

◇ Wade's Rules (recap)

For a cluster B_nH_m^k :

- Skeletal electron pairs (SEP) =
(total valence e for bonding – e used in terminal B–H bonds)/2
- Then compare with n (number of skeletal atoms, usually B atoms).
- Types:
 - **Closo**: $\text{SEP} = n + 1$ (closed polyhedron, deltahedral)
 - **Nido**: $\text{SEP} = n + 2$ (one vertex missing from closo)
 - **Arachno**: $\text{SEP} = n + 3$ (two vertices missing)
 - **Hypho**: $\text{SEP} = n + 4$ (three vertices missing)

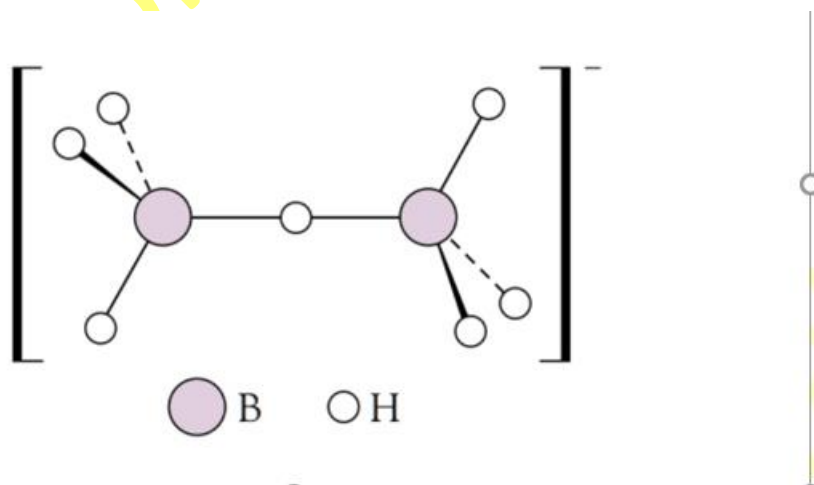
1. $[\text{B}_2\text{H}_7]^-$

- Valence e^- : $2 \times 3 + 7 \times 1 + 1 = 14$
- Terminal B–H: 6 bonds $\rightarrow 12 e^-$
- Left for framework: $14 - 12 = 2 e^- = \mathbf{1 \text{ pair}}$

➡ This is essentially two **BH_3 units bridged by an H^- ion**.

- Structure: linear or bent (**H-B-H-B-H with bridging H**).
- It is **not a polyhedral cluster**, but a simple bridged dimer.

☞ **Structure**: a 3-center-2-electron ($3c-2e$) bridge across B–H–B.



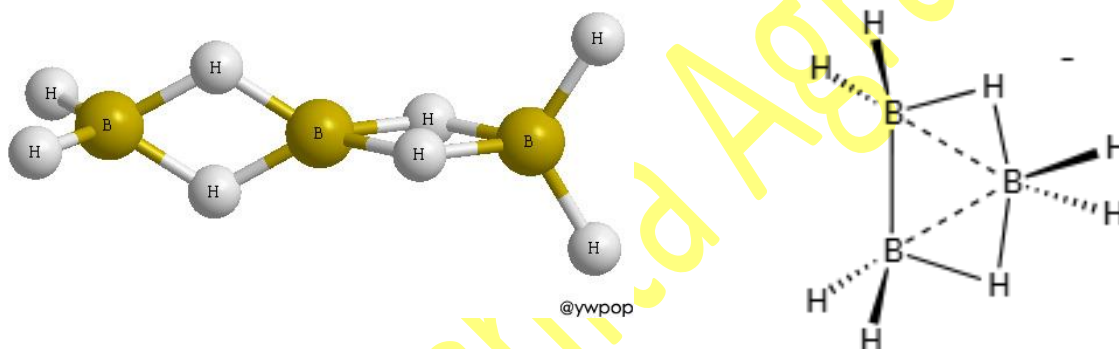
2. $[\text{B}_3\text{H}_8]^-$

- Valence e^- : $3 \times 3 + 8 \times 1 + 1 = 3 \times 3 + 8 \times 1 + 1 = 18$
- Terminal B–H: $7 \rightarrow 14 e^-$
- Left = $4 e^- = 2$ pairs

➡ For $n = 3$ boron atoms, $\text{SEP} = 2 \rightarrow$ fits $n + ?$

- $n + 2 = 5$ (not matching, too large)
Actually, this is a **dimer of $[\text{B}_2\text{H}_7]^-$ type units**, with bridging hydrogens.
- **Structure:** Two BH_2 terminal groups and one bridging BH_2 with hydrogens making bridges.

☯ **Known structure:** chainlike, with bridging hydrogens giving stability (not a closed deltahedron).



