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Atomic scattering factors for *K*-shell and *L*-shell ionization by fast electrons

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Atomic scattering factors have been calculated for *K*-shell ionization for elements in the range $Z = 6$ (carbon) to $Z = 50$ (tin) and for *L*-shell ionization in the range $Z = 20$ (calcium) to $Z = 60$ (neodymium). The calculations are based on relativistic Hartree–Fock wave functions for the atomic bound states and Hartree–Slater wave functions for the continuum wave functions. The results are presented in tabular form such that accurate values of the scattering factors can be obtained by cubic spline interpolation for incident electron energies between 50 and 400 keV and for scattering vectors with magnitude $s = \sin\theta/\lambda$ up to 2.5 Å^{-1} (2θ is the scattering angle and λ the wavelength of the incident electrons). A separate parameterization of the form factors is given for $2.5 \leq s \leq 20$ Å^{-1}, where they are small. In addition, a simpler but less accurate parameterization of the atomic scattering factors in an exponential form has been obtained by fitting the calculated form factors in the region $s \leq 2.5$ Å^{-1}. The scattering factors are suitable for the calculation of ionization cross sections for use in atom location by channelling-enhanced microanalysis (ALCHEMI).

1. Introduction

Precisely known atomic scattering factors are essential for accurate atom location by channelling-enhanced microanalysis (ALCHEMI) (see Oxley *et al.*, 1999, and references therein). First principles calculations of ionization cross sections, which realistically model the delocalization of the ionization cross sections, give excellent agreement with experiment – see, for example, Oxley & Allen (1998) and Oxley *et al.* (1999). However, such calculations are complex and computationally intensive and the calculation of the inelastic scattering coefficients for a many-beam simulation of a channelling pattern can take several hours on current desktop computer systems. Hence, simple analytic forms are often assumed to describe the scattering factors, in particular those that, in one dimension, correspond to Gaussian (Nüchter & Sigle, 1995) and Lorentzian forms (Rossouw *et al.*, 1996) of the effective ionization potential. However, the use of such analytic forms requires prior knowledge of the delocalization of the effective ionization interaction. Such an approach assumes that the precise shape of the ionization potential is not crucial but that the half-width at half-maximum height (HWHM) should be accurately estimated. This can be performed by approximating the HWHM using root-mean-square impact parameters for ionization (Pennycook, 1988; Oxley & Allen, 1999). However, this is not usually a good approximation (Oxley & Allen, 1998), as the results presented here will confirm.

Several parameterizations of elastic scattering factors for X-rays and electrons have been published (Strand & Bonham, 1963; Doyle & Turner, 1968; Rez *et al.*, 1994; Meyer *et al.*, 1995; Waasmaier & Kirfel, 1995; Wang *et al.*, 1995; Peng *et al.*, 1996*a*; Su & Coppens, 1997; Peng, 1998). [The scattering factors for X-rays and electrons are related to each other *via* the Mott formula – see, for example, Peng (1998)]. Similar parameterizations are also available for thermal diffuse scattering (TDS) of electrons (Bird & King, 1990; Peng *et al.*, 1996*a*,*b*). In this paper, atomic scattering form factors for *K*- and *L*-shell ionization are calculated from first principles using relativistic Hartree–Fock wave functions for atomic bound states and Hartree–Slater wave functions for the continuum states. It is assumed that the effective ionization interaction may be approximated by an equivalent local potential (Allen & Josefsson, 1995), in practice an excellent approximation. Atomic scattering factors are presented for *K*-shell ionization for elements in the range $Z = 6$ (carbon) to $Z = 50$ (tin) and for *L*-shell ionization in the range $Z = 20$ (calcium) to $Z = 60$ (neodymium). The results are presented in tabular form such that accurate values of the scattering factors can be obtained by interpolation of the *natural logarithm* of the form factor for incident electron energies between 50 and 400 keV and for scattering vectors $s = \sin\theta/\lambda$ up to 2.5 Å^{-1} (2θ is the angle between the wavevectors of the incident and scattered electrons and λ is the wavelength of the incident electrons). A separate parameterization of the form factors is given for $2.5 \leq s \leq 20$ Å^{-1}, where they are small, so that estimates may

be made for these larger scattering angles. In addition, a simpler but less-accurate parameterization of the atomic scattering factors in an exponential form has been obtained by fitting the calculated form factors in the region $s \leq 2.5$ Å^{-1}. The atomic scattering factors are suitable for the calculation of ionization cross sections for use in ALCHEMI.

2. Theory

2.1. Atomic scattering form factors

The atomic scattering form factor for inner-shell ionization is given by (Allen & Josefsson, 1995)

$$f(\mathbf{s}) = (1/2\pi^3 a_0^2) \int k'\kappa^2 \times \left\{ \int \left[\sum_{l,m_l} n_{m_l} \int F^{\beta *}_{l,m_l}(\mathbf{Q}_\mathbf{s}, \boldsymbol{\kappa}) F^{\beta}_{l,m_l}(\mathbf{Q}_\mathbf{0}, \boldsymbol{\kappa}) \, \mathrm{d}\Omega_\kappa \right] \times \mathrm{d}\Omega_{k'}/|\mathbf{Q}_\mathbf{s}|^2 |\mathbf{Q}_\mathbf{0}|^2 \right\} \mathrm{d}\kappa, \quad (1)$$

where the scattering vector $\mathbf{s}$ has magnitude given by $s = k \sin\theta/2\pi$ and k is the magnitude of the incident wavevector $\mathbf{k}$. We use the convention $k = 2\pi/\lambda$, with λ the wavelength of the incident radiation. The relativistic Bohr radius is denoted by a_0. The symbol k' is the magnitude of the wavevector $\mathbf{k}'$ of the scattered electron. The wavevector of the ejected electron is denoted by $\boldsymbol{\kappa}$ (magnitude κ). The quantum number associated with orbital angular momentum is denoted by l. The sum over the azimuthal quantum number m_l of the initial bound state of the atom is required for other than s orbitals. The number of electrons in each suborbital is taken into account by the factor n_{m_l}. The integration over the solid angle $\mathrm{d}\Omega_{k'} = \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi$ extends over all space. The range of integration over κ is determined by the threshold energy E_t for ionization. The atomic transition matrix elements F^{β}_{l,m_l} (where β labels the atomic species) will be defined in detail below and are functions of $\mathbf{Q}_\mathbf{s} = \mathbf{q} + 4\pi\mathbf{s}$, where $\hbar\mathbf{q} = \hbar(\mathbf{k}' - \mathbf{k})$ is the momentum transfer. The factor of 4π in the definition of $\mathbf{Q}_\mathbf{s}$ ensures that $\mathbf{s}$ is similar, for example, to that in the commonly used parameterizations of elastic scattering factors of Doyle & Turner (1968).

The atomic transition matrix element for a specific suborbital in atom species β is given by

$$F^{\beta}_{l,m_l}(\mathbf{Q}_\mathbf{s}, \boldsymbol{\kappa}) = \int b^{\beta *}(\boldsymbol{\kappa}, \mathbf{r}) \exp(i\mathbf{Q}_\mathbf{s} \cdot \mathbf{r}) u_0^{\beta}(\mathbf{r}) \, \mathrm{d}\mathbf{r}. \quad (2)$$

Here, $u_0^{\beta}(\mathbf{r})$ and $b^{\beta}(\boldsymbol{\kappa}, \mathbf{r})$ are the wave functions for the bound and continuum states, respectively. Analytic evaluations of the integral inside the square brackets in equation (1), for K-shell ionization in a linear-momentum representation and using a screened hydrogenic model, have been presented previously (Maslen, 1983). This integral may be calculated in an angular-momentum representation (Saldin & Rez, 1987; Oxley & Allen, 1998), which allows the use of more realistic atomic wave functions and is not limited to K-shell ionization.

The use of a central potential model results in the following form for the bound-state wave function:

$$u_0^{\beta}(\mathbf{r}) = (1/r) u_{nl}(r) Y_{lm_l}(\hat{\mathbf{r}}). \quad (3)$$

Here, $u_{nl}(r)$ denotes the radial wave function for the orbital specified by the quantum numbers n and l. We use a hat to denote a unit vector in the argument of the spherical harmonic $Y_{lm_l}(\hat{\mathbf{r}})$. The appropriate form of the continuum wave function is (Landau & Lifshitz, 1977)

$$b^{\beta}(\boldsymbol{\kappa}, \mathbf{r}) = (1/2\kappa r) \sum_{l'=0}^{\infty} i^{l'} (2l' + 1) \exp(i\delta_{l'}) u_{\kappa l'}(r) P_{l'}(\hat{\boldsymbol{\kappa}} \cdot \hat{\mathbf{r}}), \quad (4)$$

where $\delta_{l'}$ is the partial-wave phase shift. The continuum wave function is normalized as

$$\int b^{\beta *}(\boldsymbol{\kappa}, \mathbf{r}) b^{\beta}(\boldsymbol{\kappa}', \mathbf{r}) \, \mathrm{d}\mathbf{r} = (2\pi)^3 \delta(\boldsymbol{\kappa}' - \boldsymbol{\kappa}) \quad (5)$$

with the radial wave function $u_{\kappa l'}(r)$ satisfying

$$\int u_{\kappa' l'}(r) u_{\kappa l'}(r) \, \mathrm{d}r = 2\pi\delta(\kappa' - \kappa). \quad (6)$$

The $u_{\kappa l'}(r)$ are normalized by matching the asymptotic form (Landau & Lifshitz, 1977)

$$u_{\kappa l'}(r \rightarrow \infty) = 2 \sin[\kappa r + (1/\kappa) \log 2\kappa r - \tfrac{1}{2} l'\pi + \delta_{l'}] \quad (7)$$

to Coulomb functions at a suitably large radius.

Expansion of the exponential term in equation (2) and the Legendre polynomial in equation (4) in terms of spherical harmonics means that equation (2) can be written in the form

$$F^{\beta}_{l,m_l}(\mathbf{Q}_\mathbf{s}, \boldsymbol{\kappa}) = (8\pi^2/\kappa) \sum_{l'=0}^{\infty} \sum_{m_{l'}=-l'}^{l'} (-i)^{l'} \exp(-i\delta_{l'}) Y_{l'm_{l'}}(\hat{\boldsymbol{\kappa}}) \times \sum_{\lambda=0}^{\infty} \sum_{m_\lambda=-\lambda}^{\lambda} i^{\lambda} Y^*_{\lambda m_\lambda}(\hat{\mathbf{Q}}_\mathbf{s}) \int (1/r^2) u_{\kappa l'}(r) j_\lambda(Q_\mathbf{s} r) \times u_{nl}(r) Y^*_{l'm_{l'}}(\hat{\mathbf{r}}) Y_{lm_l}(\hat{\mathbf{r}}) Y_{\lambda m_\lambda}(\hat{\mathbf{r}}) \, \mathrm{d}\mathbf{r}, \quad (8)$$

where the index λ (not to be confused with wavelength) arises from the expansion for the exponential. Introducing the notation

$$G^{\lambda}_{nl,\kappa l'}(Q_\mathbf{s}) = \int u_{\kappa l'}(r) j_\lambda(Q_\mathbf{s} r) u_{nl}(r) \, \mathrm{d}r \quad (9)$$

and using the properties of the spherical harmonics, we can write the atomic transition matrix element in the form

$$F^{\beta}_{l,m_l}(\mathbf{Q}_\mathbf{s}, \boldsymbol{\kappa}) = \frac{8\pi^2}{\kappa} \sum_{l'=0}^{\infty} \sum_{m_{l'}=-l'}^{l'} (-1)^{m_{l'}} (-i)^{l'} \exp(-i\delta_{l'}) Y_{l'm_{l'}}(\hat{\boldsymbol{\kappa}}) \times \sum_{\lambda=0}^{\infty} \sum_{m_\lambda=-\lambda}^{\lambda} i^{\lambda} Y^*_{\lambda m_\lambda}(\hat{\mathbf{Q}}_\mathbf{s}) G^{\lambda}_{nl,\kappa l'}(Q_\mathbf{s}) \times \left[\frac{(2l' + 1)(2\lambda + 1)(2l + 1)}{4\pi} \right]^{1/2} \begin{pmatrix} l' & \lambda & l \\ 0 & 0 & 0 \end{pmatrix} \times \begin{pmatrix} l' & \lambda & l \\ -m_{l'} & m_\lambda & m_l \end{pmatrix}. \quad (10)$$

The arrays are Wigner 3j symbols.

The term in square brackets in equation (1) can now be evaluated using the orthonormality of the spherical harmonics and the orthogonality relations for the 3j symbols (Oxley & Allen, 1998). This yields

$$I(\mathbf{Q}_s, \mathbf{Q}_0, \boldsymbol{\kappa}) = \sum_{l,m_l} n_{m_l} \int F^{\beta *}_{l,m_l}(\mathbf{Q}_s, \boldsymbol{\kappa}) F^{\beta}_{l,m_l}(\mathbf{Q}_0, \boldsymbol{\kappa})\, \mathrm{d}\Omega_\kappa$$
$$= \left(\frac{4\pi}{\kappa}\right)^2 (2l+1) \sum_{l'=0}^{\infty} (2l'+1) \sum_{\lambda=0}^{\infty} (2\lambda+1)$$
$$\times G^{\lambda}_{nl,\kappa l'}(Q_s) G^{\lambda}_{nl,\kappa l'}(Q_0) \begin{pmatrix} l' & \lambda & l \\ 0 & 0 & 0 \end{pmatrix}^2$$
$$\times P_\lambda(\hat{\mathbf{Q}}_s \cdot \hat{\mathbf{Q}}_0). \qquad (11)$$

Bound-state radial wave functions were calculated using Cowan's program *RCN* (Cowan, 1981), which calculates Hartree–Fock wave functions with relativistic corrections. Continuum wave functions were calculated by solving Schrödinger's equation using a Hartree–Slater potential (Cowan, 1981). Calculation of the continuum wave functions describing the ejected electron for kinetic energies of the order of hundreds of keV required careful numerical analysis and extensive stability and accuracy checks have been undertaken. Convergence of all integrations and partial-wave summations has been carefully checked. The partial-wave summation over l' in equation (11) was truncated if the last three partial waves added changed $I(\mathbf{Q}_s, \mathbf{Q}_0, \boldsymbol{\kappa})$ by less than 0.1%. Typically, 20 to 50 partial waves were used, more being needed for more delocalized bound-state orbitals and for higher incident energies.

The atomic scattering form factor for ionization may be approximately parameterized in the form

$$f_L(s) = f(0) \exp(-4\pi c s), \qquad (12)$$

where c is a constant. In one dimension, this parameterization corresponds to an atomic ionization potential $V_L(x)$ of Lorentzian form, *i.e.* which goes as $(x^2 + c^2)^{-1}$, with the HWHM given by the parameter c.

2.2. Use of atomic form factors to calculate cross sections for inner-shell ionization in crystals

The diffraction of incident electrons in a crystalline environment makes the cross section for ionization a function of incident-beam orientation, the site of the inelastic event within the unit cell and the depth within the crystal. The phase of the atomic transition-matrix elements is an essential part of the physics. A general expression, describing the cross section for inelastic scattering from a crystal of thickness t, based on the one-particle Schrödinger equation and which implicitly assumes integration over all final states of the scattered electron, is as follows (Allen & Rossouw, 1993; Allen & Josefsson, 1995, 1996):

$$\sigma = NV_c \left\{ \left[1 - \sum_{i,j} B^{ij}(t) \sum_{\mathbf{g}} C^i_{\mathbf{g}} C^{j*}_{\mathbf{g}} \right] \mu_{\mathbf{0},\mathbf{0}} + \sum_{i,j} B^{ij}(t) \sum_{\mathbf{g},\mathbf{h}} C^i_{\mathbf{g}} C^{j*}_{\mathbf{h}} \mu_{\mathbf{h},\mathbf{g}} \right\}, \qquad (13)$$

where NV_c is the total crystal volume and

$$B^{ij}(t) = \alpha^i \alpha^{j*} \frac{\exp[i(\lambda^i - \lambda^{j*})t] - 1}{i(\lambda^i - \lambda^{j*})t}. \qquad (14)$$

The Bloch-wave eigenvalues λ^i in the $B^{ij}(t)$, the Bloch-state amplitudes α^i and Fourier coefficients $C^i_{\mathbf{g}}$, which represent the eigenvector of the i'th state, come from solution of the Bethe scattering equations (Allen & Josefsson, 1995), where $\mathbf{g}$ denotes a reciprocal-lattice vector. This result can also be obtained with suitable approximations from the formalism of Dudarev *et al.* (1993). While in this paper the $\mu_{\mathbf{h},\mathbf{g}}$ describe inner-shell ionization, they may in general describe any specific inelastic scattering under consideration. It is important to note that, while the $\mu_{\mathbf{h},\mathbf{g}}$ refer to a specific form of absorptive scattering, the eigenvector components $C^i_{\mathbf{g}}$ in equation (13) and complex eigenvalues λ^i in equation (14) come from solution of the total scattering equations (Allen & Josefsson, 1995) and hence, in principle, take into account all forms of absorptive scattering concurrently occurring. In particular, the inclusion of thermal diffuse scattering (TDS) is

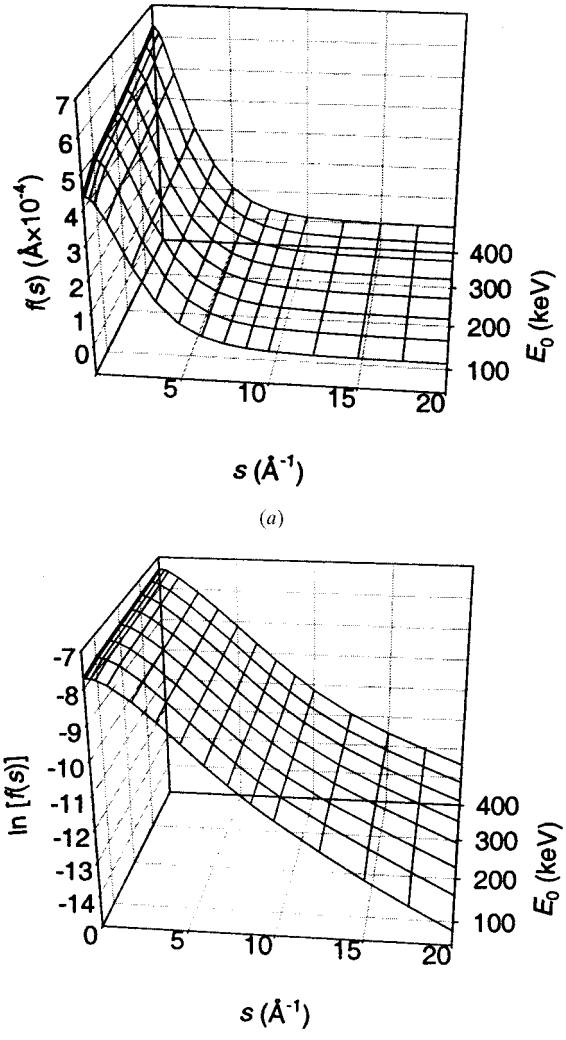

Figure 1
(*a*) Atomic inner-shell ionization form factors $f(s)$ for ionization of the Ga K shell as a function of s and incident energy. (*b*) Natural logarithm of $f(s)$ as a function of s and incident energy.

