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Note

Average Electronic Form Factors for Neutral Atoms with $40 < Z < 90$

Introduction

An atomic form factor or atomic scattering factor is used to describe the major variations of scattering power with angles. These form factors thus provide a basis for the comparison of theoretical calculations with experimental measurements. Experimentally, form factors are determined using X-ray and neutron diffraction methods. In this regard they are usually calculated as a function of $\sin \theta/\lambda$, where θ is the scattering angle and λ is the wavelength of the incident particle. However, if one needs to know the variation of the total scattering cross section with the energy of the incident particle for particle atom scattering, (the variation might be due to different electronic structure of the atom), one has to know the variation of the average electronic form factor (over all angles of scattering) as a function of the incident particle energy. For example, in the measurement of neutron–electron potential interaction [1, 2] knowledge of the average electronic form factor is needed in order to interpret the strength of the neutron–electron interaction potential from the experimental data. Whatever the need may be, the calculation of the electronic form factor is limited to the choice of the atomic model and, for fairly heavy neutral atoms, it is justified to use the Thomas–Fermi model [12, 13].

Average electronic form factors were calculated using the Thomas–Fermi model and an analytical fit to these form factors was obtained. This expression provides the average form factor as a function of $\lambda z^{1/3}$, a variable often used in connection with the Thomas–Fermi model.

Theoretical Considerations

Even though the mathematical details of the Thomas–Fermi model have been discussed in the literature [3, 4], the necessary formulas for understanding this note will be reviewed.

The form factor defined as the Fourier transform of the charge distribution can be written as

$$f(\mathbf{q}) = \int_0^\infty \rho(r) \exp(i\mathbf{q} \cdot \mathbf{r}) \, d\mathbf{r} \tag{1}$$

where $\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i$ the change in momentum; $\mathbf{k}_i$ and $\mathbf{k}_f$ are initial and final momenta of the incident particle, respectively. For elastic scattering, $|\mathbf{k}_i| = |\mathbf{k}_f| = k$, and $|\mathbf{q}| = 2k \sin(\theta/2)$, where θ is the scattering angle. Expressing q in terms of the wavelength of the incident particle ($k = 2\pi/\lambda$), one obtains

$$f(\lambda) = \lambda \int_0^\infty r\rho(r)[\sin[4\pi r \sin(\theta/2)/\lambda]/\sin(\theta/2)]\, dr. \tag{2}$$

The average of $f(\lambda)$ over all angles of scattering is given by

$$\langle f(\lambda)\rangle = \lambda \int_0^\infty r\rho(r) \int_0^\pi \sin[4\pi r \sin(\theta/2)/\lambda] \cos(\theta/2)\, d\theta\, dr \tag{3}$$

$\rho(r)$, the charge density must be known in order to calculate $f(\lambda)$. Using the Thomas–Fermi model $\rho(r)$ can be expressed in terms of the spherically symmetrical potential energy $V(r)$, such that

$$\rho(r) = \tfrac{1}{3}[2m/\pi^{4/3}\hbar^2]^{3/2} \times [-V(r)]^{3/2}. \tag{4}$$

The Poisson equation then connects the electrostatic potential $-(1/e)\, V(r)$ with the charge density $e\rho(r)$ resulting in

$$\nabla^2 V(r) = -4\pi e^2 \rho(r). \tag{5}$$

Equation (5) leads to the Thomas–Fermi equation in terms of the variables $x = r/b$ with $b = (3\pi)^{2/3}\hbar^2 z^{-1/3}/2^{7/3}\, me^2$ (or $b = .88534\, a_0 z^{-1/3}$ where $a_0 = \hbar^2/me^2 = 5.292 \times 10^{-11}$ m, the Bohr radius, and e, m, $\hbar$, z have the usual meaning) and $rV = -ze^2\phi$

