MOLECULAR STRUCTURE OF $B_{18}H_{22}$

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A three-dimensional X-ray diffraction study of a single crystal has yielded the complete molecular geometry of a new boron hydride, $B_{18}H_{22}$, recently prepared by Pitochelli and Hawthorne[1] from the $B_{20}H_{18}^{-2}$ ion.[2]

The unit cell of the crystal is orthorhombic in the space group Pccn, with dimensions $a = 10.844 \pm 0.003$, $b = 12.107 \pm 0.003$, and $c = 10.803 \pm 0.004$ A. The measured density of 1.012 gm/cm^3 requires four molecules of $B_{18}H_{22}$ per unit cell and yields a molecular weight of 216 ± 1 units. A total of 1,299 independent X-ray diffraction maxima were used in the structure determination and refinement, which now has progressed to $R = \Sigma||F_o| - |F_c||/\Sigma|F_o| = 0.13$.

The boron atoms were located by use of three-dimensional vector superposition methods and by Fourier refinement. All H atoms were located without chemical assumptions as the highest peaks on three-dimensional electron density maps from which the boron atoms had been subtracted. The structure is shown in Figure 1, where the molecule has been slightly flattened in order to show the close relation to decaborane. The valence structure is not unique but is shown as most nearly like that in decaborane.[3]

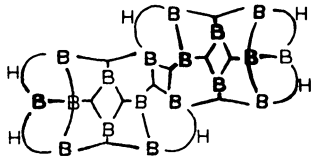

FIG. 1.—Geometrical structure and a valence structure of $B_{18}H_{22}$. The molecule is centrosymmetric with one terminal H atom (omitted from the drawing) on each of the 16 three-bonded B atoms. Open three-center bonds are shown by curved lines, and central three-center bonds are shown as triply connected. The two four-bonded B atoms correspond to the 8,9 positions in decaborane.

The unusual and new structural feature is the coordination of each of the two B atoms nearest the center of symmetry to six other B atoms. In the bonding scheme (Fig. 1), a bridge H atom, a seventh neighbor, serves to connect each unusual B atom to one of its six neighboring B atoms. Nevertheless, the valence structure is consistent with the extended valence theory[4] in which a B atom may occur without a terminal H atom, a feature first observed[5] in $B_{10}H_{16}$. Also, the steric arrangement is much like the typical apex boron coordinated to five basal borons, where the usual terminal hydrogen is replaced by the hydrogen bridge to a sixth boron.

The only known reaction of $B_{18}H_{22}$ is its dissociation to form H^+ and $B_{18}H_{21}^-$. The similarity of the outer regions of the structure to decaborane suggests that a bridge proton is lost and that the remaining adjacent bridge rearranges to yield a BH_2 group. However, there are structural reasons to expect ligand substitution reactions,[4] which may occur only with difficulty, to form $B_{18}H_{20}L$. In addition, a search for $B_{18}H_{22}^{-2}$ may be worth the effort.

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[3] Lipscomb, W. N., in *Advances in Inorganic and Radiochemistry*, ed. H. J. Emeleus and A. G. Sharpe (New York: Academic Press, 1959), vol. 1, p. 117.
[4] Lipscomb, W. N., these PROCEEDINGS, **47**, 1791 (1961).
[5] Grimes, R., F. E. Wang, R. Lewin, and W. N. Lipscomb, these PROCEEDINGS, **47**, 969 (1961).

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*IN VITRO COMPLEMENTATION BETWEEN NONALLELIC DROSOPHILA MUTANTS DEFICIENT IN XANTHINE DEHYDROGENASE**

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There are at least two loci (*ma-1* and *ry*) which control xanthine dehydrogenase in *Drosophila melanogaster*.[1, 2, 13] The fact that either locus can cause the deficiency of xanthine dehydrogenase while the other is normal indicates that each locus has a different function in the genetic control of this enzyme. This is further indicated by the fact that the *ma-1* and *ry* mutants can complement each other *in vivo* through the maternal effect of *ma-1*$^+$ on *ma-1*.[3, 4] If this is the case, one might expect that incubating extracts prepared from these mutants together under the proper conditions should produce xanthine dehydrogenase activity where none existed before. This paper is concerned with the production of xanthine dehydrogenase activity when extracts of *ma-1* and *ry* mutants are incubated together. No enzyme activity has been detected in control mutant extracts incubated singly and treated in the same way.

Methods.—Drosophila mutants and culture media have been described.[14]

Chemicals: 2-Amino-4-hydroxypteridine (2,4-compd) and isoxanthopterin (isox) were gifts of the Lederle Laboratories. The 2,4-compd was also prepared by the method of Cain *et al.*[5] and purified by the method described by Glassman and Mitchell.[2] Tris (hydroxymethyl) aminomethane (Tris) buffer was purchased from the Sigma Chemical Company. Uric acid was purchased from the Mann Research Laboratories.

Preparation of the extracts: All procedures were carried out at less than 5°C. Adult flies (usually 10 gm) were homogenized in 2.5 volumes (w/v) of 0.1 *M* Tris buffer, pH 8, and the resulting homogenate was centrifuged at 17,000 × *g* for 30 min. The supernatant solution was adjusted to pH 5 with 1*M* acetic acid and was then centrifuged immediately at 17,000 × *g* for 10 min. The precipitate was discarded. The supernatant was adjusted to pH 8 with sodium hydroxide and stored at −15°C until used. This solution will be referred to as the pH5-supernatant. Extracts stored under these conditions are usable for at least one week after preparation.

Charcoal treatment: Norite-A was added to the pH5-supernatant to give a concentration of 100 mg/ml. The mixture was stirred occasionally for 60 min, after which it was centrifuged twice at 17,000 × *g* for 20 min to remove all traces of charcoal.