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Note on the Atomformfactor Calculated from the THOMAS-FERMI Model

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Using the ROZENTAL approximate formula for the THOMAS-FERMI function, the dependence of the atomformfactor of the TF atom on atomic number as well as on $(\sin \theta)/\lambda$ was expressed in closed form by elementary function.

Since the exact values of the THOMAS-FERMI function $\varphi(x)$ are given only for the discrete values of argument x , the evaluation of the atomformfactor of the TF atom of atomic number Z :

$$F(Z, \kappa) = \int_0^\infty \frac{\sin 4\pi\kappa r}{4\pi\kappa r} \rho \, 4\pi r^2 dr, \quad (1)$$

$$= Z \left[1 - 4\pi\kappa\mu \int_0^\infty \sin 4\pi\kappa\mu x \cdot \varphi(x) dx \right], \quad (2)$$

where $\kappa \equiv (\sin \theta)/\lambda$ and μ is the TF unit, was carried out by BRAGG and WEST⁽¹⁾ in such a way as *exact* values are taken for φ and the integral is *approximated* by sum. The results can be given naturally only in tabular form, so that its dependence on Z as well as on κ is at first sight not clear except the similarity rule that the F -curve for an atom Z_0 is transformed so as to be suitable for any other atom Z by multiplying F and κ by Z/Z_0 and $(Z/Z_0)^{1/3}$ respectively. Moreover, owing to the oscillating nature of sine, it is necessary to take the summation in as small steps as possible.

Hence it is worthwhile to consider an alternative way, i. e. *approximation* for φ and *exact* performance of integral. Along this line B. v. SZ. NAGY⁽²⁾ took for ρ in Eq. (1) the JENSEN approximate formula, but the results cannot be expressed by elementary function. When we start from Eq. (2), on the other hand, the ROZENTAL⁽³⁾ approximate formulae for φ in 2 and 3 terms:

$$\varphi^{(2)} = 0.7345 e^{-0.562x} + 0.2655 e^{-3.392x}, \quad (3)$$

$$\varphi^{(3)} = 0.255 e^{-0.246x} + 0.581 e^{-0.947x} + 0.164 e^{-4.356x}, \quad (4)$$

are more advantageous than the well-known SOMMERFELD⁽⁴⁾ asymptotic formula on account of the accuracy in small x 's which contribute mainly to the integral and of the possibility of the analytical integration by the simple relation:

$$\int_0^\infty e^{-px} \sin qx \, dx = \frac{q}{p^2 + q^2}.$$

Eqs. (3) and (4) afford from Eq. (2) the dependence of the atomformfactor on Z as well as κ (λ in 10^{-8} cm) in closed form by elementary function:

$$F^{(2)} = Z \left[1 - \kappa^2 \left(\frac{0.7345}{\kappa^2 + 0.009112 Z^{2/3}} + \frac{0.2655}{\kappa^2 + 0.3319 Z^{2/3}} \right) \right], \quad (5)$$

$$F^{(3)} = Z \left[1 - \kappa^2 \left(\frac{0.255}{\kappa^2 + 0.001746 Z^{2/3}} + \frac{0.581}{\kappa^2 + 0.02587 Z^{2/3}} + \frac{0.164}{\kappa^2 + 0.5474 Z^{2/3}} \right) \right], \quad (6)$$

respectively, where the value $a_0 = 0.52920 \cdot 10^{-8}$ cm⁽⁵⁾ is adopted. The atomformfactor per electron, i. e. the bracketed expression above, is obviously a function of $\xi \equiv \kappa Z^{-1/3}$ alone, as BETHE⁽⁶⁾ pointed out. For small values of ξ , F is quadratic in κ :

$$F^{(2)}(\xi \ll 1) = Z[1 - \kappa^2 Z^{-2/3} 81.41], \quad (7)$$

$$F^{(3)}(\xi \ll 1) = Z[1 - \kappa^2 Z^{-2/3} 168.81], \quad (8)$$

while according to BETHE the exact evaluation of $\int_0^\infty x \varphi(x) dx$ results

$$F_{\text{exact}}(\xi \ll 1) = Z[1 - \kappa^2 Z^{-2/3} 160]. \quad (9)$$

For large values of ξ , F vanishes inverse-quadratically in κ :

$$F^{(2)}(\xi \gg 1) = \kappa^{-2} Z^{5/3} 0.09481, \quad (10)$$

$$F^{(3)}(\xi \gg 1) = \kappa^{-2} Z^{5/3} 0.10525. \quad (11)$$

In TABLE I the values by Eqs. (5) and (6) are compared to the standard values given by BRAGG and WEST.

TABLE I. Values of the atomformfactor for Cs ($Z=55$) by Eqs. (5) and (6), and their deviations from the standard values given by BRAGG and WEST.

$(\sin \theta)/\lambda \text{ \AA}^{-1}$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
BRAGG & WEST	50.7	43.8	37.6	32.4	28.7	25.8	23.2	20.8	18.8	17.0
Eq. (5)	52.1	45.5	38.3	32.4	27.8	24.4	21.8	19.8	18.1	16.8
Eq. (5) - BW*	1.4	1.7	0.7	0.0	-0.9	-1.4	-1.4	-1.0	-0.7	-0.2
Eq. (6)	50.2	43.3	37.8	33.1	29.2	25.8	23.0	20.7	18.7	17.1
Eq. (6) - BW	-0.5	-0.5	0.2	0.7	0.5	0.0	-0.2	-0.1	-0.1	0.1

$(\sin \theta)/\lambda \text{ \AA}^{-1}$	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0
BRAGG & WEST	15.6	14.5	13.2	12.3	11.3	10.4	9.6	9.2	8.6	8.1
Eq. (5)	15.6	14.6	13.7	12.9	12.2	11.5	10.9	10.3	9.8	9.3
Eq. (5) - BW	0.0	0.1	0.5	0.6	0.8	1.1	1.3	1.1	1.2	1.2
Eq. (6)	15.7	14.5	13.4	12.5	11.7	11.0	10.4	9.8	9.3	8.8
Eq. (6) - BW	0.1	0.0	0.2	0.2	0.4	0.6	0.8	0.6	0.7	0.7

* BW denotes the value of BRAGG & WEST.

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