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Atomic scattering factors of helium-like systems from analytic Hartree-Fock wave functions.

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Recently Hurst, Miller & Matsen (1958) and Womack, Silverman & Matsen (1961) have calculated atomic scattering factors for the two-electron systems, H^- through C^{4+}, using the radial-correlated wave analytic wave functions of Shull & Löwdin (1956) and the analytical self consistent field (SCF) functions of Roothan, Sachs & Weiss (1960). Similar calculations on atomic scattering factors have also been made by Freeman (1959), Hurst (1960) and Rustgi, Shukla & Tripathi (1963). In the present note, atomic scattering factors of He and the helium-like ions have been calculated by means of the less elaborate wave functions of Green, Mulder, Lewis & Woll (1954) and the results have been compared with the already published results.

The scattering factors are calculated from (James, 1948)

$$f=\frac{1}{N}\int \Psi^*\{\sum_k \exp\,[i\mu r_k\cos\theta_k]\}\Psi d\tau\,, \qquad (1\cdot1)$$

where

$$\mu=\frac{4\pi\sin\theta}{\lambda} \qquad (1\cdot2)$$

$$N=\int \Psi^*\Psi d\tau \qquad (1\cdot3)$$

$$d\tau=d\tau_1 d\tau_2 \qquad (1\cdot4)$$

$$d\tau_k=r_k^2 dr_k \sin\theta_k d\theta_k d\varphi_k\,. \qquad (1\cdot5)$$

The $1S$ normalized wave function used in the calculation is

$$\Psi=\psi(1)\psi(2)x(1,\,2) \qquad (2\cdot1)$$

where $x(1, 2)$ is the antisymmetric spin function given by

$$x(1,\,2)=\frac{1}{\sqrt{2}}[\alpha(1)\beta(2)-\alpha(2)\beta(1)] \qquad (2\cdot2)$$

and following Green *et al.* (1954),

$$\psi(j)=\frac{1}{\sqrt{(4\pi)}}Nr_j(\exp\,[-zr_j]+c\exp\,[-kzr_j])\,. \qquad (2\cdot3)$$

The parameters N, c, z, and k have been determined by Green *et al.* for H^-–C^{4+}. The expression for the scattering factor is found to be

Table 1. *Scattering factors computed from analytical SCF wave functions of Green et al.* (1954)

$\sin\theta/\lambda$ (Å^{-1})	H^-	He	Li^+	Be^{2+}	B^{3+}	C^{4+}
0	2·0000	2·0000	2·0000	2·0000	2·0000	2·0000
0·025	1·9192	1·9892	1·9959	1·9979	1·9987	1·9991
0·050	1·7116	1·9572	1·9837	1·9915	1·9948	1·9965
0·075	1·4499	1·9058	1·9636	1·9809	1·9883	1·9921
0·100	1·1936	1·8375	1·9361	1·9663	1·9793	1·9860
0·125	0·9707	1·7555	1·9015	1·9477	1·9677	1·9781
0·150	0·7872	1·6631	1·8606	1·9254	1·9538	1·9686
0·175	0·6393	1·5638	1·8140	1·8995	1·9375	1·9575
0·200	0·5209	1·4608	1·7625	1·8703	1·9190	1·9448
0·225	0·4263	1·3569	1·7069	1·8380	1·8983	1·9305
0·250	0·3503	1·2544	1·6480	1·8030	1·8756	1·9147
0·275	0·2893	1·1552	1·5866	1·7655	1·8510	1·8975
0·300	0·2400	1·0604	1·5233	1·7258	1·8246	1·8790
0·325	0·2000	0·9709	1·4590	1·6842	1·7966	1·8591
0·350	0·1675	0·8873	1·3943	1·6410	1·7671	1·8380
0·375	0·1409	0·8098	1·3296	1·5965	1·7362	1·8158
0·400	0·1191	0·7384	1·2656	1·5510	1·7042	1·7925
0·425	0·1012	0·6729	1·2027	1·5047	1·6710	1·7681
0·450	0·08628	0·6131	1·1412	1·4579	1·6369	1·7429
0·475	0·07391	0·5586	1·0815	1·4109	1·6020	1·7168
0·500	0·06358	0·5090	1·0236	1·3639	1·5665	1·6899
0·550	0·04762	0·4234	0·9145	1·2705	1·4940	1·6342
0·600	0·03622	0·3530	0·8146	1·1792	1·4203	1·5764
0·650	0·02794	0·2954	0·7242	1·0910	1·3465	1·5171
0·700	0·02184	0·2481	0·6430	1·0068	1·2732	1·4567
0·750	0·01727	0·2093	0·5707	0·9271	1·2011	1·3960
0·800	0·01382	0·1773	0·5065	0·8523	1·1308	1·3352
0·850	0·01117	0·1508	0·4497	0·7824	1·0627	1·2749
0·900	0·009115	0·1288	0·3996	0·7176	0·9972	1·2154
0·950	0·007504	0·1105	0·3554	0·6576	0·9344	1·1570
1·000	0·006228	0·09517	0·3165	0·6024	0·8746	1·0999
1·100	0·004388	0·07145	0·2522	0·5054	0·7643	0·9909
1·200	0·003173	0·05445	0·2022	0·4242	0·6662	0·8894
1·300	0·002348	0·04208	0·1633	0·3567	0·5800	0·7961
1·400	0·001772	0·03294	0·1328	0·3007	0·5047	0·7112
1·500	0·001362	0·02610	0·1087	0·2543	0·4393	0·6346

