8.2 Electron Configurations

- **Building-up (aufbau) principle** – as new electrons are added to the atom, they are placed in the lowest energy available orbital (minimization of the total energy of the atom)
  - Electron configuration – a list of the occupied subshells and the number of electrons on them
  - Orbital diagrams – each orbital is represented by a box; the electrons are shown as up or down arrows depending on the spin quantum number (+1/2 or -1/2)

- **Closed shell** configuration represents a completely filled principal shell (He → 1s²)

- **Degenerate orbitals** – orbitals with equal energies
  - All orbitals in a subshell are degenerate (same n and l) → the three 2p-orbitals are degenerate

- **Hund’s rule** – in filling degenerate orbitals, electrons enter the empty orbitals having identical spins before pairing in one of them (minimization of the repulsion between the electrons)

- **Outer electrons** – electrons in the outermost occupied principal shell
- **Inner (core) electrons** – inner shells
- **Condensed e⁻ configurations** – inner shells (or part of them) can be abbreviated with the symbol of the previous noble gas in brackets 1s² → abbreviated as [He]
**Example:** Predict the electron configurations of F and Ne.

**orbital order:** 1s, 2s, 2p, 3s, 3p, ...

F ($Z = 9$, 9 e\(^-\)) → 1s\(^2\)2s\(^2\)2p\(^5\) → [He]2s\(^2\)2p\(^5\)

Ne ($Z = 10$, 10 e\(^-\)) → 1s\(^2\)2s\(^2\)2p\(^6\) → [He]2s\(^2\)2p\(^6\)

[He]2s\(^2\)2p\(^6\) → closed shell → abbreviated as [Ne]

<table>
<thead>
<tr>
<th>Atomic Number/Element</th>
<th>Partial Orbital Diagram (3s and 3p Sublevels Only)</th>
<th>Full Electron Configuration</th>
<th>Condensed Electron Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>11/Na</td>
<td><img src="image1.png" alt="Diagram" /></td>
<td>[1s(^2)2s(^2)2p(^6)] 3(^{+})</td>
<td>[Ne] 3(^{+})</td>
</tr>
<tr>
<td>12/Mg</td>
<td><img src="image2.png" alt="Diagram" /></td>
<td>[1s(^2)2s(^2)2p(^6)] 3(^{2})</td>
<td>[Ne] 3(^{2})</td>
</tr>
<tr>
<td>13/Al</td>
<td><img src="image3.png" alt="Diagram" /></td>
<td>[1s(^2)2s(^2)2p(^6)] 3(^{+})</td>
<td>[Ne] 3(^{+}) 3(^{2})</td>
</tr>
<tr>
<td>14/Si</td>
<td><img src="image4.png" alt="Diagram" /></td>
<td>[1s(^2)2s(^2)2p(^6)] 3(^{2})</td>
<td>[Ne] 3(^{2}) 3(^{2})</td>
</tr>
<tr>
<td>15/P</td>
<td><img src="image5.png" alt="Diagram" /></td>
<td>[1s(^2)2s(^2)2p(^6)] 3(^{+})</td>
<td>[Ne] 3(^{+}) 3(^{2})</td>
</tr>
<tr>
<td>16/Si</td>
<td><img src="image6.png" alt="Diagram" /></td>
<td>[1s(^2)2s(^2)2p(^6)] 3(^{+})</td>
<td>[Ne] 3(^{+}) 3(^{2}) 3(^{2})</td>
</tr>
<tr>
<td>17/Cl</td>
<td><img src="image7.png" alt="Diagram" /></td>
<td>[1s(^2)2s(^2)2p(^6)] 3(^{+})</td>
<td>[Ne] 3(^{+}) 3(^{2}) 3(^{2})</td>
</tr>
</tbody>
</table>

- **How to remember the energy order of the orbitals:**
  1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 5f < 6d < 7p

