

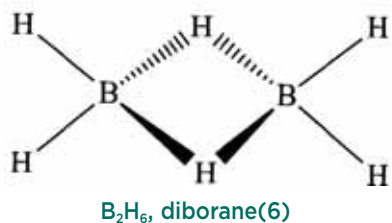
The Special Case of Boron Hydrides

by Jeffery Leigh

When writing down chemical structures, chemists feel happiest if they can depict how atoms are arranged in space and join them together appropriately with lines, each of which represents a two-electron bond. Unfortunately, though this type of model is adequate for many structures and compounds, it is not true for all. Organic chemists have developed methods that allow for the fact that aromatic compounds are not always adequately represented by names and structure based solely upon two-center two-electron bonds, and inorganic chemists have faced similar problems with certain classes of inorganic compound, such as boron hydrides. This edition of *Principles* carries a completely new chapter devoted to such compounds.

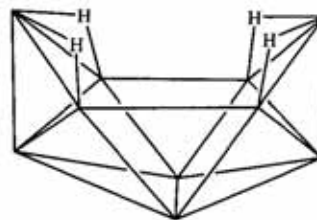
Like aromatic rings, boron hydrides are often not satisfactorily represented by structures consisting solely of two-center electron-pair bonds, though Nature still aims for full shells. The simplest boron hydride, B_2H_6 , contains 12 valence electrons, and formally four pairs are localized in two-electron B-H bonds, with a further four in two three-center two-electron B-H-B bonds, as in example (a). The complete name specifies both the number of boron atoms and the number of hydrogen atoms, which differs from organic practice, which assumes that the number of hydrogen atoms in the carbon analog of diborane would be obvious.

Example (a)



This method is extended to other boron hydrides as shown in example (b). All the apices represent B-H groups, and four three-center B-H-B bonds are designated. The name specifies the number of hydrogen atoms. In general, the polyboranes adopt the conformations of triangulated polyhedra, each of which has its own numbering convention.

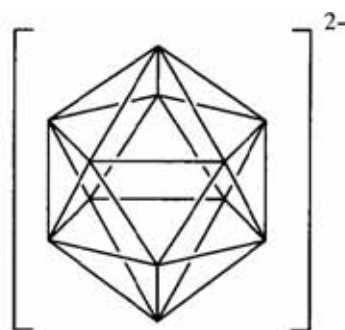
Example (b)



$B_{10}H_{14}$, decaborane(14)

These polyboranes may formally lose hydrons to yield anions, of which Example (c) is typical.

Example (c)

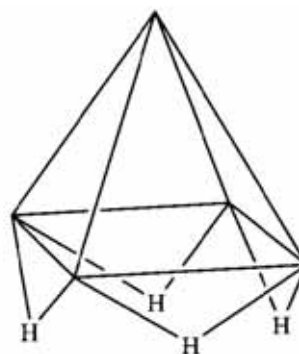


$[B_{12}H_{12}]^{2-}$, dodecahydridododecaborate(2-)

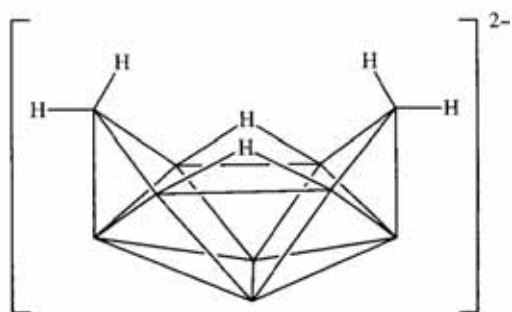
Note that in this particular case, there are no bridging hydrogen atoms, and the number of hydrogen atoms is specified in the name.

The variations chemists can produce in these materials generate a wide range of different structures. A neutral borane can lose a one or two boron hydrides to yield so-called *nido* and *arachno* structures as depicted in example (d).

Example (d)



nido- B_5H_9 , *nido*-pentaborane(9)

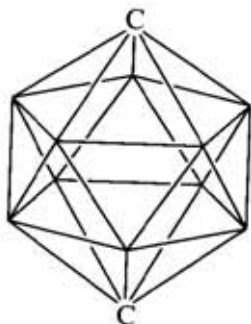


arachno-[B₁₀H₁₄]²⁻, tetradecahydro-*arachno*-decaborate(2-)

In addition to these variations, hydrogen atoms may be substituted. The names of resultant products must contain locants to specify at which skeletal positions substitutions have occurred.

Skeletal boron atoms may also be replaced by other atoms, operations termed subrogations by many boron chemists, yielding materials of which example (e) is an instance. There is an exo hydrogen atom, not shown, attached to each apical atom, carbon as well as boron.

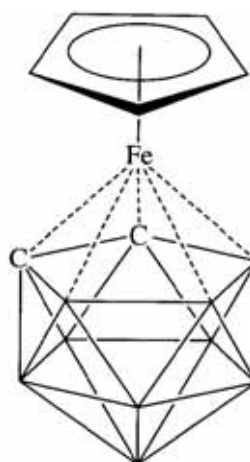
Example (e)



closo-1,12-C₂B₁₀H₁₂, 1,12-dicarpa-*closo*-dodecaborane(12)

Finally, the boranes may be considered to be similar to electronic delocalized aromatic systems, and like benzene and related derivatives they can also form sandwich compounds, as shown in example (f).

Example (f)



3-(η^5 -C₅H₅-*closo*-1,2,3-C₂FeB₉H₁₁,
3-(η^5 -cyclopentadienyl)-1,2-dicarpa-3-ferra-*closo*-
dodecaborane

Sometimes all these variations may occur in the same structure, so that considerable care is required in determining the appropriate parent borane and the number of hydrogen atoms. Example (f) is derived from a parent dodecaborane, although there are only nine boron atoms in the actual structure, the three other apical positions being occupied by an iron atom and two carbon atoms. Consequently, an accurate structural diagram and the corresponding name can be rather large and complex. *Principles* summarizes all these structural types and the appropriate methods for naming them, together with references to the original literature.

Jeffery Leigh is the editor and contributing author of *Principles of Chemical Nomenclature—A Guide to IUPAC Recommendations*, 2011 Edition (RSC 2011, ISBN 978-1-84973-007-5). Leigh is emeritus professor at the University of Sussex and has been active in IUPAC nomenclature since 1973.

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