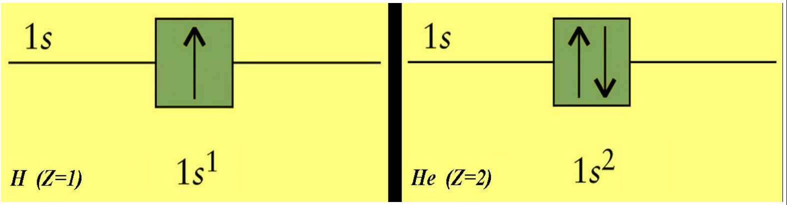
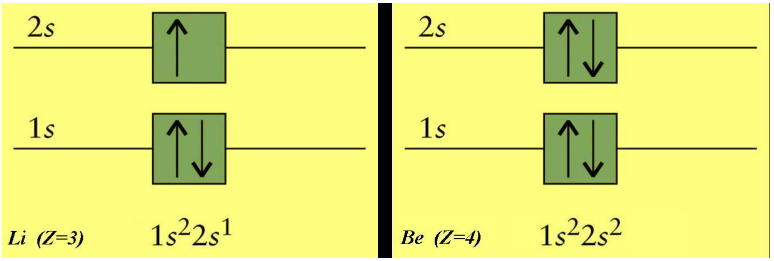
8.2 Electron Configurations

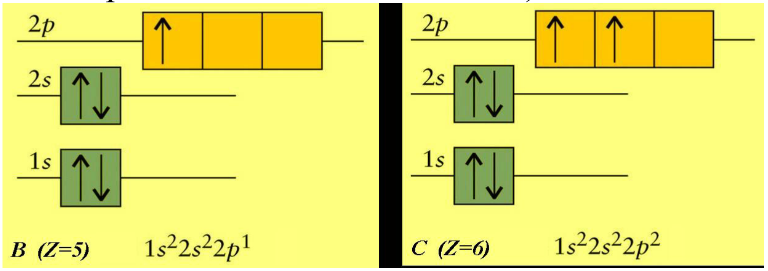
- **Building-up (aufbau) principle** – as new electrons are added to the atom, they are placed in the lowest energy available orbital (minimization of the total energy of the atom)
  - **Electron configuration** – a list of the occupied subshells and the number of electrons on them
  - **Orbital diagrams** – 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)

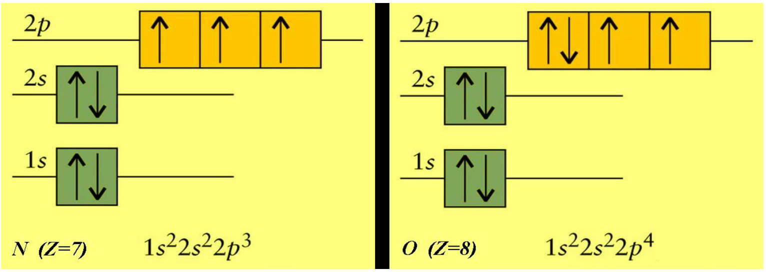


- **Closed shell** configuration represents a completely filled principal shell **(He → 1s^2)**



- **Degenerate orbitals** – orbitals with equal energies
  - All orbitals in a subshell are degenerate (same ***n*** and ***l***) → the three **2*p***-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
  1s^2 → abbreviated as **[He]**

Example: Predict the electron configurations of **F** and **Ne**.

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

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]

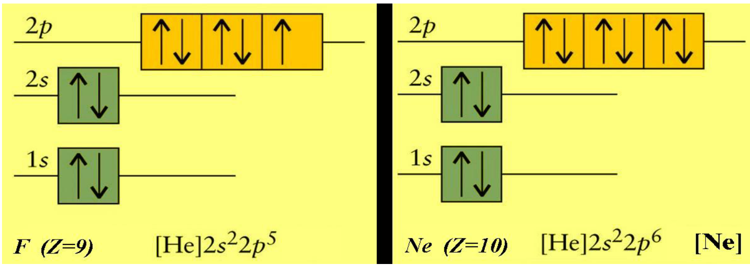


Table 8.3 Partial Orbital Diagrams and Electron Configurations* for the Elements in Period 3

Atomic Number/ Element	Partial Orbital Diagram (3s and 3p Sublevels Only) 3s	3p	Full Electron Configuration	Condensed Electron Configuration
11/Na	↑		[$1s^2 2s^2 2p^6$] $3s^1$	[Ne] $3s^1$
12/Mg	↑↓		[$1s^2 2s^2 2p^6$] $3s^2$	[Ne] $3s^2$
13/Al	↑↓	↑	[$1s^2 2s^2 2p^6$] $3s^2 3p^1$	[Ne] $3s^2 3p^1$
14/Si	↑↓	↑ ↑	[$1s^2 2s^2 2p^6$] $3s^2 3p^2$	[Ne] $3s^2 3p^2$
15/P	↑↓	↑ ↑ ↑	[$1s^2 2s^2 2p^6$] $3s^2 3p^3$	[Ne] $3s^2 3p^3$
16/S	↑↓	↑↓ ↑ ↑	[$1s^2 2s^2 2p^6$] $3s^2 3p^4$	[Ne] $3s^2 3p^4$
17/Cl	↑↓	↑↓ ↑↓ ↑	[$1s^2 2s^2 2p^6$] $3s^2 3p^5$	[Ne] $3s^2 3p^5$
18/Ar	↑↓	↑↓ ↑↓ ↑↓	[$1s^2 2s^2 2p^6$] $3s^2 3p^6$	[Ne] $3s^2 3p^6$

