0.7700	0.5888	1.2651	0.8257	0.1326	0.1242
Zn	f' =	-0.3524	-0.6166	-0.9134	-1.0843	-1.5491	0.2839	0.3242	0.0722	0.0648
	f'' =	1.8861	1.3712	1.0193	0.8857	0.6778	1.4301	0.9375	0.1526	0.1430
Ga	f' =	-0.2524	-0.4989	-0.7701	-0.9200	-1.2846	0.2307	0.3179	0.0800	0.0721
	f'' =	2.1518	1.5674	1.1663	1.0138	0.7763	1.6083	1.0589	0.1745	0.1636
Ge	f' =	-0.1549	-0.3858	-0.6412	-0.7781	-1.0885	0.1547	0.3016	0.0880	0.0796
	f'' =	2.4445	1.7841	1.3291	1.1557	0.8855	1.8001	1.1903	0.1987	0.1863
As	f' =	-0.0687	-0.2871	-0.5260	-0.6523	-0.9300	0.0499	0.2758	0.0962	0.0873
	f'' =	2.7627	2.0194	1.5069	1.3109	1.0051	2.0058	1.3314	0.2252	0.2112
Se	f' =	0.0052	-0.1919	-0.4179	-0.5390	-0.7943	-0.0929	0.2367	0.1047	0.0954
	f'' =	3.1131	2.2784	1.7027	1.4821	1.1372	2.2259	1.4831	0.2543	0.2386
Br	f' =	0.0592	-0.1095	-0.3244	-0.4363	-0.6763	-0.2901	0.1811	0.1106	0.1026
	f'' =	3.4901	2.5578	1.9140	1.6673	1.2805	2.4595	1.6452	0.2858	0.2682
Kr	f' =	0.1009	-0.0316	-0.2303	-0.3390	-0.5657	-0.5574	0.1067	0.1180	0.1082
	f'' =	3.9083	2.8669	2.1472	1.8713	1.4385	2.7079	1.8192	0.3197	0.3003

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Table 4.2.6.8. Dispersion corrections for forward scattering (cont.)

