Photoelectric Atomic Absorption Cross Sections for Elements $Z = 6$ to 54 in the Medium Energy X-Ray Range (5 to 25 keV) — Part I

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Photoelectric atomic absorption cross sections have been calculated by means of hydrogen-like eigenfunctions for the atomic K, L, M and N sub-shells of the elements $Z = 6$ to 54, using revised screening constants and an extension of the theory. The absorption cross sections have been further separated into dipole and quadrupole components so that the numerical data can also be applied to the Borrmann effect.

1. Introduction

Theoretical computations of photoelectric absorption coefficients for silicon and germanium have been reported in an earlier paper [1] and shown to be in satisfactory agreement with experimental normal and anomalous X-ray absorption coefficients using perfect single crystals. In order to account for the angular dependence of the Borrmann effect it is convenient to expand the transition probabilities of the photoeffect into a series in which each term represents a certain multipole transition. This is based on Hönl's [2] treatment of the so called generalized scattering factor, i. e. the normal scattering factor which includes effects due to anomalous X-ray dispersion. The transition probabilities of each multipole transition are evaluated by means of hydrogen-like eigenfunctions. Theoretical calculations have been carried out for different atomic sub-shells by many authors [2]. The surprisingly good agreement, found between our theoretical and experimental data in [1], has encouraged us to extend the calculations to elements of atomic number $Z = 6$ to 54 using 18 characteristic wavelengths between CrK_α (5.4 keV) and AgK_β (24.9 keV), with the restriction that the X-ray energy must be above the theoretical (hydrogen-like) energy of a 2s electron. This is due to the fact that hydrogen-like eigenfunctions are only approximately valid for the outer shell electrons.

The accuracy of the results is strongly dependent on the choice of appropriate screening constants. The method used to determine these screening constants is described in Chapt. 2 of this paper. Since the hydrogen-like energy eigenvalue of each sub-shell is higher than the actual ionization energy, we have used an extension to the theory which accounts for cross sections between the theoretical and ionization edges. This extension is theoretically unjustified but a comparison with experimental data [1] shows that it works quite well for the K-shell.

Although more rigorous and better theoretical absorption cross sections exist, it is emphasized that our computations are particularly useful for the theoretical calculation of the Borrmann effect. The agreement between the photoelectric absorption cross section data presented in this paper and those derived from alternative theories and also those deducible from experimental linear absorption coefficients is in many cases better than 5%; this will be shown in a following paper [Part II] [3].

2. Atomic Sub-shell Screening Constants

The atomic sub-shell screening constants are determined by a semi-empirical method using Sommerfeld's approach [4] and precise spectroscopic data. Spin doublets which are found in the X-ray spectrum of each element are grouped according to their (almost constant) experimental term differences. Sommerfeld shows for hydrogen, that these groups are accurately explained by means of selected electron transitions applied to a fine structure formula in which relativistic and electron spin terms are also considered. For the many electron atom, similar agreement is possible only, if the nuclear charge of the element Z is replaced by a reduced charge $Z - s_{nl}$; s_{nl} is an average screening constant for an electron in a sub-shell of quantum numbers n and l which is screened from the nuclear field by intermediary electrons. Figure 1 shows the transitions used in these calculations where it can be seen that each kind of spin doublet is related to a particular sub-shell (n, l) according to appropriate selection

rules. A more detailed list of these transitions, in terms of Bohr and Coster's notation, is given in Table 1. Experimental term differences are obtained from the X-ray wavelength tables of Bearden [5] and substituted in the Sommerfeld term difference equations which are tabulated in the appendix of this paper. The sets of screening constants are listed in Table 2. In regions, where experimental spin doublets are not available, we have taken a mean value (bracketed) of the first ten neighbouring screening constants within the same sub-shell. This can introduce errors in the cross sections calculated for elements with low atomic numbers.

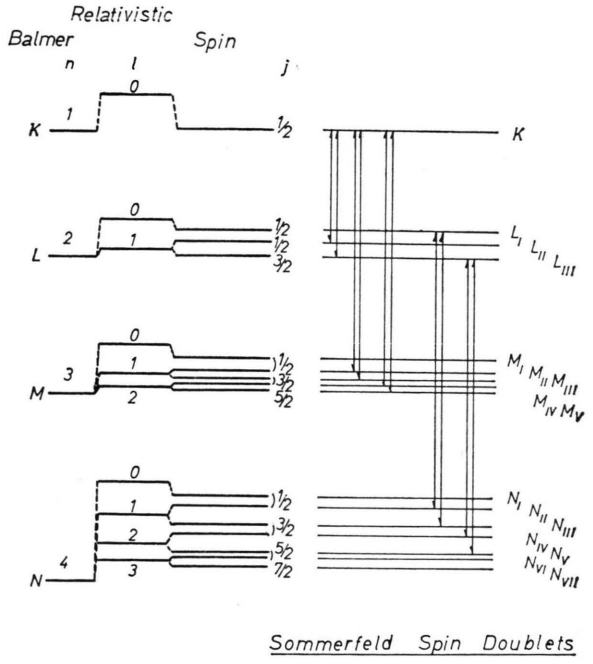

Fig. 1. Grotrian diagram showing a series of spin-doublet transitions.

Table 1. Spin doublet transitions selected for the evaluation of the average screening constants within each sub-shell.

Sub-shell	Screening constant (s_{nl})	Transition
(2 s, p)	s_{21}	KL_{II}-KL_{III}
(3 s, p)	s_{31}	KM_{II}-KM_{III}
(3 d)	s_{32}	KM_{IV}-KM_{V}
(4 s, p)	s_{41}	$L_{I}N_{II}$-$L_{I}N_{III}$
(4 d)	s_{42}	$L_{III}N_{IV}$-$L_{III}N_{V}$

3. Extension to the Theory for the K Shell

Previous computations of atomic absorption cross sections by Guttman and Wagenfeld [6] contain incorrect quadrupole cross sections and do not include values beyond the theoretical (H-like) absorption edges.

A convenient extension to the K-shell is obtained as follows: For the K-shell and for a region, where the incident X-ray photon wavelength λ is less than or equal to the theoretical (eigenvalue) wavelength λ_{1S}, the atomic dipole absorption cross section for

Table 2. Sub-shell screening constants. Bracketed values are averages of the following ten screening constants. For the K-shell, we have taken the theoretical value, $s_{10} = 0.30$, given by Slater.

Z	s_{21}	s_{31}	s_{32}	s_{41}
6				
7				
8	3.22			
9				
10				
11				
12				
13	3.16			
14	3.25			
15	2.88			
16	3.25			
17	3.30			
18	3.40			
19	3.34			
20	3.26	8.20		
21	3.34			
22	2.99			
23	2.87			
24	2.84			
25	2.84			
26	2.96			
27	3.12			
28	3.28		12.9	
29	3.38			
30	3.44			
31	3.42	7.89		
32	3.41	8.62		18.5
33	3.43	7.42		
34	3.40	7.98		
35	3.42	8.45		
36	3.64	8.37		
37	3.45	8.15	12.7	
38	3.45	8.34	12.8	
39	3.44	8.38	12.9	
40	3.48	8.41	12.8	
41	3.51	8.16	12.7	
42	3.46	8.26	12.7	
43	3.50	8.48	12.8	
44	3.51	8.57	12.8	
45	3.51	8.57	13.1	
46	3.51	8.60	13.0	14.5
47	3.53	8.56	12.9	
48	3.53	8.56	13.0	
49	3.54	8.54	12.9	
50	3.54	8.60	12.9	18.5
51	3.55	8.56	13.0	
52	3.56	8.50	12.9	
53	3.55	8.71	13.0	
54	3.56	8.34	13.0	

a K-shell electron is

$$\tau_{1S}^{D} = \frac{2^7}{3}\pi r_0 \lambda \left(\frac{\lambda}{\lambda_{1S}}\right)^3 \frac{\exp\{-(4/A)\arctan A\}}{1-\exp\{-2\pi/A\}}, \tag{3.1}$$

where $r_0 = e^2/m c^2 = 2.8179 \cdot 10^{-13}$ cm is the classical electron radius, $A = 1/n_1' = \sqrt{x-1}$, $x = \lambda_{1S}/\lambda$ and $\lambda_{1S} = 1/(Z-0.3)^2 R_\infty$.

Beyond this region, λ is now greater than λ_{1S} (i. e. $x<1$), and we rewrite $A = i\sqrt{|x-1|} = iB$.

The dipole cross section for this region is then

$$(\tau_{1S}^{D})' = \frac{2^7}{3}\pi r_0 \lambda \left(\frac{\lambda}{\lambda_{1S}}\right)^3 \exp\left\{-\frac{2}{B}\ln\left[\frac{(1+B)}{(1-B)}\right]\right\}, \tag{3.2}$$

where $[1-\exp\{-2\pi/A\}]$ is approximated to 1 and use is made of the following identities:

$$\arctan(iB) = i\,\operatorname{artanh}(B) = (i/2)\ln[(1+B)/(1-B)].$$

$(\tau_{1S}^{D})'$ is further substituted into the quadrupole and dipole-octupole cross section equations related to the same condition.

4. Applications

4.1. Normal Absorption

For the calculation of absorption coefficients in the X-ray energy region one has to take into account, besides the photoelectric absorption coefficient τ_0, the contributions μ_0(CS) due to Compton scattering (including plasmon excitation) and μ_0(TDS) due to thermal diffuse scattering such that

$$\mu_0 = \tau_0 + \mu_0(\mathrm{CS}) + \mu_0(\mathrm{TDS}). \tag{4.1}$$

The magnitude of these other scattering contributions to τ_0 is considered in Part II of this paper [3].

Our calculations are restricted to the photoelectric coefficient

$$\tau_0 = \frac{1}{\Omega}\sum_i N_i(\sigma_{\mathrm{tot}})_i, \tag{4.2}$$

where N_i is the number of atoms (of type i) within a unit cell of volume Ω (in Å^3), and $(\delta_{\mathrm{tot}})_i$ the total photoelectric atomic absorption coefficient for the i th atom (in barn/atom). The summation is to be taken over all types of atom within the unit cell.

In Table 3, the contributions of the K, L, M, and N shells to δ_{tot} and the ratio $Q = \sigma^Q/\sigma_{\mathrm{tot}} = \tau^Q/\tau_0$ are given, where τ^Q is the sum of the quadrupole contributions. Our calculations are based on the formulae listed in the paper by Wagenfeld [2].

The close approximation of τ_0 to μ_0 throughout the medium X-ray energy range (5 to 25 keV) has been shown for Si and Ge[1] and will be further discussed for other cases in [3].

