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Numerical Calculations of Elastic Scattering Amplitudes for High-Energy Electron Scattering by Ionized Atoms

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Abstract

The elastic electron scattering factors and phases for eleven alkali and halide ionized atoms, Li^+, Li^{2+}, Li^{3+}, Na^+, K^+, Rb^+, Cs^+, F^-, Cl^-, Br^- and I^-, have been calculated by the partial wave method for impact energies of 10, 40, 70 and 100 keV. Clementi analytic Hartree–Fock wavefunctions were used except for Li^{2+} whose wavefunction was hydrogen-like, Li^{3+} whose potential was purely Coulombic, and Rb^+, Cs^+, Br^- and I^- for which potential functions estimated from the X-ray scattering factors were used. The calculated scattering factors and phases for the ionized atoms have been compared with those for neutral atoms in *International Tables for X-ray Crystallography* [(1974). Vol. IV, pp. 176–269. Birmingham: Kynoch Press]. It has been found that the difference in the scattering phase between the neutral and ionized atom is almost constant except for small *s* and that the magnitude of the difference for a given valence of the ionized atom and a particular impact energy is nearly independent of the atomic number.

Introduction

It is well known in the field of gas electron diffraction that values of molecular parameters obtained from diffraction data depend on a particular set of theoretically calculated scattering factors and phases used in the analysis (Schomaker & Glauber, 1952; Glauber & Schomaker, 1953). It has been pointed out that for analysis of electron diffraction data of ionic molecules (Turman, Ingrams & Hanson, 1968) and of ion-bonded molecules such as alkali halide vapors (Miki, Kakumoto, Ino, Kodera & Kakinoki, 1980), precise values of the scattering factor and phase are essential. To our best knowledge, scattering amplitudes for ionized atoms are available only for O^-, Ne^+ and Na^+ for an impact energy of 40 keV by the partial wave method (Peixoto, 1969), although scattering factors for ions in the first Born approximation are listed in the latest *International Tables for X-ray Crystallography* (1974).

In the present study, scattering factors and phases were calculated for alkali and halogen ionized atoms, Li^+, Li^{2+}, Li^{3+}, Na^+, K^+, Rb^+, Cs^+, F^-, Cl^-, Br^- and I^- by a partial wave method similar to Peixoto's (1969) for impact energies of 10, 40, 70 and 100 keV. Clementi analytic wavefunctions were used for Li^+, Na^+, K^+, F^- and Cl^-. Since no such analytic wavefunctions were available for Rb^+, Cs^+, Br^- and I^-, analytic potential functions for these ionized atoms were determined using X-ray scattering factors.

For negatively ionized atoms F^-, Cl^-, Br^- and I^-, non-vanishing minimum values and their positions (value of *s*) of the scattering factor were carefully determined. Almost constant difference in scattering phase between neutral and ionized atoms was obtained for $s > 3$ Å^{-1}. Values of scattering phase for positively (negatively) ionized atoms were found to be smaller (larger) than those for neutral atoms.

Theory and calculation

The problem of elastic scattering of electrons by an ionized atom can be treated as the scattering by a modified Coulomb field (Mott & Massey, 1965). A scattering amplitude $f(\theta)$ at scattering angle θ is given as a sum of a pure Coulomb term $f_c(\theta)$ and a residual term $f_m(\theta)$:

$$f(\theta) = f_c(\theta) + f_m(\theta), \tag{1}$$

with

$$f_c(\theta) = [\beta/2k \sin^2(\theta/2)] \exp\{-i\beta \ln[\sin^2(\theta/2)] + i\pi + 2i\sigma_0\} \tag{2}$$

and

$$f_m(\theta) = \frac{1}{2ik} \sum_{L=0}^{\infty} (2L+1) \exp(2i\sigma_L) [\exp(2i\delta_L) - 1] \times P_L(\cos\theta), \tag{3}$$

where σ_L is a pure Coulomb phase shift and δ_L is an additional phase shift due to a departure from pure Coulomb field. The quantities σ_L and β are expressed as