Wavelength (Å)	2.748510	2.289620	1.935970	1.788965	1.540520	0.709260	0.559360	0.215947	0.209010	0.180195	
Rb	$f' =$	0.1056	0.0247	-0.1516	-0.2535	-0.4688	-0.9393	0.0068	0.1247	0.1146	0.0717
	$f'' =$	4.3505	3.1954	2.3960	2.0893	1.6079	2.9676	2.0025	0.3561	0.3346	0.2514
Sr	$f' =$	0.1220	0.1037	-0.0489	-0.1448	-0.3528	-1.5307	-0.1172	0.1321	0.1219	0.0769
	$f'' =$	4.8946	3.6029	2.7060	2.3614	1.8200	3.2498	2.2025	0.3964	0.3726	0.2805
Y	$f' =$	0.0654	0.1263	0.0138	-0.0720	-0.2670	-2.7962	-0.2879	0.1380	0.1278	0.0819
	$f'' =$	5.4198	3.9964	3.0054	2.6241	2.0244	3.5667	2.4099	0.4390	0.4128	0.3112
Zr	$f' =$	-0.0304	0.1338	0.0659	-0.0066	-0.1862	-2.9673	-0.5364	0.1431	0.1329	0.0863
	$f'' =$	5.9818	4.4226	3.3301	2.9086	2.2449	0.5597	2.6141	0.4852	0.4562	0.3443
Nb	$f' =$	-0.1659	0.1211	0.1072	0.0496	-0.1121	-2.0727	-0.8282	0.1471	0.1371	0.0905
	$f'' =$	6.5803	4.8761	3.6768	3.2133	2.4826	0.6215	2.8404	0.5342	0.5025	0.3797
Mo	$f' =$	-0.3487	0.0801	0.1301	0.0904	-0.0483	-1.6832	-1.2703	0.1487	0.1391	0.0934
	$f'' =$	7.2047	5.3484	4.0388	3.5326	2.7339	0.6857	3.0978	0.5862	0.5517	0.4177
Tc	$f' =$	-0.6073	-0.0025	0.1314	0.1164	0.0057	-1.4390	-2.0087	0.1496	0.1406	0.0960
	$f'' =$	7.8739	5.8597	4.4331	3.8799	3.0049	0.7593	3.3490	0.6424	0.6047	0.4582
Ru	$f' =$	-0.9294	-0.1091	0.1220	0.1331	0.0552	-1.2594	-5.3630	0.1491	0.1409	0.0981
	$f'' =$	8.5988	6.4069	4.8540	4.2509	3.2960	0.8363	3.6506	0.7016	0.6607	0.5014
Rh	$f' =$	-1.3551	-0.2630	0.0861	0.1305	0.0927	-1.1178	-2.5280	0.1445	0.1373	0.0970
	$f'' =$	9.3504	6.9820	5.2985	4.6432	3.6045	0.9187	0.5964	0.7639	0.7195	0.5469
Pd	$f' =$	-1.9086	-0.4640	0.0279	0.1128	0.1215	-0.9988	-1.9556	0.1387	0.1327	0.0959
	$f'' =$	10.1441	7.5938	5.7719	5.0613	3.9337	1.0072	0.6546	0.8302	0.7822	0.5955
Ag	$f' =$	-2.5003	-0.7387	-0.0700	0.0634	0.1306	-0.8971	-1.6473	0.1295	0.1251	0.0928
	$f'' =$	10.9916	8.2358	6.2709	5.5027	4.2820	1.1015	0.7167	0.9001	0.8484	0.6469
Cd	$f' =$	-3.5070	-1.1086	-0.2163	-0.0214	0.1185	-0.8075	-1.4396	0.1171	0.1147	0.0881
	$f'' =$	11.9019	8.9174	6.8017	5.9728	4.6533	1.2024	0.7832	0.9741	0.9185	0.7013
In	$f' =$	-5.1325	-1.5975	-0.4165	-0.1473	0.0822	-0.7276	-1.2843	0.1013	0.1012	0.0816
	$f'' =$	12.6310	9.6290	7.3594	6.4674	5.0449	1.3100	0.8542	1.0519	0.9922	0.7587
Sn	$f' =$	-7.5862	-2.2019	-0.6686	-0.3097	0.0259	-0.6537	-1.1587	0.0809	0.0839	0.0728
	$f'' =$	13.5168	10.3742	7.9473	6.9896	5.4591	1.4246	0.9299	1.1337	1.0697	0.8192
Sb	$f' =$	-9.2145	-3.0637	-0.9868	-0.5189	-0.0562	-0.5866	-1.0547	0.0559	0.0619	0.0613
	$f'' =$	12.7661	11.1026	8.5620	7.5367	5.8946	1.5461	1.0104	1.2196	1.1512	0.8830
Te	$f' =$	-11.6068	-4.2407	-1.4022	-0.7914	-0.1759	-0.5308	-0.9710	0.0216	0.0316	0.0435
	$f'' =$	-10.1013	11.8079	9.2067	8.1113	6.3531	1.6751	1.0960	1.3095	1.2366	0.9499
I	$f' =$	-13.9940	-5.6353	1.9032	1.1275	-0.3257	-0.4742	-0.8919	-0.0146	-0.0001	0.0259
	$f'' =$	3.4071	12.6156	9.8852	8.7159	6.8362	1.8119	1.1868	1.4037	1.3259	1.0201
