positional parameters), but to the poor quality of the intensity measurements as a result of the absorption effects. The standard deviations of the atomic positions indicate that the carbon atom has been located rather imprecisely in the presence of the heavier I and As atoms.

The arsenic atom has the usual pyramidal configuration. The As–I distance (2·54 ± 0·01 Å) is similar to corresponding lengths in AsI_3 (2·52 Å), Me_2AsI (2·54 Å), and Ph_2AsI (2·53 Å) (*Tables of Interatomic Distances and Configuration in Molecules and Ions*, 1958; Trotter, 1963). The I–As–I angle (104° ± 0·4°) is a little larger than the angles in AsI_3 (*Tables of Interatomic Distances and Configuration in Molecules and Ions*, 1958). Bonds and angles involving the carbon atom have been determined less precisely, and do not differ significantly from normal values.

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Calculation of Atomic Scattering Factors for the Helium Atom by means of the Six-Term Hylleraas Wave Function

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Atomic scattering factors have been calculated for the helium atom by means of the six-term Hylleraas wave function. The results are in good agreement with the calculations of Matsen and collaborators.

Introduction

In their classic work on the atomic scattering factors, James & Brindley (1931) employed the Hartree self-consistent field wave functions which were then available only for a few atoms. These wave functions were also limited in numerical accuracy owing to the lack of computing facilities at that time. In order to extend their work to other atoms for which the Hartree solutions were then not available, James & Brindley (1931) resorted to an interpolation scheme which has been found to be unreliable in the light of some recent experimental and theoretical developments (McWeeny, 1951; Hoerni & Ibers, 1954; Bacon, 1952; Cochran, 1953).

Recently efforts have been made by Matsen and collaborators to improve upon the values of atomic scattering factors of James & Brindley (Hurst, Miller & Matsen, 1958; Hurst & Matsen, 1959; Silverman, Platas & Matsen, 1960; Hurst, 1960). These authors have also studied the effects of radial and angular correlation on the form factor. The effects of aspherical charge distributions on the scattering factor have been studied by McWeeny (1951) and Freeman (1959). In this paper, calculations have been made on the scattering factor for the helium atom by means of the six-term Hylleraas wave function.

The Hylleraas wave function, which is essentially an expansion in terms of the positions of electrons from each other and the nucleus, is given by (Hylleraas, 1929; Bethe & Salpeter, 1957):

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$$\varphi(ks, kt, ku) = \exp[-ks/2] \sum_{l,n,m=0}^{\infty} C_{n,2l,m} s^n t^{2l} u^m (k)^{n+2l+m} . \quad (1)$$

Taking the first six terms of this expression, the Hylleraas wave function without the normalization constant may be written as

$$\psi = \exp[-\alpha s][1 + c_1 u + c_2 t^2 + c_3 s + c_4 s^2 + c_5 u^2] X(1,2) \quad (2)$$

where

$$s = r_1 + r_2 \quad (2a)$$

$$u = r_{12} \quad (2b)$$

$$t = r_2 - r_1 \quad (2c)$$

and $X(1, 2)$ is the antisymmetric spin function given by

$$X(1,2) = 1/(\sqrt{2})[\alpha(1)\beta(2) - \alpha(2)\beta(1)] . \quad (2d)$$

Theory

The scattering factors are computed from (James, 1948)

$$f = \frac{\int \psi^* \left[\sum_{k=1}^{2} \exp[(i\mu r_k \cos\theta_k)] \right] \psi d\tau}{N} \quad (3a)$$

where

$$\mu = 4\pi \sin\theta/\lambda \quad (3b)$$

$$N = \int \psi^* \psi d\tau . \quad (3c)$$

Here θ is the Bragg angle and θ_k is the co-latitude angle of the kth electron and λ is the wavelength of the X-ray beam.

