THE CRYSTAL STRUCTURE OF DECABORANE

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The crystal structure of decaborane, $B_{10}H_{14}$, has been determined from single-crystal oscillation photographs, using CoKα x-radiation.

Crystals prepared by sublimation at room temperature, or above, show a high degree of polysynthetic twinning, giving rise to diffuseness of reflections for which h and k are odd. In the untwinned condition, the crystal is monoclinic,[1] but pseudo-orthorhombic, and it is convenient to choose the two-fold axis in the c direction. The space group is then $C_{2h}^4-C11\ 2/a$. With $a_0=14.37$ Å, $b_0=20.98$ Å, $c_0=5.69$ Å, $\beta=90.0°$, the cell contains eight molecules of $B_{10}H_{14}$, and the calculated density is 0.96.

The individual crystals, which make up the actual, highly twinned, crystalline edifice, are so short in the b-direction (a few unit translations, at most) that it is convenient to consider the system as a partially ordered crystal, the disordered state of which is described by a unit cell one-fourth the size of the one mentioned above. The dimensions of this small cell are: $a_0=7.18$ Å, $b_0=10.49$ Å, $c_0=5.69$ Å; and it contains $2B_{10}H_{14}$ or $(1/2\ B)_{20}$ $(1/2\ H)_{28}$. The "disordered" structure based on this cell explains *all* the sharp spots observed—its space-group is $D_{2h}^{12}-P_{nnm}$.

The boron parameters have been established by means of Fourier methods, including a three-dimensional synthesis of the complete unit cell. They have not varied more than $\pm.001$ in the last two refinements. Hydrogen atoms contribute significantly to many reflections, and it appears that all of them are resolved in Fourier sections. However, a total of 18 peaks, each possible for a hydrogen, has been obtained in the electron density functions for the molecule and the 14 hydrogen positions have not been assigned unequivocally at the present time. Consequently, only the boron parameters will be given. They are as follows (for the large unit cell of the ordered structure):

8B at 000; $\frac{1}{2}\frac{1}{2}0$ +
xyz $\quad \frac{1}{2}+x, y, \bar{z}$
$\bar{x}\bar{y}\bar{z}$ $\quad \frac{1}{2}-x, \bar{y}, z$

	x	y	z		x	y	z
B_I	.033	.328	0	B_I'	.217	.078	.500
B_{II}	.109	.276	.142	B_{II}'	.141	.026	.642
B_{III}	.109	.276	−.142	B_{III}'	.141	.026	.358
B_{IV}	.097	.202	0	B_{IV}'	.153	−.048	.500
B_V	.019	.210	.228	B_V'	.231	−.040	.728

The molecules are required by the space group to have only a two-fold axis, but appear to have two mirror-planes as well; thus, they exhibit the symmetry $C_{2v}-mm2$. From the coordinates listed above, the molecule of $B_{10}H_{14}$ has a novel, open-clam-shell type of structure which has not been postulated heretofore. Each boron atom is bound to five or six other atoms, but the bonds are not all equivalent. Tentatively, it appears that ten of the hydrogen atoms are each bound to a single boron atom; the four remaining ones may have a higher coordination number.

[1] Möller (*Zeit. Krist.*, **76,** 500–516, 1931) concluded incorrectly that the crystal class was orthorhombic. The correct space group, $C11\ 2/a$, is a sub-group of the one C_{mma}, given by Möller.