by checking, by means of equation (2), the diffraction conditions in both cases*.

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* It is worthwhile to note that equation (2) is a geometrical condition of simultaneous diffraction and does not take into account the fact that the 'reciprocal-lattice points' are not geometrical points.

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A Theoretical Calculation of X-ray Absorption Cross Sections

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Numerical values of X-ray absorption cross-sections for atoms are given for 10 commonly used X-ray wavelengths. The calculations are based on a multipole expansion of the appropriate matrix elements, using hydrogen-like eigenfunctions, for the *K*, *L*, *M* and *N* electrons. For the given figures, agreement with experiment is in general better than 5%.

Photoelectric absorption cross-sections for X-rays have been calculated by several authors using hydrogen-like eigenfunctions (Bethe & Salpeter, 1957). These calculations have been made for the *K*- and *L*-shells using the dipole approximation. Recently one of us discussed the angular dependence of the Borrmann effect, and it was found that apart from the influence of thermal vibrations within the crystal, this angular dependence is caused by electrical quadrupole transitions (Wagenfeld, 1966).* Here the methods, and to some extent the results of Hönl's (1933) and Eisenlohr & Müller's (1954) calculations of the generalized atomic scattering factor for the region of anomalous dispersion have been used, but the calculations have been extended for the *M*- and *N*-shells as well. A further complication has been the inaccuracy of the screening constants which are needed for the hydrogen-like eigenvalues. Since Bearden (1964) has measured, or given best values for, the X-ray wave length for most elements with high precision, one can determine the screening constants from his data, using Sommerfeld's fine structure formulae for the term values. Since the calculations are based on hydrogen-like eigenfunctions, the eigenvalues for the energies do not agree exactly with the energies of the measured absorption edges. Hence one cannot expect that this calculation will hold for the wavelength region near to and below an absorption edge. In the following tables we therefore publish only the numerical values for the atomic absorption cross-sections which we believe are theoretically justified. For this reason we also do not give cross-sections for the wave length region longer than the *L*-shell absorption edge. However, we compared some of the values with experimental data, and found agreement within 5%. The comparisons showed that these values are significantly better than the theoretical values given in *International Tables for X-ray Crystallography* (1962).

* Dipole–octupole transitions, which give a smaller contribution than quadrupole transitions, are also included. It can be proved that electrical octupole transitions are very weak. Magnetic transitions do not occur in this case.

Table 1. *X-ray absorption cross-sections* ($cm^2 \times 10^{21}$)

