

❖ 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**: SEP = n + 1 (closed polyhedron, deltahedral)
 - **Nido**: SEP = n + 2 (one vertex missing from closo)
 - **Arachno**: SEP = n + 3 (two vertices missing)
 - **Hypho**: SEP = n + 4 (three vertices missing)

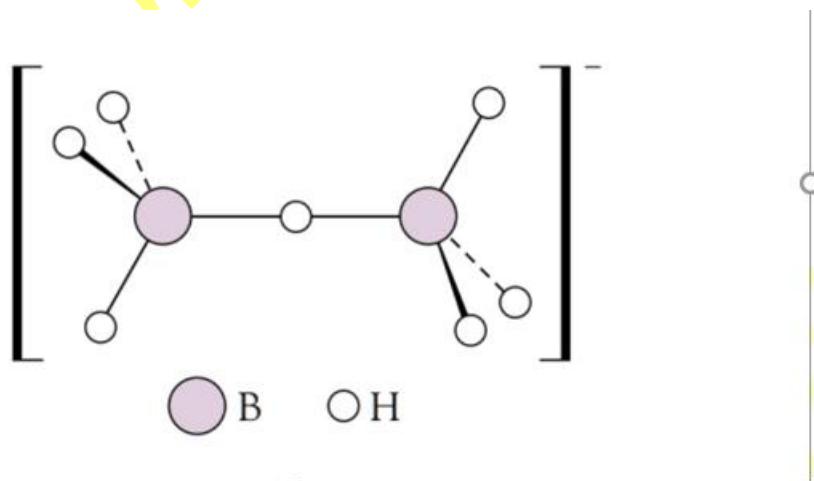
1. $[\text{B}_2\text{H}_7]^-$

- 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⁻ = **1 pair**

→ This is essentially two **BH₃** 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.



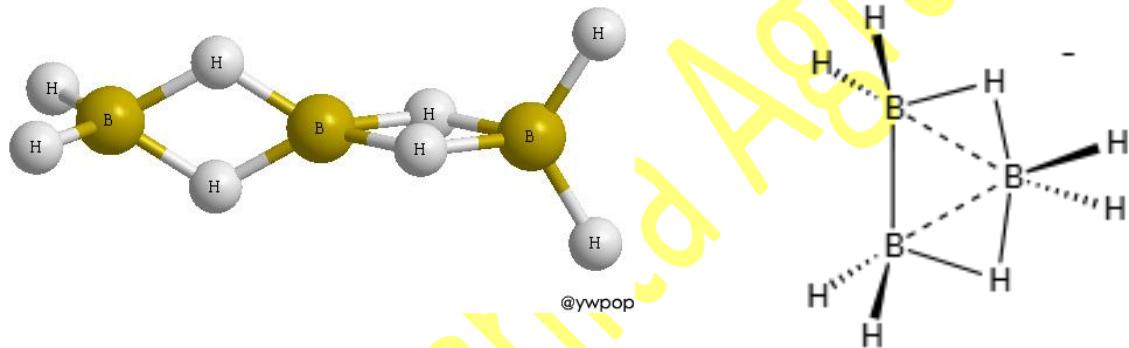
2. $[\text{B}_3\text{H}_8]^-$

- 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, SEP = 2 → 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

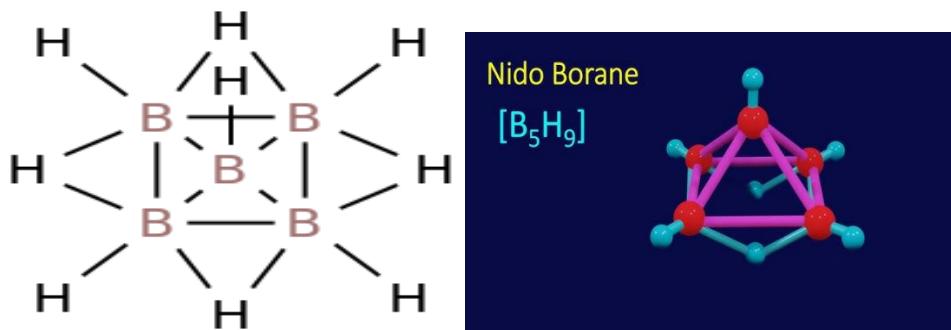
→ $n = 5$

- For **nido**: SEP = $n + 2 = 7$
- For **arachno**: 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.