Xe	$f' =$	-9.6593	-8.1899	-2.6313	-1.5532	-0.5179	-0.4205	-0.8200	-0.0565	-0.0367	0.0057
	$f'' =$	3.7063	11.7407	10.5776	9.3585	7.3500	1.9578	1.2838	1.5023	1.4195	1.0938
Cs	$f' =$	-8.1342	-10.3310	-3.5831	-2.1433	-0.7457	-0.3680	-0.7527	-0.1070	-0.0809	0.0194
	$f'' =$	4.0732	12.8551	11.2902	10.0454	7.9052	2.1192	1.3916	1.6058	1.5179	1.1714
Ba	$f' =$	-7.2079	-11.0454	-4.6472	-2.7946	-1.0456	-0.3244	-0.6940	-0.1670	-0.1335	-0.0494
	$f'' =$	4.4110	10.0919	12.0003	10.7091	8.4617	2.2819	1.5004	1.7127	1.6194	1.2517
La	$f' =$	-6.5722	-12.8190	-6.3557	-3.6566	-1.4094	-0.2871	-0.6411	-0.2363	-0.1940	-0.0835
	$f'' =$	4.7587	3.5648	12.8927	11.4336	9.0376	2.4523	1.6148	1.8238	1.7250	1.3353
Ce	$f' =$	-6.0641	-9.3304	-8.0962	-4.8792	-1.8482	-0.2486	-0.5890	-0.3159	-0.2633	-0.1222
	$f'' =$	5.1301	3.8433	11.8734	12.1350	9.6596	2.6331	1.7358	1.9398	1.8353	1.4227
Pr	$f' =$	-5.6727	-7.9841	-10.9279	-6.7923	-2.4164	-0.2180	-0.5424	-0.4096	-0.3443	-0.1666
	$f'' =$	5.5091	4.1304	9.2394	12.8653	10.2820	2.8214	1.8624	2.0599	1.9496	1.5136
Nd	$f' =$	-5.3510	-7.1451	-10.5249	-8.1618	-3.1807	-0.1943	-0.5012	-0.5194	-0.4389	-0.2183
	$f'' =$	5.9005	4.4278	9.9814	11.9121	10.9079	3.0179	1.9950	2.1843	2.0679	1.6077
Pm	$f' =$	-5.0783	-6.5334	-13.2062	-10.0720	-4.0598	-0.1753	-0.4626	-0.6447	-0.5499	-0.2776
	$f'' =$	6.3144	4.7422	3.6278	9.2324	11.5523	3.2249	2.1347	2.3143	2.1906	1.7056
Sm	$f' =$	-4.8443	-6.0570	-9.3497	-10.2609	-5.3236	-0.1638	-0.4287	-0.7989	-0.6734	-0.3455
	$f'' =$	6.7524	5.0744	3.8839	9.9412	12.2178	3.4418	2.2815	2.4510	2.3197	1.8069
Eu	$f' =$	-4.6288	-5.6630	-7.9854	-13.5405	-8.9294	-0.1578	-0.3977	-0.9903	-0.8137	-0.4235
	$f'' =$	7.2035	5.4178	4.1498	3.6550	11.1857	3.6682	2.4351	2.5896	2.4526	1.9120
Gd	$f' =$	-4.5094	-5.3778	-7.1681	-9.3863	-8.8380	-0.1653	-0.3741	-1.2279	-1.0234	-0.5140
	$f'' =$	7.6708	5.7756	4.4280	3.9016	11.9157	3.9035	2.5954	2.7304	2.5878	2.0202
Tb	$f' =$	-4.3489	-5.0951	-6.5583	-8.0413	-9.1472	-0.1723	-0.3496	-1.5334	-1.2583	-0.6165
	$f'' =$	8.1882	6.1667	4.7292	4.1674	9.1891	4.1537	2.7654	2.8797	2.7310	2.1330
Dy	$f' =$	-4.1616	-4.8149	-6.0597	-7.1503	-9.8046	-0.1892	-0.3302	-1.9594	-1.5632	-0.7322
	$f'' =$	8.6945	6.5527	5.0280	4.4320	9.8477	4.4098	2.9404	3.0274	2.8733	2.2494
Ho	$f' =$	-4.0280	-4.5887	-5.6628	-6.5338	-14.9734	-0.2175	-0.3168	-2.6705	-1.9886	-0.8709
	$f'' =$	9.2302	6.9619	5.3451	4.7129	3.7046	4.6783	3.1241	3.1799	3.0218	2.3711
Er	$f' =$	-3.9471	-4.4106	-5.3448	-6.0673	-9.4367	-0.2586	-0.3091	-5.5645	-2.6932	-1.0386
	$f'' =$	9.7921	7.3910	5.6776	5.0074	3.9380	4.9576	3.3158	0.6167	3.1695	2.4949
Tm	$f' =$	-3.9079	-4.2698	-5.0823	-5.6969	-8.0393	-0.3139	-0.3084	-2.8957	-5.6057	-1.2397
	$f'' =$	10.3763	7.8385	6.0249	5.3151	4.1821	5.2483	3.5155	0.6569	0.6192	2.6240
Yb	$f' =$	-3.8890	-4.1523	-4.8591	-5.3940	-7.2108	-0.3850	-0.3157	-2.4144	-2.9190	-1.4909
	$f'' =$	10.9742	8.2969	6.3813	5.6309	4.4329	5.5486	3.7229	0.6994	0.6592	2.7538