AT. NO.	WAVELENGTH	Cr $K\alpha_1$ 2.2897 Å	Cr $K\beta_1$ 2.0849 Å	Fe $K\alpha_1$ 1.9360 Å	Fe $K\beta_1$ 1.7566 Å	Cu $K\alpha_1$ 1.5406 Å	Cu $K\beta_1$ 1.3922 Å	Mo $K\alpha_1$ 0.7093 Å	Mo $K\beta_1$ 0.6323 Å	Ag $K\alpha_1$ 0.5594 Å	Ag $K\beta_1$ 0.4976 Å
	DIPOLE	3.411	2.582	2.070	1.546	1.040	0.765	0.095	0.067	0.045	0.032
11	QUADRUPOLE	0.045	0.039	0.034	0.028	0.022	0.018	0.005	0.004	0.003	0.002
	TOTAL	3.456	2.621	2.103	1.574	1.063	0.783	0.100	0.070	0.048	0.034
	DIPOLE	4.859	3.690	2.965	2.221	1.501	1.107	0.140	0.098	0.067	0.047
12	QUADRUPOLE	0.061	0.053	0.046	0.039	0.031	0.026	0.007	0.005	0.004	0.003
	TOTAL	4.920	3.742	3.011	2.260	1.532	1.133	0.147	0.104	0.071	0.050
	DIPOLE	6.670	5.080	4.091	3.075	2.085	1.542	0.199	0.139	0.095	0.066
13	QUADRUPOLE	0.079	0.068	0.061	0.052	0.042	0.035	0.010	0.008	0.006	0.005
	TOTAL	6.749	5.149	4.152	3.127	2.127	1.577	0.209	0.147	0.101	0.071
	DIPOLE	8.895	6.795	5.484	4.133	2.814	2.087	0.273	0.192	0.132	0.092
14	QUADRUPOLE	0.098	0.086	0.077	0.067	0.054	0.046	0.013	0.010	0.008	0.006
	TOTAL	8.993	6.881	5.561	4.200	2.868	2.132	0.286	0.203	0.140	0.098
	DIPOLE	11.694	8.958	7.246	5.476	3.741	2.781	0.370	0.261	0.179	0.125
15	QUADRUPOLE	0.118	0.105	0.095	0.083	0.068	0.058	0.017	0.014	0.011	0.009
	TOTAL	11.812	9.063	7.341	5.559	3.809	2.840	0.387	0.275	0.190	0.134
	DIPOLE	14.969	11.499	9.321	7.063	4.842	3.610	0.487	0.344	0.237	0.166
16	QUADRUPOLE	0.137	0.124	0.114	0.101	0.084	0.072	0.023	0.018	0.014	0.011
	TOTAL	15.106	11.623	9.434	7.163	4.926	3.682	0.510	0.362	0.251	0.177
	DIPOLE	18.558	14.297	11.615	8.826	6.073	4.539	0.623	0.440	0.304	0.213
17	QUADRUPOLE	0.151	0.140	0.130	0.117	0.099	0.086	0.028	0.023	0.018	0.014
	TOTAL	18.710	14.437	11.745	8.943	6.172	6.625	0.651	0.463	0.322	0.227
	DIPOLE	22.843	17.644	14.364	10.943	7.555	5.661	0.788	0.559	0.386	0.271
18	QUADRUPOLE	0.162	0.154	0.146	0.133	0.115	0.101	0.035	0.028	0.023	0.018
	TOTAL	23.005	17.799	14.509	11.076	7.670	5.763	0.823	0.587	0.409	0.289
	DIPOLE	27.755	21.493	17.531	13.391	9.276	6.968	0.984	0.699	0.485	0.341
19	QUADRUPOLE	0.166	0.164	0.158	0.148	0.131	0.117	0.042	0.035	0.028	0.022