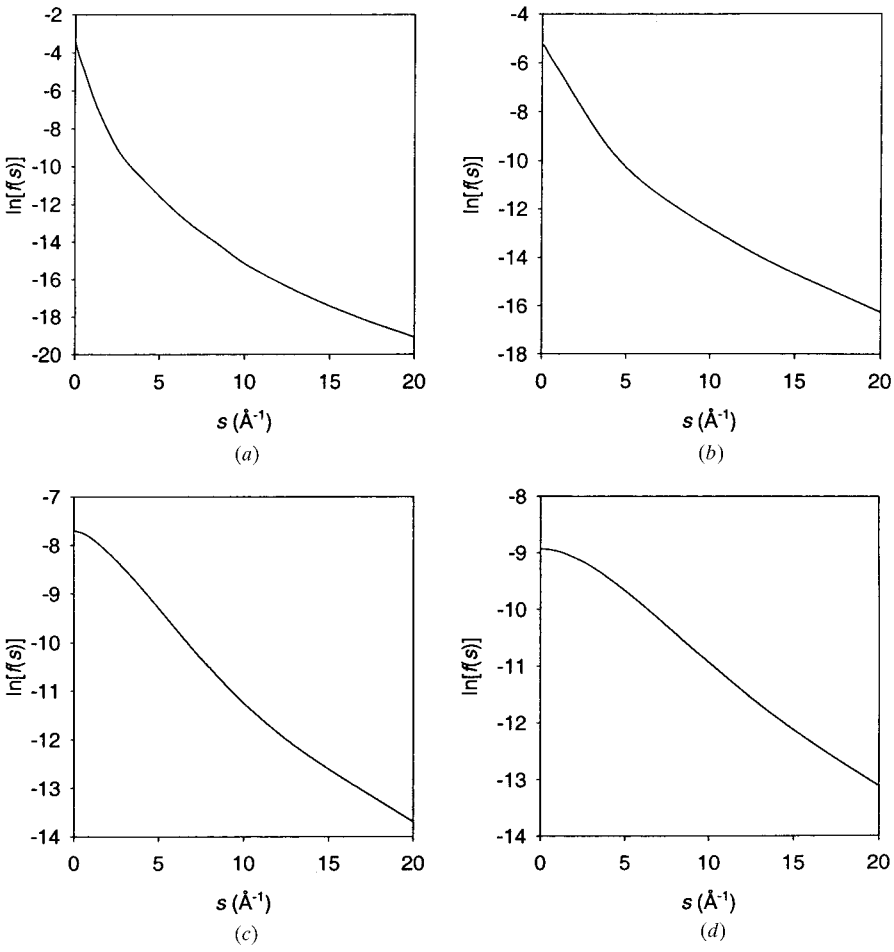

Figure 2
Natural logarithm of inner-shell ionization form factors $f(s)$ for 200 keV incident electrons as a function of s for (*a*) ionization of the carbon K shell ($E_t = 309$ eV), (*b*) ionization of the aluminium K shell ($E_t = 1.59$ keV), (*c*) ionization of the arsenic K shell ($E_t = 11.95$ keV) and (*d*) ionization of the tin K shell ($E_t = 29.35$ keV).

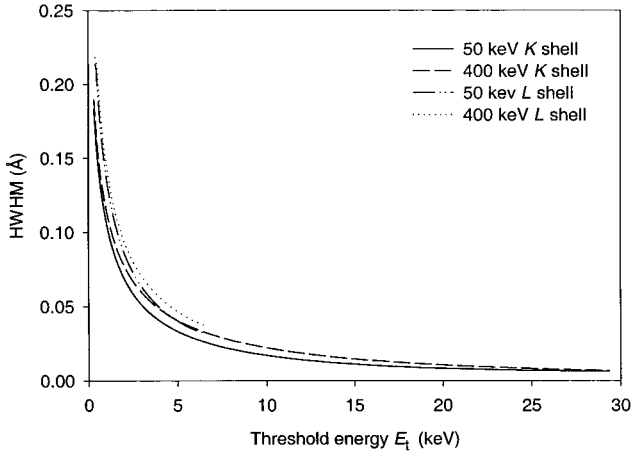

Figure 3
The best-fit parameters for calculation of form factors using equation (12), which in one dimension correspond to the half-width at half-maximum (HWHM) of a Lorentzian form of the atomic ionization potential, plotted as a function of threshold energy E_t.

crucially important to obtain accurate cross sections (Allen & Rossouw, 1993; Allen & Josefsson, 1995). The first term in equation (13) (the factor in square brackets multiplied by $\mu_{\mathbf{0},\mathbf{0}}$) accounts for ionization by electrons that have been 'dechannelled' or absorbed from the dynamical elastic beams by wide-angle (mainly TDS) scattering. The second term represents the dynamical contribution to σ (which is attenuated by the absorptive scattering).

The inelastic scattering coefficients for ionization required to calculate ionization cross sections as a function of orientation of the incident beam in a particular crystal can be expressed, in a local approximation (Allen & Josefsson, 1995), as

$$\begin{aligned}\mu_{\mathbf{h},\mathbf{g}} &\approx \mu_{\mathbf{h}-\mathbf{g},\mathbf{0}} \\ &= (1/kV_c)\sum_{\beta_n}\exp[-M_\beta(\mathbf{g}-\mathbf{h})] \\ &\quad\times\exp[i(\mathbf{g}-\mathbf{h})\cdot\boldsymbol{\tau}_{\beta_n}] \\ &\quad\times f_\beta[(\mathbf{h}-\mathbf{g})/4\pi],\end{aligned} \tag{15}$$

where $\mathbf{g}$ and $\mathbf{h}$ are reciprocal-lattice vectors and the vectors $\boldsymbol{\tau}_{\beta_n}$ describe the position of each atom of type β within the unit cell and the Debye–Waller factor for atoms of type β, $M_\beta(\mathbf{g}-\mathbf{h}) = \frac{1}{2}|\mathbf{g}-\mathbf{h}|^2\langle u_\beta^2\rangle$, is given in terms of the projected mean-square thermal displacement $\langle u_\beta^2\rangle$. The effective (local) potential for ionization in the crystal can be expressed as

$$V_L(\mathbf{r}) = (\hbar^2 k/2m)\sum_{\mathbf{s}=(\mathbf{h}-\mathbf{g})/4\pi}\mu_{\mathbf{s},\mathbf{0}}\exp(i4\pi\mathbf{s}\cdot\mathbf{r}), \tag{16}$$

where the summation occurs over the discrete scattering vectors $\mathbf{s} = (\mathbf{h}-\mathbf{g})/4\pi$ relevant to the crystal under consideration.

3. Results

Atomic scattering factors have been calculated for K-shell ionization for elements in the range $Z = 6$ (carbon) to $Z = 50$ (tin) and for L-shell ionization in the range $Z = 20$ (calcium) to $Z = 60$ (neodymium). To an excellent approximation, $f(\mathbf{s}) \approx f(s)$ for all $\mathbf{s}$, *i.e.* the scattering factor depends only on the magnitude of $\mathbf{s}$. For each energy, $f(s)$ has been calculated for $s = 0.0$, 0.125, 0.375, 0.625, 1.25 and 2.5 Å^{-1}. These values of s are such that *their natural logarithm* can be accurately interpolated using cubic splines, a point on which we will elaborate below.

The scattering factors for K-shell ionization are presented in Table 1 and for L-shell ionization in Table 2. The parameters a

and b in Tables 1 and 2 can be used to estimate the scattering factors for s in the range 2.5 to 20 Å^{-1} using $f(s) \approx a\exp(-bs)$. For each element, the first row is for 50 keV incident electrons and for each subsequent row the incident energy is incremented by 50 keV so that the final row corresponds to an energy of 400 keV.

Shown in Fig. 1(*a*) is the atomic form factor for Ga K-shell ionization as a function of incident energy and s. In Fig. 1(*b*), the natural logarithm of $f(s)$ is plotted as a function of the incident energy and s. This provides a much smoother surface for cubic spline interpolation than direct interpolation on $f(s)$. This not only allows us to minimize the number of data points

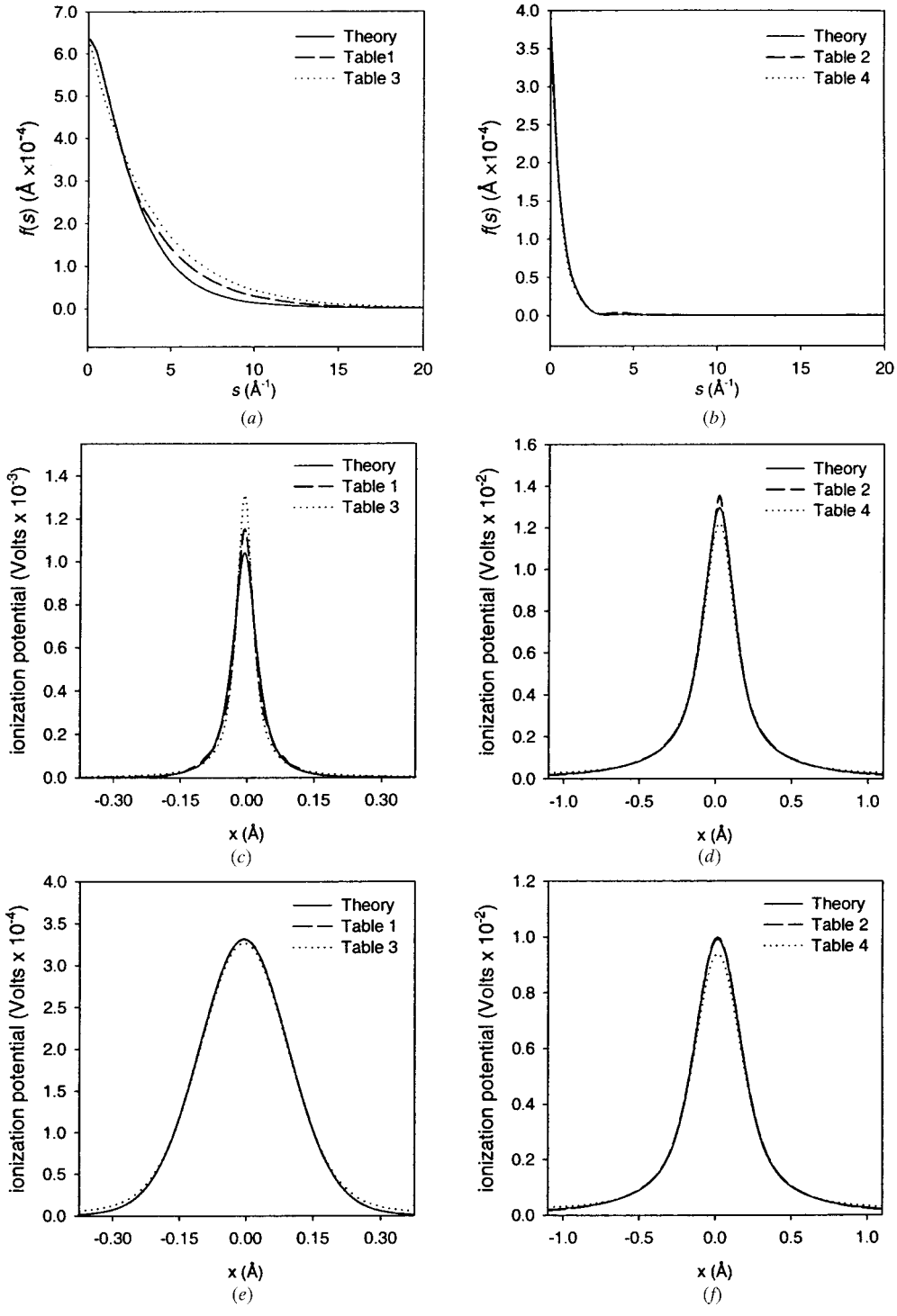

Figure 4
Scattering factors for inner-shell ionization as a function of s for ionization of (*a*) the Ga K shell ($E_t = 10.45$ keV) and (*b*) the Ga L shell ($E_t = 1.20$ keV) for 400 keV incident electrons. Static potentials for ionization of the Ga K shell are shown in (*c*) and for the L shell in (*d*). Ionization potentials that incorporate the effects of thermal smearing are shown in (*e*) for the K shell and (*f*) for the L shell. Theory results are those calculated from first principles and these are compared with parameterizations in Tables 1 to 4 or to potentials calculated using them.

Table 1
Atomic scattering factors $f(s)$ (in Å) for K-shell ionization for elements in the range $Z = 6$ (carbon) to $Z = 50$ (tin) at selected values of s between 0 and 2.5 Å^{-1}.

For each element, the first row is for 50 keV incident electrons and for each subsequent row the incident energy is incremented by 50 keV so that the final row corresponds to an energy of 400 keV. The natural logarithm of these values can be accurately interpolated in s and in energy using cubic splines. The parameters a and b can be used to estimate the scattering factors for s in the range 2.5 to 20 Å^{-1} using $f(s) \approx a\exp(-bs)$.

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
C $Z = 6$	K shell						
0.381041E−1	0.274758E−1	0.141170E−1	0.760704E−2	0.157186E−2	0.150749E−3	0.679205E−3	0.602123E+0
0.338843E−1	0.225720E−1	0.115095E−1	0.629539E−2	0.130138E−2	0.126478E−3	0.553458E−3	0.590448E+0
0.329878E−1	0.211993E−1	0.107574E−1	0.587506E−2	0.122366E−2	0.119592E−3	0.513212E−3	0.582642E+0
0.331263E−1	0.207403E−1	0.105339E−1	0.572490E−2	0.120453E−2	0.118079E−3	0.495721E−3	0.573863E+0
0.337120E−1	0.208403E−1	0.105749E−1	0.576033E−2	0.120907E−2	0.118756E−3	0.500981E−3	0.575797E+0
0.345108E−1	0.212554E−1	0.107190E−1	0.586399E−2	0.123489E−2	0.120725E−3	0.470262E−3	0.543912E+0
0.354308E−1	0.218505E−1	0.110228E−1	0.599869E−2	0.127792E−2	0.124507E−3	0.589425E−3	0.621915E+0
0.364199E−1	0.222232E−1	0.112941E−1	0.618702E−2	0.129356E−2	0.128379E−3	0.565017E−3	0.592747E+0
N $Z = 7$	K shell						
0.269768E−1	0.213115E−1	0.118833E−1	0.699304E−2	0.180845E−2	0.186855E−3	0.801266E−3	0.582344E+0
0.240846E−1	0.177221E−1	0.970645E−2	0.577172E−2	0.149915E−2	0.156878E−3	0.652362E−3	0.570052E+0
0.234825E−1	0.166956E−1	0.907290E−2	0.537453E−2	0.140673E−2	0.147857E−3	0.601297E−3	0.561138E+0
0.236490E−1	0.163902E−1	0.889296E−2	0.524791E−2	0.138505E−2	0.146184E−3	0.583244E−3	0.553495E+0
0.241535E−1	0.164679E−1	0.890415E−2	0.528558E−2	0.138734E−2	0.147373E−3	0.582554E−3	0.549783E+0
0.248429E−1	0.167726E−1	0.903794E−2	0.536624E−2	0.141728E−2	0.150459E−3	0.562024E−3	0.527141E+0
0.256335E−1	0.172250E−1	0.927998E−2	0.549584E−2	0.147183E−2	0.155119E−3	0.615258E−3	0.551139E+0
0.264771E−1	0.176150E−1	0.952930E−2	0.566292E−2	0.150023E−2	0.159958E−3	0.642511E−3	0.556189E+0
O $Z = 8$	K shell						
0.199030E−1	0.167854E−1	0.100990E−1	0.632028E−2	0.194440E−2	0.226882E−3	0.934613E−3	0.566282E+0
0.178531E−1	0.141890E−1	0.826524E−2	0.521138E−2	0.161357E−2	0.192048E−3	0.766015E−3	0.553383E+0
0.174276E−1	0.134152E−1	0.772623E−2	0.484836E−2	0.151042E−2	0.180284E−3	0.702324E−3	0.543946E+0
0.175629E−1	0.132138E−1	0.757747E−2	0.473898E−2	0.148539E−2	0.178691E−3	0.682641E−3	0.536125E+0
0.179572E−1	0.132988E−1	0.758783E−2	0.477020E−2	0.148993E−2	0.180138E−3	0.680010E−3	0.531355E+0
0.185094E−1	0.135485E−1	0.770932E−2	0.484650E−2	0.151926E−2	0.183962E−3	0.675361E−3	0.520208E+0
0.191435E−1	0.138831E−1	0.789949E−2	0.495992E−2	0.156477E−2	0.189389E−3	0.710840E−3	0.529057E+0
0.198294E−1	0.142806E−1	0.811541E−2	0.510907E−2	0.160344E−2	0.194464E−3	0.751296E−3	0.540620E+0
F $Z = 9$	K shell						
0.151665E−1	0.134043E−1	0.864964E−2	0.568310E−2	0.200049E−2	0.270473E−3	0.107696E−2	0.552690E+0
0.136679E−1	0.115093E−1	0.711132E−2	0.469141E−2	0.165474E−2	0.229262E−3	0.881976E−3	0.538920E+0
0.133675E−1	0.109429E−1	0.664905E−2	0.436218E−2	0.155149E−2	0.215358E−3	0.808571E−3	0.529186E+0
0.134789E−1	0.108173E−1	0.651887E−2	0.426353E−2	0.152756E−2	0.213064E−3	0.783716E−3	0.520981E+0
0.137922E−1	0.109099E−1	0.653508E−2	0.428500E−2	0.153022E−2	0.215986E−3	0.783088E−3	0.515213E+0
0.142181E−1	0.111258E−1	0.663816E−2	0.435488E−2	0.156044E−2	0.219262E−3	0.784601E−3	0.509963E+0
0.147198E−1	0.114187E−1	0.680328E−2	0.446253E−2	0.160614E−2	0.226348E−3	0.816098E−3	0.512984E+0
0.152649E−1	0.117612E−1	0.699359E−2	0.459294E−2	0.165299E−2	0.233958E−3	0.880982E−3	0.530358E+0
Ne $Z = 10$	K shell						
0.118638E−1	0.108326E−1	0.744714E−2	0.510410E−2	0.199736E−2	0.313574E−3	0.121076E−2	0.540388E+0
0.107435E−1	0.944284E−2	0.616541E−2	0.421500E−2	0.165573E−2	0.266007E−3	0.990527E−3	0.525887E+0
0.105254E−1	0.903052E−2	0.577880E−2	0.392518E−2	0.155088E−2	0.250387E−3	0.908969E−3	0.515721E+0
0.106229E−1	0.895956E−2	0.566524E−2	0.383967E−2	0.152439E−2	0.247812E−3	0.881555E−3	0.507607E+0
0.108726E−1	0.906082E−2	0.568394E−2	0.385527E−2	0.153029E−2	0.250358E−3	0.876915E−3	0.501408E+0
0.112098E−1	0.924819E−2	0.577262E−2	0.391897E−2	0.155812E−2	0.255212E−3	0.887474E−3	0.498513E+0
0.116059E−1	0.950650E−2	0.591545E−2	0.401393E−2	0.160163E−2	0.262354E−3	0.919010E−3	0.501441E+0
0.120432E−1	0.980528E−2	0.608537E−2	0.413442E−2	0.163801E−2	0.271011E−3	0.953247E−3	0.503086E+0
Na $Z = 11$	K shell						
0.911548E−2	0.853946E−2	0.628098E−2	0.449834E−2	0.194558E−2	0.353370E−3	0.132574E−2	0.528885E+0
0.828673E−2	0.754199E−2	0.524903E−2	0.372789E−2	0.161411E−2	0.300526E−3	0.108556E−2	0.513726E+0
0.812953E−2	0.725538E−2	0.492906E−2	0.347730E−2	0.151055E−2	0.283313E−3	0.996678E−3	0.503150E+0
0.821134E−2	0.723022E−2	0.484682E−2	0.341016E−2	0.148741E−2	0.280702E−3	0.968032E−3	0.495188E+0
0.840779E−2	0.733234E−2	0.486300E−2	0.341990E−2	0.149553E−2	0.283157E−3	0.961580E−3	0.489031E+0
0.866670E−2	0.749255E−2	0.494398E−2	0.347611E−2	0.151899E−2	0.289442E−3	0.979020E−3	0.487439E+0
0.897515E−2	0.771595E−2	0.506626E−2	0.356081E−2	0.156365E−2	0.297376E−3	0.101359E−2	0.490501E+0
0.931196E−2	0.796711E−2	0.521400E−2	0.366768E−2	0.160051E−2	0.306022E−3	0.104504E−2	0.491261E+0
Mg $Z = 12$	K shell						
0.716728E−2	0.683343E−2	0.531745E−2	0.396146E−2	0.186513E−2	0.388681E−3	0.141882E−2	0.517929E+0
0.654213E−2	0.610325E−2	0.449703E−2	0.329836E−2	0.155141E−2	0.331433E−3	0.116289E−2	0.502096E+0
0.642798E−2	0.590421E−2	0.423715E−2	0.308789E−2	0.145148E−2	0.312805E−3	0.106847E−2	0.491359E+0
0.649716E−2	0.590425E−2	0.417185E−2	0.302898E−2	0.142754E−2	0.309770E−3	0.103683E−2	0.483236E+0
0.665611E−2	0.600333E−2	0.419628E−2	0.304183E−2	0.143725E−2	0.312824E−3	0.103159E−2	0.477285E+0
0.686079E−2	0.614218E−2	0.426551E−2	0.309211E−2	0.146148E−2	0.319486E−3	0.104699E−2	0.474784E+0
0.710806E−2	0.633851E−2	0.437646E−2	0.317000E−2	0.150429E−2	0.328504E−3	0.108847E−2	0.479192E+0
0.737374E−2	0.654924E−2	0.450265E−2	0.326628E−2	0.154077E−2	0.338246E−3	0.111154E−2	0.475893E+0