4.2. Anomalous Absorption

In diffraction experiments with perfect (or nearly perfect) crystals, wavefields are created with different absorption coefficients which are larger or smaller than μ_0. The fields with small coefficients are able to traverse much thicker crystals (Borrmann effect) than in the normal absorption case. Similar to Eq. (4.1), two absorption coefficients related to fields with minimum absorption can be expressed by

$$\mu_{\mathrm{min}}^{C} = \tau_{\mathrm{min}}^{C} + \mu_{\mathrm{min}}(\mathrm{CS}) + \mu_{\mathrm{min}}(\mathrm{TDS}). \tag{4.3}$$

$C = \perp$ or $\parallel$ refers to polarization perpendicular or parallel to the plane defined by the wave vectors $\boldsymbol{K}_0$, $\boldsymbol{K}_H$ (2-beam case). In the theoretical case of a crystal with extreme thickness, only the wave field with $\mu_{\mathrm{min}}^{\perp}$ will survive.

In transmission experiments with perfect crystals of finite thickness, μ_{min}^{C} must be known in order to calculate the integrated intensities of the reflexions.

One important fact is that the relative contributions due to Compton and thermal diffuse scattering are larger in (4.3) than in (4.1) and should be considered. Corresponding theory and data for μ(CS) and μ(TDS), for both normal and anomalous absorption, have been calculated by Dederichs [7] and Sano, Ohtaka and Ohtsuki [8].

The photoelectric contribution for the general two beam case can be written

$$\tau_{\mathrm{min}}^{C} = \tau_0\left(1 - \left|\frac{\chi_{iH}^{C}}{\chi_{i0}}\right|\right)\Big/\cos\Theta_B, \tag{4.4}$$

with Θ_B the Bragg angle of the diffracting planes $H = h_1, h_2, h_3$ and χ_{iH}, χ_{i0} the imaginary parts of the Fourier components of the dielectric susceptibility.

The angular dependence of χ_{iH}/χ_{i0} is discussed by Wagenfeld [2, *]. In the case of the diamond type

* The formulae given in this paper are invalid near an experimental absorption edge where for instance Kronig-Kramer fine structure becomes important.

Table 3. H-like photoelectric atomic absorption cross sections for the K, L, M and N sub-shells and total values T, given in barn/atom ($= 10^{-24}$ cm^2/atom), together with the quantity $\tau^Q/\tau_0 = Q$ used in anomalous transmission. Dashed and full line boundaries denote energy regions below the theoretical and experimental absorption edges, E(1s) [– – –], E(2s) and K [———], L, respectively.

Z	CrKα1	CrKβ1	FeKα1	CoKα1	FeKβ1	NiKα1	CoKβ1	CuKα1	NiKβ1	ZnKα1	CuKβ1	ZnKβ1	GeKα1	GeKβ1	MoKα1	MoKβ1	AgKα1	AgKβ1	line
	5.415	5.947	6.404	6.930	7.058	7.478	7.649	8.048	8.265	8.639	8.905	9.572	9.886	10.982	17.479	19.608	22.163	24.942	keV
6	2.46 2	1.83 2	1.45 2	1.13 2	1.07 2	8.88 1	8.26 1	7.03 1	6.46 1	5.61 1	5.09 1	4.05 1	3.65 1	2.61 1	5.85	4.04	2.72	1.86	K
	1.23	9.03 -1	7.07 -1	5.45 -1	5.13 -1	4.24 -1	3.93 -1	3.33 -1	3.05 -1	2.63 -1	2.38 -1	1.87 -1	1.69 -1	1.19 -1	2.54 -2	1.73 -2	1.15 -2	7.80 -3	L
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	2.47 2	1.84 2	1.46 2	1.14 2	1.07 2	8.92 1	8.30 1	7.06 1	6.49 1	5.64 1	5.12 1	4.07 1	3.67 1	2.62 1	5.88	4.06	2.73	1.86	T
	1.56 -2	1.72 -2	1.86 -2	2.02 -2	2.05 -2	2.18 -2	2.23 -2	2.35 -2	2.41 -2	2.52 -2	2.60 -2	2.79 -2	2.89 -2	3.20 -2	5.03 -2	5.62 -2	6.30 -2	7.03 -2	Q
7	4.91 2	3.67 2	2.92 2	2.28 2	2.15 2	1.80 2	1.67 2	1.43 2	1.31 2	1.14 2	1.04 2	8.26 1	7.46 1	5.35 1	1.22 1	8.45	5.71	3.91	K
	4.99	3.69	2.90	2.25	2.12	1.75	1.63	1.38	1.27	1.10	9.92 -1	7.84 -1	7.05 -1	5.00 -1	1.09 -1	7.46 -2	4.99 -2	3.38 -2	L
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	4.96 2	3.71 2	2.94 2	2.30 2	2.17 2	1.81 2	1.69 2	1.44 2	1.33 2	1.15 2	1.05 2	8.34 1	7.53 1	5.40 1	1.23 1	8.52	5.76	3.94	T
	1.53 -2	1.69 -2	1.82 -2	1.98 -2	2.02 -2	2.14 -2	2.19 -2	2.31 -2	2.38 -2	2.49 -2	2.56 -2	2.76 -2	2.85 -2	3.17 -2	5.00 -2	5.58 -2	6.27 -2	7.00 -2	Q
8	8.79 2	6.60 2	5.26 2	4.12 2	3.89 2	3.26 2	3.04 2	2.59 2	2.39 2	2.08 2	1.89 2	1.51 2	1.37 2	9.84 1	2.28 1	1.58 1	1.07 1	7.37	K
	1.43 1	1.06 1	8.36	6.49	6.12	5.09	4.73	4.02	3.69	3.20	2.90	2.30	2.07	1.47	3.26 -1	2.24 -1	1.50 -1	1.02 -1	L
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	8.93 2	6.70 2	5.34 2	4.19 2	3.96 2	3.31 2	3.08 2	2.63 2	2.43 2	2.11 2	1.92 2	1.54 2	1.39 2	9.99 1	2.31 1	1.60 1	1.09 1	7.47	T
	1.48 -2	1.64 -2	1.78 -2	1.94 -2	1.98 -2	2.10 -2	2.15 -2	2.27 -2	2.33 -2	2.44 -2	2.52 -2	2.72 -2	2.81 -2	3.13 -2	4.96 -2	5.55 -2	6.23 -2	6.97 -2	Q
9	1.45 3	1.09 3	8.73 2	6.86 2	6.49 2	5.44 2	5.08 2	4.35 2	4.01 2	3.50 2	3.18 2	2.55 2	2.31 2	1.67 2	3.91 1	2.72 1	1.85 1	1.28 1	K
	3.31 1	2.46 1	1.95 1	1.52 1	1.43 1	1.19 1	1.11 1	9.43	8.66	7.52	6.83	5.42	4.89	3.49	7.83 -1	5.41 -1	3.64 -1	2.49 -1	L
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	1.48 3	1.12 3	8.93 2	7.02 2	6.64 2	5.56 2	5.19 2	4.44 2	4.09 2	3.57 2	3.25 2	2.60 2	2.36 2	1.70 2	3.98 1	2.78 1	1.89 1	1.30 1	T
	1.44 -2	1.60 -2	1.73 -2	1.89 -2	1.93 -2	2.05 -2	2.10 -2	2.22 -2	2.29 -2	2.40 -2	2.48 -2	2.67 -2	2.76 -2	3.08 -2	4.92 -2	5.50 -2	6.19 -2	6.97 -2	Q
0	2.25 3	1.70 3	1.36 3	1.07 3	1.02 3	8.53 2	7.96 2	6.83 2	6.30 2	5.51 2	5.02 2	4.03 2	3.65 2	2.64 2	6.28 1	4.39 1	3.00 1	2.07 1	K
	6.58 1	4.91 1	3.90 1	3.04 1	2.87 1	2.40 1	2.23 1	1.90 1	1.75 1	1.52 1	1.38 1	1.10 1	9.93	7.11	1.62	1.12	7.57 -1	5.19 -1	L
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	2.31 3	1.75 3	1.40 3	1.10 3	1.04 3	8.77 2	8.19 2	7.02 2	6.47 2	5.66 2	5.16 2	4.14 2	3.75 2	2.72 2	6.44 1	4.50 1	3.07 1	2.12 1	T
	1.38 -2	1.54 -2	1.68 -2	1.84 -2	1.88 -2	2.00 -2	2.05 -2	2.17 -2	2.23 -2	2.35 -2	2.42 -2	2.62 -2	2.71 -2	3.03 -2	4.87 -2	5.46 -2	6.14 -2	6.88 -2	Q
1	3.31 3	2.51 3	2.02 3	1.60 3	1.51 3	1.27 3	1.19 3	1.02 3	9.42 2	8.24 2	7.52 2	6.05 2	5.48 2	3.99 2	9.59 1	6.73 1	4.60 1	3.19 1	K
	1.18 2	8.84 1	7.02 1	5.50 1	5.19 1	4.34 1	4.04 1	3.45 1	3.18 1	2.77 1	2.51 1	2.01 1	1.81 1	1.30 1	3.00	2.09	1.41	9.71 -1	L
	1.86 -1	1.37 -1	1.07 -1	8.29 -2	7.80 -2	6.45 -2	5.99 -2	5.07 -2	4.64 -2	4.01 -2	3.63 -2	2.86 -2	2.57 -2	1.82 -2	3.91 -3	2.67 -3	1.78 -3	1.21 -3	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	3.43 3	2.60 3	2.09 3	1.65 3	1.56 3	1.31 3	1.23 3	1.05 3	9.73 2	8.52 2	7.77 2	6.25 2	5.66 2	4.12 2	9.89 1	6.93 1	4.74 1	3.29 1	T
	1.32 -2	1.48 -2	1.62 -2	1.78 -2	1.82 -2	1.94 -2	1.99 -2	2.11 -2	2.18 -2	2.29 -2	2.37 -2	2.56 -2	2.66 -2	2.98 -2	4.82 -2	5.40 -2	6.09 -2	6.83 -2	Q
2	4.68 3	3.56 3	2.87 3	2.27 3	2.16 3	1.82 3	1.70 3	1.46 3	1.35 3	1.18 3	1.08 3	8.71 2	7.90 2	5.76 2	1.40 2	9.87 1	6.77 1	4.71 1	K
	1.96 2	1.47 2	1.17 2	9.18 1	8.68 1	7.26 1	6.77 1	5.79 1	5.33 1	4.65 1	4.23 1	3.38 1	3.06 1	2.20 1	5.14	3.58	2.43	1.68	L
	1.48	1.10	8.65 -1	6.71 -1	6.32 -1	5.25 -1	4.88 -1	4.14 -1	3.80 -1	3.29 -1	2.98 -1	2.36 -1	2.12 -1	1.51 -1	3.31 -2	2.27 -2	1.52 -2	1.04 -2	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	4.88 3	3.71 3	2.99 3	2.37 3	2.24 3	1.89 3	1.77 3	1.52 3	1.40 3	1.23 3	1.12 3	9.05 2	8.21 2	5.98 2	1.46 2	1.02 2	7.02 1	4.88 1	T
	1.26 -2	1.42 -2	1.56 -2	1.72 -2	1.76 -2	1.88 -2	1.93 -2	2.05 -2	2.12 -2	2.23 -2	2.31 -2	2.50 -2	2.59 -2	2.91 -2	4.76 -2	5.35 -2	6.04 -2	6.78 -2	Q
3	6.40 3	4.89 3	3.94 3	3.13 3	2.97 3	2.51 3	2.35 3	2.02 3	1.87 3	1.64 3	1.50 3	1.21 3	1.10 3	8.04 2	1.98 2	1.40 2	9.62 1	6.70 1	K
	3.14 2	2.36 2	1.88 2	1.48 2	1.40 2	1.17 2	1.09 2	9.35 1	8.62 1	7.52 1	6.85 1	5.49 1	4.97 1	3.59 1	8.47	5.91	4.03	2.78	L
	4.18	3.11	2.46	1.91	1.81	1.50	1.40	1.19	1.09	9.48 -1	8.60 -1	6.83 -1	6.16 -1	4.39 -1	9.83 -2	6.78 -2	4.56 -2	3.11 -2	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	6.72 3	5.12 3	4.13 3	3.28 3	3.11 3	2.63 3	2.46 3	2.12 3	1.96 3	1.72 3	1.57 3	1.27 3	1.15 3	8.41 2	2.07 2	1.46 2	1.00 2	6.99 1	T
	1.19 -2	1.35 -2	1.49 -2	1.65 -2	1.69 -2	1.81 -2	1.86 -2	1.98 -2	2.05 -2	2.16 -2	2.24 -2	2.44 -2	2.53 -2	2.85 -2	4.70 -2	5.29 -2	5.98 -2	6.72 -2	Q