	TOTAL	27.921	21.657	17.690	13.539	9.407	7.085	1.026	0.734	0.513	0.363
	DIPOLE	33.385	25.913	21.176	16.214	11.268	8.485	1.215	0.865	0.601	0.423
20	QUADRUPOLE	0.160	0.167	0.166	0.160	0.146	0.132	0.051	0.042	0.034	0.027
	TOTAL	33.545	26.079	21.342	16.374	11.414	8.617	1.266	0.907	0.635	0.450
	DIPOLE		30.783	25.200	19.341	13.485	10.178	1.478	1.055	0.734	0.518
21	QUADRUPOLE		0.160	0.166	0.167	0.157	0.146	0.060	0.050	0.040	0.033
	TOTAL		30.943	25.367	19.508	13.642	10.324	1.538	1.104	0.775	0.551
	DIPOLE				22.964	16.057	12.147	1.787	1.278	0.892	0.630
22	QUADRUPOLE				0.168	0.166	0.158	0.070	0.059	0.048	0.039
	TOTAL				23.132	16.223	12.305	1.858	1.337	0.939	0.669
	DIPOLE	6.003				18.884	14.317	2.135	1.529	1.069	0.757
23	QUADRUPOLE	0.035				0.170	0.166	0.081	0.068	0.056	0.046
	TOTAL	6.038				19.053	14.483	2.216	1.598	1.125	0.803
	DIPOLE	7.302	5.553			21.966	16.689	2.522	1.810	1.268	0.899
24	QUADRUPOLE	0.038	0.035			0.166	0.170	0.092	0.078	0.064	0.053
	TOTAL	7.340	5.588			22.132	16.859	2.614	1.888	1.332	0.953
	DIPOLE	8.780	6.683	5.383			19.295	2.954	2.124	1.491	1.059
25	QUADRUPOLE	0.042	0.039	0.036			0.168	0.103	0.088	0.074	0.061
	TOTAL	8.822	6.721	5.419			19.463	3.057	2.212	1.565	1.121
	DIPOLE	10.282	7.831	6.311	4.752			3.427	2.469	1.737	1.236
26	QUADRUPOLE	0.045	0.042	0.039	0.036			0.115	0.099	0.083	0.069
	TOTAL	10.327	7.873	6.351	4.788			3.541	2.568	1.820	1.306
	DIPOLE	11.885	9.058	7.304	5.503			3.946	2.849	2.007	1.432
27	QUADRUPOLE	0.047	0.044	0.042	0.039			0.126	0.109	0.093	0.078
	TOTAL	11.932	9.103	7.346	5.541			4.071	2.958	2.100	1.510
	DIPOLE	13.670	10.424	8.408	6.338	4.324		4.514	3.265	2.305	1.647
28	QUADRUPOLE	0.049	0.047	0.045	0.042	0.037		0.136	0.120	0.103	0.087
	TOTAL	13.719	10.471	8.453	6.380	4.361		4.650	3.385	2.408	1.734
	DIPOLE	15.794	12.051	9.726	7.336	5.009	3.728	5.139	3.724	2.635	1.886
29	QUADRUPOLE	0.051	0.049	0.047	0.044	0.040	0.036	0.146	0.130	0.113	0.097
	TOTAL	15.845	12.101	9.773	7.381	5.049	3.765	5.285	3.855	2.747	1.982
	DIPOLE	18.175	13.876	11.206	8.458	5.780	4.305	5.819	4.225	2.995	2.147
30	QUADRUPOLE	0.052	0.051	0.049	0.047	0.043	0.039	0.155	0.140	0.123	0.106
	TOTAL	18.228	13.929	11.255	8.505	5.823	4.344	5.974	4.365	3.117	2.253