Table 1 (continued)

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Al $Z = 13$	K shell						
0.574590E−2	0.554308E−2	0.451868E−2	0.349026E−2	0.176733E−2	0.417449E−3	0.148339E−2	0.507168E+0
0.526707E−2	0.499978E−2	0.386812E−2	0.292693E−2	0.147506E−2	0.356525E−3	0.121591E−2	0.490737E+0
0.518306E−2	0.485986E−2	0.366257E−2	0.274988E−2	0.138200E−2	0.337206E−3	0.111891E−2	0.479767E+0
0.524234E−2	0.487620E−2	0.361559E−2	0.270113E−2	0.136051E−2	0.334049E−3	0.108621E−2	0.471663E+0
0.537437E−2	0.496767E−2	0.364226E−2	0.271339E−2	0.136833E−2	0.337145E−3	0.108068E−2	0.465933E+0
0.554176E−2	0.509612E−2	0.370654E−2	0.275826E−2	0.139232E−2	0.344614E−3	0.109767E−2	0.463409E+0
0.574142E−2	0.526066E−2	0.380389E−2	0.282918E−2	0.143183E−2	0.354034E−3	0.112774E−2	0.463433E+0
0.596011E−2	0.544245E−2	0.391797E−2	0.291859E−2	0.147069E−2	0.365734E−3	0.116630E−2	0.463873E+0
Si $Z = 14$	K shell						
0.468451E−2	0.455743E−2	0.385694E−2	0.307548E−2	0.166143E−2	0.438957E−3	0.151982E−2	0.496779E+0
0.431557E−2	0.414591E−2	0.334627E−2	0.260678E−2	0.139335E−2	0.376378E−3	0.124879E−2	0.479733E+0
0.425195E−2	0.404851E−2	0.318401E−2	0.245586E−2	0.130871E−2	0.357184E−3	0.115287E−2	0.468705E+0
0.430693E−2	0.407263E−2	0.315178E−2	0.241590E−2	0.128740E−2	0.352961E−3	0.111591E−2	0.460426E+0
0.441601E−2	0.415558E−2	0.317952E−2	0.242803E−2	0.129435E−2	0.356628E−3	0.111215E−2	0.454944E+0
0.456064E−2	0.427532E−2	0.324304E−2	0.247343E−2	0.131793E−2	0.365071E−3	0.113158E−2	0.452509E+0
0.472170E−2	0.441427E−2	0.332846E−2	0.253589E−2	0.135486E−2	0.374569E−3	0.116127E−2	0.452598E+0
0.489965E−2	0.456667E−2	0.342733E−2	0.261362E−2	0.138967E−2	0.384921E−3	0.119553E−2	0.453323E+0
P $Z = 15$	K shell						
0.387436E−2	0.379092E−2	0.330589E−2	0.271559E−2	0.155137E−2	0.453282E−3	0.152993E−2	0.486584E+0
0.358901E−2	0.347783E−2	0.290812E−2	0.232527E−2	0.130993E−2	0.390371E−3	0.126079E−2	0.468959E+0
0.354190E−2	0.340932E−2	0.278122E−2	0.219915E−2	0.123131E−2	0.370742E−3	0.116424E−2	0.457727E+0
0.359015E−2	0.343688E−2	0.276110E−2	0.216823E−2	0.121332E−2	0.366693E−3	0.112828E−2	0.449569E+0
0.368437E−2	0.351309E−2	0.279121E−2	0.218166E−2	0.122052E−2	0.370266E−3	0.112409E−2	0.444202E+0
0.380660E−2	0.361987E−2	0.285116E−2	0.222421E−2	0.124278E−2	0.379046E−3	0.114368E−2	0.441741E+0
0.394363E−2	0.374170E−2	0.292971E−2	0.228200E−2	0.127922E−2	0.389551E−3	0.117431E−2	0.441377E+0
0.409333E−2	0.387518E−2	0.302027E−2	0.235305E−2	0.131228E−2	0.401319E−3	0.121316E−2	0.442491E+0
S $Z = 16$	K shell						
0.324306E−2	0.318748E−2	0.284670E−2	0.239874E−2	0.144279E−2	0.460974E−3	0.151752E−2	0.476596E+0
0.302110E−2	0.294781E−2	0.253750E−2	0.207980E−2	0.122701E−2	0.399514E−3	0.125709E−2	0.458522E+0
0.298942E−2	0.289834E−2	0.244001E−2	0.197469E−2	0.115559E−2	0.378695E−3	0.115765E−2	0.446967E+0
0.303100E−2	0.292865E−2	0.242994E−2	0.195140E−2	0.113912E−2	0.375937E−3	0.112672E−2	0.439058E+0
0.311374E−2	0.299773E−2	0.246106E−2	0.196653E−2	0.114714E−2	0.379915E−3	0.112384E−2	0.433824E+0
0.321722E−2	0.309244E−2	0.251800E−2	0.200628E−2	0.116909E−2	0.388223E−3	0.114106E−2	0.431251E+0
0.333749E−2	0.319973E−2	0.259074E−2	0.206045E−2	0.120236E−2	0.399934E−3	0.117363E−2	0.430622E+0
0.346508E−2	0.331739E−2	0.267398E−2	0.212543E−2	0.123626E−2	0.412217E−3	0.120935E−2	0.430516E+0
Cl $Z = 17$	K shell						
0.274238E−2	0.270448E−2	0.246234E−2	0.212113E−2	0.133670E−2	0.463112E−3	0.148789E−2	0.466857E+0
0.257236E−2	0.252143E−2	0.222352E−2	0.186349E−2	0.114689E−2	0.403795E−3	0.123867E−2	0.448356E+0
0.254966E−2	0.248686E−2	0.214968E−2	0.177756E−2	0.108304E−2	0.383440E−3	0.114239E−2	0.436677E+0
0.258796E−2	0.251750E−2	0.214731E−2	0.176139E−2	0.106873E−2	0.380726E−3	0.111233E−2	0.428854E+0
0.265998E−2	0.258072E−2	0.218006E−2	0.177807E−2	0.107706E−2	0.384610E−3	0.110917E−2	0.423654E+0
0.275074E−2	0.266464E−2	0.223343E−2	0.181551E−2	0.109870E−2	0.393658E−3	0.112882E−2	0.421380E+0
0.285392E−2	0.275911E−2	0.229991E−2	0.186517E−2	0.113055E−2	0.405117E−3	0.115881E−2	0.420391E+0
0.296285E−2	0.286130E−2	0.237486E−2	0.192343E−2	0.116144E−2	0.417937E−3	0.119518E−2	0.420288E+0
Ar $Z = 18$	K shell						
0.233942E−2	0.231305E−2	0.213817E−2	0.187784E−2	0.123466E−2	0.460224E−3	0.144395E−2	0.457368E+0
0.221023E−2	0.217437E−2	0.195583E−2	0.167223E−2	0.106979E−2	0.404086E−3	0.120949E−2	0.438530E+0
0.219531E−2	0.215109E−2	0.190161E−2	0.160407E−2	0.101415E−2	0.384319E−3	0.111686E−2	0.426720E+0
0.223154E−2	0.218191E−2	0.190522E−2	0.159336E−2	0.100168E−2	0.382224E−3	0.108946E−2	0.418971E+0
0.229460E−2	0.223959E−2	0.193797E−2	0.161129E−2	0.101048E−2	0.386223E−3	0.108722E−2	0.413986E+0
0.237391E−2	0.231264E−2	0.198744E−2	0.164595E−2	0.103094E−2	0.395757E−3	0.110756E−2	0.411647E+0
0.246402E−2	0.239791E−2	0.204977E−2	0.169342E−2	0.106154E−2	0.407257E−3	0.113735E−2	0.410805E+0
0.256061E−2	0.248852E−2	0.211895E−2	0.174741E−2	0.109135E−2	0.419588E−3	0.117039E−2	0.410329E+0
K $Z = 19$	K shell						
0.200094E−2	0.198243E−2	0.185618E−2	0.165789E−2	0.113432E−2	0.452682E−3	0.138781E−2	0.448118E+0
0.190545E−2	0.187962E−2	0.171931E−2	0.149803E−2	0.994637E−3	0.400912E−3	0.117176E−2	0.429009E+0
0.189726E−2	0.186522E−2	0.167999E−2	0.144393E−2	0.945772E−3	0.381703E−3	0.108277E−2	0.417054E+0
0.193062E−2	0.189497E−2	0.168875E−2	0.143900E−2	0.936450E−3	0.380266E−3	0.105851E−2	0.409499E+0
0.198619E−2	0.194687E−2	0.172131E−2	0.145804E−2	0.944951E−3	0.384528E−3	0.105743E−2	0.404631E+0
0.205608E−2	0.201206E−2	0.176784E−2	0.149121E−2	0.964897E−3	0.393940E−3	0.107671E−2	0.402186E+0
0.213477E−2	0.208752E−2	0.182575E−2	0.153587E−2	0.993515E−3	0.405661E−3	0.110642E−2	0.401346E+0
0.221919E−2	0.216771E−2	0.188812E−2	0.158572E−2	0.102298E−2	0.418063E−3	0.113832E−2	0.400671E+0

Table 1 (continued)

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Ca $Z = 20$	K shell						
0.172296E−2	0.170923E−2	0.161664E−2	0.146561E−2	0.103948E−2	0.441554E−3	0.132354E−2	0.439107E+0
0.165478E−2	0.163619E−2	0.151695E−2	0.134403E−2	0.923665E−3	0.394921E−3	0.112767E−2	0.419690E+0
0.165139E−2	0.162857E−2	0.149000E−2	0.130267E−2	0.881840E−3	0.377318E−3	0.104593E−2	0.407829E+0
0.168263E−2	0.165627E−2	0.150139E−2	0.130096E−2	0.874142E−3	0.375700E−3	0.102189E−2	0.400248E+0
0.173268E−2	0.170385E−2	0.153377E−2	0.132168E−2	0.883575E−3	0.380251E−3	0.102211E−2	0.395518E+0
0.179400E−2	0.176170E−2	0.157726E−2	0.135399E−2	0.902817E−3	0.389865E−3	0.104179E−2	0.393160E+0
0.186328E−2	0.182932E−2	0.163074E−2	0.139513E−2	0.929573E−3	0.401402E−3	0.107006E−2	0.392202E+0
0.193769E−2	0.190112E−2	0.168834E−2	0.144120E−2	0.958065E−3	0.414234E−3	0.110272E−2	0.391642E+0
Sc $Z = 21$	K shell						
0.149640E−2	0.148644E−2	0.141711E−2	0.130055E−2	0.952280E−3	0.428226E−3	0.125589E−2	0.430379E+0
0.145101E−2	0.143692E−2	0.134756E−2	0.121085E−2	0.858122E−3	0.386954E−3	0.108068E−2	0.410817E+0
0.145171E−2	0.143430E−2	0.132940E−2	0.117971E−2	0.822730E−3	0.371131E−3	0.100622E−2	0.398959E+0
0.148154E−2	0.146179E−2	0.134372E−2	0.118258E−2	0.817906E−3	0.369749E−3	0.983865E−3	0.391466E+0
0.152672E−2	0.150471E−2	0.137464E−2	0.120224E−2	0.827128E−3	0.374864E−3	0.986172E−3	0.386907E+0
0.158162E−2	0.155845E−2	0.141702E−2	0.123447E−2	0.845946E−3	0.383865E−3	0.100374E−2	0.384481E+0
0.164356E−2	0.161802E−2	0.146537E−2	0.127286E−2	0.871966E−3	0.395540E−3	0.103167E−2	0.383472E+0
0.171000E−2	0.168319E−2	0.151944E−2	0.131684E−2	0.898951E−3	0.408388E−3	0.106365E−2	0.382896E+0
Ti $Z = 22$	K shell						
0.130633E−2	0.129886E−2	0.124641E−2	0.115589E−2	0.871200E−3	0.412694E−3	0.118491E−2	0.421888E+0
0.127966E−2	0.126928E−2	0.120100E−2	0.109277E−2	0.797255E−3	0.377253E−3	0.103125E−2	0.402246E+0
0.128465E−2	0.127096E−2	0.119029E−2	0.107050E−2	0.767599E−3	0.362974E−3	0.963257E−3	0.390396E+0
0.131251E−2	0.129708E−2	0.120665E−2	0.107652E−2	0.764646E−3	0.362181E−3	0.943414E−3	0.382944E+0
0.135356E−2	0.133655E−2	0.123628E−2	0.109668E−2	0.774590E−3	0.367375E−3	0.946282E−3	0.378463E+0
0.140308E−2	0.138581E−2	0.127651E−2	0.112730E−2	0.792892E−3	0.376428E−3	0.963938E−3	0.376120E+0
0.145904E−2	0.143977E−2	0.132175E−2	0.116413E−2	0.818203E−3	0.387869E−3	0.990343E−3	0.374953E+0
0.151756E−2	0.149718E−2	0.137046E−2	0.120428E−2	0.843051E−3	0.400946E−3	0.102236E−2	0.374418E+0
V $Z = 23$	K shell						
0.114553E−2	0.113969E−2	0.109955E−2	0.102866E−2	0.795891E−3	0.395655E−3	0.111283E−2	0.413649E+0
0.113476E−2	0.112683E−2	0.107424E−2	0.987773E−3	0.739970E−3	0.366332E−3	0.980895E−3	0.393970E+0
0.114271E−2	0.113164E−2	0.106955E−2	0.973390E−3	0.716269E−3	0.353634E−3	0.919348E−3	0.382161E+0
0.116931E−2	0.115787E−2	0.108748E−2	0.982170E−3	0.715542E−3	0.352803E−3	0.900281E−3	0.374719E+0
0.120685E−2	0.119448E−2	0.111686E−2	0.100329E−2	0.726370E−3	0.358420E−3	0.904664E−3	0.370343E+0
0.125235E−2	0.123814E−2	0.115302E−2	0.103147E−2	0.743746E−3	0.368473E−3	0.925090E−3	0.368209E+0
0.130155E−2	0.128722E−2	0.119525E−2	0.106611E−2	0.767461E−3	0.379343E−3	0.949485E−3	0.366991E+0
0.135455E−2	0.133933E−2	0.124048E−2	0.110394E−2	0.791349E−3	0.391887E−3	0.979181E−3	0.366297E+0
Cr $Z = 24$	K shell						
0.101004E−2	0.100560E−2	0.974438E−3	0.918432E−3	0.727038E−3	0.377796E−3	0.104149E−2	0.405623E+0
0.101281E−2	0.100663E−2	0.965541E−3	0.896300E−3	0.687496E−3	0.354633E−3	0.930828E−3	0.385996E+0
0.102354E−2	0.101496E−2	0.966307E−3	0.887923E−3	0.668334E−3	0.343759E−3	0.876164E−3	0.374246E+0
0.104883E−2	0.103966E−2	0.984365E−3	0.898532E−3	0.669975E−3	0.343411E−3	0.859402E−3	0.366923E+0
0.108386E−2	0.107440E−2	0.101301E−2	0.920019E−3	0.681403E−3	0.349355E−3	0.864897E−3	0.362609E+0
0.112483E−2	0.111426E−2	0.104715E−2	0.947297E−3	0.698613E−3	0.358829E−3	0.883463E−3	0.360401E+0
0.117090E−2	0.115893E−2	0.108655E−2	0.980119E−3	0.721350E−3	0.369993E−3	0.908322E−3	0.359246E+0
0.121914E−2	0.120706E−2	0.112908E−2	0.101633E−2	0.744523E−3	0.382512E−3	0.937369E−3	0.358527E+0
Mn $Z = 25$	K shell						
0.889847E−3	0.886526E−3	0.862291E−3	0.818064E−3	0.661462E−3	0.358464E−3	0.969007E−3	0.397777E+0
0.904017E−3	0.899331E−3	0.867198E−3	0.811592E−3	0.636751E−3	0.341727E−3	0.879764E−3	0.378256E+0
0.916791E−3	0.909926E−3	0.871802E−3	0.808728E−3	0.622782E−3	0.332697E−3	0.831909E−3	0.366596E+0
0.941432E−3	0.933847E−3	0.890323E−3	0.820676E−3	0.625946E−3	0.333106E−3	0.818055E−3	0.359388E+0
0.973751E−3	0.966299E−3	0.918020E−3	0.842285E−3	0.637377E−3	0.339234E−3	0.824399E−3	0.355186E+0
0.101187E−2	0.100306E−2	0.950198E−3	0.868423E−3	0.654730E−3	0.349102E−3	0.843841E−3	0.353039E+0
0.105310E−2	0.104381E−2	0.986552E−3	0.899402E−3	0.676255E−3	0.359701E−3	0.866747E−3	0.351790E+0
0.109641E−2	0.108605E−2	0.102454E−2	0.932031E−3	0.698219E−3	0.371501E−3	0.893327E−3	0.350960E+0
Fe $Z = 26$	K shell						
0.787668E−3	0.785007E−3	0.765926E−3	0.730664E−3	0.601910E−3	0.339101E−3	0.899394E−3	0.390169E+0
0.811534E−3	0.807718E−3	0.782276E−3	0.737523E−3	0.590330E−3	0.328560E−3	0.830211E−3	0.370785E+0
0.826527E−3	0.820749E−3	0.790415E−3	0.739139E−3	0.580937E−3	0.321538E−3	0.789412E−3	0.359269E+0
0.850225E−3	0.843792E−3	0.809299E−3	0.752380E−3	0.585844E−3	0.322585E−3	0.777963E−3	0.352125E+0
0.880501E−3	0.873454E−3	0.835045E−3	0.772941E−3	0.597579E−3	0.328840E−3	0.784974E−3	0.348031E+0
0.915314E−3	0.908355E−3	0.866241E−3	0.799177E−3	0.614777E−3	0.338347E−3	0.803226E−3	0.345825E+0
0.952964E−3	0.945621E−3	0.899968E−3	0.828180E−3	0.634905E−3	0.349171E−3	0.826513E−3	0.344661E+0
0.992445E−3	0.984458E−3	0.935357E−3	0.858980E−3	0.656422E−3	0.360869E−3	0.852412E−3	0.343822E+0

Table 1 (continued)