Z	CrKα1	CrKβ1	FeKα1	CoKα1	FeKβ1	NiKα1	CoKβ1	CuKα1	NiKβ1	ZnKα1	CuKβ1	ZnKβ1	GeKα1	GeKβ1	MoKα1	MoKβ1	AgKα1	AgKβ1	line
	5.415	5.947	6.404	6.930	7.058	7.478	7.649	8.048	8.265	8.639	8.905	9.572	9.886	10.982	17.479	19.608	22.163	24.942	keV
14	8.49 3	6.50 3	5.26 3	4.19 3	3.98 3	3.36 3	3.15 3	2.72 3	2.51 3	2.21 3	2.02 3	1.64 3	1.49 3	1.09 3	2.72 2	1.92 2	1.33 2	9.26 1	K
	4.51 2	3.40 2	2.72 2	2.14 2	2.02 2	1.70 2	1.58 2	1.36 2	1.25 2	1.09 2	9.95 1	7.98 1	7.22 1	5.23 1	1.25 1	8.72	5.96	4.12	L
	9.52	7.11	5.64	4.41	4.16	3.47	3.23	2.76	2.54	2.21	2.00	1.59	1.44	1.03	2.35 -1	1.62 -1	1.10 -1	7.51 -2	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	8.95 3	6.85 3	5.54 3	4.41 3	4.18 3	3.54 3	3.31 3	2.85 3	2.64 3	2.32 3	2.12 3	1.72 3	1.56 3	1.14 3	2.85 2	2.01 2	1.39 2	9.68 1	T
	1.12 -2	1.28 -2	1.42 -2	1.57 -2	1.61 -2	1.74 -2	1.79 -2	1.91 -2	1.97 -2	2.09 -2	2.17 2	2.36 -2	2.46 -2	2.78 -2	4.63 -2	5.22 -2	5.91 -2	6.65 -2	Q
15	1.10 4	8.45 3	6.85 3	5.47 3	5.19 3	4.40 3	4.12 3	3.56 3	3.30 3	2.90 3	2.66 3	2.15 3	1.96 3	1.44 3	3.63 2	2.57 2	1.78 2	1.25 2	K
	7.32 2	5.53 2	4.42 2	3.49 2	3.30 2	2.77 2	2.59 2	2.22 2	2.05 2	1.79 2	1.63 2	1.31 2	1.19 2	8.64 1	2.08 1	1.46 1	1.00 1	6.95	L
	1.89 1	1.42 1	1.13 1	8.82	8.34	5.97	6.49	5.54	5.10	4.44	4.04	3.22	2.91	2.10	4.83 -1	3.35 -1	2.27 -1	1.56 -1	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	1.18 4	9.01 3	7.30 3	5.82 3	5.53 3	4.68 3	4.39 3	3.79 3	3.51 3	3.08 3	2.82 3	2.29 3	2.08 3	1.53 3	3.85 2	2.72 2	1.88 2	1.32 2	T
	1.04 -2	1.20 -2	1.34 -2	1.50 -2	1.54 -2	1.67 -2	1.72 -2	1.84 -2	1.90 -2	2.01 -2	2.09 -2	2.29 -2	2.38 -2	2.70 -2	4.56 -2	5.15 -2	5.85 -2	6.59 -2	Q
16	1.39 4	1.07 4	8.73 3	6.98 3	6.63 3	5.63 3	5.28 3	4.56 3	4.23 3	3.73 3	3.42 3	2.77 3	2.53 3	1.86 3	4.75 2	3.37 2	2.34 2	1.64 2	K
	8.98 2	6.79 2	5.44 2	4.29 2	4.06 2	3.41 2	3.19 2	2.73 2	2.52 2	2.21 2	2.01 2	1.62 2	1.47 2	1.07 2	2.59 1	1.82 1	1.25 1	8.67	L
	3.41 1	2.56 1	2.04 1	1.60 1	1.51 1	1.27 1	1.18 1	1.01 1	9.29	8.10	7.37	5.89	5.33	3.84	8.96 -1	6.24 -1	4.24 -1	2.92 -1	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	1.49 4	1.14 4	9.29 3	7.43 3	7.05 3	5.98 3	5.61 3	4.85 3	4.49 3	3.96 3	3.62 3	2.94 3	2.68 3	1.97 3	5.01 2	3.56 2	2.47 2	1.73 2	T
	9.51 -3	1.11 -2	1.25 -2	1.41 -2	1.45 -2	1.58 -2	1.63 -2	1.75 -2	1.81 -2	1.92 -2	2.00 -2	2.20 -2	2.30 -2	2.62 -2	4.48 -2	5.07 -2	5.77 -2	6.51 -2	Q
17	1.73 4	1.34 4	1.09 4	8.75 3	8.31 3	7.07 3	6.63 3	5.74 3	5.33 3	4.70 3	4.31 3	3.51 3	3.20 3	2.36 3	6.08 2	4.33 2	3.01 2	2.12 2	K
	1.20 3	9.08 2	7.28 2	5.75 2	5.44 2	4.58 2	4.28 2	3.67 2	3.39 2	2.97 2	2.71 2	2.18 2	1.98 2	1.44 2	3.51 1	2.48 1	1.70 1	1.19 1	L
	5.73 1	4.31 1	3.44 1	2.70 1	2.55 1	2.14 1	1.99 1	1.71 1	1.57 1	1.37 1	1.25 1	9.99 1	9.05	6.53	1.54	1.07	7.31 -1	5.05 -1	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	1.86 4	1.43 4	1.17 4	9.35 3	8.88 3	7.54 3	7.08 3	6.13 3	5.68 3	5.01 3	4.59 3	3.73 3	3.40 3	2.51 3	6.45 2	4.59 2	3.19 2	2.24 2	T
	8.60 -3	1.02 -2	1.16 -2	1.32 -2	1.36 -2	1.49 -2	1.54 -2	1.66 -2	1.72 -2	1.84 -2	1.92 -2	2.11 -2	2.21 -2	2.53 -2	4.40 -2	4.99 -2	5.69 -2	6.43 -2	Q
18	2.12 4	1.64 4	1.34 4	1.08 4	1.03 4	8.72 3	8.19 3	7.11 3	6.60 3	5.82 3	5.35 3	4.36 3	3.98 3	2.95 3	7.67 2	5.47 2	3.81 2	2.69 2	K
	1.55 3	1.17 3	9.39 2	7.42 2	7.03 2	5.91 2	5.53 2	4.75 2	4.39 2	3.84 2	3.51 2	2.83 2	2.56 2	1.87 2	4.59 1	3.24 1	2.23 1	1.56 1	L
	9.16 1	6.89 1	5.50 1	4.32 1	4.08 1	3.42 1	3.19 1	2.73 1	2.52 1	2.20 1	2.00 1	1.60 1	1.45 1	1.05 1	2.48	1.74	1.19	8.20 -1	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	2.28 4	1.77 4	1.44 4	1.16 4	1.10 4	9.35 3	8.77 3	7.61 3	7.06 3	6.23 3	5.72 3	4.66 3	4.25 3	3.14 3	8.15 2	5.81 2	4.05 2	2.85 2	T
	7.63 -3	9.26 -3	1.07 -2	1.23 -2	1.26 -2	1.39 -2	1.44 -2	1.56 -2	1.63 -2	1.74 -2	1.82 -2	2.02 -2	2.11 -2	2.44 -2	4.31 -2	4.90 -2	5.60 -2	6.35 -2	Q
19	2.55 4	1.99 4	1.62 4	1.31 4	1.25 4	1.06 4	9.97 3	8.66 3	8.05 3	7.11 3	6.53 3	5.34 3	4.87 3	3.62 3	9.52 2	6.81 2	4.76 2	3.36 2	K
	2.04 3	1.54 3	1.24 3	9.81 2	9.29 2	7.82 2	7.31 2	6.29 2	5.81 2	5.09 2	4.65 2	3.75 2	3.40 2	2.49 2	6.14 1	4.34 1	3.00 1	2.09 1	L
	1.36 2	1.03 2	8.21 1	6.46 1	6.11 1	5.13 1	4.78 1	4.10 1	3.78 1	3.30 1	3.01 1	2.41 1	2.19 1	1.59 1	3.79	2.66	1.82	1.26	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	2.77 4	2.15 4	1.76 4	1.41 4	1.34 4	1.15 4	1.08 4	9.33 3	8.67 3	7.65 3	7.03 3	5.74 3	5.23 3	3.88 3	1.02 3	7.27 2	5.07 2	3.58 2	T
	6.64 -3	8.26 -3	9.66 -3	1.13 -2	1.16 -2	1.29 -2	1.34 -2	1.46 -2	1.53 -2	1.64 -2	1.72 -2	1.92 -2	2.02 -2	2.34 -2	4.22 -2	4.81 -2	5.51 -2	6.26 -2	Q
20	3.04 4	2.37 4	1.94 4	1.57 4	1.49 4	1.27 4	1.20 4	1.04 4	9.69 3	8.57 3	7.88 3	6.45 3	5.89 3	4.39 3	1.17 3	8.36 2	5.85 2	4.14 2	K
	2.65 3	2.01 3	1.62 3	1.28 3	1.21 3	1.02 3	9.56 2	8.22 2	7.60 2	6.66 2	6.09 2	4.91 2	4.46 2	3.26 2	8.11 1	5.74 1	3.97 1	2.78 1	L
	1.95 2	1.47 2	1.18 2	9.29 1	8.79 1	7.38 1	6.89 1	5.91 1	5.45 1	4.77 1	4.35 1	3.49 1	3.17 1	2.30 1	5.54	3.89	2.67	1.86	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	3.32 4	2.58 4	2.11 4	1.71 4	1.62 4	1.38 4	1.30 4	1.13 4	1.05 4	9.29 3	8.53 3	6.97 3	6.37 3	4.74 3	1.25 3	8.97 2	6.28 2	4.44 2	T
	5.60 -3	7.23 -3	8.62 -3	1.02 -2	1.06 -2	1.19 -2	1.24 -2	1.36 -2	1.43 -2	1.54 -2	1.62 -2	1.82 -2	1.91 -2	2.24 -2	4.12 -2	4.72 -2	5.42 -2	6.17 -2	Q
21	3.58 4	2.79 4	2.29 4	1.86 4	1.77 4	1.51 4	1.42 4	1.24 4	1.15 4	1.02 4	9.39 3	7.70 3	7.04 3	5.26 3	1.41 3	1.01 3	7.11 2	5.05 2	K
	3.27 3	2.48 3	2.00 3	1.58 3	1.50 3	1.26 3	1.18 3	1.02 3	9.40 2	8.24 2	7.53 2	6.08 2	5.53 2	4.05 2	1.01 2	7.17 1	4.96 1	3.48 1	L
	2.70 2	2.04 2	1.64 2	1.29 2	1.22 2	1.03 2	9.61 1	8.25 1	7.61 1	6.66 1	6.08 1	4.89 1	4.43 1	3.23 1	7.84	5.52	3.79	2.64	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	3.93 4	3.06 4	2.51 4	2.03 4	1.93 4	1.65 4	1.55 4	1.35 4	1.25 4	1.11 4	1.02 4	8.36 3	7.64 3	5.69 3	1.52 3	1.10 3	7.64 2	5.42 2	T
	4.48 -3	6.10 -3	7.50 -3	9.11 -3	9.49 -3	1.08 -2	1.13 -2	1.25 -2	1.32 -2	1.43 -2	1.51 -2	1.71 -2	1.80 -2	2.13 -2	4.02 -2	4.61 -2	5.32 -2	6.08 -2	Q