$$\sigma_L = \arg \Gamma(L + 1 + i\beta) \tag{4}$$

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and

$$\beta = -\frac{mZ'}{\hbar^2 k} e^2, \tag{5}$$

where Z' is the valence of the ionized atom, m the reduced mass of the projectile electron and the ion, and k the wave number of the electron. Corrections for relativistic effects in the reduced mass and the wave number were made in the present calculation. The value of σ_L can be readily computed with the following recurrence formula and the value of σ_0 can be accurately approximated over the entire range of β as follows (Melkanoff, Sawada & Raynal, 1966):

$$\sigma_{L+1} = \tan^{-1}[\beta/(L+1)] + \sigma_L, \tag{6}$$

$$\begin{aligned}\sigma_0 = {} & -\beta + \frac{\beta}{2}\ln(\beta^2+16) + \frac{7}{2}\tan^{-1}\left(\frac{\beta}{4}\right) \\ & - \left[\tan^{-1}\beta + \tan^{-1}\left(\frac{\beta}{2}\right) + \tan^{-1}\left(\frac{\beta}{3}\right)\right] \\ & - \frac{\beta}{12(\beta^2+16)}\left[1 + \frac{\beta^2-48}{30(\beta^2+16)^2}\right. \\ & \left. + \frac{\beta^4 - 160\beta^2 + 1280}{105(\beta^2+16)^4}\right].\end{aligned} \tag{7}$$

The additional phase shift δ_L can be obtained from the solution for the radial equation

$$[\mathrm{d}^2/\mathrm{d}r^2 + k^2 - U(r) - L(L+1)/r^2]\,\psi_L(r) = 0 \tag{8}$$

with $U(r) = (2m/\hbar^2)V(r)$, where $V(r)$ is the potential energy which asymptotically behaves as $-Z'e^2/r$ at large r. Since at $r = r_m = 15a_B$ (a_B is the Bohr radius) the potential of the ion agrees with purely Coulombic potential to five significant figures in the present calculation, the asymptotic solution is matched to a linear combination of the regular and irregular Coulomb wave functions, $F_L(\beta{:}k,r)$ and $G_L(\beta{:}k,r)$, as follows (Melkanoff, Sawada & Raynal, 1966):

$$\psi_L(\beta{:}k,r) = F_L(\beta{:}k,r) + C_L[G_L(\beta{:}k,r) + iF_L(\beta{:}k,r)] \tag{9}$$

for $r \simeq r_m$. The value of δ_L can be obtained from C_L through the equation

$$C_L = \frac{1}{2i}[\exp(2i\delta_L) - 1]. \tag{10}$$

Equation (8) was solved by Cowell's method modified by Melkanoff, Sawada & Raynal (1966), where the mesh space used in the numerical integration is $0{\cdot}001a_B$. The Coulomb wave functions F_L and G_L ($L = 0,1$) for $r = r_m$ were obtained using the asymptotic solution given by Fröberg (1955), since the criteria for the solution, $\beta^2 \ll kr_m$, $L^2 \ll kr_m$, hold well. The calculation of wavefunctions with higher L for $r = r_m$ was carried out with an upwards recurrence relation.

Using $s = 2k\sin(\theta/2)$, the scattering amplitude (1) is expressed as

$$\begin{aligned}f(s) = {} & \frac{2k\beta}{s^2}\exp[-2i\beta\ln(s/2k) + i\pi + 2i\sigma_0] \\ & + \frac{1}{2ik}\sum_{L=0}^{\infty}(2L+1)\exp(2i\sigma_L)[\exp(2i\delta_L) - 1] \\ & \times P_L\{\cos[2\sin^{-1}(s/2k)]\}.\end{aligned} \tag{11}$$

In the present work, the scattering amplitude was calculated as a function of s. The upper limits of the azimuthal quantum number L used in this partial wave calculation are listed in Table 1. In the table, the figures show the number taken for a satisfactory convergence, while those with asterisks give the maximum number available for the present computational facilities. The fluctuation in $f(s)$ due to the poor convergence was successfully eliminated by a smoothing-out method. It is noted that the curve $f(s)$, obtained by smoothing-out, of Na^+ for $L = 100$ at 40 keV agreed well with the smooth curve calculated with $L = 160$.