4.2. X-RAYS

Table 4.2.6.8. Dispersion corrections for forward scattering (cont.)

Wavelength (Å)	2.748510	2.289620	1.935970	1.788965	1.540520	0.709260	0.559360	0.215947	0.209010	0.180195	
Lu	f'	-3.9056	-4.0630	-4.6707	-5.1360	-6.6179	-0.4720	-0.3299	-2.1535	-2.4402	-1.8184
	f''	11.5787	8.7649	6.7484	5.9574	4.6937	5.8584	3.9377	0.7436	0.7010	2.8890
Hf	f'	-4.0452	-4.0564	-4.4593	-4.9466	-6.1794	-0.5830	-0.3548	-1.9785	-2.1778	-2.2909
	f''	12.2546	9.2832	7.1518	6.3150	4.9776	6.1852	4.1643	0.7905	0.7454	3.0246
Ta	f'	-4.0905	-3.9860	-4.3912	-4.7389	-5.7959	-0.7052	-0.3831	-1.8534	-2.0068	-3.1639
	f''	12.9479	9.8171	7.5686	6.6850	5.2718	6.5227	4.3992	0.8392	0.7915	3.1610
W	f'	-4.1530	-3.9270	-4.2486	-4.5529	-5.4734	-0.8490	-0.4201	-1.7565	-1.8819	-3.8673
	f''	13.6643	10.3696	8.0005	7.0688	5.5774	6.8722	4.6430	0.8905	0.8388	0.6433
Re	f'	-4.2681	-3.9052	-4.1390	-4.4020	-5.2083	-1.0185	-0.4693	-1.6799	-1.7868	-2.8429
	f''	14.3931	10.9346	8.4435	7.4631	5.8923	7.2310	4.8944	0.9441	0.8907	0.6827
Os	f'	-4.4183	-3.9016	-4.0478	-4.2711	-4.9801	-1.2165	-0.5280	-1.6170	-1.7107	-2.4688
	f''	15.1553	11.5251	8.9067	7.8753	6.2216	7.6030	5.1558	1.0001	0.9437	0.7238
Ir	f'	-4.5860	-3.9049	-3.9606	-4.1463	-4.7710	-1.4442	-0.5977	-1.5648	-1.6486	-2.2499
	f''	15.9558	12.1453	9.3923	8.3074	6.5667	7.9887	5.4269	1.0589	0.9993	0.7669
Pt	f'	-4.8057	-3.9435	-3.8977	-4.0461	-4.5932	-1.7033	-0.6812	-1.5228	-1.5998	-2.1036
	f''	16.7870	12.7910	9.8985	8.7578	6.9264	8.3905	5.7081	1.1193	1.0565	0.8116
Au	f'	-5.0625	-3.9908	-3.8356	-3.9461	-4.4197	-2.0133	-0.7638	-1.4693	-1.5404	-1.9775
	f''	17.6400	13.4551	10.4202	9.2222	7.2980	8.8022	5.9978	1.1833	1.1171	0.8589
Hg	f'	-5.4327	-4.1029	-3.8228	-3.8921	-4.2923	-2.3894	-0.8801	-1.4389	-1.5055	-1.8958
	f''	18.5241	14.1473	10.9650	9.7076	7.6849	9.2266	6.2989	1.2483	1.1796	0.9080
Tl	f'	-5.8163	-4.2233	-3.8103	-3.8340	-4.1627	-2.8358	-1.0117	-1.4111	-1.4740	-1.8288
	f''	19.4378	14.8643	11.5300	10.2108	8.0900	9.6688	6.6090	1.3189	1.2456	0.9594
Pb	f'	-6.4779	-4.4167	-3.8519	-3.8236	-4.0753	-3.3944	-1.1676	-1.3897	-1.4497	-1.7773
	f''	20.3336	15.5987	12.1106	10.7292	8.5060	10.1111	6.9287	1.3909	1.3137	1.0127
Bi	f'	-7.0419	-4.6533	-3.9228	-3.8408	-4.0111	-4.1077	-1.3494	-1.3721	-1.4290	-1.7346
	f''	21.2196	16.3448	12.7017	11.2575	8.9310	10.2566	7.2566	1.4661	1.3851	1.0685
Po	f'	-7.7195	-4.9604	-4.0267	-3.8855	-3.9670	-5.1210	-1.5613	-1.3584	-1.4133	-1.7005