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Co $Z = 27$	K shell						
0.698660E−3	0.696627E−3	0.681484E−3	0.653226E−3	0.547098E−3	0.319491E−3	0.831783E−3	0.382737E+0
0.730991E−3	0.727910E−3	0.707583E−3	0.671204E−3	0.547281E−3	0.315158E−3	0.782121E−3	0.363574E+0
0.747643E−3	0.742933E−3	0.718731E−3	0.676785E−3	0.542142E−3	0.309789E−3	0.747025E−3	0.352083E+0
0.770598E−3	0.765330E−3	0.737717E−3	0.691188E−3	0.548554E−3	0.312063E−3	0.739741E−3	0.345237E+0
0.798959E−3	0.793122E−3	0.762328E−3	0.711210E−3	0.560453E−3	0.318792E−3	0.748150E−3	0.341226E+0
0.831048E−3	0.825458E−3	0.791662E−3	0.736252E−3	0.577342E−3	0.327630E−3	0.764605E−3	0.338990E+0
0.865898E−3	0.859817E−3	0.823058E−3	0.763733E−3	0.597134E−3	0.338043E−3	0.786398E−3	0.337717E+0
0.902551E−3	0.895858E−3	0.856407E−3	0.793095E−3	0.617992E−3	0.350119E−3	0.812933E−3	0.336950E+0
Ni $Z = 28$	K shell						
0.620883E−3	0.619285E−3	0.607180E−3	0.584389E−3	0.496798E−3	0.300050E−3	0.767175E−3	0.375507E+0
0.660192E−3	0.657330E−3	0.641443E−3	0.611727E−3	0.507272E−3	0.301577E−3	0.735457E−3	0.356586E+0
0.678456E−3	0.674423E−3	0.654910E−3	0.620473E−3	0.505818E−3	0.298113E−3	0.706711E−3	0.345260E+0
0.700582E−3	0.696082E−3	0.673795E−3	0.635324E−3	0.513174E−3	0.301163E−3	0.702027E−3	0.338529E+0
0.727365E−3	0.723071E−3	0.698044E−3	0.655992E−3	0.526299E−3	0.307530E−3	0.709645E−3	0.334477E+0
0.757277E−3	0.752295E−3	0.724981E−3	0.679215E−3	0.542114E−3	0.316916E−3	0.727470E−3	0.332374E+0
0.789327E−3	0.784275E−3	0.754623E−3	0.705438E−3	0.561179E−3	0.327517E−3	0.749514E−3	0.331154E+0
0.823393E−3	0.817311E−3	0.785393E−3	0.732885E−3	0.581460E−3	0.339099E−3	0.774516E−3	0.330378E+0
Cu $Z = 29$	K shell						
0.553396E−3	0.552122E−3	0.542359E−3	0.523849E−3	0.451268E−3	0.281102E−3	0.706194E−3	0.368468E+0
0.598921E−3	0.596460E−3	0.583174E−3	0.558741E−3	0.470693E−3	0.288166E−3	0.690964E−3	0.349820E+0
0.618444E−3	0.615009E−3	0.599069E−3	0.569984E−3	0.472514E−3	0.286710E−3	0.668633E−3	0.338705E+0
0.640146E−3	0.636130E−3	0.617967E−3	0.586052E−3	0.481027E−3	0.290348E−3	0.665952E−3	0.332055E+0
0.665236E−3	0.661152E−3	0.640874E−3	0.605776E−3	0.493828E−3	0.296913E−3	0.674354E−3	0.328126E+0
0.693263E−3	0.689055E−3	0.666772E−3	0.628508E−3	0.509990E−3	0.306279E−3	0.691899E−3	0.325978E+0
0.723185E−3	0.718816E−3	0.694601E−3	0.653560E−3	0.528385E−3	0.316753E−3	0.713390E−3	0.324762E+0
0.754744E−3	0.749236E−3	0.723155E−3	0.679300E−3	0.547473E−3	0.327846E−3	0.736820E−3	0.323920E+0
Zn $Z = 30$	K shell						
0.492282E−3	0.491257E−3	0.483381E−3	0.468350E−3	0.408336E−3	0.261997E−3	0.646875E−3	0.361528E+0
0.542805E−3	0.540856E−3	0.530028E−3	0.509904E−3	0.435194E−3	0.274456E−3	0.647324E−3	0.343222E+0
0.563425E−3	0.560128E−3	0.547184E−3	0.523668E−3	0.440819E−3	0.274514E−3	0.629889E−3	0.332217E+0
0.584561E−3	0.581164E−3	0.566364E−3	0.539831E−3	0.450080E−3	0.279100E−3	0.630120E−3	0.325736E+0
0.608178E−3	0.605432E−3	0.588898E−3	0.559774E−3	0.463016E−3	0.285987E−3	0.639483E−3	0.321886E+0
0.634434E−3	0.630881E−3	0.612704E−3	0.581151E−3	0.478855E−3	0.295306E−3	0.656904E−3	0.319810E+0
0.662156E−3	0.658608E−3	0.638852E−3	0.604702E−3	0.496546E−3	0.305630E−3	0.677779E−3	0.318578E+0
0.691385E−3	0.686779E−3	0.665487E−3	0.628959E−3	0.514899E−3	0.316466E−3	0.700255E−3	0.317691E+0
Ga $Z = 31$	K shell						
0.438071E−3	0.437257E−3	0.430875E−3	0.418632E−3	0.368930E−3	0.243354E−3	0.590728E−3	0.354736E+0
0.492889E−3	0.491234E−3	0.482398E−3	0.465770E−3	0.402618E−3	0.260806E−3	0.605319E−3	0.336792E+0
0.514423E−3	0.511594E−3	0.500985E−3	0.481575E−3	0.410832E−3	0.262715E−3	0.593514E−3	0.325996E+0
0.535086E−3	0.532077E−3	0.519938E−3	0.497985E−3	0.421059E−3	0.267977E−3	0.595845E−3	0.319632E+0
0.557702E−3	0.554591E−3	0.541036E−3	0.516800E−3	0.434115E−3	0.275100E−3	0.605938E−3	0.315857E+0
0.581740E−3	0.579084E−3	0.564175E−3	0.537721E−3	0.449602E−3	0.284303E−3	0.622995E−3	0.313800E+0
0.608129E−3	0.604993E−3	0.588780E−3	0.559868E−3	0.466498E−3	0.294534E−3	0.643426E−3	0.312564E+0
0.634744E−3	0.631535E−3	0.614059E−3	0.583204E−3	0.484620E−3	0.305349E−3	0.665620E−3	0.311706E+0
Ge $Z = 32$	K shell						
0.390045E−3	0.389343E−3	0.384149E−3	0.374142E−3	0.332976E−3	0.225309E−3	0.537898E−3	0.348078E+0
0.448349E−3	0.446162E−3	0.438872E−3	0.425112E−3	0.371702E−3	0.246818E−3	0.563770E−3	0.330398E+0
0.470662E−3	0.468315E−3	0.459522E−3	0.443291E−3	0.382940E−3	0.251050E−3	0.558645E−3	0.319944E+0
0.490525E−3	0.488466E−3	0.478450E−3	0.460045E−3	0.393754E−3	0.256797E−3	0.562561E−3	0.313686E+0
0.512420E−3	0.509635E−3	0.498457E−3	0.478206E−3	0.407109E−3	0.264235E−3	0.573526E−3	0.309986E+0
0.535439E−3	0.532739E−3	0.520444E−3	0.498358E−3	0.422309E−3	0.273497E−3	0.590633E−3	0.307962E+0
0.559660E−3	0.556954E−3	0.543577E−3	0.519732E−3	0.438959E−3	0.283539E−3	0.610394E−3	0.306701E+0
0.584038E−3	0.581126E−3	0.566711E−3	0.541156E−3	0.455773E−3	0.294061E−3	0.631638E−3	0.305811E+0
As $Z = 33$	K shell						
0.347366E−3	0.346796E−3	0.342552E−3	0.334342E−3	0.300134E−3	0.207964E−3	0.488452E−3	0.341550E+0
0.408637E−3	0.406682E−3	0.400646E−3	0.389177E−3	0.343819E−3	0.233777E−3	0.525918E−3	0.324311E+0
0.431602E−3	0.429498E−3	0.422244E−3	0.408644E−3	0.357056E−3	0.239642E−3	0.525465E−3	0.314055E+0
0.451035E−3	0.449263E−3	0.440954E−3	0.425590E−3	0.368562E−3	0.246030E−3	0.531248E−3	0.307910E+0
0.472020E−3	0.469801E−3	0.460525E−3	0.443528E−3	0.382250E−3	0.253681E−3	0.542825E−3	0.304284E+0
0.493595E−3	0.491246E−3	0.481043E−3	0.462447E−3	0.396875E−3	0.262855E−3	0.559661E−3	0.302292E+0
0.516241E−3	0.513811E−3	0.502706E−3	0.482708E−3	0.412849E−3	0.272718E−3	0.578793E−3	0.301003E+0
0.539596E−3	0.536555E−3	0.524584E−3	0.503034E−3	0.429076E−3	0.283144E−3	0.599605E−3	0.300126E+0

Table 1 (continued)

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Se $Z = 34$	K shell						
0.309320E−3	0.308828E−3	0.305349E−3	0.298618E−3	0.270177E−3	0.191377E−3	0.442349E−3	0.335142E+0
0.372909E−3	0.370511E−3	0.365506E−3	0.355916E−3	0.317378E−3	0.220797E−3	0.489300E−3	0.318292E+0
0.396539E−3	0.394618E−3	0.388570E−3	0.377172E−3	0.332932E−3	0.228441E−3	0.493779E−3	0.308324E+0
0.415636E−3	0.414082E−3	0.407154E−3	0.394289E−3	0.345114E−3	0.235518E−3	0.501426E−3	0.302268E+0
0.435567E−3	0.433456E−3	0.425717E−3	0.411472E−3	0.358415E−3	0.243288E−3	0.513419E−3	0.298738E+0
0.456012E−3	0.453928E−3	0.445416E−3	0.429768E−3	0.372777E−3	0.252514E−3	0.530306E−3	0.296794E+0
0.477356E−3	0.475173E−3	0.465996E−3	0.449079E−3	0.388131E−3	0.262049E−3	0.548473E−3	0.295443E+0
0.499170E−3	0.496328E−3	0.486426E−3	0.468280E−3	0.404243E−3	0.272256E−3	0.568543E−3	0.294534E+0
Br $Z = 35$	K shell						
0.275375E−3	0.274972E−3	0.272111E−3	0.266541E−3	0.242868E−3	0.175581E−3	0.399502E−3	0.328848E+0
0.340455E−3	0.338646E−3	0.334449E−3	0.326415E−3	0.293548E−3	0.208500E−3	0.455382E−3	0.312480E+0
0.364612E−3	0.362957E−3	0.357890E−3	0.348041E−3	0.310072E−3	0.217315E−3	0.463149E−3	0.302680E+0
0.383634E−3	0.382344E−3	0.376174E−3	0.365253E−3	0.323204E−3	0.225027E−3	0.472557E−3	0.296774E+0
0.402767E−3	0.400868E−3	0.394345E−3	0.382356E−3	0.336505E−3	0.233159E−3	0.485459E−3	0.293349E+0
0.422221E−3	0.420233E−3	0.413096E−3	0.399928E−3	0.350546E−3	0.242321E−3	0.502053E−3	0.291376E+0
0.442245E−3	0.440440E−3	0.432601E−3	0.417936E−3	0.365435E−3	0.251768E−3	0.519901E−3	0.290052E+0
0.462665E−3	0.460111E−3	0.451743E−3	0.436483E−3	0.380792E−3	0.262058E−3	0.539977E−3	0.289185E+0
Kr $Z = 36$	K shell						
0.245016E−3	0.244395E−3	0.242037E−3	0.237438E−3	0.217994E−3	0.160618E−3	0.359853E−3	0.322668E+0
0.311471E−3	0.309870E−3	0.306345E−3	0.299549E−3	0.271189E−3	0.196351E−3	0.422716E−3	0.306719E+0
0.336032E−3	0.334296E−3	0.330030E−3	0.321888E−3	0.289246E−3	0.206758E−3	0.434677E−3	0.297222E+0
0.354721E−3	0.353260E−3	0.348366E−3	0.339088E−3	0.302797E−3	0.214982E−3	0.445506E−3	0.291462E+0
0.373063E−3	0.371298E−3	0.365829E−3	0.355668E−3	0.316046E−3	0.223323E−3	0.458875E−3	0.288063E+0
0.391567E−3	0.389902E−3	0.383888E−3	0.372431E−3	0.329763E−3	0.232391E−3	0.475191E−3	0.286118E+0
0.410494E−3	0.408829E−3	0.402287E−3	0.390115E−3	0.344469E−3	0.241910E−3	0.493068E−3	0.284833E+0
0.429627E−3	0.427275E−3	0.420228E−3	0.407272E−3	0.358799E−3	0.251778E−3	0.511947E−3	0.283870E+0
Rb $Z = 37$	K shell						
0.217629E−3	0.216596E−3	0.214654E−3	0.211335E−3	0.194926E−3	0.146368E−3	0.322958E−3	0.316560E+0
0.285023E−3	0.283590E−3	0.280621E−3	0.274601E−3	0.250605E−3	0.184812E−3	0.392365E−3	0.301142E+0
0.309915E−3	0.308324E−3	0.304721E−3	0.297810E−3	0.269707E−3	0.196407E−3	0.407430E−3	0.291873E+0
0.328614E−3	0.326953E−3	0.322816E−3	0.314941E−3	0.283570E−3	0.205116E−3	0.419534E−3	0.286229E+0
0.345851E−3	0.344280E−3	0.339655E−3	0.330906E−3	0.296745E−3	0.213369E−3	0.432749E−3	0.282855E+0
0.363578E−3	0.361941E−3	0.356855E−3	0.347278E−3	0.310218E−3	0.222582E−3	0.449274E−3	0.280935E+0
0.381456E−3	0.379923E−3	0.374396E−3	0.364029E−3	0.324255E−3	0.232016E−3	0.466812E−3	0.279647E+0
0.399599E−3	0.397435E−3	0.391446E−3	0.380187E−3	0.338051E−3	0.241691E−3	0.485102E−3	0.278679E+0
Sr $Z = 38$	K shell						
0.193094E−3	0.192623E−3	0.191017E−3	0.187871E−3	0.174204E−3	0.132960E−3	0.289007E−3	0.310560E+0
0.261245E−3	0.259459E−3	0.256951E−3	0.252094E−3	0.231740E−3	0.173678E−3	0.363710E−3	0.295661E+0
0.286157E−3	0.284717E−3	0.281661E−3	0.275775E−3	0.251532E−3	0.186410E−3	0.381661E−3	0.286634E+0
0.304519E−3	0.303036E−3	0.299525E−3	0.292807E−3	0.265631E−3	0.195580E−3	0.394958E−3	0.281123E+0
0.321227E−3	0.319752E−3	0.315826E−3	0.308357E−3	0.278710E−3	0.204016E−3	0.408573E−3	0.277788E+0
0.338050E−3	0.336574E−3	0.332255E−3	0.324071E−3	0.291886E−3	0.213062E−3	0.424627E−3	0.275852E+0
0.354986E−3	0.353364E−3	0.348671E−3	0.339784E−3	0.305296E−3	0.222345E−3	0.441713E−3	0.274573E+0
0.372165E−3	0.370108E−3	0.365048E−3	0.355562E−3	0.318781E−3	0.231848E−3	0.459450E−3	0.273578E+0
Y $Z = 39$	K shell						
0.171173E−3	0.170359E−3	0.169032E−3	0.166428E−3	0.155423E−3	0.120443E−3	0.257969E−3	0.304667E+0
0.239545E−3	0.237938E−3	0.235807E−3	0.231660E−3	0.214185E−3	0.163094E−3	0.337004E−3	0.290307E+0
0.264815E−3	0.263327E−3	0.260722E−3	0.255686E−3	0.234852E−3	0.176824E−3	0.357438E−3	0.281522E+0
0.282738E−3	0.281362E−3	0.278366E−3	0.272608E−3	0.249046E−3	0.186377E−3	0.371680E−3	0.276104E+0
0.298962E−3	0.297649E−3	0.294298E−3	0.287890E−3	0.262028E−3	0.195161E−3	0.386060E−3	0.272866E+0
0.314792E−3	0.313523E−3	0.309837E−3	0.302817E−3	0.274949E−3	0.204052E−3	0.401695E−3	0.270927E+0
0.331098E−3	0.329699E−3	0.325692E−3	0.318082E−3	0.287964E−3	0.213274E−3	0.418498E−3	0.269637E+0
0.347377E−3	0.345329E−3	0.341012E−3	0.332840E−3	0.300763E−3	0.222259E−3	0.434967E−3	0.268570E+0
Zr $Z = 40$	K shell						
0.151514E−3	0.150433E−3	0.149336E−3	0.147512E−3	0.138033E−3	0.108755E−3	0.229584E−3	0.298869E+0
0.219762E−3	0.218322E−3	0.216511E−3	0.212969E−3	0.197724E−3	0.152604E−3	0.311109E−3	0.284919E+0
0.245185E−3	0.243806E−3	0.241577E−3	0.237258E−3	0.219030E−3	0.167281E−3	0.333845E−3	0.276400E+0
0.262845E−3	0.261581E−3	0.259025E−3	0.254074E−3	0.233251E−3	0.177523E−3	0.349718E−3	0.271212E+0
0.278591E−3	0.277392E−3	0.274521E−3	0.269006E−3	0.246443E−3	0.186470E−3	0.364384E−3	0.267975E+0
0.293723E−3	0.292521E−3	0.289362E−3	0.283317E−3	0.258924E−3	0.195263E−3	0.379755E−3	0.266071E+0
0.309153E−3	0.307789E−3	0.304314E−3	0.297759E−3	0.271456E−3	0.204184E−3	0.395777E−3	0.264732E+0
0.324660E−3	0.322788E−3	0.319091E−3	0.312048E−3	0.283938E−3	0.213205E−3	0.412187E−3	0.263690E+0

Table 1 (continued)