Substitution of equation (2) in (3a) and summation over the spin coordinate gives

$$\begin{aligned} f = \frac{1}{N}[&k_{0,0}(\mu,\alpha) + c_1^2 k_{0,2}(\mu,\alpha) + c_2^2 k_{4,0}(\mu,\alpha) + c_5^2 k_{0,4}(\mu,\alpha) \\ &+ 2c_1 k_{0,1}(\mu,\alpha) + 2c_2 k_{2,0}(\mu,\alpha) + 2c_5 k_{0,2}(\mu,\alpha) \\ &+ 2c_1 c_2 k_{2,1}(\mu,\alpha) + 2c_1 c_5 k_{0,3}(\mu,\alpha) + 2c_4 L_{2,0}(\mu,\alpha) \\ &+ 2c_2 c_3 L_{1,2}(\mu,\alpha) + 2c_2 c_4 L_{2,2}(\mu,\alpha) + 2c_3 c_4 L_{3,0}(\mu,\alpha) \\ &+ 2c_2 c_5 k_{2,2}(\mu,\alpha) + c_3^2 L_{2,0}(\mu,\alpha) + c_4^2 L_{4,0}(\mu,\alpha) \\ &+ 2c_3 L_{1,0}(\mu,\alpha) + 2c_1 c_3 N_{1,1}(\mu,\alpha) + 2c_1 c_4 N_{2,1}(\mu,\alpha) \\ &+ 2c_3 c_5 N_{1,2}(\mu,\alpha) + 2c_4 c_5 N_{2,2}(\mu,\alpha)] \end{aligned} \quad (4)$$

where $k_{l,m}(\mu,\alpha)$, $L_{p,q}(\mu,\alpha)$ and $N_{a,b}(\mu,\alpha)$ are defined by

$$k_{l,m}(\mu,\alpha) = 2\int e^{(-2\alpha s + i\mu r_1 \cos\theta_1)} t^l u^m d\tau \quad (5a)$$

$$L_{p,q}(\mu,\alpha) = 2\int e^{(-2\alpha s + i\mu r_1 \cos\theta_1)} s^p t^q d\tau \quad (5b)$$

$$N_{a,b}(\mu,\alpha) = 2\int e^{(-2\alpha s + i\mu r_1 \cos\theta_1)} s^a u^b d\tau \quad (5c)$$

and as shown by Hurst (1960)

$$d\tau = 4\pi^2 r_1 dr_1 r_2 dr_2 r_{12} dr_{12} \sin\theta_1 d\theta_1 . \quad (5d)$$

Integral (5a) has already been evaluated by Hurst (1960). In this paper, Hurst's procedure has been followed to evaluate (5b) and (5c).

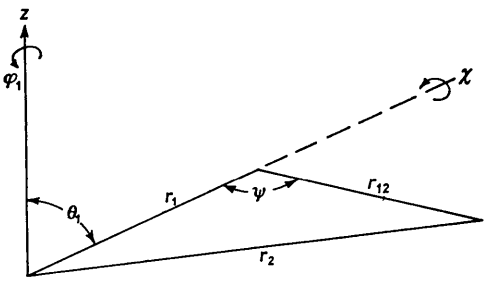

Fig. 1. Scattering factor for helium.

All the various $k_{l,m}(\mu,\alpha)$, $L_{p,q}(\mu,\alpha)$ and $N_{a,b}(\mu,\alpha)$ which occur in equation (4) are given below:

(1) $k_{0,0}(\mu,\alpha) = 32\pi^2[g_1(\alpha,\mu)h_2(\alpha)]$.

(2) $k_{0,1}(\mu,\alpha) = 32\pi^2[g_2(\alpha,\mu)h_2(\alpha) + (1/3)g_0(\alpha,\mu)h_4(\alpha) - (1/3)g_1(2\alpha,\mu)h_3(\alpha) - (1/3)g_0(2\alpha,\mu)h_4(\alpha)]$.

(3) $k_{0,2}(\mu,\alpha) = 32\pi^2[g_3(\alpha,\mu)h_2(\alpha) + g_1(\alpha,\mu)h_4(\alpha)]$.

(4) $k_{0,3}(\mu,\alpha) = 32\pi^2[g_4(\alpha,\mu)h_2(\alpha) + 2g_2(\alpha,\mu)h_4(\alpha) + (1/5)g_0(\alpha,\mu)h_6(\alpha) - (1/5)g_1(2\alpha,\mu)h_5(\alpha) - (1/5)g_0(2\alpha,\mu)h_6(\alpha)]$.