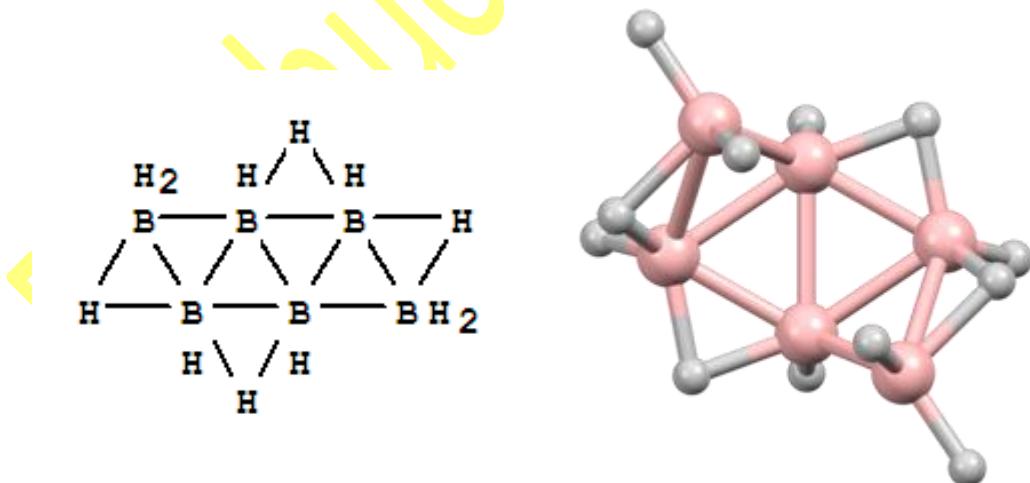
☞ Experimentally, $\mathbf{B_5H_9}$ is **nido** (square pyramidal with one open face).

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



4. $\mathbf{B_6H_{12}}$

- 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 $\mathbf{B_8}$).
- Structure: **arachno-octahedron fragment**, with bridging hydrogens.



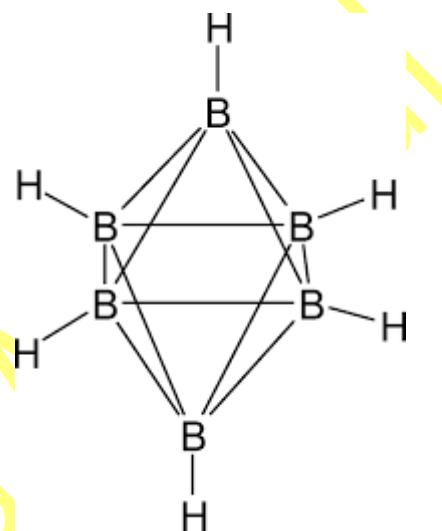
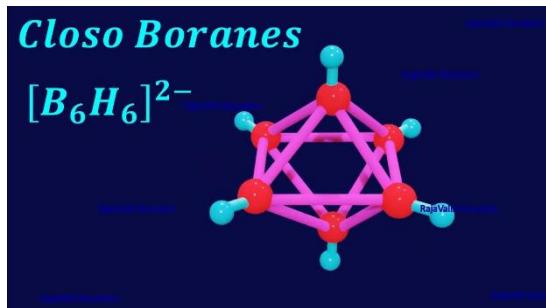
5. $\mathbf{B_6H_6^{2-}}$ (closely related to $\mathbf{B_6H_6}$ neutral cluster sometimes written as $\mathbf{B_6H_6}$)

- 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.