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Nb $Z = 41$	K shell						
0.133579E−3	0.132935E−3	0.132025E−3	0.130236E−3	0.122640E−3	0.979065E−4	0.203758E−3	0.293168E+0
0.201426E−3	0.200117E−3	0.198896E−3	0.195862E−3	0.182733E−3	0.142675E−3	0.287055E−3	0.279642E+0
0.227282E−3	0.226041E−3	0.224126E−3	0.220405E−3	0.204546E−3	0.158477E−3	0.312425E−3	0.271503E+0
0.244709E−3	0.243547E−3	0.241338E−3	0.237063E−3	0.218887E−3	0.169026E−3	0.329012E−3	0.266416E+0
0.260011E−3	0.258883E−3	0.256411E−3	0.251647E−3	0.231819E−3	0.178116E−3	0.343953E−3	0.263228E+0
0.274475E−3	0.273427E−3	0.270692E−3	0.265410E−3	0.244128E−3	0.186849E−3	0.359112E−3	0.261333E+0
0.289282E−3	0.288146E−3	0.285187E−3	0.279517E−3	0.256438E−3	0.195802E−3	0.375067E−3	0.259999E+0
0.303834E−3	0.302212E−3	0.299029E−3	0.292935E−3	0.268319E−3	0.204363E−3	0.390360E−3	0.258869E+0
Mo $Z = 42$	K shell						
0.118074E−3	0.117075E−3	0.116589E−3	0.115104E−3	0.108526E−3	0.878029E−4	0.180182E−3	0.287549E+0
0.184961E−3	0.184082E−3	0.182752E−3	0.180146E−3	0.168800E−3	0.133533E−3	0.265290E−3	0.274591E+0
0.210823E−3	0.209677E−3	0.207867E−3	0.204650E−3	0.190878E−3	0.149988E−3	0.292134E−3	0.266662E+0
0.227860E−3	0.226783E−3	0.224878E−3	0.221198E−3	0.205652E−3	0.160610E−3	0.308908E−3	0.261626E+0
0.242855E−3	0.241814E−3	0.239679E−3	0.235467E−3	0.218194E−3	0.169983E−3	0.324436E−3	0.258557E+0
0.256792E−3	0.255770E−3	0.253421E−3	0.248889E−3	0.230223E−3	0.178541E−3	0.339112E−3	0.256606E+0
0.270816E−3	0.269907E−3	0.267352E−3	0.262435E−3	0.242186E−3	0.187398E−3	0.354755E−3	0.255278E+0
0.284810E−3	0.283105E−3	0.280353E−3	0.275069E−3	0.253469E−3	0.196020E−3	0.370063E−3	0.254183E+0
Tc $Z = 43$	K shell						
0.103792E−3	0.102609E−3	0.101987E−3	0.100760E−3	0.955429E−4	0.780581E−4	0.157878E−3	0.281748E+0
0.169824E−3	0.169030E−3	0.167888E−3	0.165647E−3	0.155672E−3	0.124797E−3	0.244873E−3	0.269619E+0
0.195350E−3	0.194547E−3	0.193121E−3	0.190335E−3	0.178322E−3	0.142051E−3	0.273471E−3	0.262004E+0
0.212445E−3	0.211428E−3	0.209779E−3	0.206564E−3	0.192998E−3	0.152679E−3	0.290267E−3	0.256986E+0
0.226973E−3	0.225955E−3	0.224113E−3	0.220525E−3	0.205374E−3	0.161924E−3	0.305468E−3	0.253886E+0
0.240573E−3	0.239515E−3	0.237495E−3	0.233557E−3	0.217041E−3	0.170765E−3	0.320655E−3	0.252030E+0
0.253929E−3	0.252855E−3	0.250642E−3	0.246369E−3	0.228603E−3	0.179338E−3	0.335606E−3	0.250665E+0
0.267041E−3	0.265660E−3	0.263276E−3	0.258699E−3	0.239662E−3	0.187625E−3	0.350070E−3	0.249475E+0
Ru $Z = 44$	K shell						
0.909474E−4	0.901413E−4	0.896258E−4	0.886088E−4	0.840758E−4	0.694995E−4	0.138670E−3	0.276311E+0
0.156338E−3	0.155047E−3	0.154064E−3	0.152132E−3	0.143631E−3	0.116523E−3	0.225857E−3	0.264725E+0
0.181529E−3	0.180793E−3	0.179555E−3	0.177134E−3	0.166617E−3	0.134293E−3	0.255539E−3	0.257338E+0
0.198360E−3	0.197437E−3	0.195995E−3	0.193198E−3	0.181296E−3	0.145161E−3	0.272856E−3	0.252440E+0
0.212365E−3	0.211484E−3	0.209876E−3	0.206748E−3	0.193420E−3	0.154520E−3	0.288248E−3	0.249399E+0
0.225519E−3	0.224699E−3	0.222927E−3	0.219490E−3	0.204959E−3	0.163260E−3	0.303119E−3	0.247513E+0
0.238455E−3	0.237467E−3	0.235541E−3	0.231815E−3	0.216008E−3	0.171675E−3	0.317641E−3	0.246127E+0
0.251135E−3	0.249790E−3	0.247715E−3	0.243702E−3	0.226917E−3	0.179808E−3	0.331676E−3	0.244907E+0
Rh $Z = 45$	K shell						
0.794971E−4	0.785611E−4	0.781357E−4	0.772956E−4	0.735411E−4	0.613837E−4	0.120790E−3	0.270764E+0
0.143355E−3	0.142444E−3	0.141596E−3	0.139927E−3	0.132549E−3	0.108685E−3	0.208152E−3	0.259927E+0
0.168706E−3	0.168032E−3	0.166955E−3	0.164846E−3	0.155506E−3	0.126607E−3	0.238102E−3	0.252645E+0
0.185397E−3	0.184532E−3	0.183283E−3	0.180728E−3	0.170158E−3	0.137889E−3	0.256290E−3	0.247942E+0
0.198934E−3	0.198108E−3	0.196707E−3	0.193973E−3	0.182242E−3	0.147286E−3	0.271699E−3	0.244927E+0
0.211664E−3	0.210903E−3	0.209358E−3	0.206344E−3	0.193457E−3	0.155977E−3	0.286371E−3	0.243033E+0
0.223932E−3	0.223107E−3	0.221427E−3	0.218188E−3	0.204342E−3	0.164148E−3	0.300313E−3	0.241623E+0
0.236182E−3	0.234654E−3	0.232843E−3	0.229309E−3	0.214626E−3	0.172235E−3	0.314155E−3	0.240412E+0
Pd $Z = 46$	K shell						
0.691747E−4	0.681989E−4	0.678485E−4	0.671563E−4	0.641357E−4	0.540838E−4	0.105010E−3	0.265410E+0
0.131731E−3	0.130907E−3	0.130173E−3	0.128728E−3	0.122398E−3	0.101291E−3	0.191720E−3	0.255216E+0
0.157148E−3	0.156072E−3	0.155135E−3	0.153296E−3	0.145216E−3	0.119645E−3	0.222516E−3	0.248188E+0
0.173392E−3	0.172457E−3	0.171365E−3	0.169227E−3	0.159922E−3	0.130972E−3	0.240759E−3	0.243526E+0
0.186578E−3	0.185825E−3	0.184599E−3	0.182201E−3	0.171748E−3	0.140392E−3	0.256163E−3	0.240551E+0
0.198898E−3	0.198119E−3	0.196767E−3	0.194114E−3	0.182783E−3	0.149001E−3	0.270588E−3	0.238656E+0
0.210699E−3	0.209900E−3	0.208429E−3	0.205564E−3	0.193323E−3	0.157079E−3	0.284248E−3	0.237239E+0
0.222267E−3	0.221042E−3	0.219458E−3	0.216488E−3	0.203316E−3	0.165025E−3	0.297719E−3	0.236021E+0
Ag $Z = 47$	K shell						
0.601163E−4	0.590223E−4	0.587348E−4	0.581663E−4	0.556820E−4	0.473594E−4	0.907438E−4	0.260110E+0
0.121154E−3	0.120158E−3	0.119524E−3	0.118272E−3	0.112701E−3	0.941082E−4	0.176032E−3	0.250489E+0
0.146139E−3	0.145155E−3	0.144337E−3	0.142728E−3	0.135629E−3	0.112840E−3	0.207540E−3	0.243740E+0
0.162136E−3	0.161284E−3	0.160329E−3	0.158453E−3	0.150241E−3	0.124296E−3	0.226015E−3	0.239175E+0
0.175026E−3	0.174312E−3	0.173237E−3	0.171129E−3	0.161892E−3	0.133704E−3	0.241328E−3	0.236212E+0
0.187060E−3	0.186202E−3	0.185017E−3	0.182699E−3	0.172663E−3	0.142108E−3	0.255259E−3	0.234277E+0
0.198288E−3	0.197558E−3	0.196269E−3	0.193750E−3	0.182959E−3	0.150189E−3	0.268839E−3	0.232888E+0
0.209424E−3	0.208196E−3	0.206806E−3	0.204098E−3	0.192474E−3	0.157879E−3	0.281707E−3	0.231615E+0

Table 1 (continued)

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Cd $Z = 48$	K shell						
0.517800E−4	0.507719E−4	0.505367E−4	0.501337E−4	0.480385E−4	0.411799E−4	0.778664E−4	0.254818E+0
0.110986E−3	0.110294E−3	0.109744E−3	0.108659E−3	0.103700E−3	0.874475E−4	0.161713E−3	0.245914E+0
0.135739E−3	0.135032E−3	0.134316E−3	0.132907E−3	0.126667E−3	0.106155E−3	0.193069E−3	0.239259E+0
0.151702E−3	0.150907E−3	0.150068E−3	0.148421E−3	0.141174E−3	0.117897E−3	0.212090E−3	0.234879E+0
0.164427E−3	0.163529E−3	0.162584E−3	0.160732E−3	0.152692E−3	0.127149E−3	0.227024E−3	0.231879E+0
0.175946E−3	0.175126E−3	0.174084E−3	0.172043E−3	0.163156E−3	0.135608E−3	0.240995E−3	0.230003E+0
0.186762E−3	0.185985E−3	0.184851E−3	0.182625E−3	0.172949E−3	0.143659E−3	0.254442E−3	0.228652E+0
0.197439E−3	0.196245E−3	0.195024E−3	0.192637E−3	0.182333E−3	0.151047E−3	0.266621E−3	0.227295E+0
In $Z = 49$	K shell						
0.443999E−4	0.435507E−4	0.433593E−4	0.429396E−4	0.412042E−4	0.355716E−4	0.663895E−4	0.249597E+0
0.101986E−3	0.101069E−3	0.100592E−3	0.996505E−4	0.955076E−4	0.811141E−4	0.148312E−3	0.241383E+0
0.126378E−3	0.125529E−3	0.124902E−3	0.123667E−3	0.118248E−3	0.100133E−3	0.180205E−3	0.235038E+0
0.141839E−3	0.141182E−3	0.140444E−3	0.138993E−3	0.132491E−3	0.111686E−3	0.198781E−3	0.230604E+0
0.154433E−3	0.153585E−3	0.152753E−3	0.151119E−3	0.143990E−3	0.121003E−3	0.213792E−3	0.227677E+0
0.165577E−3	0.164821E−3	0.163903E−3	0.162101E−3	0.154141E−3	0.129362E−3	0.227489E−3	0.225796E+0
0.176013E−3	0.175233E−3	0.174233E−3	0.172364E−3	0.163817E−3	0.137173E−3	0.240374E−3	0.224380E+0
0.186333E−3	0.185200E−3	0.184123E−3	0.181953E−3	0.172809E−3	0.144633E−3	0.252639E−3	0.223103E+0
Sn $Z = 50$	K shell						
0.377744E−4	0.369581E−4	0.368031E−4	0.364963E−4	0.350765E−4	0.304800E−4	0.561544E−4	0.244414E+0
0.935013E−4	0.926738E−4	0.922600E−4	0.914419E−4	0.877462E−4	0.751764E−4	0.135939E−3	0.236949E+0
0.117674E−3	0.116814E−3	0.116266E−3	0.115181E−3	0.110404E−3	0.942391E−4	0.167807E−3	0.230791E+0
0.132813E−3	0.132125E−3	0.131475E−3	0.130196E−3	0.124518E−3	0.105840E−3	0.186427E−3	0.226443E+0
0.145113E−3	0.144320E−3	0.143586E−3	0.142142E−3	0.135820E−3	0.115112E−3	0.201284E−3	0.223526E+0
0.155945E−3	0.155221E−3	0.154347E−3	0.152753E−3	0.145741E−3	0.123382E−3	0.214733E−3	0.221644E+0
0.166034E−3	0.165291E−3	0.164407E−3	0.162674E−3	0.155065E−3	0.130992E−3	0.227138E−3	0.220170E+0
0.175882E−3	0.174734E−3	0.173782E−3	0.171916E−3	0.163771E−3	0.138214E−3	0.238881E−3	0.218864E+0

required for accurate interpolation but also reduces the variation in the first and second derivatives of the surface, minimizing the possibility of rounding errors during the interpolation procedure. The smooth variation of $\ln[f(s)]$ with s is further illustrated for K-shell ionization for a range of elements with differing delocalizations in Fig. 2. Similar results can be obtained for L-shell ionization. The plots in Figs. 2(a) to 2(d) exhibit a roughly linear behaviour for moderate to large s, justifying the parameterization $f(s) \approx a\exp(-bs)$ in the range 2.5 to 20 Å^{-1}. The parameters a and b in Tables 1 and 2 are determined by matching the values of $f(s)$ at $s = 2.5$ and $s = 20$ Å^{-1}. For the more delocalized cases of the carbon and aluminium K shells [Figs. 2(a) and 2(b)], the plots are also approximately linear in the range $s = 0$ to 2.5 Å^{-1}. This suggests that an exponential form of the scattering factors, such as that defined in equation (12), may offer a suitable parameterization in this range, especially for more delocalized interactions. While simple straight-line extrapolation of the small-s behaviour of $\ln[f(s)]$ will lead to an underestimation of the form factors for large s, the value of $f(s)$ in this region is small for delocalized interactions and this should not lead to large errors in subsequent calculations of cross sections. For more localized interactions, the parameterization in equation (12) does not provide as accurate a description of the form factors, but then the effective delocalization is largely determined by the Debye–Waller factor present in equation (15), as we will illustrate by example later. The parameter c in the exponential parameterization of the atomic scattering factors $f(s)$ given by equation (12), which in one dimension corresponds to the HWHM of a Lorentzian form of the atomic ionization potential, has been found using the calculated form factors in Tables 1 and 2 and presented in Tables 3 (K shell) and 4 (L shell). These parameters were calculated by holding $f(0)$ fixed at the calculated value (which ensures that the ionization cross section for an amorphous solid is maintained) and obtaining the best straight-line fit to $\ln[f(s)]$ [*i.e.* $f(s)$ is

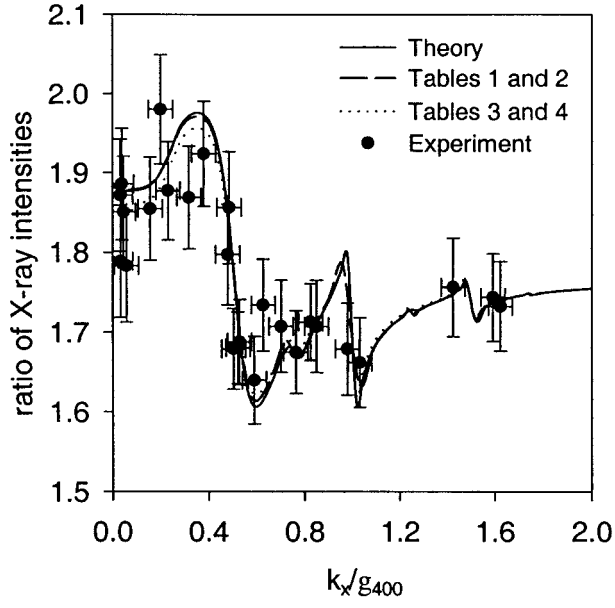

Figure 5
Ratio of X-ray intensities, Ga K shell to Ga L shell, for ⟨400⟩ systematic row conditions for 400 keV incident electrons incident on GaAs. The experimental data are those of Nüchter & Sigle (1995).

Table 2
Atomic scattering factors $f(s)$ (in Å) for L-shell ionization for elements in the range $Z = 20$ (calcium) to $Z = 60$ (neodymium) at selected values of s between 0 and 2.5 Å^{-1}.

For each element, the first row is for 50 keV incident electrons and for each subsequent row the incident energy is incremented by 50 keV so that the final row corresponds to an energy of 400 keV. The natural logarithm of these values can be accurately interpolated in s and in energy using cubic splines. The parameters a and b can be used to estimate the scattering factors in the range 2.5 to 20 Å^{-1} using $f(s) \approx a\exp(-bs)$.

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Ca $Z = 20$	L shell						
0.130603E+0	0.987798E−1	0.505557E−1	0.260202E−1	0.394482E−2	0.167751E−3	0.562715E−3	0.484117E+0
0.119556E+0	0.830633E−1	0.415631E−1	0.216253E−1	0.334859E−2	0.159092E−3	0.525016E−3	0.477579E+0
0.118752E+0	0.785777E−1	0.390158E−1	0.203395E−1	0.317842E−2	0.155422E−3	0.504110E−3	0.470659E+0
0.121046E+0	0.774311E−1	0.383249E−1	0.199570E−1	0.315371E−2	0.156857E−3	0.503886E−3	0.466806E+0
0.124403E+0	0.780676E−1	0.385126E−1	0.201018E−1	0.317655E−2	0.157795E−3	0.507581E−3	0.467345E+0
0.128219E+0	0.795731E−1	0.390613E−1	0.205003E−1	0.326434E−2	0.164099E−3	0.524714E−3	0.464953E+0
0.132418E+0	0.815994E−1	0.401768E−1	0.210279E−1	0.338432E−2	0.168379E−3	0.539244E−3	0.465580E+0
0.136544E+0	0.838502E−1	0.413489E−1	0.216998E−1	0.344531E−2	0.174413E−3	0.563767E−3	0.469286E+0
Sc $Z = 21$	L shell						
0.112155E+0	0.882719E−1	0.471458E−1	0.253900E−1	0.436017E−2	0.138789E−3	0.441953E−3	0.463301E+0
0.102480E+0	0.746633E−1	0.388194E−1	0.210715E−1	0.369596E−2	0.133238E−3	0.418092E−3	0.457426E+0
0.101544E+0	0.707289E−1	0.364097E−1	0.197911E−1	0.349742E−2	0.132143E−3	0.409127E−3	0.452056E+0
0.103487E+0	0.698161E−1	0.357987E−1	0.194268E−1	0.346862E−2	0.134160E−3	0.411753E−3	0.448556E+0
0.106563E+0	0.704359E−1	0.359574E−1	0.195874E−1	0.349647E−2	0.137286E−3	0.421681E−3	0.448874E+0
0.110106E+0	0.717734E−1	0.364816E−1	0.199400E−1	0.358582E−2	0.141027E−3	0.427343E−3	0.443453E+0
0.113858E+0	0.736754E−1	0.375064E−1	0.204497E−1	0.371725E−2	0.143564E−3	0.437782E−3	0.445976E+0
0.117780E+0	0.757752E−1	0.385969E−1	0.210995E−1	0.377654E−2	0.149658E−3	0.461140E−3	0.450138E+0
Ti $Z = 22$	L shell						
0.973807E−1	0.792194E−1	0.440406E−1	0.246430E−1	0.474643E−2	0.174997E−3	0.563158E−3	0.467516E+0
0.889048E−1	0.673779E−1	0.363209E−1	0.204502E−1	0.401282E−2	0.143164E−3	0.443539E−3	0.452319E+0
0.879373E−1	0.639994E−1	0.340582E−1	0.191807E−1	0.379889E−2	0.134450E−3	0.407701E−3	0.443737E+0
0.895549E−1	0.632683E−1	0.335014E−1	0.188383E−1	0.376261E−2	0.132031E−3	0.395051E−3	0.438392E+0
0.922602E−1	0.638574E−1	0.336302E−1	0.189804E−1	0.379380E−2	0.133051E−3	0.397871E−3	0.438157E+0
0.954799E−1	0.650401E−1	0.341865E−1	0.193200E−1	0.388657E−2	0.135820E−3	0.399814E−3	0.431867E+0
0.989360E−1	0.668635E−1	0.350712E−1	0.198173E−1	0.401989E−2	0.140363E−3	0.415129E−3	0.433744E+0
0.102482E+0	0.688204E−1	0.360879E−1	0.204333E−1	0.408676E−2	0.144725E−3	0.429433E−3	0.435051E+0
V $Z = 23$	L shell						
0.853107E−1	0.713769E−1	0.412072E−1	0.238478E−1	0.509208E−2	0.212308E−3	0.687406E−3	0.469955E+0
0.778676E−1	0.610963E−1	0.340336E−1	0.197818E−1	0.430060E−2	0.175844E−3	0.548646E−3	0.455143E+0
0.769363E−1	0.581539E−1	0.319126E−1	0.185524E−1	0.406856E−2	0.168190E−3	0.515018E−3	0.447643E+0
0.782703E−1	0.575178E−1	0.313897E−1	0.182076E−1	0.402274E−2	0.163964E−3	0.495724E−3	0.442549E+0
0.806257E−1	0.581400E−1	0.315031E−1	0.183500E−1	0.405306E−2	0.165475E−3	0.500245E−3	0.442512E+0
0.835108E−1	0.592307E−1	0.320375E−1	0.186732E−1	0.415841E−2	0.168865E−3	0.502453E−3	0.436162E+0
0.866597E−1	0.609522E−1	0.328747E−1	0.191549E−1	0.429167E−2	0.174705E−3	0.522899E−3	0.438515E+0
0.899243E−1	0.627944E−1	0.338158E−1	0.197428E−1	0.437971E−2	0.180336E−3	0.536308E−3	0.435956E+0
Cr $Z = 24$	L shell						
0.775385E−1	0.661744E−1	0.392310E−1	0.232469E−1	0.541472E−2	0.254885E−3	0.829799E−3	0.472149E+0
0.708414E−1	0.569577E−1	0.324311E−1	0.192811E−1	0.455925E−2	0.212539E−3	0.667758E−3	0.457920E+0
0.699787E−1	0.543434E−1	0.304224E−1	0.180755E−1	0.431425E−2	0.202189E−3	0.623075E−3	0.450186E+0
0.711414E−1	0.537992E−1	0.299157E−1	0.177213E−1	0.426030E−2	0.198213E−3	0.604977E−3	0.446339E+0
0.732663E−1	0.544302E−1	0.300270E−1	0.178637E−1	0.429324E−2	0.201193E−3	0.613710E−3	0.446104E+0
0.759122E−1	0.555218E−1	0.304705E−1	0.181846E−1	0.439510E−2	0.206638E−3	0.620295E−3	0.439691E+0
0.788269E−1	0.571273E−1	0.313274E−1	0.186513E−1	0.454781E−2	0.212753E−3	0.644413E−3	0.443283E+0
0.819084E−1	0.588955E−1	0.322459E−1	0.192265E−1	0.466267E−2	0.219454E−3	0.661776E−3	0.441514E+0
Mn $Z = 25$	L shell						
0.669551E−1	0.585425E−1	0.362126E−1	0.221863E−1	0.565578E−2	0.293878E−3	0.958121E−3	0.472723E+0
0.611732E−1	0.507471E−1	0.300236E−1	0.184095E−1	0.476112E−2	0.247479E−3	0.779691E−3	0.459028E+0
0.603813E−1	0.485217E−1	0.281779E−1	0.172523E−1	0.450181E−2	0.235125E−3	0.726622E−3	0.451316E+0
0.613267E−1	0.481150E−1	0.277104E−1	0.169223E−1	0.444399E−2	0.231524E−3	0.709278E−3	0.447825E+0
0.631220E−1	0.487257E−1	0.278254E−1	0.170494E−1	0.447709E−2	0.235563E−3	0.721028E−3	0.447481E+0
0.653849E−1	0.496926E−1	0.282997E−1	0.173557E−1	0.458133E−2	0.240976E−3	0.726294E−3	0.441303E+0
0.679173E−1	0.511858E−1	0.290293E−1	0.177990E−1	0.473042E−2	0.248695E−3	0.748542E−3	0.440761E+0
0.706163E−1	0.528125E−1	0.298878E−1	0.183483E−1	0.485496E−2	0.255525E−3	0.770392E−3	0.441431E+0
Fe $Z = 26$	L shell						
0.598642E−1	0.532315E−1	0.340026E−1	0.213555E−1	0.587231E−2	0.338240E−3	0.110434E−2	0.473299E+0
0.547433E−1	0.464440E−1	0.282609E−1	0.177278E−1	0.493949E−2	0.286373E−3	0.903572E−3	0.459624E+0
0.540331E−1	0.445039E−1	0.265380E−1	0.166123E−1	0.466582E−2	0.272205E−3	0.843265E−3	0.452291E+0
0.548523E−1	0.442211E−1	0.260985E−1	0.162948E−1	0.460623E−2	0.269523E−3	0.829398E−3	0.449618E+0
0.564377E−1	0.448012E−1	0.262077E−1	0.164211E−1	0.464083E−2	0.273967E−3	0.843403E−3	0.449775E+0
0.584505E−1	0.457259E−1	0.266721E−1	0.167113E−1	0.474287E−2	0.280683E−3	0.850117E−3	0.443259E+0
0.607235E−1	0.471296E−1	0.273632E−1	0.171411E−1	0.489782E−2	0.289340E−3	0.879622E−3	0.444756E+0
0.631610E−1	0.486599E−1	0.281745E−1	0.176671E−1	0.503243E−2	0.298700E−3	0.901490E−3	0.441844E+0

