6.5: Wade’s Rules

Ken Wade (Figure 6.5.1) developed a method for the prediction of shapes of borane clusters; however, it may be used for a wide range of substituted boranes (such as carboranes) as well as other classes of cluster compounds.

Figure 6.5.1: Chemist Ken Wade FRS.

Wade’s rules are used to rationalize the shape of borane clusters by calculating the total number of **skeletal electron pairs (SEP)** available for cluster bonding. In using Wade’s rules it is key to understand structural relationship of various boranes (Figure 6.5.2).

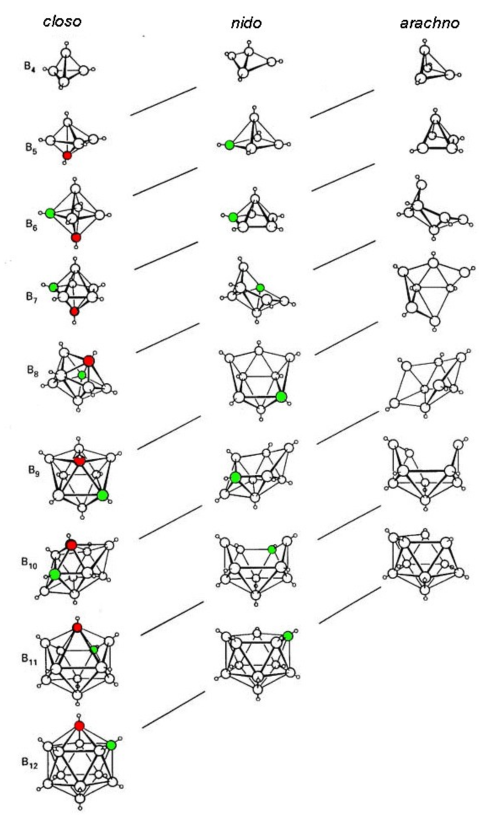

Figure 6.5.2: Structural relationship between *closo*, *nido*, and *arachno* boranes (and hetero-substituted boranes). The diagonal lines connect species that have the same number of skeletal electron pairs (SEP). Hydrogen atoms except those of the B-H framework are omitted. The red atom is omitted first, the green atom removed second. Adapted from R. W. Rudolph, *Acc. Chem. Res.*, 1976, **9**, 446.

The general methodology to be followed when applying Wade’s rules is as follows:

1. Determine the total number of valence electrons from the chemical formula, i.e., 3 electrons per B, and 1 electron per H.

2. Subtract 2 electrons for each B-H unit (or C-H in a carborane).
3. Divide the number of remaining electrons by 2 to get the number of skeletal electron pairs (SEP).
4. A cluster with *n* vertices (i.e., *n* boron atoms) and *n*+1 SEP for bonding has a *closo* structure.
5. A cluster with *n*-1 vertices (i.e., *n*-1 boron atoms) and *n*+1 SEP for bonding has a *nido* structure.
6. A cluster with *n*-2 vertices (i.e., *n*-2 boron atoms) and *n*+1 SEP for bonding has an *arachno* structure.
7. A cluster with *n*-3 vertices (i.e., *n*-3 boron atoms) and *n*+1 SEP for bonding has an *hypho* structure.
8. If the number of boron atoms (i.e., *n*) is larger than *n*+1 SEP then the extra boron occupies a capping position on a triangular phase.

What is the structure of B_5H_{11}?

1. Total number of valence electrons = (5 x B) + (11 x H) = (5 x 3) + (11 x 1) = 26
2. Number of electrons for each B-H unit = (5 x 2) = 10
3. Number of skeletal electrons = 26 – 10 = 16
4. Number SEP = 16/2 = 8
5. If *n*+1 = 8 and *n*-2 = 5 boron atoms, then *n* = 7
6. Structure of *n* = 7 is pentagonal bipyramid (Figure 6.5.2), therefore B_5H_{11} is an *arachno* based upon a pentagonal bipyramid with two apexes missing (Figure 6.5.3).

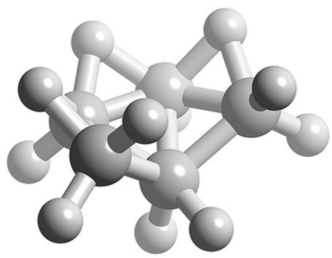

Figure 6.5.3: Ball and stick representation of the structure of B_5H_{11}.

What is the structure of B_5H_9?

1. Total number of valence electrons = (5 x B) + (9 x H) = (5 x 3) + (9 x 1) = 24
2. Number of electrons for each B-H unit = (5 x 2) = 10
3. Number of skeletal electrons = 24 – 10 = 14
4. Number SEP = 14/2 = 7
5. If *n*+1 = 7 and *n*-1 = 5 boron atoms, then *n* = 6
6. Structure of *n* = 6 is octahedral (Figure 6.5.2), therefore B_5H_9 is a *nido* structure based upon an octahedral structure with one apex missing (Figure 6.5.4).

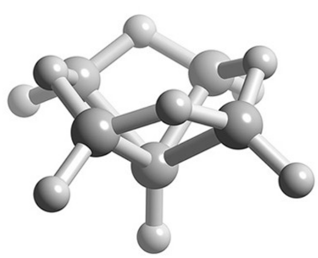

Figure 6.5.4: Ball and stick representation of the structure of B_5H_9.

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What is the structure of $B_6H_6^{2-}$?

Solution

1. Total number of valence electrons = (6 x B) + (3 x H) = (6 x 3) + (6 x 1) + 2 = 26
2. Number of electrons for each B-H unit = (6 x 2) = 12

3. Number of skeletal electrons = 26 – 12 = 14
4. Number SEP = 14/2 = 7
5. If n+1 = 7 and n boron atoms, then n = 6
6. Structure of n = 6 is octahedral (Figure 6.5.2), therefore $B_6H_6^{2-}$ is a *closo* structure based upon an octahedral structure (Figure 6.5.5).

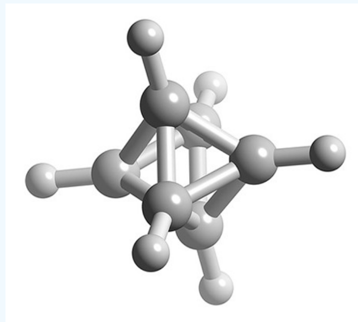

Figure 6.5.5: Ball and stick representation of the structure of $B_6H_6^{2-}$.

Table 6.5.1 provides a summary of borane cluster with the general formula $B_nH_n^{x-}$ and their structures as defined by Wade's rules.

Table 6.5.1: Wade's rules for boranes.

Type	Basic formula	Example	# of verticies	# of vacancies	# of e- in B + charge	# of bonding MOs
Closo	$B_nH_n^{2-}$	$B_6H_6^{2-}$	n	0	3n + 2	n + 1
Nido	$B_nH_n^{4-}$	B_5H_9	n + 1	1	3n + 4	n + 2
Arachno	$B_nH_n^{6-}$	B_4H_{10}	n + 2	2	3n + 6	n + 3
Hypho	$B_nH_n^{8-}$	$B_5H_{11}^{2-}$	n + 3	3	3n + 8	n + 4

Bibliography

- R. W. Rudolph, *Acc. Chem. Res.*, 1976, **9**, 446.
- K. Wade, *Adv. Inorg. Chem. Radiochem.*, 1976, **18**, 1.