	DIPOLE	21.028	16.067	12.981	9.805	6.707	4.999	6.563	4.774	3.390	2.434
31	QUADRUPOLE	0.053	0.052	0.051	0.049	0.045	0.042	0.163	0.149	0.133	0.116
	TOTAL	21.081	16.120	13.032	9.854	6.752	5.040	6.725	4.923	3.522	2.550
	DIPOLE	23.801	18.196	14.707	11.115	7.609	5.674	7.352	5.357	3.811	2.742
32	QUADRUPOLE	0.052	0.052	0.051	0.050	0.047	0.044	0.168	0.157	0.142	0.125
	TOTAL	23.853	18.248	14.759	11.165	7.656	5.718	7.520	5.515	3.953	2.867
	DIPOLE	27.819	21.289	17.220	13.026	8.928	6.663	8.235	6.011	4.284	3.087
33	QUADRUPOLE	0.054	0.055	0.054	0.053	0.050	0.048	0.172	0.165	0.151	0.135
	TOTAL	27.873	21.344	17.275	13.080	8.978	6.711	8.407	6.176	4.435	3.222
	DIPOLE	31.306	23.972	19.399	14.683	10.071	7.520	9.148	6.689	4.776	3.447
34	QUADRUPOLE	0.052	0.053	0.054	0.054	0.052	0.049	0.172	0.169	0.158	0.143
	TOTAL	31.358	24.025	19.453	14.736	10.122	7.570	9.321	6.859	4.934	3.591
	DIPOLE	35.101	26.893	21.773	16.489	11.318	8.457	10.124	7.415	5.303	3.834
35	QUADRUPOLE	0.049	0.052	0.053	0.053	0.052	0.050	0.169	0.172	0.164	0.151
	TOTAL	35.150	26.945	21.826	16.543	11.370	8.507	10.293	7.587	5.468	3.986
	DIPOLE	38.414	29.447	23.850	18.071	12.412	9.276		8.168	5.852	4.238
36	QUADRUPOLE	0.049	0.052	0.053	0.054	0.053	0.052		0.172	0.169	0.158
	TOTAL	38.463	29.499	23.903	18.125	12.465	9.330		8.340	6.021	4.396
	DIPOLE	44.348	34.027	27.576	20.915	14.381	10.760		9.030	6.480	4.701
37	QUADRUPOLE	0.046	0.050	0.052	0.054	0.054	0.053		0.170	0.172	0.165
	TOTAL	44.394	34.077	27.630	20.969	14.436	10.813		9.200	6.663	4.865
	DIPOLE	49.377	37.911	30.742	23.329	16.054	12.019			7.123	5.175
38	QUADRUPOLE	0.043	0.047	0.050	0.052	0.054	0.054			0.173	0.169
	TOTAL	49.420	37.958	30.791	23.381	16.108	12.073			7.296	5.344
	DIPOLE	55.038	42.289	34.311	26.056	17.947	13.445			7.810	5.682
39	QUADRUPOLE	0.041	0.045	0.048	0.051	0.054	0.054			0.171	0.172
	TOTAL	55.079	42.334	34.359	26.107	18.001	13.499			7.981	5.855
	DIPOLE	60.892	46.813	38.005	28.879	19.909	14.923	2.147		8.532	6.217
40	QUADRUPOLE	0.039	0.043	0.046	0.050	0.053	0.054	0.039		0.167	0.174
	TOTAL	60.931	46.861	38.051	28.929	19.962	14.978	2.186		8.699	6.391