Analytic forms of potential

Since the exchange effect can be neglected in high-energy scattering (Mott & Massey, 1965), the potential energy $V(r)$ in (8) may be given by

$$V(r) = -Z\frac{e^2}{r} + e^2\int \rho(\mathbf{r}')/|\mathbf{r} - \mathbf{r}'|\mathrm{d}\mathbf{r}', \tag{12}$$

where Z is the atomic number; $\rho(\mathbf{r})$ is the electron density of the ionized atom, which can be obtained from the atomic wavefunction. Analytic potentials, $V(r)$, for ionized atoms Li^+, Na^+, K^+, F^- and Cl^- were calculated using nonrelativistic analytic Hartree–Fock wavefunctions by Clementi (1965). Although relativistic Hartree–Fock atomic fields for Br^-, I^-, Rb^+ and Cs^+ obtained by Coulthard (1967) were given numerically, in the present paper analytic potentials, $V(r)$, for these ionized atoms were calculated in the

Table 1. *The upper limits of the azimuthal quantum number L taken in the partial wave sum*

	10 keV	40 keV	70 keV	100 keV
Li^+	50	130	399*	399*
Li^{2+}	50	210	399*	399*
Na^+	120	160	200*	230*
K^+	100	170	230	330
Rb^+	100	190	240	330
Cs^+	150	190	250	320
F^-	140	230	280*	330*
Cl^-	140	230	280*	330*
Br^-	140	270	399*	399*
I^-	270	399*	399*	399*

* Maximum number available for the computing facilities.

following indirect way, starting with the X-ray scattering factor $F_x(s)$. The values of $F_x(s)$ were calculated by Doyle & Turner (1968) and are tabulated in Table 2.2*A* of *International Tables for X-ray Crystallography* (1974).

The electron scattering factor, $F_B(s)$, is related to $F_x(s)$ in the first Born approximation by

$$F_B(s) = \frac{2}{a_B}[Z - F_x(s)]/s^2$$
$$= -\frac{2}{a_B e^2}\int_0^\infty V(r)\frac{\sin(sr)}{sr} r^2\,\mathrm{d}r. \tag{13}$$

Since singly ionized halogen atoms (X^-) and alkali atoms (A^+) are isoelectronic with a neutral rare-gas atom whose atomic number is $Z \pm 1$, the potential, $V(r)$, for X^- and A^+ is approximated by

$$V(r) \simeq v(r) = \pm\frac{e^2}{r} - \frac{e^2}{r}(Z \pm 1)\sum_{i=1}^{m}\gamma_i \exp(-\lambda_i r), \tag{14}$$

according to Cox & Bonham (1967). In the first Born approximation (Cox & Bonham, 1967), the electron scattering factors, $f_B(s)$, were found to be

$$f_B(s) = \mp\frac{2}{a_B s^2} + \frac{2}{a_B}(Z \pm 1)\sum_{i=1}^{m}\frac{\gamma_i}{\lambda_i^2 + s^2}. \tag{15}$$

However, it is found that the electron scattering factor, $f_B(s)$, calculated by (15) differs from $F_B(s)$ by a small amount; $F_B(s) = f_B(s) + \Delta f_B(s)$. This small difference arises from the difference between $V(r)$ and $v(r)$; $\Delta v(r) = V(r) - v(r)$. The small potential difference, $\Delta v(r)$, may be regarded as the sum of Gaussian functions:

$$\Delta v(r) = -\frac{a_B e^2}{4\sqrt{\pi}}\sum_{i=1}^{n}\frac{a_i}{b_i^3}\exp\left(-\frac{r^2}{4b_i^2}\right). \tag{16}$$

The electron scattering factor $\Delta f_B(s)$ due to $\Delta v(r)$ is calculated by

$$\Delta f_B(s) = \sum_{i=1}^{n} a_i \exp(-b_i^2 s^2). \tag{17}$$

Numerical values for $\Delta f_B(s) = F_B(s) - f_B(s)$ are used to determine a_i and b_i by a least-squares method. The values of a_i and b_i are listed together with γ_i and λ_i (Cox & Bonham, 1967) in Table 2.

