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New atomic form factors for beryllium and boron.

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Improved calculations of atomic fields for several atoms have recently become available: Kibartas, Kavetskis & Iutsis (1955) have carried out a three-configuration Hartree–Fock self-consistent field calculation for beryllium; Glembotskii, Kibartas & Iutsis (1955) have carried out a similar two-configuration calculation for boron. The multiple-configuration method considers the interaction of various configurations of the atom and is an extension of the usual Hartree–Fock single-configuration approximation. In essence, by this technique, account is taken of electron correlation, the effects of which are neglected in the more approximate single-configuration method. For the following reasons it is of interest to obtain the atomic form factors from these new field approximations. The results for beryllium may be compared with the calculations of Berghuis *et al.* (1955) for beryllium, which were based on the single-configuration approximation. The effect of electron correlation on the atomic form factor of a light atom may thus be assessed. This is important since the most recent form-factor calculations for other light atoms (Hoerni & Ibers, 1954; Berghuis *et al.*, 1955) are based on single-configuration field approximations. The results for boron are of interest, for no other form-factor calculations for boron based on the Hartree–Fock approximation are available.

The atomic form factors for beryllium and boron are given in Table 1. They were obtained by integration of the radial distribution functions given by Iutsis and his coworkers. The details and methods used in carrying out such numerical integrations have been described previously (Hoerni & Ibers, 1954). For these particular calculations the following intervals in r (in atomic units) were employed:

0·000 (0·005) 0·300; 0·300 (0·050) 4·000; 4·000 (0·500) 9·000 .

When necessary, interpolation of the radial distribution functions was done graphically. The computations were carried out on the Shell Development Company Datatron.

Table 1. *Atomic form factors for beryllium and boron*

(Values in electrons)

$\sin\theta/\lambda$	f_{Be}	f_B	$\sin\theta/\lambda$	f_{Be}	f_B
0·00	4·000	5·000	0·50	1·367	1·534
0·05	3·706	4·726	0·60	1·201	1·406
0·10	3·067	4·066	0·70	1·031	1·276
0·15	2·469	3·325	0·80	0·878	1·147
0·20	2·067	2·711	0·90	0·738	1·016
0·25	1·838	2·276	1·00	0·620	0·895
0·30	1·705	1·993	1·10	0·519	0·783
0·35	1·613	1·813	1·20	0·432	0·682
0·40	1·531	1·692	1·30	0·365	0·596

The results for beryllium are in excellent agreement with the form factors obtained by Berghuis *et al.* (1955) from the single-configuration approximation to the atomic field. The maximum deviation of 0·013 electrons in the form factors is probably not significant in view of differences in the calculational techniques employed, and particularly in view of the errors inherent in the interpolation of the radial distribution functions. (The third decimal place in the form factors in Table 1 is not significant, and is given only as an aid to interpolation.) Thus for beryllium, and presumably for other light atoms, electron correlation does not affect the form factors to an extent which can be detected experimentally.

The results for boron are in good agreement with the $\bar{f}$ values derived by McWeeny (1951) from variational wave functions. The maximum deviation is about 0·05 electrons. The results in Table 1 for boron, since they are derived from less approximate atomic fields, are in principle superior to those of McWeeny. However, the differences are probably not detectable experimentally.

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Der strukturelle Zusammenhang zwischen γ- und ε-Phase im System Kupfer–Zinn.

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Vorangegangene Untersuchungen (Hendus & Knödler, 1956) haben gezeigt, dass die kubisch raumzentrierte γ-Hochtemperaturphase im System Kupfer–Zinn geordnet ist und bei der Zusammensetzung Cu_3Sn die Überstruktur des Fe_3Al-Gitters besitzt. Die Gitterkonstante wurde für Cu_3Sn bei 700° C. zu $a_\gamma = 2a_0^* = 6{,}116_6$ Å bestimmt.

* a_0 = Gitterkonstante des kubisch raumzentrierten Gitters bei statistischer Atomverteilung.