Table 2 (continued)

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Co $Z = 27$	L shell						
0.538021E−1	0.485388E−1	0.319611E−1	0.205432E−1	0.604571E−2	0.385440E−3	0.126029E−2	0.473886E+0
0.492605E−1	0.426080E−1	0.266432E−1	0.170823E−1	0.507982E−2	0.326855E−3	0.103258E−2	0.460120E+0
0.486228E−1	0.409226E−1	0.250367E−1	0.159948E−1	0.479958E−2	0.312393E−3	0.970902E−3	0.453585E+0
0.493549E−1	0.407418E−1	0.246273E−1	0.156816E−1	0.473858E−2	0.310492E−3	0.958812E−3	0.451015E+0
0.507608E−1	0.413014E−1	0.247391E−1	0.157978E−1	0.477216E−2	0.314913E−3	0.974370E−3	0.451798E+0
0.525593E−1	0.421309E−1	0.251817E−1	0.160862E−1	0.487449E−2	0.322765E−3	0.981618E−3	0.444911E+0
0.545987E−1	0.434969E−1	0.258326E−1	0.164969E−1	0.502361E−2	0.334954E−3	0.101930E−2	0.445149E+0
0.567919E−1	0.449306E−1	0.265976E−1	0.169955E−1	0.516463E−2	0.345096E−3	0.104955E−2	0.444919E+0
Ni $Z = 28$	L shell						
0.485949E−1	0.443910E−1	0.300775E−1	0.197465E−1	0.618850E−2	0.437575E−3	0.143333E−2	0.474602E+0
0.445463E−1	0.391740E−1	0.251361E−1	0.164228E−1	0.519197E−2	0.373148E−3	0.118283E−2	0.461477E+0
0.439755E−1	0.377177E−1	0.236553E−1	0.153882E−1	0.490166E−2	0.355667E−3	0.110818E−2	0.454592E+0
0.446330E−1	0.376172E−1	0.232719E−1	0.150965E−1	0.483685E−2	0.353763E−3	0.109595E−2	0.452299E+0
0.458952E−1	0.381587E−1	0.233768E−1	0.151953E−1	0.487417E−2	0.359276E−3	0.111095E−2	0.451552E+0
0.475103E−1	0.390047E−1	0.238112E−1	0.154748E−1	0.497775E−2	0.369013E−3	0.113066E−2	0.447890E+0
0.493494E−1	0.402496E−1	0.244305E−1	0.158772E−1	0.513641E−2	0.380670E−3	0.116204E−2	0.446401E+0
0.513320E−1	0.415902E−1	0.251552E−1	0.163529E−1	0.526920E−2	0.394231E−3	0.119790E−2	0.444556E+0
Cu $Z = 29$	L shell						
0.451473E−1	0.416014E−1	0.287709E−1	0.191635E−1	0.630541E−2	0.492032E−3	0.161273E−2	0.474856E+0
0.414727E−1	0.369031E−1	0.241115E−1	0.159791E−1	0.529140E−2	0.422832E−3	0.134249E−2	0.462122E+0
0.409744E−1	0.356198E−1	0.227133E−1	0.149525E−1	0.498904E−2	0.403015E−3	0.125831E−2	0.455422E+0
0.416098E−1	0.355814E−1	0.223634E−1	0.146828E−1	0.492849E−2	0.400321E−3	0.124383E−2	0.453475E+0
0.427795E−1	0.361265E−1	0.224726E−1	0.147630E−1	0.496364E−2	0.407706E−3	0.126454E−2	0.452768E+0
0.442806E−1	0.369446E−1	0.228853E−1	0.150379E−1	0.506765E−2	0.418665E−3	0.128615E−2	0.448936E+0
0.459945E−1	0.381473E−1	0.234828E−1	0.154307E−1	0.522612E−2	0.431936E−3	0.131867E−2	0.446442E+0
0.478414E−1	0.394324E−1	0.241796E−1	0.158936E−1	0.536337E−2	0.447569E−3	0.136294E−2	0.445427E+0
Zn $Z = 30$	L shell						
0.400958E−1	0.373754E−1	0.266763E−1	0.181990E−1	0.635660E−2	0.548850E−3	0.180066E−2	0.475232E+0
0.368785E−1	0.333266E−1	0.224671E−1	0.151983E−1	0.533603E−2	0.471379E−3	0.149773E−2	0.462418E+0
0.364399E−1	0.322452E−1	0.211917E−1	0.142424E−1	0.502946E−2	0.449765E−3	0.140734E−2	0.456294E+0
0.370002E−1	0.322654E−1	0.208819E−1	0.139936E−1	0.496552E−2	0.447132E−3	0.139194E−2	0.454239E+0
0.380341E−1	0.327946E−1	0.209852E−1	0.140668E−1	0.500597E−2	0.456374E−3	0.141723E−2	0.453258E+0
0.393624E−1	0.335957E−1	0.213834E−1	0.143284E−1	0.510781E−2	0.467739E−3	0.143815E−2	0.449281E+0
0.408806E−1	0.346751E−1	0.219420E−1	0.147025E−1	0.526403E−2	0.480627E−3	0.147024E−2	0.447236E+0
0.425167E−1	0.358566E−1	0.225978E−1	0.151503E−1	0.541597E−2	0.498257E−3	0.152026E−2	0.446209E+0
Ga $Z = 31$	L shell						
0.356905E−1	0.335816E−1	0.247047E−1	0.172413E−1	0.636675E−2	0.604982E−3	0.198546E−2	0.475363E+0
0.328609E−1	0.300987E−1	0.209102E−1	0.144640E−1	0.535533E−2	0.522219E−3	0.166060E−2	0.462740E+0
0.324761E−1	0.291973E−1	0.197581E−1	0.135437E−1	0.504177E−2	0.496963E−3	0.155631E−2	0.456622E+0
0.329747E−1	0.292584E−1	0.194859E−1	0.133115E−1	0.498060E−2	0.495198E−3	0.154450E−2	0.455000E+0
0.338959E−1	0.297636E−1	0.196040E−1	0.133845E−1	0.502058E−2	0.505669E−3	0.157124E−2	0.453496E+0
0.350758E−1	0.305688E−1	0.199697E−1	0.136328E−1	0.512118E−2	0.518489E−3	0.159738E−2	0.450081E+0
0.364202E−1	0.315196E−1	0.204990E−1	0.139892E−1	0.527588E−2	0.534566E−3	0.163480E−2	0.447128E+0
0.378803E−1	0.326118E−1	0.211183E−1	0.144246E−1	0.543144E−2	0.553145E−3	0.168780E−2	0.446225E+0
Ge $Z = 32$	L shell						
0.319296E−1	0.302841E−1	0.228976E−1	0.163264E−1	0.635005E−2	0.662836E−3	0.217434E−2	0.475181E+0
0.294328E−1	0.272658E−1	0.194878E−1	0.137326E−1	0.534490E−2	0.573271E−3	0.182383E−2	0.462934E+0
0.291007E−1	0.265131E−1	0.184405E−1	0.128767E−1	0.503379E−2	0.547161E−3	0.171509E−2	0.456991E+0
0.295459E−1	0.266060E−1	0.182029E−1	0.126574E−1	0.496941E−2	0.544911E−3	0.170157E−2	0.455473E+0
0.303710E−1	0.270998E−1	0.183357E−1	0.127342E−1	0.501196E−2	0.557725E−3	0.173357E−2	0.453628E+0
0.314246E−1	0.278491E−1	0.186784E−1	0.129740E−1	0.511433E−2	0.570551E−3	0.175791E−2	0.450111E+0
0.326270E−1	0.287338E−1	0.191783E−1	0.133131E−1	0.526223E−2	0.588383E−3	0.180065E−2	0.447409E+0
0.339217E−1	0.297363E−1	0.197545E−1	0.137206E−1	0.541933E−2	0.608561E−3	0.185703E−2	0.446255E+0
As $Z = 33$	L shell						
0.286995E−1	0.274029E−1	0.212413E−1	0.154552E−1	0.630612E−2	0.721029E−3	0.236367E−2	0.474917E+0
0.264930E−1	0.247824E−1	0.181809E−1	0.130312E−1	0.531633E−2	0.625666E−3	0.198983E−2	0.462795E+0
0.261994E−1	0.241438E−1	0.172343E−1	0.122413E−1	0.500835E−2	0.597691E−3	0.187410E−2	0.457124E+0
0.266044E−1	0.242633E−1	0.170303E−1	0.120464E−1	0.494602E−2	0.595682E−3	0.186044E−2	0.455544E+0
0.273494E−1	0.247387E−1	0.171671E−1	0.121205E−1	0.498699E−2	0.607791E−3	0.188876E−2	0.453537E+0
0.282962E−1	0.254425E−1	0.174953E−1	0.123500E−1	0.508787E−2	0.623482E−3	0.192324E−2	0.450580E+0
0.293781E−1	0.262691E−1	0.179707E−1	0.126765E−1	0.523704E−2	0.642537E−3	0.196351E−2	0.446827E+0
0.305452E−1	0.271939E−1	0.185149E−1	0.130674E−1	0.539283E−2	0.664754E−3	0.202810E−2	0.446174E+0

Table 2 (continued)

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Se $Z = 34$	L shell						
0.259046E−1	0.248709E−1	0.197230E−1	0.146271E−1	0.623952E−2	0.780253E−3	0.255497E−2	0.474472E+0
0.239487E−1	0.225807E−1	0.169769E−1	0.123695E−1	0.527004E−2	0.678396E−3	0.215672E−2	0.462645E+0
0.236943E−1	0.220451E−1	0.161219E−1	0.116437E−1	0.496538E−2	0.648950E−3	0.203520E−2	0.457198E+0
0.240624E−1	0.221884E−1	0.159535E−1	0.114662E−1	0.490532E−2	0.646641E−3	0.201946E−2	0.455518E+0
0.247408E−1	0.226466E−1	0.160960E−1	0.115429E−1	0.494537E−2	0.659446E−3	0.204747E−2	0.453185E+0
0.255947E−1	0.233016E−1	0.164104E−1	0.117616E−1	0.504534E−2	0.676499E−3	0.208542E−2	0.450319E+0
0.265716E−1	0.240772E−1	0.168605E−1	0.120707E−1	0.518930E−2	0.697538E−3	0.213363E−2	0.447208E+0
0.276246E−1	0.249298E−1	0.173738E−1	0.124448E−1	0.534092E−2	0.720610E−3	0.219242E−2	0.445064E+0
Br $Z = 35$	L shell						
0.234712E−1	0.226452E−1	0.183305E−1	0.138406E−1	0.615553E−2	0.838403E−3	0.274085E−2	0.473810E+0
0.217315E−1	0.206370E−1	0.158673E−1	0.117432E−1	0.520505E−2	0.730221E−3	0.231843E−2	0.462120E+0
0.215129E−1	0.201943E−1	0.151081E−1	0.110807E−1	0.491576E−2	0.699962E−3	0.219402E−2	0.456986E+0
0.218550E−1	0.203447E−1	0.149658E−1	0.109202E−1	0.485285E−2	0.696905E−3	0.217518E−2	0.455286E+0
0.224716E−1	0.207784E−1	0.151074E−1	0.109919E−1	0.489370E−2	0.710267E−3	0.220322E−2	0.452814E+0
0.232515E−1	0.213991E−1	0.154156E−1	0.112051E−1	0.499328E−2	0.729029E−3	0.224024E−2	0.449051E+0
0.241380E−1	0.221159E−1	0.158345E−1	0.114955E−1	0.513579E−2	0.751745E−3	0.229570E−2	0.446557E+0
0.250943E−1	0.229152E−1	0.163268E−1	0.118610E−1	0.528324E−2	0.777066E−3	0.235945E−2	0.444264E+0
Kr $Z = 36$	L shell						
0.213446E−1	0.206768E−1	0.170484E−1	0.130945E−1	0.605496E−2	0.895494E−3	0.292462E−2	0.473417E+0
0.198030E−1	0.189145E−1	0.148472E−1	0.111570E−1	0.513426E−2	0.782213E−3	0.247835E−2	0.461289E+0
0.196079E−1	0.185440E−1	0.141696E−1	0.105483E−1	0.484976E−2	0.749807E−3	0.234804E−2	0.456608E+0
0.199258E−1	0.186994E−1	0.140518E−1	0.104004E−1	0.478631E−2	0.746183E−3	0.232611E−2	0.454793E+0
0.204933E−1	0.191166E−1	0.141977E−1	0.104748E−1	0.482949E−2	0.761428E−3	0.235896E−2	0.452312E+0
0.212032E−1	0.196972E−1	0.144945E−1	0.106792E−1	0.492575E−2	0.780167E−3	0.239567E−2	0.448765E+0
0.220145E−1	0.203711E−1	0.148963E−1	0.109604E−1	0.506926E−2	0.804970E−3	0.245181E−2	0.445511E+0
0.228852E−1	0.211086E−1	0.153613E−1	0.113075E−1	0.521444E−2	0.832178E−3	0.252420E−2	0.443853E+0
Rb $Z = 37$	L shell						
0.193389E−1	0.187989E−1	0.157799E−1	0.123320E−1	0.592536E−2	0.947998E−3	0.308739E−2	0.472291E+0
0.179649E−1	0.172563E−1	0.138258E−1	0.105551E−1	0.503657E−2	0.831384E−3	0.262964E−2	0.460605E+0
0.178034E−1	0.169443E−1	0.132292E−1	0.100013E−1	0.476411E−2	0.796172E−3	0.248924E−2	0.455967E+0
0.180911E−1	0.171060E−1	0.131358E−1	0.986616E−2	0.470085E−2	0.793092E−3	0.246966E−2	0.454359E+0
0.186068E−1	0.175020E−1	0.132815E−1	0.993978E−2	0.474308E−2	0.807675E−3	0.249780E−2	0.451602E+0
0.192551E−1	0.180408E−1	0.135687E−1	0.101393E−1	0.484166E−2	0.829156E−3	0.254167E−2	0.448067E+0
0.199930E−1	0.186667E−1	0.139509E−1	0.104119E−1	0.498516E−2	0.855474E−3	0.260302E−2	0.445109E+0
0.207874E−1	0.193542E−1	0.143936E−1	0.107399E−1	0.512537E−2	0.884733E−3	0.267564E−2	0.442663E+0
Sr $Z = 38$	L shell						
0.175641E−1	0.171284E−1	0.146109E−1	0.116033E−1	0.578674E−2	0.998682E−3	0.324336E−2	0.471172E+0
0.163527E−1	0.157786E−1	0.128834E−1	0.998808E−2	0.493393E−2	0.876804E−3	0.276509E−2	0.459418E+0
0.162062E−1	0.155156E−1	0.123549E−1	0.947716E−2	0.466802E−2	0.841885E−3	0.262834E−2	0.455385E+0
0.164713E−1	0.156744E−1	0.122799E−1	0.935512E−2	0.460975E−2	0.838948E−3	0.260716E−2	0.453547E+0
0.169459E−1	0.160588E−1	0.124361E−1	0.943662E−2	0.465309E−2	0.854555E−3	0.263650E−2	0.450652E+0
0.175396E−1	0.165586E−1	0.127125E−1	0.962894E−2	0.474793E−2	0.876834E−3	0.267868E−2	0.446704E+0
0.182121E−1	0.171417E−1	0.130783E−1	0.989257E−2	0.488832E−2	0.903934E−3	0.273768E−2	0.443244E+0
0.189362E−1	0.177731E−1	0.134912E−1	0.102036E−1	0.502946E−2	0.934725E−3	0.281917E−2	0.441578E+0
Y $Z = 39$	L shell						
0.160680E−1	0.157106E−1	0.135870E−1	0.109512E−1	0.564747E−2	0.104614E−2	0.338530E−2	0.469734E+0
0.149954E−1	0.145241E−1	0.120565E−1	0.947729E−2	0.482969E−2	0.921968E−3	0.290059E−2	0.458463E+0
0.148733E−1	0.143030E−1	0.115911E−1	0.901177E−2	0.457385E−2	0.885313E−3	0.275748E−2	0.454452E+0
0.151242E−1	0.144647E−1	0.115381E−1	0.890615E−2	0.451876E−2	0.882860E−3	0.273814E−2	0.452747E+0
0.155586E−1	0.148326E−1	0.116957E−1	0.898721E−2	0.456101E−2	0.898479E−3	0.276400E−2	0.449492E+0
0.161062E−1	0.153009E−1	0.119633E−1	0.917533E−2	0.465587E−2	0.922103E−3	0.280946E−2	0.445637E+0
0.167248E−1	0.158472E−1	0.123142E−1	0.942633E−2	0.479347E−2	0.950689E−3	0.286822E−2	0.441704E+0
0.173895E−1	0.164343E−1	0.127069E−1	0.972642E−2	0.493396E−2	0.983285E−3	0.295331E−2	0.439914E+0
Zr $Z = 40$	L shell						
0.147453E−1	0.144473E−1	0.126522E−1	0.103373E−1	0.549824E−2	0.108958E−2	0.351606E−2	0.468620E+0
0.137887E−1	0.133981E−1	0.112889E−1	0.898870E−2	0.471815E−2	0.962074E−3	0.301640E−2	0.457091E+0
0.136825E−1	0.132120E−1	0.108794E−1	0.856406E−2	0.447146E−2	0.923811E−3	0.286952E−2	0.453357E+0
0.139169E−1	0.133733E−1	0.108450E−1	0.847466E−2	0.442152E−2	0.921085E−3	0.284970E−2	0.451767E+0
0.143186E−1	0.137189E−1	0.110010E−1	0.855473E−2	0.446201E−2	0.936774E−3	0.287258E−2	0.448210E+0
0.148248E−1	0.141600E−1	0.112626E−1	0.873892E−2	0.455476E−2	0.962411E−3	0.292030E−2	0.444000E+0
0.153916E−1	0.146682E−1	0.115962E−1	0.898077E−2	0.468841E−2	0.991732E−3	0.298104E−2	0.440231E+0
0.160066E−1	0.152219E−1	0.119762E−1	0.927207E−2	0.482939E−2	0.102570E−2	0.307091E−2	0.438641E+0

Table 2 (continued)