Z	CrKα1	CrKβ1	FeKα1	CoKα1	FeKβ1	NiKα1	CoKβ1	CuKα1	NiKβ1	ZnKα1	CuKβ1	ZnKβ1	GeKα1	GeKβ1	MoKα1	MoKβ1	AgKα1	AgKβ1	line
	5.415	5.947	6.404	6.930	7.058	7.478	7.649	8.048	8.265	8.639	8.905	9.572	9.886	10.982	17.479	19.608	22.163	24.942	keV
22	4.16 4	3.26 4	2.68 4	2.17 4	2.07 4	1.77 4	1.67 4	1.46 4	1.36 4	1.20 4	1.11 4	9.09 3	8.32 3	6.23 3	1.69 3	1.22 3	8.54 2	6.08 2	K
	4.35 3	3.31 3	2.66 3	2.11 3	2.00 3	1.69 3	1.58 3	1.36 3	1.26 3	1.10 3	1.01 3	8.16 2	7.42 2	5.44 2	1.37 2	9.71 1	6.73 1	4.73 1	L
	3.65 2	2.76 2	2.22 2	1.75 2	1.66 2	1.39 2	1.30 2	1.12 2	1.03 2	9.05 1	8.26 1	6.65 1	6.04 1	4.40 1	1.08 1	7.60	5.23	3.65	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	4.63 4	3.62 4	2.97 4	2.40 4	2.28 4	1.96 4	1.84 4	1.60 4	1.49 4	1.32 4	1.22 4	9.97 3	9.12 3	6.82 3	1.83 3	1.32 3	9.27 2	6.59 2	T
	3.41 -3	5.04 -3	6.43 -3	8.04 -3	8.43 -3	9.70 -3	1.02 -2	1.14 -2	1.21 -2	1.32 -2	1.40 -2	1.60 -2	1.70 -2	2.03 -2	3.92 -2	4.52 -2	5.22 -2	5.98 -2	Q
23	0.0	3.77 4	3.10 4	2.52 4	2.40 4	2.06 4	1.94 4	1.70 4	1.58 4	1.40 4	1.29 4	1.06 4	9.74 3	7.31 3	2.00 1	1.44 3	1.02 3	7.24 2	K
	5.44 3	4.14 3	3.33 3	2.65 3	2.51 3	2.12 3	1.98 3	1.71 3	1.58 3	1.39 3	1.27 3	1.03 3	9.32 2	6.84 2	1.73 2	1.23 2	8.54 1	6.01 1	L
	4.81 2	3.64 2	2.93 2	2.32 2	2.19 2	1.85 2	1.73 2	1.48 2	1.37 2	1.20 2	1.10 2	8.84 1	8.03 1	5.86 1	1.45 1	1.02 1	7.04	4.92	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	5.92 3	4.22 4	3.47 4	2.81 4	2.68 4	2.29 4	2.16 4	1.88 4	1.75 4	1.55 4	1.43 4	1.18 4	1.08 4	8.05 3	2.19 3	1.58 3	1.11 3	7.89 2	T
	1.65 -2	3.87 -3	5.27 -3	6.87 -3	7.26 -3	8.54 -3	9.06 -3	1.03 -2	1.09 -2	1.21 -2	1.29 -2	1.49 -2	1.58 -2	1.91 -2	3.81 -2	4.41 -2	5.12 -2	5.88 -2	Q
24	0.0	0.0	3.56 4	2.90 4	2.77 4	2.38 4	2.24 4	1.96 4	1.83 4	1.62 4	1.50 4	1.23 4	1.13 4	8.50 3	2.35 3	1.70 3	1.20 3	8.56 2	K
	6.60 3	5.02 3	4.05 3	3.21 3	3.05 3	2.57 3	2.41 3	2.08 3	1.92 3	1.69 3	1.54 3	1.25 3	1.14 3	8.34 2	2.12 2	1.51 2	1.05 2	7.38 1	L
	6.21 2	4.72 2	3.79 2	3.00 2	2.84 2	2.40 2	2.24 2	1.93 2	1.78 2	1.56 2	1.43 2	1.15 2	1.05 2	7.64 1	1.90 1	1.34 1	9.28	6.50	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	7.22 3	5.49 3	4.01 4	3.25 4	3.10 4	2.66 4	2.50 4	2.19 4	2.03 4	1.81 4	1.66 4	1.37 4	1.25 4	9.41 3	2.58 3	1.86 3	1.31 3	9.36 2	T
	1.63 -2	1.80 -2	4.03 -3	5.63 -3	6.02 -3	7.30 -3	7.82 -3	9.03 -3	9.69 -3	1.08 -2	1.16 -2	1.37 -2	1.46 -2	1.79 -2	3.69 -2	4.29 -2	5.01 -2	5.77 -2	Q
25	0.0	0.0	0.0	3.31 4	3.16 4	2.72 4	2.56 4	2.24 4	2.09 4	1.86 4	1.72 4	1.42 4	1.30 4	9.80 3	2.73 3	1.98 3	1.40 3	1.00 2	K
	7.87 3	5.99 3	4.83 3	3.84 3	3.64 3	3.08 3	2.88 3	2.48 3	2.30 3	2.02 3	1.85 3	1.49 3	1.36 3	9.99 2	2.55 2	1.81 2	1.26 2	8.90 1	L
	7.89 2	6.00 1	4.83 2	3.83 2	3.62 2	3.06 2	2.86 2	2.46 2	2.28 2	2.00 2	1.82 2	1.47 2	1.34 2	9.79 1	2.44 1	1.73 1	1.20 1	8.41	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	8.65 3	6.59 3	5.31 3	3.73 4	3.56 4	3.06 4	2.88 4	2.52 4	2.34 4	2.08 4	1.92 4	1.58 4	1.45 4	1.09 4	3.01 3	2.18 3	1.54 3	1.10 3	T
	1.61 -2	1.78 -2	1.93 -2	4.33 -3	4.72 -3	6.00 -3	6.52 -3	7.74 -3	8.39 -3	9.53 -3	1.03 -2	1.24 -2	1.33 -2	1.66 -2	3.57 -2	4.17 -2	4.89 -2	5.65 -2	Q
26	0.0	0.0	0.0	0.0	0.0	3.08 4	2.91 4	2.55 4	2.38 4	2.12 4	1.96 4	1.62 4	1.48 4	1.12 4	3.15 3	2.29 3	1.63 3	1.17 3	K
	9.15 3	6.97 3	5.62 3	4.47 3	4.24 3	3.58 3	3.35 3	2.89 3	2.68 3	2.35 3	2.15 3	1.74 3	1.59 3	1.17 3	2.98 2	2.13 2	1.48 2	1.05 2	L
	9.87 2	7.51 2	6.05 2	4.80 2	4.55 2	3.84 2	3.59 2	3.09 2	2.86 2	2.51 2	2.30 2	1.85 2	1.69 2	1.24 2	3.10 1	2.20 1	1.53 1	1.07 1	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	1.01 4	7.72 3	6.23 3	4.95 3	4.69 3	3.48 4	3.28 4	2.87 4	2.67 4	2.38 4	2.19 4	1.81 4	1.66 4	1.25 4	3.48 3	2.53 3	1.79 3	1.28 3	T
	1.59 -2	1.76 -2	1.91 -2	2.07 -2	2.11 -2	4.62 -3	5.14 -3	6.35 -3	7.01 -3	8.15 -3	8.96 -3	1.10 -2	1.19 -2	1.52 -2	3.44 -2	4.04 -2	4.76 -2	5.53 -2	Q
27	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.88 4	2.69 4	2.39 4	2.21 4	1.83 4	1.68 4	1.27 4	3.62 3	2.63 3	1.87 3	1.34 3	K
	1.05 4	7.99 3	6.45 3	5.13 3	4.87 3	4.11 3	3.85 3	3.32 3	3.08 3	2.70 3	2.47 3	2.01 3	1.82 3	1.34 3	3.44 2	2.45 2	1.71 2	1.21 2	L
	1.22 3	9.28 2	7.48 2	5.94 2	5.63 2	4.76 2	4.45 2	3.83 2	3.55 2	3.11 2	2.85 2	2.30 2	2.09 2	1.54 2	3.87 1	2.75 1	1.91 1	1.34 1	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	1.17 4	8.92 3	7.20 3	5.72 3	5.43 3	4.59 3	4.30 3	3.25 4	3.03 4	2.70 4	2.49 4	2.06 4	1.89 4	1.42 4	4.00 3	2.91 3	2.06 3	1.48 3	T
	1.57 -2	1.74 -2	1.89 -2	2.05 -2	2.09 -2	2.23 -2	2.28 -2	4.90 -3	5.56 -3	6.70 -3	7.51 -3	9.53 -3	1.05 -2	1.38 -2	3.30 -2	3.91 -2	4.63 -2	5.40 -2	Q
28	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.69 4	2.49 4	2.06 4	1.90 4	1.44 4	4.12 3	3.01 3	2.14 3	1.54 3	K
	1.20 4	9.12 3	7.37 3	5.86 3	5.56 3	4.70 3	4.40 3	3.80 3	3.52 3	3.09 3	2.83 3	2.29 3	2.09 3	1.54 3	3.95 2	2.82 2	1.97 2	1.39 2	L
	1.49 3	1.13 3	9.14 2	7.27 2	6.89 2	5.82 2	5.45 2	4.70 2	4.35 2	3.82 2	3.49 2	2.83 2	2.57 2	1.89 2	4.78 1	3.40 1	2.36 1	1.67 1	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	N
	1.34 4	1.03 4	8.28 3	6.59 3	6.25 3	5.28 3	4.95 3	4.27 3	3.95 3	3.04 4	2.81 4	2.32 4	2.13 4	1.61 4	4.56 3	3.32 3	2.36 3	1.70 3	T
	1.55 -2	1.72 -2	1.87 -2	2.03 -2	2.07 -2	2.20 -2	2.26 -2	2.38 -2	2.45 -2	5.19 -3	6.00 -3	8.03 -3	8.98 -3	1.23 -2	3.15 -2	3.77 -2	4.49 -2	5.26 -2	Q
29	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.31 4	2.12 4	1.61 4	4.67 3	3.41 3	2.43 3	1.76 3	K
	1.37 4	1.05 4	8.44 3	6.72 3	6.37 3	5.39 3	5.05 3	4.36 3	4.04 3	3.55 3	3.25 3	2.63 3	2.40 3	1.77 3	4.55 2	3.25 2	2.27 2	1.61 2	L
	1.80 3	1.37 3	1.11 3	8.80 2	8.35 2	7.05 2	6.60 2	5.70 2	5.27 2	4.63 2	4.24 2	3.43 2	3.12 2	2.29 2	5.83 1	4.15 1	2.89 1	2.04 1	M
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	9.02 1	6.86 1	0.0	0.0	0.0	0.0	0.0	0.0	9.02 1	6.86 1	N
	1.55 4	1.18 4	9.55 3	7.60 3	7.21 3	6.10 3	5.71 3	4.93 3	4.65 3	4.08 3	3.67 3	2.61 4	2.39 4	1.81 4	5.18 3	3.78 3	2.78 3	2.01 3	T
	1.52 -2	1.70 -2	1.84 -2	2.01 -2	2.05 -2	2.18 -2	2.24 -2	2.36 -2	2.38 -2	2.50 -2	2.62 -2	6.49 -3	7.44 -3	1.08 -2	3.01 -2	3.62 -2	4.21 -2	4.95 -2	Q