Using the analytic potential $V(r) = v(r) + \Delta v(r)$ obtained above, electron scattering factors for Br$^-$, I$^-$, Rb$^+$ and Cs$^+$ were calculated by the partial wave method. In order to check the accuracy of the scattering factors, scattering factors for K$^+$ and Cl$^-$ were calculated by the indirect method and were found to agree within 1% with the corresponding ones calculated using Clementi's (1965) analytic wavefunction. It is expected that scattering factors for Br$^-$, I$^-$, Rb$^+$ and Cs$^+$ are accurate to a similar degree.

For Li^{2+}, the potential was derived from the ground-state wavefunction of the hydrogen-like atom.

Numerical results and discussion

Using the theory and the potentials obtained in the preceding sections, scattering factor $|f|$ and phase η of ionized atoms, Li$^+$, Li^{2+}, Na$^+$, K$^+$, Rb$^+$, Cs$^+$, F$^-$, Cl$^-$, Br$^-$ and I$^-$, were computed* by the partial wave method for impact electron energies 10, 40, 70 and 100

Table 2. *The potential parameters γ_i and λ_i (a.u.) determined by Cox & Bonham (1967) and parameters a_i and b_i (Å) obtained in the present study*

	γ	λ	a	b
Br$^-$	4·1201	7·2511	0·0026	0·0080
	−0·0553	85·3351	0·0211	0·0746
	11·8935	12·8260	0·2179	0·2163
	13·7167	36·0695	1·8339	0·5415
	−1·3169	2·6894	0·2139	1·2192
	−14·3716	11·2830		
	−14·2991	35·2590		
	1·3121	1·9907		
Rb$^+$	4·1201	7·2511	−0·0112	0·3309
	−0·0553	85·3351	−0·1006	0·1669
	11·8935	12·8260	−1·3976	0·4369
	13·7167	36·0695	−0·0074	0·1844
	−1·3169	2·6894		
	−14·3716	11·2830		
	−14·2991	35·2590		
	1·3121	1·9907		
Cs$^+$	7·6397	13·6666	0·0145	54·9604
	−0·0299	137·4095	−0·1125	0·0855
	21·5995	24·0007	−0·3158	0·1896
	20·8424	48·7608	−2·0852	0·4789
	−5·1302	7·8087	−5·5334	0·6872
	−25·0317	21·1625	−1·3543	1·2156
	−22·8271	47·4972		
	1·5368	9·1558		
	2·1983	4·9962		
	0·2210	0·8904		
I$^-$	7·6397	13·6666	−0·0075	0·0212
	−0·0299	137·4095	0·0071	0·0275
	21·5995	24·0007	−0·0062	0·0387
	20·8424	48·7608	−0·0182	0·0661
	−5·1352	7·8087	0·0066	0·0816
	−25·0317	21·1625	−0·0426	0·1403
	−22·8271	47·4972	−0·0499	0·1946
	1·5368	9·1558	−0·9825	0·4244
	2·1983	4·9962	540·8258	0·5914
	0·2210	0·8904	−7372·5131	0·6573
			85065·750	0·7188
			−203928·42	0·7469
			154890·39	0·7721
			−41105·347	0·8404
			32767·088	0·9313
			−21236·090	0·9554
			5·6320	1·0336
			610·3093	1·1636
			−384·1653	1·2727
			143·0639	1·3297

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* Tables of the results have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34894 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

keV over the range $1 \le s \le 60$ Å^{-1} with an interval $\Delta s = 1$ Å^{-1}. To check the accuracy of the numerical results, the values of $|f|$ and η of Na^+ and O^- for impact energy 40 keV were calculated and were found to agree with the corresponding values calculated by Peixoto (1969) within ±1·5%.

The values of $|f|$ for the singly ionized atoms agree well with those for the neutral atoms tabulated in Table 2.5*A* of *International Tables for X-ray Crystallography* (1974) for $s > 3$ Å^{-1}, but deviate considerably from the values for neutral atoms for $s < 3$ Å^{-1}. It is noted that a similar tendency has been observed for the values of $|f|$ calculated in the first Born approximation (Doyle & Turner, 1968). For example, the scattering factors for Na^+ and Na and for Cl^- and Cl are illustrated in Figs. 1 and 2, respectively.