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Nb $Z = 41$	L shell						
0.136296E−1	0.133804E−1	0.118449E−1	0.979722E−2	0.536247E−2	0.113284E−2	0.364018E−2	0.466924E+0
0.127813E−1	0.124532E−1	0.106326E−1	0.856922E−2	0.461827E−2	0.100333E−2	0.313443E−2	0.455648E+0
0.126948E−1	0.123002E−1	0.102735E−1	0.817989E−2	0.438324E−2	0.964923E−3	0.298759E−2	0.452070E+0
0.129187E−1	0.124643E−1	0.102588E−1	0.810662E−2	0.433650E−2	0.962168E−3	0.296863E−2	0.450667E+0
0.132964E−1	0.127921E−1	0.104132E−1	0.818690E−2	0.437591E−2	0.979131E−3	0.299282E−2	0.446923E+0
0.137693E−1	0.132141E−1	0.106712E−1	0.836750E−2	0.446948E−2	0.100549E−2	0.303999E−2	0.442550E+0
0.143009E−1	0.136907E−1	0.109903E−1	0.860033E−2	0.460297E−2	0.103637E−2	0.310587E−2	0.439027E+0
0.148723E−1	0.142137E−1	0.113559E−1	0.888262E−2	0.473992E−2	0.107202E−2	0.319510E−2	0.436832E+0
Mo $Z = 42$	L shell						
0.125751E−1	0.123671E−1	0.110581E−1	0.925528E−2	0.520829E−2	0.116992E−2	0.374373E−2	0.465258E+0
0.118244E−1	0.115494E−1	0.998430E−2	0.814444E−2	0.450527E−2	0.103970E−2	0.323562E−2	0.454117E+0
0.117556E−1	0.114219E−1	0.967081E−2	0.779030E−2	0.428097E−2	0.100056E−2	0.308667E−2	0.450614E+0
0.119665E−1	0.115861E−1	0.967195E−2	0.772928E−2	0.423802E−2	0.997948E−3	0.306944E−2	0.449420E+0
0.123195E−1	0.118980E−1	0.982855E−2	0.781207E−2	0.427811E−2	0.101604E−2	0.309532E−2	0.445590E+0
0.127583E−1	0.122973E−1	0.100779E−1	0.798691E−2	0.436960E−2	0.104268E−2	0.314189E−2	0.441212E+0
0.132528E−1	0.127457E−1	0.103871E−1	0.821576E−2	0.449906E−2	0.107526E−2	0.321002E−2	0.437486E+0
0.137860E−1	0.132359E−1	0.107356E−1	0.848308E−2	0.463690E−2	0.111070E−2	0.329516E−2	0.434987E+0
Tc $Z = 43$	L shell						
0.115798E−1	0.114055E−1	0.102933E−1	0.871766E−2	0.504520E−2	0.120217E−2	0.383081E−2	0.463579E+0
0.109192E−1	0.106914E−1	0.935130E−2	0.771787E−2	0.438268E−2	0.107188E−2	0.332155E−2	0.452408E+0
0.108642E−1	0.105843E−1	0.907737E−2	0.739636E−2	0.417104E−2	0.103284E−2	0.317674E−2	0.449418E+0
0.110638E−1	0.107458E−1	0.909386E−2	0.734975E−2	0.413109E−2	0.103037E−2	0.315943E−2	0.448187E+0
0.113922E−1	0.110384E−1	0.924675E−2	0.743138E−2	0.417027E−2	0.104943E−2	0.318657E−2	0.444278E+0
0.118035E−1	0.114183E−1	0.949091E−2	0.760525E−2	0.426261E−2	0.107604E−2	0.322982E−2	0.439654E+0
0.122631E−1	0.118381E−1	0.978802E−2	0.782501E−2	0.438808E−2	0.111056E−2	0.330254E−2	0.435931E+0
0.127558E−1	0.122962E−1	0.101211E−1	0.808286E−2	0.452329E−2	0.114677E−2	0.338587E−2	0.433065E+0
Ru $Z = 44$	L shell						
0.107787E−1	0.106307E−1	0.966910E−2	0.826748E−2	0.490240E−2	0.123114E−2	0.390277E−2	0.461497E+0
0.101938E−1	0.999838E−2	0.883274E−2	0.736289E−2	0.427597E−2	0.110268E−2	0.340223E−2	0.450675E+0
0.101527E−1	0.991359E−2	0.859576E−2	0.707387E−2	0.407553E−2	0.106164E−2	0.325137E−2	0.447706E+0
0.103450E−1	0.100729E−1	0.862168E−2	0.703854E−2	0.403818E−2	0.106038E−2	0.324062E−2	0.446854E+0
0.106557E−1	0.103551E−1	0.877969E−2	0.712475E−2	0.408179E−2	0.107978E−2	0.326634E−2	0.442765E+0
0.110408E−1	0.107088E−1	0.901198E−2	0.729002E−2	0.417031E−2	0.110764E−2	0.331162E−2	0.438084E+0
0.114724E−1	0.111119E−1	0.930188E−2	0.750637E−2	0.429287E−2	0.114332E−2	0.338717E−2	0.434423E+0
0.119357E−1	0.115433E−1	0.962200E−2	0.775305E−2	0.442679E−2	0.118091E−2	0.347416E−2	0.431626E+0
Rh $Z = 45$	L shell						
0.100062E−1	0.987909E−2	0.905153E−2	0.781515E−2	0.474655E−2	0.125659E−2	0.396724E−2	0.459869E+0
0.949446E−2	0.932664E−2	0.831735E−2	0.700465E−2	0.416172E−2	0.112884E−2	0.346734E−2	0.448879E+0
0.946368E−2	0.926245E−2	0.811583E−2	0.674575E−2	0.397073E−2	0.108772E−2	0.331499E−2	0.445748E+0
0.964869E−2	0.941731E−2	0.815218E−2	0.672081E−2	0.393821E−2	0.108750E−2	0.331336E−2	0.445634E+0
0.994229E−2	0.968854E−2	0.830971E−2	0.681031E−2	0.398174E−2	0.110690E−2	0.333601E−2	0.441284E+0
0.103037E−1	0.100215E−1	0.853443E−2	0.696989E−2	0.406902E−2	0.113595E−2	0.338256E−2	0.436464E+0
0.107080E−1	0.104010E−1	0.881238E−2	0.717890E−2	0.419100E−2	0.117220E−2	0.345777E−2	0.432697E+0
0.111411E−1	0.108083E−1	0.911921E−2	0.741669E−2	0.432067E−2	0.121088E−2	0.354501E−2	0.429677E+0
Pd $Z = 46$	L shell						
0.935253E−2	0.924505E−2	0.852401E−2	0.742191E−2	0.460240E−2	0.127738E−2	0.401158E−2	0.457748E+0
0.890517E−2	0.875918E−2	0.787557E−2	0.669345E−2	0.405535E−2	0.115146E−2	0.351899E−2	0.446857E+0
0.888558E−2	0.871059E−2	0.770239E−2	0.646096E−2	0.387411E−2	0.111100E−2	0.336924E−2	0.443769E+0
0.906335E−2	0.886450E−2	0.774987E−2	0.644704E−2	0.384775E−2	0.111097E−2	0.337060E−2	0.443943E+0
0.934150E−2	0.912010E−2	0.790483E−2	0.653715E−2	0.389238E−2	0.113134E−2	0.339632E−2	0.439717E+0
0.968220E−2	0.944028E−2	0.812539E−2	0.669419E−2	0.397964E−2	0.116148E−2	0.344469E−2	0.434856E+0
0.100646E−1	0.980017E−2	0.839195E−2	0.689590E−2	0.409795E−2	0.119798E−2	0.351999E−2	0.431129E+0
0.104735E−1	0.101868E−1	0.868960E−2	0.712721E−2	0.422507E−2	0.123869E−2	0.361261E−2	0.428149E+0
Ag $Z = 47$	L shell						
0.867163E−2	0.857980E−2	0.796030E−2	0.699362E−2	0.443891E−2	0.129457E−2	0.404512E−2	0.455734E+0
0.828738E−2	0.816323E−2	0.740064E−2	0.634911E−2	0.393218E−2	0.117154E−2	0.356210E−2	0.444812E+0
0.827842E−2	0.812843E−2	0.725588E−2	0.614514E−2	0.376339E−2	0.113130E−2	0.341331E−2	0.441726E+0
0.844780E−2	0.827809E−2	0.730873E−2	0.613826E−2	0.374011E−2	0.113164E−2	0.341638E−2	0.441964E+0
0.871096E−2	0.852214E−2	0.746288E−2	0.623174E−2	0.378640E−2	0.115224E−2	0.344699E−2	0.438316E+0
0.903186E−2	0.882496E−2	0.767758E−2	0.638515E−2	0.387198E−2	0.118411E−2	0.349847E−2	0.433332E+0
0.938922E−2	0.916537E−2	0.793437E−2	0.657940E−2	0.398802E−2	0.122166E−2	0.357708E−2	0.429733E+0
0.977176E−2	0.952750E−2	0.821695E−2	0.680132E−2	0.411268E−2	0.126296E−2	0.366913E−2	0.426599E+0

Table 2 (continued)

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Cd $Z = 48$	L shell						
0.805432E−2	0.797587E−2	0.744195E−2	0.659124E−2	0.427523E−2	0.130720E−2	0.406286E−2	0.453600E+0
0.772507E−2	0.762021E−2	0.695931E−2	0.602417E−2	0.380908E−2	0.118804E−2	0.359379E−2	0.442762E+0
0.772704E−2	0.759938E−2	0.684020E−2	0.584582E−2	0.365209E−2	0.114872E−2	0.344705E−2	0.439550E+0
0.788952E−2	0.774415E−2	0.689866E−2	0.584665E−2	0.363215E−2	0.114965E−2	0.345337E−2	0.439958E+0
0.813684E−2	0.797686E−2	0.705279E−2	0.594232E−2	0.367960E−2	0.117075E−2	0.348987E−2	0.436888E+0
0.844023E−2	0.826501E−2	0.726268E−2	0.609482E−2	0.376499E−2	0.120318E−2	0.354045E−2	0.431716E+0
0.877435E−2	0.858510E−2	0.750671E−2	0.628140E−2	0.387763E−2	0.124188E−2	0.362382E−2	0.428360E+0
0.913446E−2	0.892531E−2	0.777711E−2	0.649479E−2	0.400016E−2	0.128380E−2	0.371546E−2	0.425072E+0
In $Z = 49$	L shell						
0.748555E−2	0.741879E−2	0.695735E−2	0.620874E−2	0.411108E−2	0.131630E−2	0.406749E−2	0.451280E+0
0.720946E−2	0.711782E−2	0.654445E−2	0.571343E−2	0.368603E−2	0.120096E−2	0.361425E−2	0.440704E+0
0.721834E−2	0.710927E−2	0.644922E−2	0.555877E−2	0.354064E−2	0.116294E−2	0.347168E−2	0.437477E+0
0.737382E−2	0.724824E−2	0.651270E−2	0.556834E−2	0.352400E−2	0.116396E−2	0.347940E−2	0.438012E+0
0.760959E−2	0.747142E−2	0.666470E−2	0.566502E−2	0.357268E−2	0.118620E−2	0.352396E−2	0.435532E+0
0.789441E−2	0.774430E−2	0.686806E−2	0.581409E−2	0.365664E−2	0.121915E−2	0.357632E−2	0.430472E+0
0.820940E−2	0.804625E−2	0.710214E−2	0.599533E−2	0.376902E−2	0.125846E−2	0.365695E−2	0.426695E+0
0.854635E−2	0.836798E−2	0.736142E−2	0.619978E−2	0.388764E−2	0.130107E−2	0.375026E−2	0.423457E+0
Sn $Z = 50$	L shell						
0.697136E−2	0.691247E−2	0.651219E−2	0.585259E−2	0.395098E−2	0.132170E−2	0.406221E−2	0.449123E+0
0.674044E−2	0.666310E−2	0.616506E−2	0.542536E−2	0.356498E−2	0.121075E−2	0.362407E−2	0.438542E+0
0.675752E−2	0.666072E−2	0.608545E−2	0.528959E−2	0.343103E−2	0.117351E−2	0.348517E−2	0.435406E+0
0.690757E−2	0.679887E−2	0.615772E−2	0.530891E−2	0.342091E−2	0.117575E−2	0.349563E−2	0.435844E+0
0.713014E−2	0.701188E−2	0.630628E−2	0.540530E−2	0.346816E−2	0.119789E−2	0.354690E−2	0.434205E+0
0.739919E−2	0.726991E−2	0.650277E−2	0.555051E−2	0.355214E−2	0.123201E−2	0.360116E−2	0.429044E+0
0.769662E−2	0.755617E−2	0.672924E−2	0.572737E−2	0.366097E−2	0.127196E−2	0.368209E−2	0.425168E+0
0.801277E−2	0.786074E−2	0.697664E−2	0.592491E−2	0.377788E−2	0.131540E−2	0.377490E−2	0.421693E+0
Sb $Z = 51$	L shell						
0.650138E−2	0.644970E−2	0.610190E−2	0.552029E−2	0.379597E−2	0.132245E−2	0.404103E−2	0.446804E+0
0.631278E−2	0.624652E−2	0.581269E−2	0.515334E−2	0.344729E−2	0.121686E−2	0.362218E−2	0.436322E+0
0.633865E−2	0.625417E−2	0.575142E−2	0.503874E−2	0.332591E−2	0.118060E−2	0.348671E−2	0.433176E+0
0.648113E−2	0.638774E−2	0.582503E−2	0.506144E−2	0.331796E−2	0.118501E−2	0.350520E−2	0.433798E+0
0.669442E−2	0.659106E−2	0.597227E−2	0.515987E−2	0.336670E−2	0.120708E−2	0.356143E−2	0.432782E+0
0.694878E−2	0.683588E−2	0.616284E−2	0.530355E−2	0.345014E−2	0.124176E−2	0.361935E−2	0.427905E+0
0.722921E−2	0.710876E−2	0.638248E−2	0.547592E−2	0.355851E−2	0.128165E−2	0.369765E−2	0.423819E+0
0.752832E−2	0.739593E−2	0.661837E−2	0.566430E−2	0.367101E−2	0.132620E−2	0.379195E−2	0.420224E+0
Te $Z = 52$	L shell						
0.606816E−2	0.602403E−2	0.572078E−2	0.520592E−2	0.364232E−2	0.131923E−2	0.400843E−2	0.444541E+0
0.591996E−2	0.586018E−2	0.548090E−2	0.489301E−2	0.333011E−2	0.122079E−2	0.361394E−2	0.434122E+0
0.595087E−2	0.587740E−2	0.543723E−2	0.479733E−2	0.322002E−2	0.118535E−2	0.348161E−2	0.430984E+0
0.609247E−2	0.600976E−2	0.551607E−2	0.482949E−2	0.321651E−2	0.119053E−2	0.350037E−2	0.431389E+0
0.629501E−2	0.620562E−2	0.566226E−2	0.492950E−2	0.326796E−2	0.121373E−2	0.356024E−2	0.430453E+0
0.653546E−2	0.643739E−2	0.584620E−2	0.506889E−2	0.334931E−2	0.124856E−2	0.362754E−2	0.426624E+0
0.680115E−2	0.669600E−2	0.605703E−2	0.523639E−2	0.345603E−2	0.128921E−2	0.370591E−2	0.422361E+0
0.708375E−2	0.697071E−2	0.628573E−2	0.542151E−2	0.356767E−2	0.133422E−2	0.380141E−2	0.418810E+0
I $Z = 53$	L shell						
0.567342E−2	0.563469E−2	0.536946E−2	0.491368E−2	0.349480E−2	0.131291E−2	0.396667E−2	0.442272E+0
0.556060E−2	0.550924E−2	0.517667E−2	0.465248E−2	0.321846E−2	0.122191E−2	0.359708E−2	0.431881E+0
0.559784E−2	0.553236E−2	0.514603E−2	0.457269E−2	0.311896E−2	0.118816E−2	0.347047E−2	0.428754E+0
0.573222E−2	0.565985E−2	0.522598E−2	0.460886E−2	0.311741E−2	0.119421E−2	0.349151E−2	0.429139E+0
0.592759E−2	0.584874E−2	0.537055E−2	0.470960E−2	0.316979E−2	0.121715E−2	0.355086E−2	0.428271E+0
0.615394E−2	0.606825E−2	0.554781E−2	0.484501E−2	0.325038E−2	0.125255E−2	0.362753E−2	0.425350E+0
0.640724E−2	0.631395E−2	0.575105E−2	0.500768E−2	0.335613E−2	0.129413E−2	0.370423E−2	0.420653E+0
0.667274E−2	0.657495E−2	0.597090E−2	0.518778E−2	0.346529E−2	0.133943E−2	0.378889E−2	0.415932E+0
Xe $Z = 54$	L shell						
0.530988E−2	0.527639E−2	0.504383E−2	0.463955E−2	0.335154E−2	0.130382E−2	0.391683E−2	0.439994E+0
0.522988E−2	0.518591E−2	0.489324E−2	0.442451E−2	0.310936E−2	0.122009E−2	0.357093E−2	0.429559E+0
0.527108E−2	0.521568E−2	0.487592E−2	0.436108E−2	0.302050E−2	0.118892E−2	0.345394E−2	0.426589E+0
0.540355E−2	0.534274E−2	0.496057E−2	0.440329E−2	0.302461E−2	0.119438E−2	0.347108E−2	0.426734E+0
0.558935E−2	0.552103E−2	0.509939E−2	0.450230E−2	0.307575E−2	0.121941E−2	0.353897E−2	0.426187E+0
0.580525E−2	0.573023E−2	0.527045E−2	0.463507E−2	0.315568E−2	0.125500E−2	0.361237E−2	0.422890E+0
0.604410E−2	0.596305E−2	0.546604E−2	0.479256E−2	0.325879E−2	0.129677E−2	0.368651E−2	0.417922E+0
0.629539E−2	0.620834E−2	0.567468E−2	0.496470E−2	0.336421E−2	0.134280E−2	0.377216E−2	0.413158E+0

Table 2 (continued)