Z	CrKα1	CrKβ1	FeKα1	CoKα1	FeKβ1	NiKα1	CoKβ1	CuKα1	NiKβ1	ZnKα1	CuKβ1	ZnKβ1	GeKα1	GeKβ1	MoKα1	MoKβ1	AgKα1	AgKβ1	line
	5.415	5.947	6.404	6.910	7.058	7.478	7.649	8.048	8.265	8.639	8.905	9.572	9.886	10.982	17.479	19.608	22.163	24.942	keV
30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.37 4	1.80 4	5.26 3	3.85 3	2.75 3	1.99 3	K
	1.57 4	1.20 4	9.68 3	7.71 3	7.32 3	6.19 3	5.80 3	5.01 3	4.64 3	4.08 3	3.73 3	3.03 3	2.76 3	2.03 3	5.25 2	3.76 2	2.63 2	1.86 2	L
	2.15 3	1.64 3	1.33 3	1.05 3	1.00 3	8.46 2	7.92 2	6.83 2	6.32 2	5.56 2	5.09 2	4.12 2	3.75 2	2.76 2	7.05 1	5.02 1	3.50 1	2.47 1	M
	5.53 1	4.38 1	4.15 1	3.50 1	3.27 1	2.82 1	2.60 1	2.28 1	1.40 2	1.06 2	5.53 1	4.38 1	4.15 1	3.50 1	3.27 1	2.82 1	1.40 2	1.06	N
	1.79 4	1.37 4	1.11 4	8.80 3	8.35 3	7.06 3	6.62 3	5.71 3	5.41 3	4.74 3	4.30 3	3.49 3	2.68 4	2.04 4	5.88 3	4.30 3	3.19 3	2.31 3	T
	1.49 -2	1.67 -2	1.81 -2	1.98 -2	2.02 -2	2.15 -2	2.20 -2	2.33 -2	2.34 -2	2.47 -2	2.57 -2	2.77 -2	5.86 -3	9.18 -3	2.84 -2	3.45 -2	4.02 -2	4.75 -2	Q
31	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.00 4	5.89 3	4.32 3	3.10 3	2.24 3	K
	1.81 4	1.38 4	1.12 4	8.90 3	8.45 3	7.15 3	6.70 3	5.79 3	5.36 3	4.72 3	4.32 3	3.51 3	3.19 3	2.35 3	6.10 2	4.36 2	3.05 2	2.16 2	L
	2.68 3	2.05 3	1.65 3	1.32 3	1.25 3	1.06 3	9.91 2	8.55 2	7.92 2	6.97 2	6.38 2	5.17 2	4.71 2	3.47 2	8.90 1	6.35 1	4.43 1	3.13 1	M
	9.02 1	6.86 1	5.53 1	4.38 1	4.15 1	3.50 1	3.27 1	2.82 1	2.60 1	2.28 1	2.08 1	1.68 1	1.52 1	1.11 1	2.69	1.88	1.28	8.87 -1	N
	2.09 4	1.59 4	1.29 4	1.03 4	9.74 3	8.24 3	7.72 3	6.67 3	6.18 3	5.43 3	4.98 3	4.04 3	3.68 3	2.27 4	6.59 3	4.82 3	3.45 3	2.49 3	T
	1.46 -2	1.63 -2	1.78 -2	1.95 -2	1.99 -2	2.12 -2	2.17 -2	2.30 -2	2.36 -2	2.48 -2	2.56 -2	2.76 -2	2.86 -2	7.60 -3	2.70 -2	3.32 -2	4.05 -2	4.83 -2	Q
32	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0 K	0.0	6.56 3	4.82 3	3.47 3	2.51 3	K
	2.07 4	1.58 4	1.28 4	1.02 4	9.68 3	8.20 3	7.68 3	6.64 3	6.15 3	5.41 3	4.96 3	4.02 3	3.66 3	2.70 3	7.02 2	5.03 2	3.52 2	2.50 2	L
	2.81 3	2.15 3	1.73 3	1.38 3	1.31 3	1.11 3	1.04 3	8.96 2	8.30 2	7.30 2	6.68 2	5.42 2	4.93 2	3.63 2	9.32 1	6.65 1	4.64 1	3.28 1	M
	1.40 2	1.06 2	8.47 1	6.68 1	6.32 1	5.31 1	4.96 1	4.25 1	3.92 1	3.43 1	3.13 1	2.51 1	2.27 1	1.65 1	3.92	2.74	1.86	1.28	N
	2.36 4	1.81 4	1.46 4	1.17 4	1.11 4	9.36 3	8.77 3	7.57 3	7.02 3	6.17 3	5.65 3	4.59 3	4.18 3	3.08 3	7.36 3	5.39 3	3.87 3	2.80 3	T
	1.44 -2	1.62 -2	1.76 -2	1.93 -2	1.97 -2	2.11 -2	2.16 -2	2.29 -2	2.36 -2	2.47 -2	2.56 -2	2.76 -2	2.86 -2	3.19 -2	2.54 -2	3.16 -2	3.89 -2	4.68 -2	Q
33	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	7.28 3	5.36 3	3.86 3	2.80 3	K
	2.35 4	1.80 4	1.45 4	1.16 4	1.10 4	9.32 3	8.73 3	7.54 3	6.99 3	6.15 3	5.64 3	4.58 3	4.17 3	3.08 3	8.02 2	5.74 2	4.03 2	2.86 2	L
	3.90 3	2.99 3	2.42 3	1.93 3	1.83 3	1.55 3	1.46 3	1.26 3	1.17 3	1.03 3	9.40 2	7.64 2	6.96 2	5.13 2	1.33 2	9.50 1	6.65 1	4.71 1	M
	2.14 2	1.61 2	1.28 2	1.01 -2	9.50 1	7.95 1	1.41 1	6.34 1	5.84 1	5.09 1	4.63 1	3.70 1	3.35 1	2.42 1	5.63	3.92	2.66	1.83	N
	2.76 4	2.11 4	1.71 4	1.36 4	1.29 4	1.10 4	1.03 4	8.87 3	8.21 3	7.23 3	6.62 3	5.38 3	4.90 3	3.62 3	8.22 3	6.03 3	4.33 3	3.14 3	T
	1.38 -2	1.56 -2	1.70 -2	1.87 -2	1.91 -2	2.05 -2	2.10 -2	2.22 -2	2.29 -2	2.41 -2	2.49 -2	2.69 -2	2.79 -2	3.12 -2	2.37 -2	3.00 -2	3.73 -2	4.52 -2	Q
34	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.04 3	5.93 3	4.28 3	3.11 3	K
	2.67 4	2.04 4	1.65 4	1.32 4	1.25 4	1.06 4	9.94 3	8.59 3	7.96 3	7.01 3	6.43 3	5.22 3	4.76 3	3.51 3	9.17 2	6.57 2	4.61 2	3.27 2	L
	4.18 3	3.20 3	2.59 3	2.07 3	1.96 3	1.66 3	1.56 3	1.35 3	1.25 3	1.10 3	1.01 3	8.17 2	7.44 2	5.49 2	1.42 2	1.02 2	7.12 1	5.04 1	M
	3.21 2	2.40 2	1.90 2	1.49 2	1.41 2	1.17 2	1.09 2	9.32 1	8.57 1	7.46 1	6.78 1	5.40 1	4.88 1	3.50 1	7.99	5.54	3.74	2.56	N
	3.12 4	2.39 4	1.93 4	1.54 4	1.46 4	1.24 4	1.16 4	1.00 4	9.30 3	8.18 3	7.50 3	6.09 3	5.55 3	4.10 3	9.11 3	6.70 3	4.81 3	3.49 3	T
	1.36 -2	1.53 -2	1.68 -2	1.85 -2	1.89 -2	2.03 -2	2.08 -2	2.21 -2	2.28 -2	2.39 -2	2.48 -2	2.68 -2	2.78 -2	3.11 -2	2.20 -2	2.83 -2	3.57 -2	4.36 -2	Q
35	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.84 3	6.54 3	4.72 3	3.44 3	K
	3.00 4	2.30 4	1.86 4	1.49 4	1.41 4	1.20 4	1.12 4	9.69 3	8.98 3	7.91 3	7.25 3	5.89 3	5.37 3	3.97 3	1.04 3	7.44 2	5.22 2	3.71 2	L
	4.53 3	3.47 3	2.81 3	2.24 3	2.13 3	1.80 3	1.69 3	1.46 3	1.35 3	1.19 3	1.09 3	8.85 2	8.06 2	5.95 2	1.54 2	1.10 2	7.72 1	5.47 1	M
	4.71 2	3.51 2	2.78 2	1.17 2	2.04 2	1.70 2	1.58 2	1.35 2	1.24 2	1.08 2	9.77 1	7.76 1	7.00 1	5.00 1	1.12 1	7.74	5.21	3.55	N
	3.50 4	2.68 4	2.17 4	1.73 4	1.64 4	1.39 4	1.31 4	1.13 4	1.05 4	9.20 3	8.43 3	6.85 3	6.24 3	4.61 3	1.00 4	7.40 3	5.33 3	3.87 3	T
	1.33 -2	1.51 -2	1.66 -2	1.83 -2	1.87 -2	2.00 -2	2.06 -2	2.18 -2	2.25 -2	2.37 -2	2.45 -2	2.66 -2	2.76 -2	3.09 -2	2.02 -2	2.65 -2	3.39 -2	4.19 -2	Q
36	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	9.69 3	7.18 3	5.20 3	3.80 3	K
	3.28 4	2.51 4	2.04 4	1.63 4	1.54 4	1.31 4	1.23 4	1.06 4	9.83 3	8.66 3	7.94 3	6.45 3	5.88 3	4.35 3	1.14 3	8.18 2	5.74 2	4.08 2	L
	5.25 3	4.02 3	3.26 3	2.60 3	2.47 3	2.09 3	1.96 3	1.70 3	1.57 3	1.38 3	1.27 3	1.03 3	9.38 2	6.93 2	1.80 2	1.29 2	9.03 1	6.41 1	M
	6.77 2	5.03 2	3.98 2	3.10 2	2.92 2	2.43 2	2.26 2	1.92 2	1.76 2	1.53 2	1.39 2	1.10 2	9.90 1	7.05 1	1.56 1	1.07 1	7.17	4.87	N
	3.87 4	2.97 4	2.40 4	1.92 4	1.82 4	1.54 4	1.45 4	1.25 4	1.16 4	1.02 4	9.35 3	7.59 3	6.92 3	5.11 3	1.10 4	8.13 3	5.86 3	4.27 3	T
	1.29 -2	1.47 -2	1.62 -2	1.79 -2	1.83 -2	1.96 -2	2.02 -2	2.14 -2	2.21 -2	2.33 -2	2.41 -2	2.62 -2	2.71 -2	3.05 -2	1.83 -2	2.46 -2	3.21 -2	4.00 -2	Q
37	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.06 4	7.85 3	5.70 3	4.17 3	K
	3.75 4	2.87 4	2.33 4	1.86 4	1.77 4	1.50 4	1.41 4	1.22 4	1.13 4	9.93 3	9.11 3	7.41 3	6.75 3	5.00 3	1.31 3	9.42 2	6.62 2	4.71 2	L
	6.16 3	4.73 3	3.83 3	3.06 3	2.91 3	2.46 3	2.31 3	2.00 3	1.85 3	1.63 3	1.49 3	1.21 3	1.11 3	8.18 2	2.13 2	1.53 2	1.07 2	7.60 1	M
	8.58 2	6.39 2	5.06 2	3.94 2	3.72 2	3.10 2	2.88 2	2.45 2	2.25 2	1.95 2	1.77 2	1.41 2	1.27 2	9.03 1	2.00 1	1.38 1	9.22	6.27	N
	4.45 4	3.41 4	2.76 4	2.21 4	2.10 4	1.78 4	1.67 4	1.44 4	1.34 4	1.18 4	1.08 4	8.76 3	7.98 3	5.90 3	1.21 4	8.96 3	6.47 3	4.72 3	T
	1.24 -2	1.42 -2	1.57 -2	1.74 -2	1.78 -2	1.92 -2	1.97 -2	2.10 -2	2.17 -2	2.29 -2	2.37 -2	2.58 -2	2.68 -2	3.01 -2	1.65 -2	2.28 -2	3.03 -2	3.83 -2	Q