(5) $k_{0,4}(\mu,\alpha) = 32\pi^2[g_1(\alpha,\mu)h_6(\alpha) + (10/3)g_3(\alpha,\mu)h_4(\alpha) + g_5(\alpha,\mu)h_2(\alpha)]$.

(6) $k_{2,0}(\mu,\alpha) = 32\pi^2[g_3(\alpha,\mu)h_2(\alpha) - 2g_2(\alpha,\mu)h_3(\alpha) + g_1(\alpha,\mu)h_4(\alpha)]$.

(7) $k_{2,1}(\mu,\alpha) = 32\pi^2[g_4(\alpha,\mu)h_2(\alpha) - 2g_3(\alpha,\mu)h_3(\alpha) + (4/3)g_2(\alpha,\mu)h_4(\alpha) - (2/3)g_1(\alpha,\mu)h_5(\alpha) + (1/3)g_0(\alpha,\mu)h_6(\alpha) - (1/3)g_1(2\alpha,\mu)h_5(\alpha) - (1/3)g_0(2\alpha,\mu)h_6(\alpha)]$.

(8) $k_{2,2}(\mu,\alpha) = 32\pi^2[g_1(\alpha,\mu)h_6(\alpha) + 2g_3(\alpha,\mu)h_4(\alpha) - 2g_2(\alpha,\mu)h_5(\alpha) - 2g_4(\alpha,\mu)h_3(\alpha) + g_5(\alpha,\mu)h_2(\alpha)]$.

(9) $k_{4,0}(\mu,\alpha) = 32\pi^2[g_5(\alpha,\mu)h_2(\alpha) - 4g_4(\alpha,\mu)h_3(\alpha) + 6g_3(\alpha,\mu)h_4(\alpha) - 4g_2(\alpha,\mu)h_5(\alpha) + g_1(\alpha,\mu)h_6(\alpha)]$.

(10) $L_{1,0}(\mu,\alpha) = 32\pi^2[g_1(\alpha,\mu)h_3(\alpha) + g_2(\alpha,\mu)h_2(\alpha)]$.

(11) $L_{2,0}(\mu,\alpha) = 32\pi^2[g_1(\alpha,\mu)h_4(\alpha) + 2g_2(\alpha,\mu)h_3(\alpha) + g_3(\alpha,\mu)h_2(\alpha)]$.

(12) $L_{3,0}(\mu,\alpha) = 32\pi^2[g_1(\alpha,\mu)h_5(\alpha) + 3g_2(\alpha,\mu)h_2(\alpha) + 3g_3(\alpha,\mu)h_3(\alpha) + g_4(\alpha,\mu)h_2(\alpha)]$.

(13) $L_{4,0}(\mu,\alpha) = 32\pi^2[g_1(\alpha,\mu)h_6(\alpha) + 4g_2(\alpha,\mu)h_5(\alpha) + 6g_3(\alpha,\mu)h_4(\alpha) + 4g_4(\alpha,\mu)h_3(\alpha) + g_5(\alpha,\mu)h_2(\alpha)]$.

(14) $L_{1,2}(\mu,\alpha) = 32\pi^2[g_1(\alpha,\mu)h_5(\alpha) - g_2(\alpha,\mu)h_4(\alpha) - g_3(\alpha,\mu)h_3(\alpha) + g_4(\alpha,\mu)h_2(\alpha)]$.

(15) $L_{2,2}(\mu,\alpha) = 32\pi^2[g_1(\alpha,\mu)h_6(\alpha) - 2g_3(\alpha,\mu)h_4(\alpha) + g_5(\alpha,\mu)h_2(\alpha)]$.

(16) $N_{1,1}(\mu,\alpha) = 32\pi^2[g_2(\alpha,\mu)h_3(\alpha) + g_3(\alpha,\mu)h_2(\alpha) + (1/3)g_1(\alpha,\mu)h_4(\alpha) + (1/3)g_0(\alpha,\mu)h_5(\alpha) - (2/3)g_2(2\alpha,\mu)h_3(\alpha) - (1/3)g_1(2\alpha,\mu)h_4(\alpha) - (1/3)g_0(2\alpha,\mu)h_5(\alpha)]$.