s (Å^{-1})							
0.0	0.125	0.375	0.625	1.25	2.5	a	b
Cs $Z = 55$	L shell						
0.494777E−2	0.491861E−2	0.471557E−2	0.435808E−2	0.319745E−2	0.128968E−2	0.385177E−2	0.437656E+0
0.490456E−2	0.486408E−2	0.460770E−2	0.419009E−2	0.299082E−2	0.121439E−2	0.353412E−2	0.427288E+0
0.494925E−2	0.489966E−2	0.460178E−2	0.414127E−2	0.291263E−2	0.118515E−2	0.342369E−2	0.424341E+0
0.507898E−2	0.502320E−2	0.468754E−2	0.418829E−2	0.291927E−2	0.119242E−2	0.344421E−2	0.424283E+0
0.525428E−2	0.519362E−2	0.482292E−2	0.428655E−2	0.297077E−2	0.121631E−2	0.350826E−2	0.423721E+0
0.546081E−2	0.539395E−2	0.498993E−2	0.441807E−2	0.305196E−2	0.125283E−2	0.358577E−2	0.420627E+0
0.568657E−2	0.561394E−2	0.517638E−2	0.456936E−2	0.315092E−2	0.129401E−2	0.365484E−2	0.415324E+0
0.592435E−2	0.584891E−2	0.537896E−2	0.473759E−2	0.325646E−2	0.134065E−2	0.374059E−2	0.410435E+0
Ba $Z = 56$	L shell						
0.462522E−2	0.459935E−2	0.442139E−2	0.410534E−2	0.305567E−2	0.127402E−2	0.378356E−2	0.435394E+0
0.460886E−2	0.457472E−2	0.434991E−2	0.397710E−2	0.288082E−2	0.120658E−2	0.349096E−2	0.424955E+0
0.466345E−2	0.461789E−2	0.435591E−2	0.394374E−2	0.281360E−2	0.118061E−2	0.339120E−2	0.422060E+0
0.478600E−2	0.473577E−2	0.444029E−2	0.399213E−2	0.282274E−2	0.118744E−2	0.340924E−2	0.421875E+0
0.495473E−2	0.489973E−2	0.457317E−2	0.409083E−2	0.287612E−2	0.121344E−2	0.347887E−2	0.421299E+0
0.515156E−2	0.509245E−2	0.473644E−2	0.422020E−2	0.295672E−2	0.124982E−2	0.355463E−2	0.418102E+0
0.536587E−2	0.530187E−2	0.491650E−2	0.436832E−2	0.305460E−2	0.129149E−2	0.362500E−2	0.412823E+0
0.559185E−2	0.552454E−2	0.511005E−2	0.452983E−2	0.315703E−2	0.133849E−2	0.371064E−2	0.407865E+0
La $Z = 57$	L shell						
0.433539E−2	0.431175E−2	0.415486E−2	0.387425E−2	0.292255E−2	0.125675E−2	0.371134E−2	0.433147E+0
0.434734E−2	0.431536E−2	0.411686E−2	0.378369E−2	0.277906E−2	0.119876E−2	0.344927E−2	0.422749E+0
0.440332E−2	0.436099E−2	0.413177E−2	0.376091E−2	0.272084E−2	0.117497E−2	0.335691E−2	0.419912E+0
0.452429E−2	0.447909E−2	0.421774E−2	0.381390E−2	0.273327E−2	0.118368E−2	0.337934E−2	0.419620E+0
0.468173E−2	0.463748E−2	0.434831E−2	0.391166E−2	0.278798E−2	0.120841E−2	0.344320E−2	0.418838E+0
0.487132E−2	0.481958E−2	0.450377E−2	0.403701E−2	0.286624E−2	0.124539E−2	0.351979E−2	0.415582E+0
0.507503E−2	0.501834E−2	0.467733E−2	0.418105E−2	0.296235E−2	0.128722E−2	0.358958E−2	0.410221E+0
0.528996E−2	0.523024E−2	0.486320E−2	0.433758E−2	0.306320E−2	0.133373E−2	0.367384E−2	0.405304E+0
Ce $Z = 58$	L shell						
0.409313E−2	0.407233E−2	0.393255E−2	0.367981E−2	0.280885E−2	0.124125E−2	0.364596E−2	0.431000E+0
0.413006E−2	0.410158E−2	0.392406E−2	0.362212E−2	0.269393E−2	0.119253E−2	0.341396E−2	0.420718E+0
0.418931E−2	0.415129E−2	0.394394E−2	0.360781E−2	0.264155E−2	0.117061E−2	0.332716E−2	0.417839E+0
0.430895E−2	0.427019E−2	0.403586E−2	0.366791E−2	0.266113E−2	0.118110E−2	0.335481E−2	0.417579E+0
0.446419E−2	0.442000E−2	0.416037E−2	0.376270E−2	0.271368E−2	0.120592E−2	0.341622E−2	0.416518E+0
0.464378E−2	0.459723E−2	0.431330E−2	0.388697E−2	0.279197E−2	0.124332E−2	0.349152E−2	0.413023E+0
0.483938E−2	0.478909E−2	0.448293E−2	0.402855E−2	0.288794E−2	0.128603E−2	0.356612E−2	0.407966E+0
0.504606E−2	0.499179E−2	0.466216E−2	0.418106E−2	0.298694E−2	0.133210E−2	0.364567E−2	0.402712E+0
Pr $Z = 59$	L shell						
0.385800E−2	0.383934E−2	0.371459E−2	0.348771E−2	0.269304E−2	0.122167E−2	0.357172E−2	0.429131E+0
0.391618E−2	0.389245E−2	0.373352E−2	0.346065E−2	0.260290E−2	0.118115E−2	0.336543E−2	0.418825E+0
0.398056E−2	0.394685E−2	0.376084E−2	0.345554E−2	0.255937E−2	0.116184E−2	0.328775E−2	0.416081E+0
0.409747E−2	0.405984E−2	0.385030E−2	0.351575E−2	0.258024E−2	0.117230E−2	0.331463E−2	0.415752E+0
0.424738E−2	0.420729E−2	0.397520E−2	0.361325E−2	0.263581E−2	0.119849E−2	0.337735E−2	0.414410E+0
0.441894E−2	0.437670E−2	0.412313E−2	0.373450E−2	0.271274E−2	0.123589E−2	0.345207E−2	0.410874E+0
0.460620E−2	0.456125E−2	0.428677E−2	0.387274E−2	0.280786E−2	0.127814E−2	0.352474E−2	0.405762E+0
0.480228E−2	0.475469E−2	0.445959E−2	0.402010E−2	0.290376E−2	0.132461E−2	0.360577E−2	0.400566E+0
Nd $Z = 60$	L shell						
0.363591E−2	0.361925E−2	0.350792E−2	0.330431E−2	0.257986E−2	0.120147E−2	0.349456E−2	0.427065E+0
0.371527E−2	0.369322E−2	0.355094E−2	0.330452E−2	0.251537E−2	0.117057E−2	0.331956E−2	0.416938E+0
0.378464E−2	0.375205E−2	0.358637E−2	0.330989E−2	0.248074E−2	0.115361E−2	0.324815E−2	0.414076E+0
0.389729E−2	0.386674E−2	0.367923E−2	0.337563E−2	0.250403E−2	0.116493E−2	0.327604E−2	0.413590E+0
0.404221E−2	0.400774E−2	0.379991E−2	0.347094E−2	0.256167E−2	0.119226E−2	0.334119E−2	0.412189E+0
0.420728E−2	0.417077E−2	0.394352E−2	0.358969E−2	0.263808E−2	0.122952E−2	0.341339E−2	0.408432E+0
0.438677E−2	0.434689E−2	0.410094E−2	0.372323E−2	0.272988E−2	0.127220E−2	0.348822E−2	0.403459E+0
0.457472E−2	0.453185E−2	0.426741E−2	0.386620E−2	0.282389E−2	0.131834E−2	0.356742E−2	0.398188E+0

assumed to be of the form given by equation (12)] for the tabulated form factors in the range $0 \leq s \leq 2.5$ Å^{-1}. Atomic numbers Z and the threshold energies E_t found using Cowan's program *RCN* (Cowan, 1981) when calculating the form factors in Tables 1 and 2 are also shown in Tables 3 and 4. The parameters c in equation (12) are plotted as a function of threshold energy E_t in Fig. 3 for both K and L shells and for incident energies of 50 and 400 keV. It is clear by comparison with Fig. 1 in Oxley & Allen (1999) that root-mean-square impact parameters do not provide an immediate estimate of the HWHM of the one-dimensional atomic ionization potential.

Atomic scattering factors as a function of s for ionization of the Ga K and L shells for 400 keV incident electrons are shown in Figs. 4(a) and 4(b), respectively. Results calculated from first principles are compared with the cubic spline plus exponential parameterization of the calculated form factors in Tables 1 and 2 and the parameterization provided in Tables 3 and 4, based on equation (12). For the Ga K shell, the use of the cubic spline procedure provides an excellent

Table 3
Parameters c in the exponential parameterization of the atomic scattering factors $f(s)$ given by equation (12) for K-shell ionization for elements in the range $Z = 6$ to $Z = 50$ and for the incident energies E_0 shown.

The values of c are obtained by fitting the calculated form factors in the range $0 \leq s \leq 2.5$ Å^{-1}, as described in the text. Atomic numbers Z and the threshold energies E_t obtained in the calculation of the form factors in Table 1 are also shown.

			E_0 (keV)							
Element	Z	E_t (keV)	50	100	150	200	250	300	350	400
C	6	0.3095	0.1831	0.1862	0.1877	0.1887	0.1893	0.1895	0.1893	0.1894
N	7	0.4274	0.1617	0.1649	0.1667	0.1677	0.1684	0.1688	0.1688	0.1691
O	8	0.5641	0.1436	0.1468	0.1487	0.1497	0.1505	0.1510	0.1512	0.1516
F	9	0.7196	0.1279	0.1313	0.1333	0.1343	0.1350	0.1356	0.1359	0.1361
Ne	10	0.8939	0.1145	0.1180	0.1200	0.1210	0.1218	0.1224	0.1227	0.1231
Na	11	1.1040	0.1013	0.1049	0.1069	0.1079	0.1087	0.1092	0.1096	0.1100
Mg	12	1.3377	0.0900	0.0936	0.0956	0.0967	0.0974	0.0980	0.0983	0.0987
Al	13	1.5963	0.0803	0.0839	0.0858	0.0869	0.0877	0.0882	0.0886	0.0889
Si	14	1.8785	0.0719	0.0755	0.0773	0.0785	0.0793	0.0798	0.0802	0.0806
P	15	2.1841	0.0647	0.0682	0.0700	0.0712	0.0720	0.0725	0.0729	0.0733
S	16	2.5133	0.0583	0.0617	0.0637	0.0648	0.0656	0.0661	0.0665	0.0668
Cl	17	2.8662	0.0528	0.0561	0.0581	0.0591	0.0599	0.0604	0.0608	0.0612
Ar	18	3.2428	0.0479	0.0512	0.0531	0.0541	0.0549	0.0554	0.0558	0.0562
K	19	3.6523	0.0435	0.0466	0.0485	0.0495	0.0503	0.0508	0.0512	0.0515
Ca	20	4.0874	0.0396	0.0426	0.0444	0.0454	0.0462	0.0467	0.0470	0.0474
Sc	21	4.5424	0.0362	0.0391	0.0408	0.0418	0.0425	0.0430	0.0434	0.0437
Ti	22	5.0214	0.0331	0.0359	0.0376	0.0386	0.0393	0.0398	0.0401	0.0404
V	23	5.5245	0.0304	0.0330	0.0347	0.0357	0.0363	0.0368	0.0371	0.0375
Cr	24	6.0473	0.0280	0.0305	0.0321	0.0331	0.0337	0.0341	0.0345	0.0348
Mn	25	6.6041	0.0258	0.0281	0.0297	0.0306	0.0312	0.0317	0.0320	0.0323
Fe	26	7.1807	0.0238	0.0260	0.0275	0.0284	0.0290	0.0294	0.0298	0.0301
Co	27	7.7821	0.0220	0.0241	0.0255	0.0264	0.0270	0.0274	0.0277	0.0280
Ni	28	8.4085	0.0204	0.0223	0.0237	0.0245	0.0251	0.0255	0.0258	0.0261
Cu	29	9.0534	0.0189	0.0208	0.0221	0.0229	0.0234	0.0238	0.0241	0.0245
Zn	30	9.7362	0.0176	0.0193	0.0206	0.0213	0.0218	0.0222	0.0225	0.0228
Ga	31	10.4480	0.0164	0.0180	0.0192	0.0198	0.0204	0.0207	0.0210	0.0213
Ge	32	11.1868	0.0152	0.0168	0.0179	0.0185	0.0190	0.0193	0.0196	0.0198
As	33	11.9526	0.0142	0.0157	0.0167	0.0173	0.0178	0.0181	0.0183	0.0186
Se	34	12.7456	0.0133	0.0147	0.0156	0.0161	0.0166	0.0169	0.0172	0.0174
Br	35	13.5658	0.0124	0.0138	0.0146	0.0151	0.0155	0.0158	0.0161	0.0163
Kr	36	14.4134	0.0117	0.0129	0.0137	0.0141	0.0145	0.0148	0.0151	0.0153
Rb	37	15.2958	0.0110	0.0121	0.0128	0.0133	0.0136	0.0139	0.0141	0.0143
Sr	38	16.2067	0.0103	0.0114	0.0120	0.0125	0.0128	0.0131	0.0133	0.0135
Y	39	17.1433	0.0097	0.0107	0.0113	0.0117	0.0120	0.0122	0.0124	0.0127
Zr	40	18.1076	0.0092	0.0102	0.0107	0.0110	0.0113	0.0115	0.0117	0.0119
Nb	41	19.0970	0.0086	0.0096	0.0101	0.0104	0.0106	0.0108	0.0110	0.0112
Mo	42	20.1174	0.0083	0.0090	0.0095	0.0098	0.0100	0.0102	0.0103	0.0105
Tc	43	21.1702	0.0080	0.0086	0.0089	0.0092	0.0094	0.0096	0.0098	0.0099
Ru	44	22.2443	0.0076	0.0082	0.0084	0.0087	0.0089	0.0090	0.0092	0.0094
Rh	45	23.3514	0.0073	0.0077	0.0080	0.0083	0.0084	0.0085	0.0087	0.0089
Pd	46	24.4838	0.0070	0.0073	0.0076	0.0078	0.0079	0.0081	0.0082	0.0084
Ag	47	25.6537	0.0069	0.0071	0.0072	0.0074	0.0075	0.0077	0.0077	0.0079
Cd	48	26.8548	0.0066	0.0067	0.0068	0.0070	0.0072	0.0073	0.0073	0.0075
In	49	28.0885	0.0065	0.0064	0.0065	0.0067	0.0068	0.0069	0.0070	0.0071
Sn	50	29.3533	0.0063	0.0061	0.0062	0.0063	0.0065	0.0065	0.0066	0.0068

fit for small $s \leq 2.5$ Å^{-1}. The fit using equation (12) underestimates the form factors in this region. Both the parameterization given in Table 1 for $2.5 \leq s \leq 20.0$ Å^{-1} and the extrapolation of equation (12) to that region overestimate the form factors for large s, that given by equation (12) the more so. The parameterizations defined in Tables 2 and 4 both offer an excellent fit to the Ga L-shell scattering factors. The one-dimensional ⟨400⟩ static and thermally smeared ionization potentials calculated from first principles are compared with those obtained from parameterized form factors in Figs. 4(c) to 4(f). For the static case in Figs. 4(c) and 4(d) [the Debye–Waller factor in equation (15) is set to zero], the potentials calculated using Tables 1 and 2 are slightly too high but the shape of the first-principles potentials are closely matched. When thermal smearing is included, with $\langle \mu_\beta^2 \rangle = 0.0082$ Å^2, then the differences between the exact results and those obtained using Tables 1 and 2 are indiscernible on the scale of Figs. 4(e) and 4(f). The Lorentzian static ionization potentials (from Tables 3 and 4) are slightly less accurate than those obtained from the form factors defined in Tables 1 and 2, especially for the Ga K shell, but the addition of thermal smearing improves agreement with the exact result. We note that, while the assumption of a Gaussian form of the ionization potential provides an adequate description of localized interactions, it provides a poor description of

Table 4
Parameters c in the exponential parameterization of the atomic scattering factors $f(s)$ given by equation (12) for L-shell ionization for elements in the range $Z = 20$ to $Z = 60$ and for the incident energies E_0 shown.

The values of c are obtained by fitting the calculated form factors in the range $0 \leq s \leq 2.5$ Å^{-1}, as described in the text. Atomic numbers Z and the threshold energies E_t obtained in the calculation of the form factors in Table 2 are also shown.

			E_0 (keV)							
Element	Z	E_t (keV)	50	100	150	200	250	300	350	400
Ca	20	0.3901	0.2134	0.2145	0.2160	0.2170	0.2180	0.2179	0.2181	0.2181
Sc	21	0.4472	0.2102	0.2109	0.2120	0.2128	0.2135	0.2139	0.2143	0.2144
Ti	22	0.5070	0.1977	0.2022	0.2045	0.2061	0.2071	0.2077	0.2079	0.2083
V	23	0.5698	0.1866	0.1909	0.1927	0.1944	0.1954	0.1961	0.1963	0.1967
Cr	24	0.6304	0.1775	0.1817	0.1836	0.1852	0.1861	0.1866	0.1870	0.1874
Mn	25	0.7049	0.1675	0.1714	0.1734	0.1748	0.1756	0.1762	0.1765	0.1771
Fe	26	0.7773	0.1591	0.1629	0.1648	0.1661	0.1669	0.1675	0.1679	0.1683
Co	27	0.8531	0.1513	0.1551	0.1569	0.1580	0.1588	0.1594	0.1597	0.1601
Ni	28	0.9321	0.1438	0.1475	0.1494	0.1506	0.1513	0.1518	0.1522	0.1526
Cu	29	1.0076	0.1378	0.1414	0.1433	0.1445	0.1452	0.1457	0.1461	0.1464
Zn	30	1.1004	0.1303	0.1339	0.1358	0.1370	0.1376	0.1382	0.1386	0.1389
Ga	31	1.2005	0.1233	0.1268	0.1287	0.1298	0.1304	0.1310	0.1314	0.1317
Ge	32	1.3058	0.1167	0.1201	0.1220	0.1231	0.1237	0.1243	0.1247	0.1250
As	33	1.4161	0.1105	0.1139	0.1158	0.1169	0.1175	0.1180	0.1184	0.1187
Se	34	1.5316	0.1047	0.1081	0.1099	0.1110	0.1116	0.1121	0.1125	0.1129
Br	35	1.6521	0.0993	0.1026	0.1044	0.1055	0.1061	0.1066	0.1070	0.1073
Kr	36	1.7777	0.0942	0.0975	0.0992	0.1003	0.1009	0.1015	0.1019	0.1022
Rb	37	1.9153	0.0893	0.0924	0.0942	0.0953	0.0959	0.0964	0.0968	0.0971
Sr	38	2.0589	0.0846	0.0877	0.0894	0.0905	0.0911	0.0916	0.0920	0.0923
Y	39	2.2051	0.0804	0.0834	0.0851	0.0862	0.0868	0.0873	0.0877	0.0880
Zr	40	2.3558	0.0764	0.0794	0.0811	0.0822	0.0828	0.0833	0.0837	0.0840
Nb	41	2.5082	0.0728	0.0757	0.0774	0.0784	0.0791	0.0796	0.0800	0.0803
Mo	42	2.6684	0.0693	0.0722	0.0738	0.0749	0.0755	0.0760	0.0764	0.0767
Tc	43	2.8374	0.0659	0.0687	0.0704	0.0714	0.0720	0.0726	0.0729	0.0733
Ru	44	3.0038	0.0630	0.0657	0.0674	0.0684	0.0690	0.0695	0.0699	0.0702
Rh	45	3.1793	0.0601	0.0628	0.0644	0.0654	0.0661	0.0666	0.0669	0.0673
Pd	46	3.3557	0.0575	0.0602	0.0618	0.0628	0.0634	0.0639	0.0643	0.0646
Ag	47	3.5457	0.0548	0.0574	0.0590	0.0600	0.0606	0.0611	0.0615	0.0618
Cd	48	3.7424	0.0523	0.0548	0.0564	0.0574	0.0580	0.0585	0.0588	0.0592
In	49	3.9468	0.0499	0.0524	0.0539	0.0549	0.0555	0.0560	0.0563	0.0566
Sn	50	4.1575	0.0476	0.0501	0.0516	0.0525	0.0531	0.0536	0.0539	0.0543
Sb	51	4.3742	0.0455	0.0479	0.0494	0.0503	0.0509	0.0514	0.0517	0.0520
Te	52	4.5972	0.0435	0.0458	0.0473	0.0482	0.0488	0.0493	0.0496	0.0499
I	53	4.8265	0.0417	0.0439	0.0454	0.0462	0.0469	0.0473	0.0476	0.0479
Xe	54	5.0621	0.0399	0.0421	0.0435	0.0444	0.0450	0.0454	0.0457	0.0460
Cs	55	5.3094	0.0381	0.0403	0.0417	0.0425	0.0431	0.0436	0.0439	0.0442
Ba	56	5.5636	0.0365	0.0386	0.0400	0.0408	0.0414	0.0418	0.0422	0.0424
La	57	5.8221	0.0350	0.0370	0.0383	0.0392	0.0397	0.0402	0.0405	0.0408
Ce	58	6.0784	0.0337	0.0356	0.0369	0.0377	0.0384	0.0387	0.0391	0.0394
Pr	59	6.3446	0.0324	0.0343	0.0356	0.0364	0.0370	0.0374	0.0377	0.0380
Nd	60	6.6153	0.0311	0.0330	0.0343	0.0351	0.0356	0.0360	0.0363	0.0366

delocalized interactions such as those associated with the ionization of the carbon K shell.

Ionization cross sections calculated from the form factors in Tables 1 and 2 and also using the data in Tables 3 and 4 [based on equation (12)] are shown in Fig. 5. Ratios of X-ray intensities, Ga K shell to Ga L shell, with each assumed proportional to the ionization cross section, have been calculated and compared to the experimental data of Nüchter & Sigle (1995). The calculations have been carried out as described by Oxley & Allen (1998). Excellent agreement is obtained between the exactly calculated theoretical result and that calculated using the data in Tables 1 and 2 and also with the experimental data. The parameterization in Tables 3 and 4 provides a less accurate result, but still falls well within the error bars of the experimental data.

4. Conclusions

Atomic scattering form factors have been calculated from first principles for K-shell ionization for elements in the range $Z = 6$ (carbon) to $Z = 50$ (tin) and for L-shell ionization in the range $Z = 20$ (calcium) to $Z = 60$ (neodymium). The results are presented in tabular form such that accurate values of the scattering factors can be obtained by interpolation on the natural logarithm of the form factors for incident electron energies between 50 and 400 keV and for scattering vectors with magnitude $s = \sin\theta/\lambda$ up to 2.5 Å^{-1}. A separate parameterization of the form factors is given for s in the range $2.5 \leq s \leq 20$ Å^{-1}, where they are small. A simpler but less accurate parameterization of the form factors, corresponding to the assumption of a Lorentzian form of the atomic ioniza-

tion potential in one dimension, is also presented. The scattering factors are suitable for the calculation of ionization cross sections for use in atom location by channelling-enhanced microanalysis (ALCHEMI).

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