Table 1 (*cont.*)

AT. NO	WAVELENGTH	Cr $K\alpha_1$ 2.2897 Å	Cr $K\beta_1$ 2.0849 Å	Fe $K\alpha_1$ 1.9360 Å	Fe $K\beta_1$ 1.7568 Å	Cu $K\alpha_1$ 1.5406 Å	Cu $K\beta_1$ 1.3922 Å	Mo $K\alpha_1$ 0.7093 Å	Mo $K\beta_1$ 0.6323 Å	Ag $K\alpha_1$ 0.5594 Å	Ag $K\beta_1$ 0.4975 Å
41	DIPOLE	67.660	52.061	42.285	32.155	22.187	16.643	2.404			6.790
	QUADRUPOLE	0.038	0.041	0.044	0.048	0.053	0.055	0.041			0.173
	TOTAL	67.698	52.102	42.329	32.203	22.240	16.697	2.445			6.962
42	DIPOLE	74.480	57.345	46.600	35.459	24.487	18.378	2.664	1.911		7.388
	QUADRUPOLE	0.037	0.039	0.042	0.046	0.051	0.053	0.043	0.039		0.169
	TOTAL	74.516	57.384	46.642	35.505	24.538	18.432	2.707	1.950		7.557
43	DIPOLE		63.107	51.299	39.050	26.981	20.359	2.945	2.113		
	QUADRUPOLE		0.038	0.040	0.044	0.049	0.053	0.045	0.041		
	TOTAL		63.144	51.338	29.094	27.030	20.312	2.990	2.154		
44	DIPOLE		68.969	56.093	42.727	29.547	22.199	3.238	2.325		
	QUADRUPOLE		0.037	0.038	0.042	0.047	0.051	0.047	0.043		
	TOTAL		69.006	56.131	42.769	29.594	22.250	3.285	2.368		
45	DIPOLE			61.452	46.840	32.419	24.372	3.568	2.564	1.801	
	QUADRUPOLE			0.037	0.040	0.045	0.049	0.048	0.045	0.040	
	TOTAL			61.489	46.880	32.464	24.421	3.617	2.608	1.841	
46	DIPOLE			67.186	51.242	35.494	26.699	3.923	2.820	1.982	
	QUADRUPOLE			0.037	0.038	0.043	0.048	0.050	0.046	0.042	
	TOTAL			67.223	51.281	35.537	26.747	3.973	2.867	2.024	
47	DIPOLE				56.241	38.999	29.360	4.334	3.118	2.193	1.564
	QUADRUPOLE				0.037	0.041	0.046	0.051	0.048	0.044	0.040
	TOTAL				56.278	39.040	29.406	4.386	3.166	2.237	1.604
48	DIPOLE				61.192	42.468	31.992	4.740	3.412	2.402	1.714
	QUADRUPOLE				0.037	0.040	0.044	0.053	0.050	0.046	0.041
	TOTAL				61.229	42.508	32.036	4.793	3.462	2.447	1.755
49	DIPOLE					46.157	34.793	5.174	3.727	2.625	1.874
	QUADRUPOLE					0.038	0.042	0.054	0.051	0.047	0.043
	TOTAL					46.195	34.835	5.228	3.778	2.672	1.917
50	DIPOLE					50.050	37.753	5.637	4.062	2.863	2.045
	QUADRUPOLE					0.038	0.040	0.055	0.052	0.049	0.045
	TOTAL					50.087	37.793	5.691	4.114	2.911	2.090
51	DIPOLE					54.196	40.905	6.129	4.419	3.116	2.228
	QUADRUPOLE					0.037	0.039	0.055	0.053	0.050	0.046
	TOTAL					54.234	40.944	6.184	4.473	3.166	2.274
52	DIPOLE						44.322	6.668	4.811	3.395	2.428
	QUADRUPOLE						0.038	0.056	0.055	0.052	0.048
	TOTAL						44.360	6.724	4.866	3.447	2.476
53	DIPOLE						47.506	7.189	5.191	3.666	2.624
	QUADRUPOLE						0.038	0.056	0.055	0.053	0.049
	TOTAL						47.543	7.245	5.247	3.719	2.674
54	DIPOLE							7.823	5.651	3.992	2.859
	QUADRUPOLE							0.056	0.056	0.054	0.051
	TOTAL							7.879	5.707	4.046	2.909
55	DIPOLE							8.402	6.072	4.292	3.075
	QUADRUPOLE							0.056	0.056	0.053	0.052
	TOTAL							8.458	6.128	4.346	3.127
56	DIPOLE							9.072	6.560	4.640	3.327
	QUADRUPOLE							0.056	0.057	0.056	0.053
	TOTAL							9.127	6.617	4.696	3.380
57	DIPOLE							9.751	7.057	4.995	3.583
	QUADRUPOLE							0.055	0.057	0.056	0.054
	TOTAL							9.806	7.113	5.051	3.638
58	DIPOLE							10.459	7.572	5.361	3.848
	QUADRUPOLE							0.054	0.056	0.056	0.055
	TOTAL							10.513	7.628	5.418	3.903
59	DIPOLE							11.229	8.133	5.762	4.137
	QUADRUPOLE							0.053	0.056	0.057	0.056
	TOTAL							11.282	8.189	5.818	4.193
60	DIPOLE							12.063	8.742	6.197	4.452
	QUADRUPOLE							0.053	0.056	0.057	0.056
	TOTAL							12.115	8.798	6.254	4.509