	f''	22.1974	17.1410	13.3329	11.8209	9.3834	11.0496	7.5986	1.5443	1.4592	1.1266
At	f'	-8.5994	-5.3399	-4.1781	-3.9706	-3.9588	-7.9122	-1.8039	-1.3540	-1.4066	-1.6784
	f''	23.2213	17.9390	13.9709	12.3915	9.8433	9.9777	7.9509	1.6260	1.5367	1.1876
Rn	f'	-10.2749	-5.7275	-4.3331	-4.0549	-3.9487	-8.0659	-2.0847	-1.3475	-1.3982	-1.6571
	f''	24.2613	18.7720	14.6313	12.9815	10.3181	10.4580	8.3112	1.7103	1.6167	1.2504
Fr	f'	-10.8938	-6.2180	-4.5387	-4.1818	-3.9689	-7.2224	-2.4129	-1.3404	-1.3892	-1.6367
	f''	24.3041	19.6009	15.3016	13.5825	10.8038	7.7847	8.6839	1.7986	1.7004	1.3162
Ra	f'	-12.3462	-6.7502	-4.7764	-4.3309	-4.0088	-6.7704	-2.8081	-1.3462	-1.3931	-1.6299
	f''	25.5374	20.4389	15.9778	14.1902	11.2969	8.1435	9.0614	1.8891	1.7863	1.3840
Ac	f'	-12.3496	-7.4161	-5.0617	-4.5270	-4.0794	-6.8494	-3.2784	-1.3473	-1.3922	-1.6190
	f''	25.1363	21.3053	16.6687	14.8096	11.7994	8.5178	9.4502	1.9845	1.8770	1.4553
Th	f'	-13.6049	-8.2118	-5.3692	-4.7310	-4.1491	-7.2400	-3.8533	-1.3524	-1.3955	-1.6136
	f''	26.2511	22.2248	17.4018	15.4642	12.3296	8.8979	9.8403	2.0819	1.9695	1.5284
Pa	f'	-14.4639	-9.4459	-5.7337	-4.9639	-4.2473	-8.0334	-4.6067	-1.3672	-1.4083	-1.6170
	f''	27.4475	23.1548	18.1406	16.1295	12.8681	9.2807	10.2413	2.1835	2.0661	1.6047
U	f'	-12.3528	-9.9362	-6.1485	-5.2392	-4.3638	-9.6767	-5.7225	-1.3792	-1.4184	-1.6188
	f''	30.1725	23.1239	18.8728	16.7952	13.4090	9.6646	10.6428	2.2876	1.1650	1.6831
Np	f'	-17.4143	-11.1080	-6.6136	-5.5633	-4.5053	-11.4937	-6.9995	-1.3941	-1.4312	-1.6231
	f''	31.7405	24.1168	19.6379	17.4837	13.9666	4.1493	9.5876	2.3958	2.2679	1.7648
Pu	f'	-18.0862	-11.4073	-6.9721	-5.8130	-4.6563	-9.4100	-13.5905	-1.4180	-1.4527	-1.6351
	f''	33.8963	23.2960	20.1548	17.9579	14.3729	4.3056	6.9468	2.4979	2.3652	1.8430
Am	f'	-19.7042	-11.7097	-7.7881	-6.2920	-4.8483	-7.8986	-6.7022	-1.4359	-1.4684	-1.6424
	f''	37.3716	24.5715	21.1738	18.8618	15.0877	4.5125	7.3108	2.6218	2.4829	1.9358
Cm	f'	-24.9307	-10.4100	-8.6102	-6.7506	-5.0611	-7.3248	-6.2891	-1.4655	-1.4952	-1.6592
	f''	41.4852	25.8115	21.8880	19.5119	15.6355	4.6980	7.6044	2.7421	2.5974	2.0271
Bk	f'	-32.8492	-9.2185	-9.3381	-7.4293	-5.3481	-6.8498	-6.3438	-1.4932	-1.5203	-1.6746
	f''	32.5421	29.3028	21.9514	20.3581	16.3190	4.9086	7.9477	2.8653	2.7147	2.1208
Cf	f'	-23.6520	-23.5202	-9.7799	-7.8616	-5.5545	-6.6561	-6.4144	-1.5323	-1.5562	-1.6984
	f''	21.9334	31.2999	22.4858	20.8536	16.7428	5.0785	8.1930	2.9807	2.8250	2.2102

