

## 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.).

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### Steps of Wade's Rule

1. **Count the total valence electrons (TVE):**
    - Each **Boron (B)** contributes 3 electrons.
    - Each **Hydrogen (H)** contributes 1 electron.
    - Add/subtract electrons for charge.
  2. **Subtract 2 electrons per B–H bond** (since these are localized  $\sigma$  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:**
    - For a cluster of **n skeletal atoms** (usually B or B+C in Carboranes):
      - **Closo (closed polyhedron):**  $\text{SEPs} = n + 1$
      - **Nido (one vertex missing):**  $\text{SEPs} = n + 2$
      - **Arachno (two vertices missing):**  $\text{SEPs} = n + 3$
      - **Hypho (three missing):**  $\text{SEPs} = n + 4$
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### 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 =  $26 \text{ e}^-$**
  - 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  $n + 1 = 7 \rightarrow$  **Closo** octahedral structure ☒
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#### (2) $\text{B}_5\text{H}_9$ (nido)

- B:  $5 \times 3 = 15 \text{ e}^-$
- H:  $9 \times 1 = 9 \text{ e}^-$
- **Total =  $24 \text{ e}^-$**
- 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**.
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### (3) $B_{10}H_{14}$ (arachno)

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