(17) $N_{1,2}(\mu,\alpha) = 32\pi^2[g_1(\alpha,\mu)h_5(\alpha) + g_2(\alpha,\mu)h_4(\alpha) + g_3(\alpha,\mu)h_3(\alpha) + g_4(\alpha,\mu)h_2(\alpha)]$.

$$(18)\ N_{2,1}(\mu,\alpha)=32\pi^2[(4/3)g_2(\alpha,\mu)h_4(\alpha)+2g_3(\alpha,\mu)h_3(\alpha)+g_4(\alpha,\mu)h_2(\alpha)+(1/3)g_0(\alpha,\mu)h_6(\alpha)+(2/3)g_1(\alpha,\mu)h_5(\alpha)-(4/3)g_3(2\alpha,\mu)h_3(\alpha)-(8/3)g_2(2\alpha,\mu)h_4(\alpha)-(5/3)g_1(2\alpha,\mu)h_5(\alpha)-(1/3)g_0(2\alpha,\mu)h_6(\alpha)].$$

$$(19)\ N_{2,2}(\mu,\alpha)=32\pi^2[g_1(\alpha,\mu)h_6(\alpha)+2g_2(\alpha,\mu)h_5(\alpha)+2g_3(\alpha,\mu)h_4(\alpha)+2g_4(\alpha,\mu)h_3(\alpha)+g_5(\alpha,\mu)h_2(\alpha)].$$

$$(20)\ g_n(\alpha,\mu)=1/\mu\int_0^\infty \exp[-2\alpha r]r^n\sin\mu r\,dr = \frac{Im}{\mu}\left(\frac{(2\alpha+i\mu)^{n+1}n!}{(4\alpha^2+\mu^2)^{n+1}}\right).$$

$$(21)\ h_n(\alpha)=\int_0^\infty \exp[-2\alpha r]r^n dr=\frac{n!}{(2\alpha)^{n+1}}.$$

In order to obtain the value of the normalization constant we put $f=2$ at $\mu=0$ in equation (4). Expressions (1), (2), (3), (6), (7) and (9) have also been derived by Hurst (1960).

To summarize, the atomic scattering factors are calculated from equation (4). The parameters α, c_1, c_2, c_3, c_4 and c_5 are taken from Slater (1960). All the computations were performed on a Marchant calculating machine and were checked by independent calculations. The values of the scattering factors are listed in Table 1.

Table 1. *Comparison of atomic scattering factors for helium*

$\sin\theta/\lambda$	Present work	Hurst (1960)	Womack (1961)	Hurst (1958)
0 Å^{-1}	2·0000	2·0000	2·0000	2·0000
0·025	1·9891	1·9892	1·9891	1·9887
0·050	0·9570	1·9573	1·9572	1·9553
0·075	1·9054	1·9060	1·9057	1·9020
0·100	1·8368	1·8378	1·8373	1·8316
0·200	1·4596	1·4612	1·4602	1·4521
0·300	1·0601	1·0607	1·0598	1·0584
0·400	0·73807	0·73877	0·7380	0·7424
0·500	0·50790	0·50949	0·5089	0·5147
0·600	0·35249	0·35351	0·3530	0·3577
0·700	0·24785	0·24855	0·2482	0·2511
0·800	0·17749	0·17759	0·1773	0·1787
0·900	0·12904	0·12904	0·1289	0·1292
1·000	0·09543	0·09533	0·09523	0·09499
1·100	0·07155	0·07155	0·07149	0·07092
1·200	0·05452	0·05452	0·05448	0·05376
1·300	0·04212	0·04210	0·04210	0·04134
1·400	0·03296	0·03294	0·03296	...
1·500	0·02610	0·02609	0·02611	...

Results

Atomic scattering factors for the helium atom have been calculated in the range

$$0 \le \sin\theta/\lambda \le 1{\cdot}5$$

at intervals of 0·025 up to 0·1 and at intervals of 0·1 upto 1·5.

From inspection of Table 1 it is evident that our values of the atomic form factor for the helium atom are in close agreement with the values of Hurst (1960), who used the three-term Hylleraas wave function. The agreement with the results of Womack, Silverman & Matsen (1961) and Hurst, Miller & Matsen (1958) is also good.

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