  **Note:**
  4s is filled before 3d

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<tr>
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<th>Condensed El. Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>19 K</td>
<td><img src="image8.png" alt="Diagram" /></td>
<td>[Ar] 4(^{+})</td>
</tr>
<tr>
<td>20 Ca</td>
<td><img src="image9.png" alt="Diagram" /></td>
<td>[Ar] 4(^{2})</td>
</tr>
<tr>
<td>21 Sc</td>
<td><img src="image10.png" alt="Diagram" /></td>
<td>[Ar] 4(^{+}) 3(^{2})</td>
</tr>
<tr>
<td>22 Ti</td>
<td><img src="image11.png" alt="Diagram" /></td>
<td>[Ar] 4(^{2}) 3(^{2})</td>
</tr>
<tr>
<td>23 V</td>
<td><img src="image12.png" alt="Diagram" /></td>
<td>[Ar] 4(^{2}) 3(^{2})</td>
</tr>
</tbody>
</table>

- **Exceptions to the building-up principle**
  - **Half-filled subshells** have exceptional stability
    - Cr → [Ar]4s\(^{1}\)3d\(^{5}\) instead of [Ar]4s\(^{2}\)3d\(^{4}\)
– Completely filled subshells have exceptional stability

\[
\text{Cu} \rightarrow [\text{Ar}]4s^13d^{10} \text{ instead of } [\text{Ar}]4s^23d^9
\]

### Electronic Structure and the Periodic Table

- The table is divided into \( s \), \( p \), \( d \), and \( f \) blocks named by the last occupied subshell being filled
- Electron configurations can be deduced from the positions of elements in the periodic table
  - Outer shell principal quantum numbers equal period numbers (\( F \rightarrow 2^{\text{nd}} \) period, \( n=2 \))
  - All elements in a period have the same noble-gas core configurations ([He], [Ne], [Ar], ...)

- Similarly, the building-up principle is used to obtain the electron configurations for periods 5, 6 and 7 (similar and even more drastic exceptions are observed)

- The filling order of the orbitals can be obtained from the periodic table:
  - The \( ns \), \( np \), \((n-1)d \) and \((n-2)f \) orbitals are filled in the \( n^{\text{th}} \) period from left to right
  - The filling order is \( ns < (n-2)f < (n-1)d < np \)
Examples:
Write the full and condensed electron configurations of galium, Ga.
(H, He) 1s² → (Li, Be) 2s² → (B-Ne) 2p⁶ → (Na, Mg) 3s² → (Al-Ar) 3p⁶ → (K, Ca) 4s² → (Sc-Zn) 3d¹⁰ → (Ga) 4p¹
⇒ Ga → 1s²2s²2p⁶3s²3p⁶4s²3d¹⁰4p¹
⇒ Ga → [Ar]4s²3d¹⁰4p¹

Write the electron configuration of osmium, Os.
Os is in the 6th period → outer shell n=6
Previous noble gas is Xe → noble-gas core is [Xe]
After Xe → 2 ns, 14 (n-2)f, and 6 (n-1)d elements
⇒ [Xe]6s²4f¹⁴5d⁶

• Valence electrons – the electrons in the outermost occupied principal shell and in partially filled subshells of lower principal shells (important in chemical reactions)
  – The number of valence electrons equals the “new” group # or (group # - 10 for p-elements)
  – All elements in a group have analogous valence shell electron configurations (F → [He]2s²2p⁵; Cl → [Ne]3s²3p⁵; all halogens → ns²np⁵)
    ➢ s and p elements → group 1 ns¹, group 2 ns², group 13 ns²np¹, ..., group 18 ns²np⁶
    ➢ d elements → group 3 (n-1)d¹ns², ..., group 12 (n-1)d¹⁰ns²

Example:
Write the electron configuration and the valence shell orbital diagram of lead, Pb.
outer shell n=6 noble-gas core [Xe]
After Xe → 2 6s, 14 4f, 10 5d, and 2 6p elements
⇒ [Xe] 6s²4f¹⁴5d¹⁰6p²
⇒ Valence shell configuration → 6s²6p²
⇒ Valence shell orbital diagram:

<table>
<thead>
<tr>
<th>6s</th>
<th>6p</th>
</tr>
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<tbody>
<tr>
<td>↑</td>
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