According to the present calculation, functions $|f(s)|$ for negatively ionized atoms F^-, Cl^-, Br^- and I^- have a minimum value at s slightly less than 1 Å^{-1}, while those for positively ionized atoms have no minimum. The minimum position is obtained at almost the same value of s as where the first Born scattering factor, $F_B(s)$, vanishes (Doyle & Turner, 1968). The minimum values are not zero in our partial wave calculation; this is also the case for O^- as pointed out by Peixoto (1969).

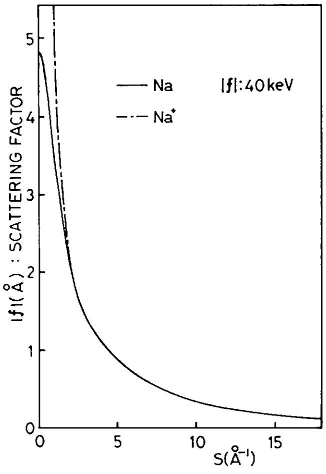

Fig. 1. The scattering factors for Na and Na^+ at 40 keV.

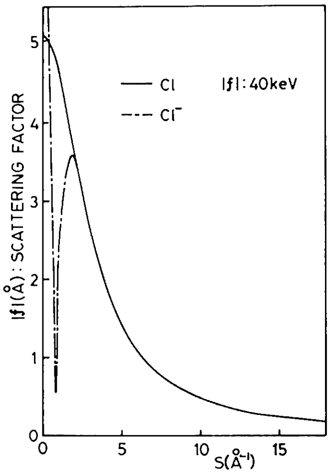

Fig. 2. The scattering factors for Cl and Cl^- at 40 keV.

In the first Born approximation, the electron scattering factor $F_B(s)$ vanishes when $F_x(s) = Z$, according to (13). In a modified Coulomb field, the amplitude is simply rewritten as

$$f = |f| \exp(i\eta) = |f_c| \exp(i\eta_c) + |f_m| \exp(i\eta_m). \quad (18)$$

One obtains for the scattering factor, $|f|$, the following relation

$$|f| = \{(|f_c| - |f_m|)^2 + 2|f_c||f_m| \times [1 + \cos(\eta_c - \eta_m)]\}^{1/2}. \quad (19)$$

As observed in the above calculation, the value of $|f|$ does not vanish except for a special case where the following relations are simultaneously satisfied:

$$\eta_c - \eta_m = (2n + 1)\pi \text{ (where } n \text{ is an integer)}, \quad (20)$$

and

$$|f_c| - |f_m| = 0. \quad (21)$$

For example, according to our present calculation for Cl^- at 40 keV impact energy, the minimum value of $|f|$ is obtained at $s = 0{\cdot}785$ Å^{-1}, where $\eta_c = 3{\cdot}3367$, $\eta_m = 0{\cdot}2790$, $|f_c| = 6{\cdot}530$ and $|f_m| = 6{\cdot}615$. It is noted that (20) with $n = 0$ and (21) do not exactly hold for these figures but are approximately satisfied.

The present calculation also shows that the minimum value of $|f|$ decreases with increasing impact energy and the minimum position approaches the value of s where $F_B(s)$ vanishes. For example, in the case of Cl^- the minimum values are 0·90372, 0·55739, 0·46765 and 0·42911 Å and the minimum positions are 0·801, 0·785, 0·783 and 0·781 Å^{-1} for impact energy 10, 40, 70 and 100 keV, respectively, while the minimum position is 0·778 Å^{-1} in the first Born approximation.

Values of $|f| = |f_c|$ for Li^{3+}, calculated directly through (2), are compared with those for Li, Li^+ and Li^{2+} in Fig. 3. One notes that for $s > 20$ Å^{-1}, the values

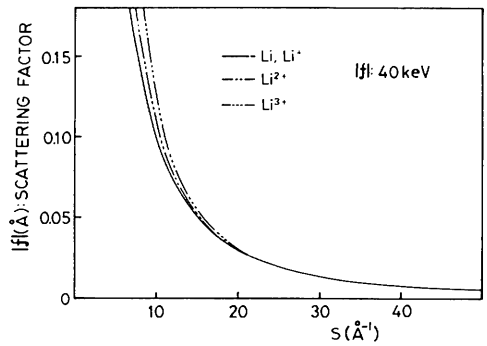

Fig. 3. The scattering factors for Li, Li^+, Li^{2+} and Li^{3+} at 40 keV.

of $|f|$ for Li^{2+} and Li^{3+} are nearly equal to those for Li and Li^+. Such a coincidence of $|f|$ for large s may be interpreted by assuming that large-angle scattering is caused mostly by the nuclear charge.