Z	CrKα1	CrKβ1	FeKα1	CoKα1	FeKβ1	NiKα1	CoKβ1	CuKα1	NiKβ1	ZnKα1	CuKβ1	ZnKβ1	GeKα1	GeKβ1	MoKα1	MoKβ1	AgKα1	AgKβ1	line
	5.415	5.947	6.404	6.930	7.058	7.478	7.649	8.048	8.265	8.639	8.905	9.572	9.886	10.982	17.479	19.608	22.163	24.942	keV
38	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.15 4	8.56 3	6.22 3	4.56 3	K
	4.17 4	3.20 4	2.60 4	2.08 4	1.97 4	1.67 4	1.57 4	1.36 4	1.26 4	1.11 4	1.02 4	8.27 3	7.54 3	5.58 3	1.47 3	1.06 3	7.42 2	5.28 2	L
	6.85 3	5.25 3	4.26 3	3.40 3	3.23 3	2.74 3	2.57 3	2.22 3	2.06 3	1.81 3	1.66 3	1.35 3	1.23 3	9.10 2	2.38 2	1.71 2	1.20 2	8.49 1	M
	1.07 3	8.00 2	6.34 2	4.95 2	4.67 2	3.89 2	3.62 2	3.08 2	2.83 2	2.46 2	2.23 2	1.77 2	1.60 2	1.14 2	2.54 1	1.74 1	1.17 1	7.96	N
	4.96 4	3.81 4	3.09 4	2.47 4	2.34 4	1.99 4	1.86 4	1.61 4	1.49 4	1.32 4	1.21 4	9.80 3	8.93 3	6.61 3	1.33 4	9.80 3	7.09 3	5.18 3	T
	1.21 -2	1.38 -2	1.54 -2	1.71 -2	1.75 -2	1.89 -2	1.94 -2	2.07 -2	2.14 -2	2.26 -2	2.34 -2	2.55 -2	2.65 -2	2.98 -2	1.46 -2	2.09 -2	2.84 -2	3.65 -2	Q
39	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.25 4	9.30 3	6.77 3	4.97 3	K
	4.63 4	3.56 4	2.89 4	2.31 4	2.19 4	1.86 4	1.75 4	1.51 4	1.40 4	1.24 4	1.13 4	9.23 3	8.41 3	6.23 3	1.64 3	1.18 3	8.31 2	5.92 2	L
	7.70 3	5.91 3	4.79 3	3.83 3	3.64 3	3.09 3	2.89 3	2.50 3	2.32 3	2.05 3	1.88 3	1.53 3	1.39 3	1.03 3	2.69 2	1.93 2	1.36 2	9.63 1	M
	1.32 3	9.88 2	7.85 2	6.13 2	5.79 2	4.83 2	4.49 2	3.83 2	3.52 2	3.06 2	2.78 2	2.21 2	1.99 2	1.42 2	3.17 1	2.18 1	1.47 1	9.97	N
	5.54 4	4.25 4	3.45 4	2.76 4	2.62 4	2.22 4	2.08 4	1.80 4	1.67 4	1.47 4	1.35 4	1.10 4	1.00 4	7.40 3	1.44 4	1.07 4	7.75 3	5.67 3	T
	1.16 -2	1.34 -2	1.49 -2	1.67 -2	1.71 -2	1.85 -2	1.90 -2	2.03 -2	2.10 -2	2.22 -2	2.30 -2	2.51 -2	2.61 -2	2.95 -2	1.26 -2	1.89 -2	2.65 -2	3.45 -2	Q
40	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.01 4	7.35 3	5.40 3	K
	5.10 4	3.92 4	3.18 4	2.55 4	2.42 4	2.05 4	1.93 4	1.67 4	1.55 4	1.36 4	1.25 4	1.02 4	9.30 3	6.89 3	1.82 3	1.31 3	9.22 2	6.57 2	L
	8.66 3	6.65 3	5.39 3	4.31 3	4.09 3	3.47 3	3.26 3	2.82 3	2.61 3	2.30 3	2.11 3	1.72 3	1.57 3	1.15 3	3.04 2	2.18 2	1.53 2	1.09 2	M
	1.61 3	1.21 3	9.59 2	7.50 2	7.09 2	5.91 2	5.51 2	4.70 2	4.32 2	3.76 2	3.41 2	2.72 2	2.45 2	1.75 2	3.93 1	2.71 1	1.82 1	1.24 1	N
	6.13 4	4.71 4	3.82 4	3.05 4	2.90 4	2.46 4	2.31 4	2.00 4	1.85 4	1.63 4	1.50 4	1.22 4	1.11 4	8.22 3	2.16 3	1.16 4	8.44 3	6.18 3	T
	1.12 -2	1.30 -2	1.45 -2	1.63 -2	1.67 -2	1.80 -2	1.86 -2	1.99 -2	2.06 -2	2.18 -2	2.26 -2	2.47 -2	2.57 -2	2.91 -2	4.82 -2	1.69 -2	2.45 -2	3.26 -2	Q
41	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.09 4	7.95 3	5.86 3	K
	5.61 4	4.32 4	3.51 4	2.81 4	2.67 4	2.27 4	2.13 4	1.84 4	1.71 4	1.51 4	1.38 4	1.13 4	1.03 4	7.61 3	2.02 3	1.45 3	1.02 3	7.28 2	L
	9.97 3	7.66 3	6.22 3	4.97 3	4.72 3	4.01 3	3.76 3	3.26 3	3.02 3	2.66 3	2.44 3	1.99 3	1.81 3	1.34 3	3.53 2	2.53 2	1.78 2	1.27 2	M
	1.94 3	1.46 3	1.16 3	9.08 2	8.58 2	7.17 2	6.68 2	5.70 2	5.25 2	4.57 2	4.15 2	3.31 2	2.98 2	2.14 2	4.81 1	3.32 1	2.23 1	1.52 1	N
	6.80 4	5.23 4	4.24 4	3.40 4	3.23 4	2.74 4	2.57 4	2.22 4	2.06 4	1.82 4	1.67 4	1.36 4	1.24 4	9.16 3	2.42 3	1.26 4	9.17 3	6.72 3	T
	1.07 -2	1.25 -2	1.40 -2	1.58 -2	1.62 -2	1.76 -2	1.81 -2	1.94 -2	2.01 -2	2.13 -2	2.21 -2	2.42 -2	2.52 -2	2.86 -2	4.77 -2	1.48 -2	K 2.24 -2	K 3.05 -2	Q
42	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.57 3	6.33 3	K
	6.19 4	4.77 4	3.88 4	3.11 4	2.95 4	2.51 4	2.35 4	2.04 4	1.89 4	1.67 4	1.53 4	1.25 4	1.14 4	8.44 3	2.24 3	1.61 3	1.14 3	8.10 2	L
	1.10 4	8.49 3	6.89 3	5.51 3	5.23 3	4.44 3	4.17 3	3.61 3	3.35 3	2.95 3	2.71 3	2.20 3	2.01 3	1.49 3	3.92 2	2.81 2	1.98 2	1.41 2	M
	2.31 3	1.74 3	1.39 3	1.09 3	1.03 3	8.61 2	8.03 2	6.86 2	6.31 2	5.50 2	5.00 2	3.98 2	3.60 2	2.58 2	5.84 1	4.03 1	2.71 1	1.85 1	N
	7.53 4	5.79 4	4.70 4	3.76 4	3.58 4	3.04 4	2.85 4	2.47 4	2.29 4	2.02 4	1.85 4	1.51 4	1.37 4	1.02 4	2.69 3	1.93 3	9.94 3	7.30 3	T
	1.03 -2	1.21 -2	1.36 -2	1.53 -2	1.58 -2	1.71 -2	1.77 -2	1.90 -2	1.97 -2	2.09 -2	2.17 -2	2.38 -2	2.48 -2	2.82 -2	4.74 -2	5.33 -2	2.03 -2	2.85 -2	Q
43	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	9.23 3	6.82 3	K
	6.76 4	5.21 4	4.24 4	3.40 4	3.23 4	2.74 4	2.57 4	2.23 4	2.07 4	1.83 4	1.68 4	1.37 4	1.25 4	9.25 3	2.46 3	1.77 3	1.25 3	8.91 2	L
	1.21 4	9.26 3	7.52 3	6.01 3	5.71 3	4.85 3	4.55 3	3.94 3	3.65 3	3.22 3	2.95 3	2.40 3	2.19 3	1.62 3	4.28 2	3.08 2	2.16 2	1.54 2	M
	2.73 3	2.06 3	1.65 3	1.29 3	1.22 3	1.02 3	9.55 2	8.17 2	7.52 2	6.55 2	5.96 2	4.76 2	4.30 2	3.09 2	7.02 1	4.85 1	3.26 1	2.23 1	N
	8.24 4	6.34 4	5.15 4	4.13 4	3.92 4	3.33 4	3.12 4	2.71 4	2.51 4	2.21 4	2.03 4	1.65 4	1.51 4	1.12 4	2.96 3	2.13 3	1.07 4	7.89 3	T
	9.82 -3	1.16 -2	1.32 -2	1.49 -2	1.53 -2	1.67 -2	1.73 -2	1.86 -2	1.93 -2	2.05 -2	2.13 -2	2.34 -2	2.44 -2	2.78 -2	4.70 -2	5.30 -2	1.81 -2	2.63 -2	Q
44		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	9.90 3	7.33 3	K
		5.70 4	4.64 4	3.72 4	3.53 4	3.00 4	2.82 4	2.44 4	2.27 4	2.00 4	1.84 4	1.50 4	1.37 4	1.02 4	2.71 3	1.95 3	1.38 3	9.82 2	L
		1.02 4	8.29 3	6.63 3	6.30 3	5.35 3	5.02 3	4.35 3	4.03 3	3.55 3	3.26 3	2.65 3	2.42 3	1.79 3	4.73 2	3.40 2	2.39 2	1.70 2	M
		2.42 3	1.94 3	1.52 3	1.44 3	1.21 3	1.13 3	9.65 2	8.89 2	7.75 2	7.06 2	5.64 2	5.10 2	3.67 2	8.38 1	5.79 1	3.90 1	2.66 1	N
		6.96 4	5.66 4	4.53 4	4.31 4	3.66 4	3.43 4	2.98 4	2.76 4	2.43 4	2.23 4	1.82 4	1.66 4	1.23 4	3.26 3	2.35 3	1.16 4	8.51 3	T
		1.12 -2	1.27 -2	1.45 -2	1.49 -2	1.63 -2	1.68 -2	1.81 -2	1.88 -2	2.00 -2	2.09 -2	2.30 -2	2.40 -2	2.74 -2	4.67 -2	5.27 -2	1.58 -2	2.41 -2	Q
45		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	7.86 3	K
		6.22 4	5.06 4	4.06 4	3.86 4	3.28 4	3.08 4	2.67 4	2.48 4	2.19 4	2.01 4	1.64 4	1.50 4	1.11 4	2.97 3	2.14 3	1.51 3	1.08 3	L
		1.13 4	9.16 3	7.33 3	6.96 3	5.91 3	5.55 3	4.81 3	4.46 3	3.93 3	3.61 3	2.94 3	2.68 3	1.99 3	5.26 2	3.78 2	2.66 2	1.90 2	M
		2.82 3	2.26 3	1.78 3	1.69 3	1.41 3	1.32 3	1.13 3	1.04 3	9.10 2	8.29 2	6.63 2	6.00 2	4.32 2	9.93 1	6.87 1	4.63 1	3.16 1	N
		7.63 4	6.20 4	4.97 4	4.72 4	4.02 4	3.77 4	3.27 4	3.03 4	2.67 4	2.45 4	2.00 4	1.82 4	1.35 4	3.60 3	2.59 3	1.82 3	9.16 3	T
	E(2s)	1.07 -2	1.22 -2	1.40 -2	1.44 -2	1.58 -2	1.63 -2	1.76 -2	1.83 -2	1.96 -2	2.04 -2	2.25 -2	2.35 -2	2.69 -2	4.63 -2	5.23 -2	5.93 -2	2.18 -2	Q