& Fischer (1994) have extended this to the description of kinematic diffraction intensities in lattices containing anisotropic anomalous scatterers. Their treatment was developed for space groups up to orthorhombic symmetry.

All the preceding treatments apply to scattering in the neighbourhood of an absorption edge, and to a fairly restricted class of crystals for which the local site symmetry of the electron density of states in the excited state is very different from the apparent crystal symmetry.

These approaches seek to treat the scattering from the crystal as though the scattering from each atomic position can be described by a symmetric second-rank tensor whose properties are determined by the point-group symmetries of those sites. Clearly, this procedure cannot be followed unless the structure has been solved by the usual method. The tensor approach can then be used to explain apparent deficiencies in that model such as the existence of 'forbidden' reflections, birefringence, and circular dichroism.

4. PRODUCTION AND PROPERTIES OF RADIATIONS

Scattering of X-rays from the electron spins in anti-ferromagnetically ordered materials can also be described by imposing a tensor description on the form factor (Blume, 1994). The tensor in this case is a fourth-rank tensor, and the strength of the interaction, even for the favourable case of resonance scattering, is several orders of magnitude lower in intensity than the polarization effects. Nevertheless, studies have been made on holmium and uranium arsenide, and significant magnetic Bragg scattering has been observed.

All the cases cited above represent exciting, state-of-the-art, scientific studies. However, none of the work will assist in the solution of crystal structures directly. Researchers should avoid the temptation, in the first instance, to ascribe anything but a scalar value to the form factor.

4.2.6.3.3.5. Summary

For the imaginary part of the dispersion correction $f''(\omega, \Delta)$, the following observations can be made.

(i) Measurements of the linear absorption coefficient μ_l from which $f'(\omega, 0)$ is deduced should follow the recommendations set out in Subsection 4.2.3.2.

(ii) There is no rational basis for preferring one set of relativistic calculations of atomic scattering cross sections over another, as Creagh & Hubbell (1987, 1990) and Kissel *et al.* (1980) have shown.

(iii) The total scattering cross section for an ensemble of atoms is not simply the sum of the individual scattering cross sections in the neighbourhood of an absorption edge and therefore $f'(\omega, 0)$ will fluctuate as $\omega \rightarrow \omega_\kappa$.

(iv) There is no dependence of $f''(\omega, \Delta)$ and Δ .

For the real part of the dispersion correction $f'(\omega, \Delta)$, the following observations can be made.

(i) The relativistic multipole values listed here tend to accord better with experiment than the non-relativistic and relativistic dipole values.

(ii) There is no dependence of $f'(\omega, \Delta)$ on Δ .

(iii) The theoretical tables are calculated for averaged polarizations.

(iv) Experimentalists wishing to compare their data with theoretical predictions should take account of the energy bandpass of their system when determining the appropriate theoretical value. They should also be aware of the fact that the position of the absorption edge depends on the oxidation state of the scattering atom, and that there is an inaccuracy in the tables of $f'(\omega, 0)$ of either $+0.20(E_{\text{tot}}/mc^2)$ or $-0.10(E_{\text{tot}}/mc^2)$.

4.2.6.4. Table of wavelengths, energies, and linewidths used in compiling the tables of the dispersion corrections

Table 4.2.6.7 lists the characteristic emission wavelengths that are commonly used by crystallographers in their experiments. Also included are the emission energies (since many systems use energy rather than wavelength discrimination) and the line widths (full width at half-maximum) of these lines (Agarwal, 1979; Stearns, 1984; Deutsch & Hart, 1984*a,b*).

4.2.6.5. Tables of the dispersion corrections for forward scattering, averaged polarization using the relativistic multipole approach

See Subsection 4.2.6.3 for comments on the accuracy of these tables. Note also that in the neighbourhood of absorption edges the values for condensed matter may be significantly different from the values in the tables due to XAFS and XANES effects. The values in Table 4.2.6.8 are for scattering by isolated atoms.