$$f = 8N^2 z \left[\frac{1}{(4z^2+\mu^2)^2} + \frac{kc^2}{(4k^2z^2+\mu^2)^2} + \frac{c(1+k)}{[z^2(1+k)^2+\mu^2]^2} \right] . \qquad (3{\cdot}1)$$

The computed scattering factors are listed in Table 1. On comparison, it is found that the scattering factors obtained in this note are in perfect agreement for Li^+–C^{4+} with the results of Womack *et al.*, obtained from a much more elaborate calculation. They differ for H^- and He but the maximum deviation is 0·0007 electron for both the systems. The present work indicates that relatively good scattering factors can be obtained from relatively poor wave functions in support of Ibers's (1959) observation.

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χ Phase in a niobium-rhenium alloy.

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Introduction

The χ phase of Nb–Re is isomorphous with α Mn. It is cubic, with space group $I\bar{4}3m$, and the 58 atoms in the unit cell occupy four crystallographically distinct sites. Greenfield & Beck (1956) were unable to conclude from their X-ray diffraction data whether there is ordering among these sites, but Niemiec & Trzebiatowski (1956) found that the intensities of two low-angle powder arcs were consistent with an ordered distribution. A single-crystal investigation was undertaken to obtain further evidence.

Experimental

The specimen had the composition Nb 25 at.%–Re 75 at.% and had been annealed in an argon arc furnace at 2200 °C for two hours.

The large linear absorption coefficient of 1660 cm^{-1} for molybdenum radiation necessitates the use of a small crystal, and a fragment of cross section 0·01 × 0·04 mm was selected. The lattice parameter was determined by the method of Farquahar & Lipson (1946). The value obtained ($a = 9{\cdot}692 \pm 0{\cdot}002$ Å) was larger than the values given by Knapton (1958) ($a = 9{\cdot}683$ Å) and Niemiec & Trzebiatowski ($a = 9{\cdot}676$ Å) for an alloy of the same composition. To check that the fragment was representative, the lattice parameter was determined from powder data, a 9 cm diameter camera and Cu $K\alpha$ radiation being used, and the value obtained was $9{\cdot}693 \pm 0{\cdot}001$ Å. The calculated density is 17·2 $g.cm^{-3}$; the measured density was $17{\cdot}6 \pm 0{\cdot}3$ $g.cm^{-3}$.

A zero-layer Weissenberg photograph was taken with Mo $K\alpha$ radiation with the use of a multiple-film pack, and the spots were integrated slightly to facilitate the measurement of intensities. After an exposure time of 190 hours, only 63 (40%) of the independent reflexions within the limiting sphere were recorded, 28 of these being so faint that their measurement was considered unsatisfactory. The structure refinement was carried out with the remaining 35 reflexions, the intensities of which were measurable with an uncertainty of less than 15%. Corrections for absorption, which were essential, were computed by the method of Rogers & Moffett (1956), and these varied by a factor of three over the range within which data were collected.

Structure determination

The four groups of sites in the α Mn structure are defined by five parameters, as shown in Table 1. Sites *a* and *c* have coordination number (C.N.) 16, and the D_1 and D_2 sites have C.N. 13 and 12 respectively.

Table 1. *Parameters defining sites in the* α Mn *structure*

Multiplicity		Parameters			
		α Mn		χ phase Nb–Re	
2(*a*)		—	—	—	—
8(*c*)		$x = 0{\cdot}317$		$x = 0{\cdot}314$	
24(*g*)	D_1	$x = 0{\cdot}356$	$z = 0{\cdot}042$	$x = 0{\cdot}360$	$z = 0{\cdot}040$
	D_2	$x = 0{\cdot}089$	$z = 0{\cdot}278$	$x = 0{\cdot}096$	$z = 0{\cdot}277$

In accordance with the alloy composition, the unit cell contains 14·5 atoms of niobium and 43·5 of rhenium. Structure factors were first computed for the arrangements A and B of Table 2, the fractional coordinates given by Bradley & Thewlis (1927) for α Mn being used;