Z	CrKα1	CrKβ1	FeKα1	CoKα1	FeKβ1	NiKα1	CoKβ1	CuKα1	NiKβ1	ZnKα1	CuKβ1	ZnKβ1	GeKα1	GeKβ1	MoKα1	MoKβ1	AgKα1	AgKβ1	line
	5.415	5.947	6.404	6.930	7.058	7.478	7.649	8.048	8.265	8.639	8.905	9.572	9.886	10.982	17.479	19.608	22.163	24.942	keV
46			0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.41 3	K
			5.51 4	4.42 4	4.20 4	3.58 4	3.36 4	2.91 4	2.70 4	2.39 4	2.19 4	1.79 4	1.63 4	1.21 4	3.25 3	2.34 3	1.65 3	1.18 3	L
			1.01 4	8.09 3	7.68 3	6.53 3	6.12 3	5.30 3	4.92 3	4.34 3	3.98 3	3.24 3	2.96 3	2.20 3	5.82 2	4.18 2	2.95 2	2.10 2	M
			2.62 3	2.07 3	1.96 3	1.64 3	1.53 3	1.32 3	1.21 3	1.06 3	9.66 2	7.74 2	7.00 2	5.06 2	1.17 2	8.09 1	5.46 1	3.73 1	N
			6.78 4	5.44 4	5.17 4	4.39 4	4.12 4	3.57 4	3.32 4	2.93 4	2.69 4	2.19 4	2.00 4	1.48 4	3.95 3	2.84 3	2.00 3	5.84 3	T
			1.17 -2	1.35 -2	1.39 -2	1.53 -2	1.59 -2	1.72 -2	1.79 -2	1.91 -2	1.99 -2	2.21 -2	2.31 -2	2.65 -2	4.58 -2	5.19 -2	5.89 -2	1.95 -2	Q
47				0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0 K	K
				4.80 4	4.56 4	3.88 4	3.65 4	3.17 4	2.94 4	2.60 4	2.38 4	1.95 4	1.78 4	1.32 4	3.55 3	2.56 3	1.81 3	1.29 3	L
				8.98 3	8.53 3	7.24 3	6.80 3	5.89 3	5.46 3	4.82 3	4.42 3	3.60 3	3.29 3	2.44 3	6.47 2	4.65 2	3.28 2	2.34 2	M
				2.38 3	2.26 3	1.90 3	1.77 3	1.52 3	1.40 3	1.23 3	1.12 3	8.97 2	8.12 2	5.87 2	1.37 2	9.46 1	6.39 1	4.37 1	N
				5.94 4	5.64 4	4.80 4	4.50 4	3.91 4	3.62 4	3.20 4	2.94 4	2.40 4	2.19 4	1.62 4	4.33 3	3.12 3	2.20 3	1.57 3	T
				1.30 -2	1.34 -2	1.48 -2	1.53 -2	1.66 -2	1.73 -2	1.86 -2	1.94 -2	2.15 -2	2.25 -2	2.60 -2	4.54 -2	5.14 -2	5.85 -2	6.60 -2	Q
48				0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	K
				5.20 4	4.95 4	4.21 4	3.96 4	3.43 4	3.19 4	2.82 4	2.59 4	2.11 4	1.93 4	1.44 4	3.86 3	2.79 3	1.97 3	1.41 3	L
				9.86 3	9.37 3	7.96 3	7.47 3	6.47 3	6.00 3	5.30 3	4.86 3	3.96 3	3.62 3	2.68 3	7.13 2	5.13 2	3.61 2	2.58 2	M
				2.73 3	2.58 3	2.18 3	2.03 3	1.75 3	1.61 3	1.41 3	1.29 3	1.03 3	9.36 2	6.78 2	1.59 2	1.10 2	7.44 1	5.09 1	N
				6.46 4	6.14 4	5.23 4	4.91 4	4.26 4	3.95 4	3.49 4	3.20 4	2.61 4	2.39 4	1.77 4	4.73 3	3.41 3	2.41 3	1.72 3	T
				1.24 -2	1.29 -2	1.42 -2	1.48 -2	1.61 -2	1.68 -2	1.80 -2	1.89 -2	2.10 -2	2.20 -2	2.55 -2	4.49 -2	5.09 -2	5.80 -2	6.56 -2	Q
49				0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	K
				5.63 4	5.35 4	4.56 4	4.28 4	3.72 4	3.45 4	3.05 4	2.80 4	2.29 4	2.09 4	1.56 4	4.20 3	3.03 3	2.14 3	1.53 3	L
				1.09 4	1.03 4	8.76 3	8.22 3	7.13 3	6.61 3	5.83 3	5.35 3	4.36 3	3.98 3	2.96 3	7.86 2	5.66 2	3.99 2	2.85 2	M
				3.11 3	2.94 3	2.48 3	2.32 3	1.99 3	1.84 3	1.61 3	1.47 3	1.18 3	1.07 3	7.79 2	1.83 2	1.27 2	8.61 1	5.90 1	N
				7.02 4	6.68 4	5.68 4	5.34 4	4.63 4	4.30 4	3.80 4	3.49 4	2.85 4	2.60 4	1.93 4	5.17 3	3.72 3	2.63 3	1.88 3	T
				1.19 -2	1.23 -2	1.37 -2	1.43 -2	1.56 -2	1.63 -2	1.75 -2	1.84 -2	2.05 -2	2.15 -2	2.50 -2	4.44 -2	5.05 -2	5.76 -2	6.51 -2	Q
50					0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	K
					4.93 4	4.63 4	4.02 4	3.73 4	3.30 4	3.03 4	2.48 4	2.27 4	1.69 4	4.56 3	3.29 3	2.33 3	1.67 3	L
					9.56 3	8.97 3	7.77 3	7.21 3	6.36 3	5.84 3	4.76 3	4.34 3	3.23 3	8.58 2	6.18 2	4.36 2	3.11 2	M
					2.81 3	2.63 3	2.27 3	2.09 3	1.83 3	1.68 3	1.35 3	1.22 3	8.89 2	2.10 2	1.46 2	9.92 1	6.80 1	N
					6.16 4	5.79 4	5.02 4	4.66 4	4.12 4	3.79 4	3.09 4	2.82 4	2.10 4	5.63 3	4.06 3	2.86 3	2.05 3	T
					1.32 -2	1.37 -2	1.51 -2	1.58 -2	1.70 -2	1.78 -2	2.00 -2	2.10 -2	2.45 -2	4.39 -2	5.00 -2	5.71 -2	6.47 -2	Q
51							0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	K
							4.34 4	4.03 4	3.56 4	3.27 4	2.68 4	2.45 4	1.82 4	4.93 3	3.57 3	2.52 3	1.81 3	L
							8.50 3	7.88 3	6.96 3	6.39 3	5.21 3	4.76 3	3.53 3	9.42 2	6.79 2	4.79 2	3.42 2	M
							2.56 3	2.37 3	2.08 3	1.90 3	1.53 3	1.39 3	1.01 3	2.40 2	1.68 2	1.14 2	7.80 1	N
							5.44 4	5.05 4	4.47 4	4.10 4	3.35 4	3.06 4	2.28 4	6.12 3	4.41 3	3.12 3	2.23 3	T
							1.45 -2	1.52 -2	1.64 -2	1.73 -2	1.94 -2	2.05 -2	2.39 -2	4.34 -2	4.95 -2	5.66 -2	6.42 -2	Q
52							0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	K
							4.67 4	4.34 4	3.83 4	3.53 4	2.88 4	2.64 4	1.97 4	5.33 3	3.85 3	2.73 3	1.95 3	L
							9.32 3	8.65 3	7.64 3	7.01 3	5.72 3	5.22 3	3.88 3	1.04 3	7.46 2	5.26 2	3.76 2	M
							3.17 3	2.94 3	2.58 3	2.36 3	1.91 3	1.73 3	1.26 3	3.05 2	2.13 2	1.45 2	9.95 1	N
							5.91 4	5.49 4	4.86 4	4.46 4	3.65 4	3.33 4	2.48 4	6.67 3	4.81 3	3.40 3	2.43 3	T
							1.39 -2	1.46 -2	1.58 -2	1.66 -2	1.88 -2	1.98 -2	2.32 -2	4.27 -2	4.88 -2	5.59 -2	6.34 -2	Q
53									0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	K
									4.13 4	3.79 4	3.11 4	2.84 4	2.12 4	5.75 3	4.16 3	2.95 3	2.11 3	L
									8.18 3	7.51 3	6.13 3	5.59 3	4.15 3	1.11 3	7.99 2	5.64 2	4.02 2	M
									2.62 3	2.40 3	1.94 3	1.76 3	1.29 3	3.10 2	2.16 2	1.47 2	1.01 2	N
									5.21 4	4.78 4	3.91 4	3.57 4	2.66 4	7.17 3	5.18 3	3.66 3	2.62 3	T
								E(2s) L_L	1.53 -2	1.62 -2	1.83 -2	1.94 -2	2.28 -2	4.25 -2	4.86 -2	5.57 -2	6.33 -2	Q

