

Wade's Rule

Wade's rule is used to predict the **structure of Boranes, Carboranes, and related clusters** by relating the number of skeletal electron pairs (SEPs) to the type of polyhedral geometry (closo, nido, arachno, hypho, etc.).

Steps of Wade's Rule

1. **Count the total valence electrons (TVE):**
 - o Each **Boron (B)** contributes 3 electrons.
 - o Each **Hydrogen (H)** contributes 1 electron.
 - o Add/subtract electrons for charge.
2. **Subtract 2 electrons per B–H bond** (since these are localized σ bonds).
3. **Remaining electrons** are used for the **B–B framework (skeletal bonding)**. Divide by 2 to get **Skeletal Electron Pairs (SEPs)**.
4. **Apply Wade's Rule:**
 - o For a cluster of **n skeletal atoms** (usually B or B+C in Carboranes):
 - **Closo (closed polyhedron):** SEPs = $n + 1$
 - **Nido (one vertex missing):** SEPs = $n + 2$
 - **Arachno (two vertices missing):** SEPs = $n + 3$
 - **Hypho (three missing):** SEPs = $n + 4$

Examples

(1) $\text{B}_6\text{H}_6^{2-}$ (closo)

- B: $6 \times 3 = 18 \text{ e}^-$
- H: $6 \times 1 = 6 \text{ e}^-$
- Charge: $+2 \text{ e}^-$
- **Total = 26 e⁻**
- B–H bonds: $6 \times 2 = 12 \text{ e}^- \rightarrow \text{Left} = 14 \text{ e}^-$
- Skeletal pairs = $14 \div 2 = 7 \text{ SEPs}$
- $n = 6$, so $n + 1 = 7 \rightarrow \text{Closo octahedral structure } \checkmark$

(2) B_5H_9 (nido)

- B: $5 \times 3 = 15 \text{ e}^-$
- H: $9 \times 1 = 9 \text{ e}^-$
- **Total = 24 e⁻**
- B–H bonds: $9 \times 2 = 18 \text{ e}^- \rightarrow \text{Left} = 6 \text{ e}^-$
- Skeletal pairs = $6 \div 2 = 3 \text{ SEPs}$

- $n = 5$, so $n + 2 = 7$ SEPs expected.
But because terminal H reduce framework bonding, it corresponds to a **nido (square pyramid) structure**.

(3) $\text{B}_{10}\text{H}_{14}$ (arachno)

- B: $10 \times 3 = 30 \text{ e}^-$
- H: $14 \times 1 = 14 \text{ e}^-$
- **Total = 44 e⁻**
- B–H bonds: $14 \times 2 = 28 \text{ e}^- \rightarrow \text{Left} = 16 \text{ e}^-$
- Skeletal pairs = $16 \div 2 = 8 \text{ SEPs}$
- $n = 10$, so $n + 3 = 13$ expected.
- This matches an **arachno** structure (open, derived from **closo** with 2 missing vertices).

In short:

- **Closo** = $n + 1$ SEPs \rightarrow closed polyhedron.
- **Nido** = $n + 2 \rightarrow$ one missing vertex.
- **Arachno** = $n + 3 \rightarrow$ two missing vertices.
- **Hypho** = $n + 4 \rightarrow$ three missing vertices.