$$d^2\phi(x)/dx^2 = \phi^{3/2}/x^{1/2}. \tag{6}$$

One thus needs $\phi(x)$ to know $\rho(r)$ which in turn is necessary to calculate the form factors. Several solutions to the Thomas–Fermi equation (6) exist. Numerical solutions as accurate as five significant figures are given by Kobayaski [7]. Other attempts have been made by various authors [5, 6, 8, 9] to obtain an anlaytic fit to the numerical solution of Eq. (6). However, none of these solutions of $\phi(x)$ can be used to obtain the expression for the form factor in an integrable form; one has to use numerical methods in order to obtain the form factors despite which form of $\phi(x)$ is used. Therefore the following integral needs to be evaluated

$$f(y) = \frac{1}{z}\langle f(\lambda)\rangle = \frac{y^2 2^{3/2}}{6\pi^2 a_0{}^2 \gamma^{1/2}} \int_0^\infty \left(\frac{\phi(x)}{x}\right)^{3/2} \cdot \left[1 - \cos\left(\frac{4\pi\gamma a_0 x}{y}\right)\right] dx \tag{7}$$

with

$$\gamma = bz^{1/3}/a_0\,; \qquad b = (1/4)\, a_0(9\pi^2/2z)^{1/3}$$

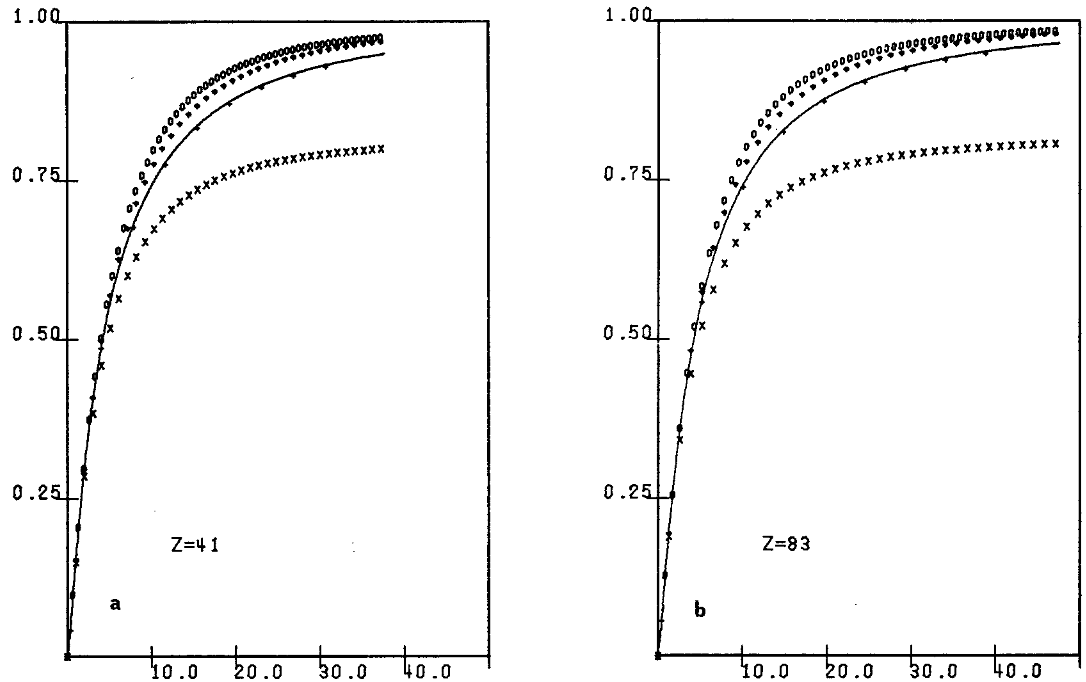

FIG. 1. Comparison of average electronic form factors. The solid line represents the form factor which is the analytic fit of $\langle f(\lambda)\rangle$ (Eq. 7) using the numerical solutions of $\phi(x)$; the symbols ($\times$), ($+$), ($*$), and ($\circ$) represent the form factors one would obtain if the solutions for $\phi(x)$ as given by: (1) $\phi(X) = \exp(-0.1837X)/(1 + 1.05X)$ [8]; (2) $\phi(X) = [\Sigma_{n=1} C_n X^{(n-1)/2}]^{-1}$ [9], with $C_1 = 1$, $C_2 = 0.02747$, $C_3 = 1.243$, $C_4 = -0.1486$, $C_5 = 0.2302$, $C_6 = 0.007298$, $C_7 = 0.006944$; (3) $\phi(X) = [a\exp(-\alpha x) + b\exp(-\beta x)]^2$ [5], with $a = 0.7111$, $\alpha = 0.175$, $b = 0.2889$, $\beta/\alpha = 9.5$; (4) $\phi(y) = \Sigma_{n=1} a_n\ y^{(n-1)/2}\exp[-y^{1/2}]$ [10], with $y = \alpha^2 x/4$, and $\alpha = 3.984329$, $a_1 = 1$, $a_2 = 1$, $a_3 = 0.2999266$, $a_4 = 0.05091369$, $a_5 = 0.005935725$, $a_6 = 0.003881420$ respectively are used. (a) for $Z = 41$, (b) for $Z = 83$.

RESULTS AND DISCUSSION

Equation (7) was evaluated (using a numerical integration method, e.g., Simpson rule) for the numerical and analytical forms of $\phi(x)$ as shown in Figs. 1(a) and 1(b). An analytical fit to the form factor $f(y)$, using numerical values for $\phi(x)$, was obtained (other attempts of analytical fit to form factors using the Hartree–Fock model can be found in the literature [11].