lattice

$$\chi_{iH}^{\perp}/\chi_{i0} = a_H D_H \,(1 - 2\,Q \sin^2 \Theta_B)\,, \qquad (4.5\,a)$$

$$\chi_{iH}^{\parallel}/\chi_{i0} = a_H D_H([1 - Q]\cos 2\,\Theta_B + Q \cos 4\,\Theta_B)\,, \qquad (4.5\,b)$$

where $a_H = 1$, if H has all even indices with $(h_1 + h_2 + h_3)/4$ an integer, or $a_H = 1/\sqrt{2}$, if H has all odd indices, otherwise $a_H = 0$; $Q = \tau^Q/\tau_0$ and $(1 - Q) = (\tau^D + \tau^{DO})/\tau_0$ where $\tau_0 = \tau^D + \tau^{DO} + \tau^Q$ is the sum of the dipole, dipole-octupole and quadrupole components of the total photoelectric absorption coefficient (τ_0). D_H is the Debye-Waller factor, whose influence (at room temperature) on the μ_{min} value is usually larger than the influence of the bracketed terms of Eqs. (4.5 a) and (4.5 b).

The value of $Q = \tau^Q/\tau_0$ increases with increase in incident photon energy and its variation for Si and Ge over the medium X-ray energy range is shown in Figure 2.

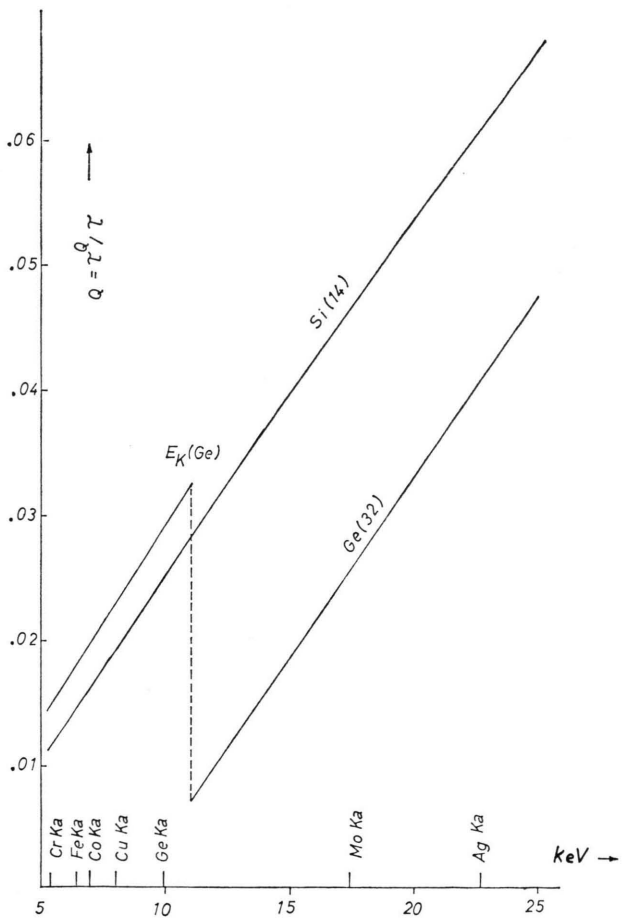

Fig. 2. The theoretical variation of $Q = \tau^Q/\tau_0$ with incident X-ray photon energy (in keV) for Si and Ge.

From experiments with thick nearly perfect crystals it is possible to obtain experimental values of $\mu_{min}^{\perp}$, but the comparison with theory is complicated by the uncertainty of the exact characteristic Debye temperature Θ_M of the crystal (which is different from the value given from specific heat measurements), and of the minimum Compton and thermal diffuse scattering contributions to Equation (4.3).

In connection with measurements of linear absorption coefficients mentioned earlier in this paper, experimental determinations of $\chi_{iH}^{\perp}/\chi_{i0}$ have also been made for germanium using several reflections and characteristic X-ray wavelengths. Taking $\tau_{min}^{\perp}$ for $\mu_{min}^{\perp}$ and using an appropriate Debye temperature, a good agreement has been obtained between theory and experiment for low order reflections [1].

5. Conclusion

Within the limits specified in this paper, the above theory provides a simple, quick and relatively accurate method for the determination of atomic photoelectric absorption cross sections and associated constants.

From the absorption cross sections given in Table 3, values of linear and anomalous absorption coefficients can be calculated with an accuracy sufficient for many purposes. Actual agreement between our figures and similar results computed from more rigorous alternate theory or those estimable from experiment is in many cases better than 5% which will be shown in Part II of this paper [3].

Appendix

The Sommerfeld Term Difference Equations used in the determination of the average screening constants (s_{nl}) given in Table 2 are:

1s: $(s_{10} = 0.3)$ (A.1)

2s, 2p: $(z - s_{21})^2 = \{(2^2/\alpha)\, V_{21}^{1/2} - 5\, V_{21}\}\{1 + (19\,\alpha^2/32)\, V_{21}\}$ (A.2)

3s, 3p: $(z - s_{31})^2 = \{(3/\alpha)\, V_{31}^{1/2} - (279/16)\, V_{31}\}\{1 + (2807\,\alpha^2/1024)\, V_{31}\}$ (A.3)*

3d: $(z - s_{32})^2 = \{(3^2/\alpha)\, V_{32}^{1/2} - (225/16)\, V_{32}\}\{1 + (589\,\alpha^2/1024)\, V_{32}\}$ (A.4)

* In (A.3) Sommerfeld incorrectly gives $(191\,\alpha^2/32)$ instead of $(2807\,\alpha^2/1024)$.

$$\mathbf{4s, 4p:}\quad (z-s_{41})^2=\{(4/\alpha)\,V_{41}{}^{1/2}-(40)\,V_{41}\}\,\{1+(191\,\alpha^2/32)\,V_{41}\} \tag{A.5}$$

$$\mathbf{4d:}\quad (z-s_{42})^2=\{(8/\alpha)\,V_{42}{}^{1/2}-(112/3)\,V_{42}\}\,\{1+(215\,\alpha^2/96)\,V_{42}\} \tag{A.6}$$

where $\alpha=1/137.04$, $R_\infty=109737.3\,\mathrm{cm}^{-1}$ and $V_{nl}=\Delta\nu_{nl}/R_\infty$.

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