3. B_5H_9

- Valence e^- : $5 \times 3 + 9 \times 1 = 5 \times 3 + 9 \times 1 = 24$
- Terminal B–H: $9 \rightarrow 18 e^-$
- Left = $6 e^- = 3$ pairs

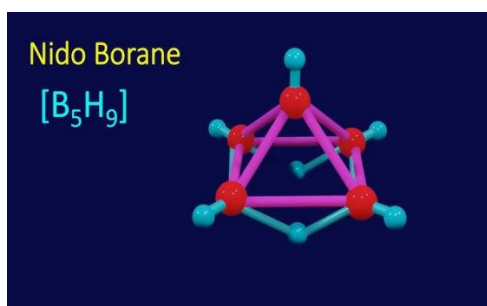
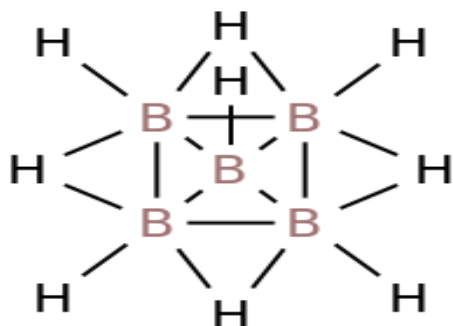
➡ $n = 5$

- For **nido**: $\text{SEP} = n + 2 = 7$
- For **arachno**: $\text{SEP} = n + 3 = 8$
But we only have 3 skeletal pairs?

⚠ Wait: In boranes, often some hydrogens are bridging (not purely terminal).
So we don't subtract *all* H bonds as terminal.

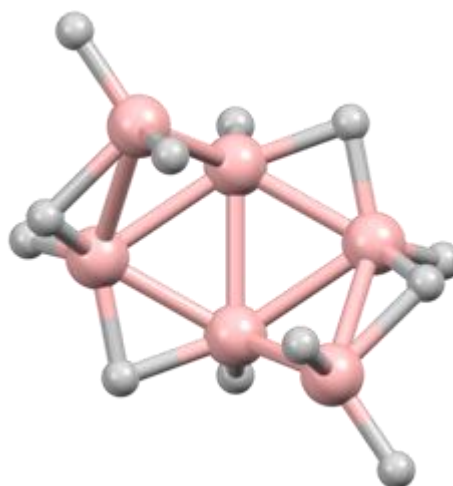
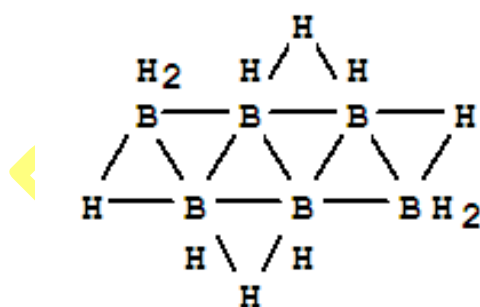
☞ Experimentally, B_5H_9 is **nido** (square pyramidal with one open face).

- Structure: looks like a square pyramid of B atoms with bridging H atoms along edges.



4. B_6H_{12}

- Valence e^- : $6 \times 3 + 12 \times 1 = 6 \times 3 + 12 \times 1 = 30$
- This is an **arachno-borane** (two missing vertices from closo B_8).
- Structure: **arachno-octahedron fragment**, with bridging hydrogens.



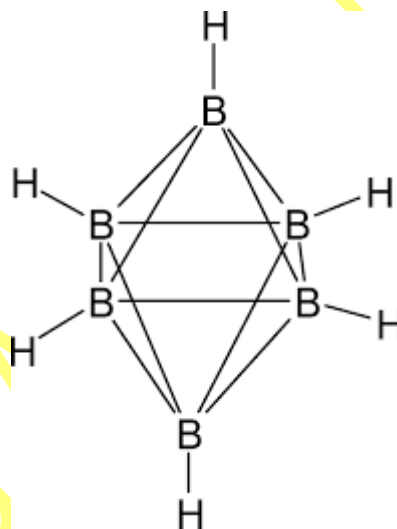
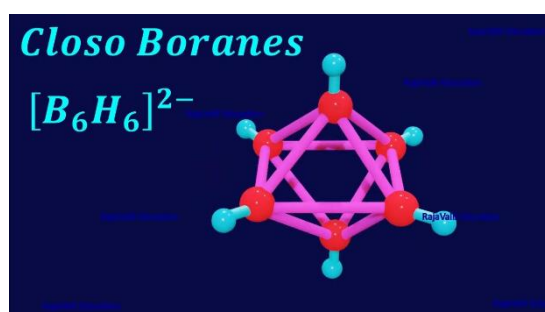
5. $\text{B}_6\text{H}_6^{2-}$ (closely related to B_6H_6 neutral cluster sometimes written as B_6H_6)

- If neutral B_6H_6 : $6 \times 3 + 6 \times 1 = 6 \times 3 + 6 \times 1 = 24$ electrons.
- Closo $n=6$ requires $SEP = 7 = 14 e^- \rightarrow$ matches $B_6H_6^{2-}$, not neutral.

Thus:

- $B_6H_6^{2-} =$ **closo octahedral cluster** (like benzene's electronic analogue).
- Neutral B_6H_6 is unstable, but the dianion is aromatic (like benzene).

♀ **Structure:** octahedron of B atoms with one H on each vertex.



☑ Summary with Figures

1. $[B_2H_7]^- \rightarrow$ two BH_3 bridged by one H^- ($B-H-B$ 3c-2e bond).
2. $[B_3H_8]^- \rightarrow$ chainlike borane with bridging H's.
3. $B_5H_9 \rightarrow$ **nido** (square pyramid fragment).
4. $B_6H_{12} \rightarrow$ **arachno** (octahedral fragment).
5. $B_6H_6^{2-} \rightarrow$ **closo** octahedron.