This polynomial fit to the form factor is written in the form

$$f(y) = \sum_{n=1}^{N} B_n y^{n-1}. \tag{8}$$

The coefficients B_n were calculated using the method of least squares for different regions of $\lambda z^{1/3}$. In order to keep the number of terms in Eq. (8) small $f(y)$ has been divided into several regions of arbitrary boundary and the end points of each region matched by extrapolation. The most accurate values of B_n as obtained by this method for various ranges of $\lambda z^{1/3}$ are presented in Table I. The power series

TABLE I

Coefficients in Form Factor Expansion

	$0 < y < 8.3315$	$8.3315 < y < 17.055$	$17.055 < y < 28.358$	$28.358 < y < 43.44$
B_1	$-0.4651391 \times 10^{-2}$	$-0.2325519 \times 10^{-1}$	-0.5275558	$+0.7303232$
B_2	$+0.1341269$	$+0.1960111$	$+0.3077992$	$+0.1118552 \times 10^{-1}$
B_3	$+0.4060494 \times 10^{-1}$	$-0.2398459 \times 10^{-1}$	$-0.3137939 \times 10^{-1}$	$-0.1844897 \times 10^{-3}$
B_4	$-0.2931862 \times 10^{-1}$	$+0.1941663 \times 10^{-2}$	$+0.1822472 \times 10^{-2}$	$+0.119529 \times 10^{-5}$
B_5	$+0.7975116 \times 10^{-2}$	$-0.9880399 \times 10^{-4}$	$-0.6113297 \times 10^{-4}$	
B_6	$+0.1145700 \times 10^{-2}$	$-0.2843516 \times 10^{-5}$	$+0.1106595 \times 10^{-5}$	
B_7	$+0.8483009 \times 10^{-4}$	$-0.3517119 \times 10^{-7}$	$-0.8390942 \times 10^{-8}$	
B_8	$-0.2543356 \times 10^{-5}$	—	—	

expansion of $f(y)$ is justified because we are using least-square fit and it is known that the most appropriate least-square polynomial approximation to a function $f(y)$ must have two characteristics: (1) it must be of sufficiently high degree so that the approximating polynomial provides a good approximation to the true function, but (2) it must not be of so high a degree that it fits the observed data too closely in the sense that the "noise" or inaccuracies in the observed data are retained in the least-square approximation.

It should be noted that the analytic solutions of $\phi(x)$ [5, 8–10] give form factors that differ from the form factor obtained using numerical values for $\phi(x)$ [7] for large values of $\lambda z^{1/3}$. Our polynomial fit corresponds to the use of the numerical solution for $\phi(x)$.

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