involving hydrogen are shown in Fig. 1; bond lengths related by the molecular symmetry are seen to agree closely.

The C–S–C bond angles (104·2 ± 1·4° and 100·6 ± 1·3°) and S–C bond lengths are within experimental error of the angle of about 105° and distance of 1·82 Å reported for $(CH_3)_2S$ by Brockway & Jenkins (1936). The S–B bond lengths are what would be expected for a normal covalent bond.

The decaborane structure has four hydrogens bridging the pairs B5–B6, B6–B7, B8–B9, B9–B10; both $B_{10}H_{12}[S(CH_3)_2]_2$ and $B_{10}H_{12}(CH_3CN)_2$ have just the two bridges B5–B10 and B7–B8. Although the corresponding distances in the two derivatives are very similar, they differ significantly from the distances in decaborane. However, the average of the 21 B–B bond lengths is 1·809 Å for $B_{10}H_{12}[S(CH_3)_2]_2$ and 1·792 Å for both $B_{10}H_{12}(CH_3CN)_2$ and $B_{10}H_{14}$. The average length of our 10 terminal B–H bonds is 1·18 Å, which is 0·08 Å greater than the corresponding average for $B_{10}H_{12}(CH_3CN)_2$ and 0·08 Å less than for decaborane.

Table 3 demonstrates the C_{2v} symmetry of the decaborane skeleton. The deviations of the $(CH_3)_2S$ groups from this symmetry may perhaps be attributed to steric effects. Reddy & Lipscomb (1959) have discussed the valence structure of $B_{10}H_{12}(CH_3CN)_2$ in terms of the topological theory of boron hydrides (Dickerson & Lipscomb, 1957). The structure is compatible with this representation if it is regarded as a substitution derivative of the $B_{10}H_{14}^{-2}$ ion, which has C_{2v} symmetry. Reddy & Lipscomb have suggested a possible mechanism for the reaction of an electron donor with this ion.

The arrangement of $B_{10}H_{12}[S(CH_3)_2]_2$ molecules in the monoclinic unit cell is shown in Fig. 2.

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Short Communications

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Atomic scattering amplitudes for electrons for some of the lighter elements.

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New values of atomic scattering amplitudes, $f_{el}(s)$ $(s = \sin\theta/\lambda)$, in the first Born approximation, have recently been derived for the neutral atoms Al to A inclusive by a process of interpolation (Dawson, 1961*a*). The interpolation procedure was concerned primarily with the derivation of values of the mean square radii $\langle r^2\rangle$ of the atomic charge distributions, and it was observed that the main uncertainty in this procedure lay in values of $\langle r^2\rangle_{3p}$ derived from curve *C* (Fig. 1 and Table 1(*B*) of Dawson, 1961*a*). To minimize this uncertainty, the upper (i.e. higher atomic number, *Z*) end of this curve was adjusted to give interpolated total $\langle r^2\rangle$ values for Cl and A in best agreement with the polydetor $\langle r^2\rangle$ result for Cl and the experimental $\langle r^2\rangle$ value for argon. A more critical appraisal of various aspects of the interpolation process is now possible in view of recent Hartree–Fock calculations by Watson & Freeman (1961) for these neutral atoms and by Sachs (1961) for

Na$^+$ and Ne, and we note here the implications of these calculations on the scattering-amplitude data presented earlier.

Table 1. *Comparison of Hartree–Fock and interpolated $\langle r^2\rangle_{3p}$ data*

	Al	Si	P	S	Cl	A
Hartree–Fock*	14·42	9·00	6·40	5·09	4·08	3·35 (3·31)
Interpolated	15·5	9·3	6·3	4·7	3·7	3·1

* From Watson & Freeman's (1961) calculations, except for the value in brackets for A from Dawson (1961*a*).