Table 1 (*cont.*)

AT. NO	WAVELENGTH	Mo $K\alpha_1$ 0.7093 Å	Mo $K\beta_1$ 0.6323 Å	Ag $K\alpha_1$ 0.5594 Å	Ag $K\beta_1$ 0.4975 Å
61	DIPOLE	12.910	9.362	6.640	4.773
	QUADRUPOLE	0.051	0.055	0.057	0.057
	TOTAL	12.962	9.416	6.697	4.830
62	DIPOLE	13.790	10.005	7.101	5.107
	QUADRUPOLE	0.050	0.054	0.056	0.057
	TOTAL	13.840	10.059	7.157	5.164
63	DIPOLE	14.758	10.713	7.608	5.475
	QUADRUPOLE	0.049	0.053	0.056	0.057
	TOTAL	14.807	10.767	7.664	5.532
64	DIPOLE	15.645	11.363	8.072	5.812
	QUADRUPOLE	0.047	0.052	0.055	0.057
	TOTAL	15.692	11.414	8.128	5.869
65	DIPOLE	16.655	12.103	8.604	6.198
	QUADRUPOLE	0.045	0.050	0.054	0.057
	TOTAL	16.700	12.153	8.658	6.254
66	DIPOLE	17.668	12.846	9.137	6.585
	QUADRUPOLE	0.044	0.049	0.053	0.056
	TOTAL	17.712	12.895	9.190	6.641
67	DIPOLE	18.693	13.597	9.675	6.976
	QUADRUPOLE	0.042	0.047	0.052	0.055
	TOTAL	18.735	13.644	9.727	7.031
68	DIPOLE	19.925	14.503	10.327	7.451
	QUADRUPOLE	0.041	0.046	0.051	0.055
	TOTAL	19.965	14.548	10.378	7.506
69	DIPOLE	20.861	15.195	10.827	7.817
	QUADRUPOLE	0.041	0.046	0.052	0.056
	TOTAL	20.902	15.241	10.879	7.873
70	DIPOLE	22.493	16.399	11.696	8.452
	QUADRUPOLE	0.039	0.044	0.049	0.054
	TOTAL	22.532	16.442	11.745	8.506
71	DIPOLE	23.643	17.244	12.304	8.895
	QUADRUPOLE	0.038	0.042	0.047	0.052
	TOTAL	23.682	17.286	12.351	8.947
72	DIPOLE	25.039	18.274	13.047	9.438
	QUADRUPOLE	0.038	0.041	0.046	0.051
	TOTAL	25.078	18.314	13.093	9.489
73	DIPOLE		19.289	13.780	9.973
	QUADRUPOLE		0.040	0.045	0.050
	TOTAL		19.328	13.825	10.023
74	DIPOLE		20.350	14.547	10.534
	QUADRUPOLE		0.039	0.043	0.049
	TOTAL		20.389	14.590	10.583
75	DIPOLE		21.497	15.377	11.142
	QUADRUPOLE		0.039	0.042	0.047
	TOTAL		21.535	15.419	11.189
76	DIPOLE		22.656	16.216	11.756
	QUADRUPOLE		0.038	0.041	0.046
	TOTAL		22.695	16.257	11.802
77	DIPOLE			17.007	12.343
	QUADRUPOLE			0.040	0.045
	TOTAL			17.047	12.388
78	DIPOLE			17.973	13.045
	QUADRUPOLE			0.039	0.043
	TOTAL			18.012	13.088
79	DIPOLE			18.894	13.720
	QUADRUPOLE			0.039	0.042
	TOTAL			18.932	13.762
80	DIPOLE			19.835	14.413
	QUADRUPOLE			0.038	0.041
	TOTAL			19.873	14.454
81	DIPOLE				14.872
	QUADRUPOLE				0.041
	TOTAL				14.912
82	DIPOLE				15.906
	QUADRUPOLE				0.039
	TOTAL				15.945
83	DIPOLE				16.656
	QUADRUPOLE				0.039
	TOTAL				16.694
84	DIPOLE				17.491
	QUADRUPOLE				0.038
	TOTAL				17.530

For a crystal composed of n_t different atoms we obtain the linear absorption coefficient from the formula

$$\tau = \sum_{i=1}^{n_t} N_i \sigma_i ,$$

where N_i is the number of atoms of the species i per cm^3, so that

$$N = \sum_{i=1}^{n_t} N_i$$

is the total number of atoms per cm^3. σ_i is the photoelectric absorption cross-section for the ith atom.

The numerical values as given in Table 1 are the atomic absorption cross-sections, split into three parts, for ten commonly used X-ray wavelengths.† For each element whose atomic number is given in the first column, the contribution to the cross-section of the dipole, dipole-octupole and Compton scattering terms is given in the row labelled *Dipole*. The cross-section due to the quadrupole term is given in the row labelled *Quadrupole*. The sum of these two, which is of course the total cross-section, is given in the row labelled *Total*.

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† The values used here are those given in Bearden's (1964) tables of X-ray wavelengths.