Values of scattering phase η for Li^+, Li^{2+} calculated by the partial wave method and for Li^{3+} calculated directly by (2) are plotted *versus* s together with that for neutral Li in Fig. 4. The phase difference between a neutral Li atom and an ionized atom is almost independent of s, except for $s < 3$, 8 and 11 $Å^{-1}$ for Li^+, Li^{2+} and Li^{3+}, respectively.

For alkali and halogen atoms, it has been noticed that the phase difference, $|\eta_z - \eta_z^{\pm 1}|$, between neutral ($\eta_z$) and ionized ($\eta_z^{\pm 1}$) atoms is almost constant in the range $s \geq 3$ $Å^{-1}$ and that this difference is about 0·19 ± 0·01 rad for an impact energy of 40 keV and is almost independent of the atomic number Z, as plotted in Fig. 5. $|\eta_z - \eta_z^{\pm 1}|$ varies with the magnitude of impact energy, being found to be about 0·32, 0·19, 0·16 and 0·15 rad for impact energies of 10, 40, 70 and 100 keV, respectively.

The fact that $|\eta_z - \eta_z^{\pm 1}|$ is almost independent of s and Z for the range $s \geq 3$ $Å^{-1}$ implies that the difference, $\eta_z^{\pm 1} - \eta_{cz}$, between the scattering phase of an ionized atom ($\eta_z^{\pm 1}$) and that of its nuclear charge (η_{cz}) has s and Z dependence similar to $\eta_z - \eta_{cz}$.

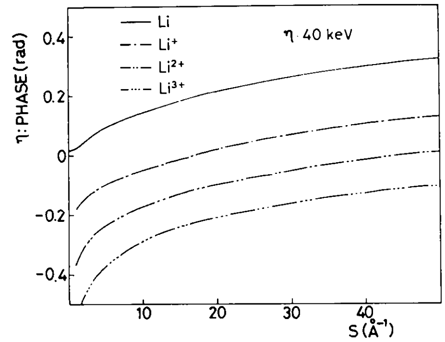

Fig. 4. The scattering phases for Li, Li^+, Li^{2+} and Li^{3+} at 40 keV.

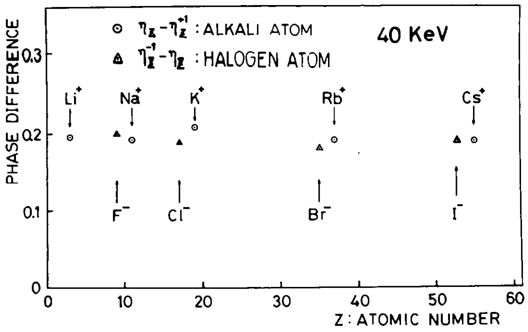

Fig. 5. The constant difference in scattering phase between the ion and its neutral atom for alkali and halogen atoms at 40 keV.

The implication is made on the following consideration. The phase difference $|\eta_z - \eta_z^{\pm 1}|$ can be rewritten as

$$|\eta_z - \eta_z^{\pm 1}| = |(\eta_z - \eta_{cz}) - (\eta_z^{\pm 1} - \eta_{cz})|. \quad (22)$$

The quantity $\eta_{cz}(s)$ is exactly given through (2) by

$$\eta_{cz}(s) = -\alpha_z \ln[\sin^2(\theta/2)] + \pi + 2\sigma_0, \quad (23)$$

where

$$\alpha_z = -Ze^2\, m/\hbar^2\, k.$$

The first term, $\eta_z - \eta_{cz}$, on the right-hand side of (22) shows s and Z dependence as plotted for halogen, rare-gas and alkali atoms in Fig. 6. It is expected from (22) that when the quantity $\eta_z^{\pm 1} - \eta_{cz}$ has s and Z dependence similar to $\eta_z - \eta_{cz}$ shown in Fig. 6, $|\eta_z - \eta_z^{\pm 1}|$ becomes independent of s and Z.