Table 1 gives a limited comparison of theoretical and interpolated results, for the important $3p$ charge distributions, by comparing $\langle r^2\rangle_{3p}$ data obtained from Watson & Freeman's (1961) calculations with the data interpolated from curve *C*. We see that the value of 15·5 (a.u.)^2 chosen arbitrarily (see Dawson, 1961*a*) for Al is too large and has resulted in a value for Si which is also above the theoretical result, but that otherwise the interpolated values are the smaller, with the greatest fractional difference occurring for Cl. Since the poly-detor $\langle r^2\rangle$ result for this atom was used as a guide, it is desirable to examine the reliability of this guide in the light of the recent Hartree–Fock calculations. If we use the simple energy criterion for assessing the relative merits of the poly-detor and Hartree–Fock calculations for Cl, then Watson & Freeman's (1961) calculation giving a total energy of $-459·4797$ a.u. is apparently preferable to that of Boys & Price (1954) with a total energy of $-458·901$ a.u. However, as Hartree (1957) and Ibers (1959) have observed, this criterion often bears little direct relation to other quantities predicted by different wave-function approximations (e.g. $\langle r^2\rangle$ values, as here); and all we may readily infer from the above comparison is that limitations in the simple basis set used by Boys & Price (1954) have had an adverse effect on the poly-detor total-energy value. A more suitable estimate of the reliability of the poly-detor $\langle r^2\rangle$ guide for Cl is obtained if we extend the poly-detor and Hartree–Fock comparison to Na$^+$ and Ne. In these cases, energy considerations this time favour the poly-detor calculations, since Bernal & Boys' (1952) energy values for Na$^+$ and Ne are $-161·8784$ and $-128·6920$ a.u. respectively while Sachs' (1961) corresponding Hartree–Fock values are $-161·6769$ and $-128·5470$ a.u. However, the significant feature of this lighter-atom comparison is that the poly-detor calculations yield more-compact charge distributions than those from Hartree–Fock calculations (Dawson, 1961*b*), which is in accord with the evidence for Cl in Table 1 above. Since this common feature of poly-detor compactness is also consistent with experimental evidence* that the outer regions of Hartree–Fock charge distributions are somewhat over-diffuse, the usefulness of the poly-detor $\langle r^2\rangle$ guide for Cl therefore still appears to outweight the above adverse energy comparison. Only more-extensive poly-detor calculations will resolve whether a better (in energy) result for Cl gives an $\langle r^2\rangle$ value significantly different from that used in the interpolation process. Meanwhile, the main conclusion to be drawn here is that the major uncertainty in the interpolated total $\langle r^2\rangle$ values as a practical source of $f_{el}(0)$ data occurs probably for Al and Si, and that a more suitable $\langle r^2\rangle_{3p}$ value for Al is that given by Biermann & Lübeck's (1948) result in Table 1(*A*) of Dawson (1961*a*).

At small scattering angles (i.e. $s=0·05$, 0·10, 0·15 Å^{-1}), $f_{el}(s)$ is sensitive to the quantities $(Z-f(s))/s^2$, where $f(s)$ is the X-ray scattering factor, and only small changes in f will produce considerable changes in f_{el}. In A, for example, where the low-angle interpolated f_{el} data were made smaller than the Hartree–Fock data of Ibers (1958) so as to conform with the differences between experimental and Hartree–Fock values of $\langle r^2\rangle$, the differences in f_{el} data for $s=0·05$ and 0·10 Å^{-1} of 3·6 and 2·5% respectively correspond to f differences of 0·11 and 0·25%. The same low trend of interpolated f_{el} values for the other third-row atoms is also found on comparison with Hartree–Fock results given by f-data from Watson & Freeman's (1961) calculations (Freeman, 1961). For the above two s-values, the average (and maximum) differences in f_{el} for all six atoms correspond to differences in f of 0·16 (0·28) and 0·53 (0·81)%. These f-differences are larger than those found between Hartree–Fock and poly-detor f-curves for Na$^+$ and Ne (Dawson, 1961*b*), but a final judgement on whether the low-angle f_{el} data obtained by interpolation have overcompensated for correlation effects neglected in Hartree–Fock treatments of complex atoms must await the derivation of f-data from more-refined calculations.

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* From diamagnetic susceptibility data (see Dawson, 1961*a*), the most recent of which is by Barter, Meisenheimer & Stevenson (1960).