The analytic form of the scattering phase for a neutral atom was derived for the first time by Glauber & Schomaker (1953). Using the second Born approximation for a neutral atom with a potential energy $-Ze^2\exp(-r/a_z)/r$ (a_z is a screening constant), they expressed the phase $\eta_z(s)$ as

$$\eta_z(s) = -2\alpha_z \frac{1 + s^2 a_z^2}{sa_z(4 + s^2 a_z^2)^{1/2}} \tanh^{-1}\left[\frac{sa_z}{(4 + s^2 a_z^2)^{1/2}}\right] \quad (24)$$

and obtained

$$\eta_z(s) = -2\alpha_z \ln(sa_z) \text{ for } s \gg 1/a_z. \quad (25)$$

The asymptotic phase difference $\eta_z - \eta_{cz}$ given by the subtraction (25) − (23) is independent of s:

$$\eta_z - \eta_{cz} = -2\alpha_z \ln(2ka_z) - \pi - 2\sigma_0 \text{ for } s \gg 1/a_z. \quad (26)$$

The s and Z dependence of $\eta_z - \eta_{cz}$, as shown in Fig. 6, may be qualitatively interpreted from (24), (25) and (26), derived with the second Born approximation.

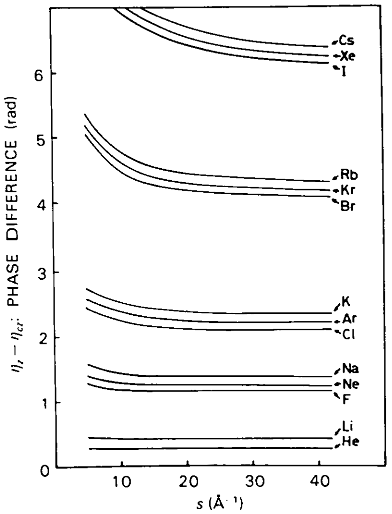

Fig. 6. The differences in scattering phase between the neutral atom and its nucleus at 40 keV plotted against s.

As a result, it could be inferred that the s and Z dependences of $\eta_z^{\pm 1} - \eta_{cz}$ are similar to the subtraction (24) − (23) and (26). An analytic form of $\eta_z^{\pm 1} - \eta_{cz}$ will be highly desirable for the interpretation of the scattering phase for ionized atoms.

The numerical computations were performed on a FACOM M-190 of the Kyoto University Computing Center and FACOM 230-60 of the Osaka City University Computing Center. The authors would like to thank Dr Y. Kudo for his help, since this study was carried out by improving his original programs in nuclear research. They would also like to thank S. Kodera for his help in the numerical calculations and are grateful to Professor H. Watanabe for his encouragement.

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Lattice Symmetry Determination

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Abstract

Transformation matrices required to obtain a conventional cell (Crystal Data cell) from the reduced cell have been applied to 47 000 crystalline compounds in the Crystal Data file. For 97% of the compounds, the calculations from the reduced cells yield conventional cells (lattice parameters, lattice type, and crystal system) that are entirely consistent with those reported in the original literature. In a few instances in which the reduced-cell matrix indicated a higher symmetry, the author has often noted that the crystal was unusual in some way or there was an error in the reported symmetry. Some implications of the results of this survey are: (1) metric symmetry as determined from the reduced cell is usually identical to the crystal-lattice symmetry; (2) determination of precise cell parameters defining any primitive cell of the lattice is valuable because from them one can conveniently determine the crystal system with a high degree of confidence (the results, however, should still be verified by checking equivalent intensities and systematic extinctions); (3) if the metric symmetry obtained from the reduced cell and the symmetry determined by other techniques do not agree, the reason should be sought as there are often important structural implications; (4) the sequence of steps in an automatic procedure for the determination of space groups could be: primitive cell, reduced cell, lattice metric symmetry, crystal-lattice symmetry, extinction conditions.

Introduction

Research on crystallographic data bases should lead to the discovery of new relationships, to new classification schemes and to better data evaluation. Such data bases will become increasingly important in scientific

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