- How to remember the energy order of the orbitals:

  1*s* < 2*s* < 2*p* < 3*s* < 3*p* < 4*s* < 3*d* < 4*p* < 5*s* < 4*d* < 5*p* < 6*s* < 4*f* < 5*d* < 6*p* < 7*s* < 5*f* < 6*d* < 7*p*

Note:

4*s* is filled before 3*d*

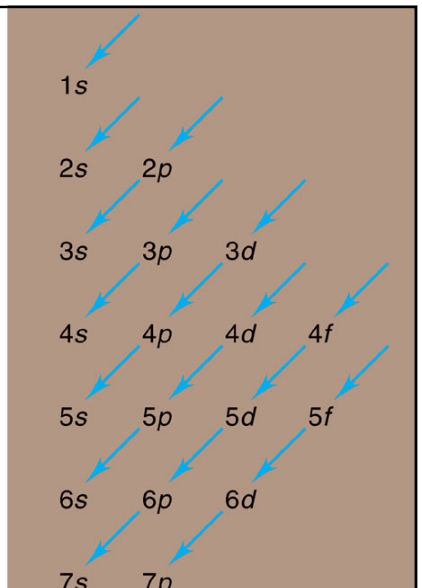


Table 8.4 Partial Orbital Diagrams and Electron Configurations* for Period 4

Atomic Number	Element	Partial Orbital Diagram (4s, 3d, and 4p Sublevels Only) 4s	3d	4p	Condensed El. Configuration
19	K	↑			[Ar] $4s^1$
20	Ca	↑↓			[Ar] $4s^2$
21	Sc	↑↓	↑		[Ar] $4s^2 3d^1$
22	Ti	↑↓	↑ ↑		[Ar] $4s^2 3d^2$
23	V	↑↓	↑ ↑ ↑		[Ar] $4s^2 3d^3$

- Exceptions to the building-up principle
  - **Half-filled subshells** have exceptional stability

    Cr → [Ar]$4s^1 3d^5$ instead of **[Ar]$4s^2 3d^4$**

Table 8.4 Partial Orbital Diagrams and Electron Configurations* for Period 4

Atomic Number	Element	Partial Orbital Diagram (4s, 3d, and 4p Sublevels Only): 4s	3d	4p	Condensed El. Configuration
24	Cr	↑	↑ ↑ ↑ ↑ ↑	_ _ _	[Ar] $4s^1 3d^5$
25	Mn	↑↓	↑ ↑ ↑ ↑ ↑	_ _ _	[Ar] $4s^2 3d^5$
26	Fe	↑↓	↑↓ ↑ ↑ ↑ ↑	_ _ _	[Ar] $4s^2 3d^6$
27	Co	↑↓	↑↓ ↑↓ ↑ ↑ ↑	_ _ _	[Ar] $4s^2 3d^7$
28	Ni	↑↓	↑↓ ↑↓ ↑↓ ↑ ↑	_ _ _	[Ar] $4s^2 3d^8$
29	Cu	↑	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	_ _ _	[Ar] $4s^1 3d^{10}$
30	Zn	↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	_ _ _	[Ar] $4s^2 3d^{10}$

– **Completely filled subshells** have exceptional stability

Cu → [Ar]$4s^1 3d^{10}$ instead of **[Ar]$4s^2 3d^9$**

Table 8.4 Partial Orbital Diagrams and Electron Configurations* for Period 4

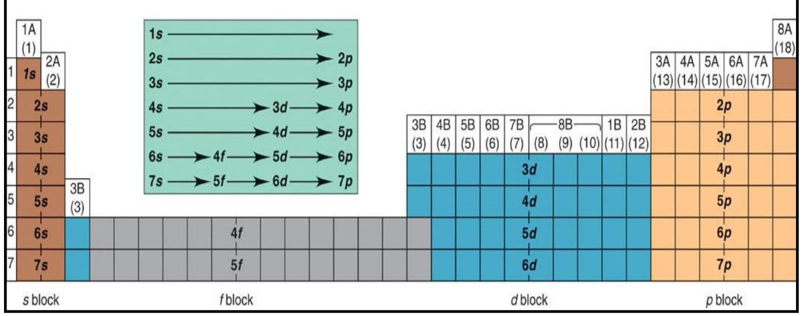
Atomic Number	Element	Partial Orbital Diagram (4s, 3d, and 4p Sublevels Only): 4s	3d	4p	Condensed El. Configuration
31	Ga	↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑ _ _	[Ar] $4s^2 3d^{10} 4p^1$
32	Ge	↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑ ↑ _	[Ar] $4s^2 3d^{10} 4p^2$
33	As	↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑ ↑ ↑	[Ar] $4s^2 3d^{10} 4p^3$
34	Se	↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓ ↑ ↑	[Ar] $4s^2 3d^{10} 4p^4$
35	Br	↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓ ↑↓ ↑	[Ar] $4s^2 3d^{10} 4p^5$
36	Kr	↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓ ↑↓ ↑↓	[Ar] $4s^2 3d^{10} 4p^6$

– 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)

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 → 2nd period, *n*=2)
  - All elements in a period have the same noble-gas core configurations ([He], [Ne], [Ar], …)

- 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^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) $1s^2$ → (Li, Be) $2s^2$ → (B-Ne) $2p^6$ → (Na, Mg) $3s^2$ → (Al-Ar) $3p^6$ → (K, Ca) $4s^2$ → (Sc-Zn) $3d^{10}$ → (Ga) $4p^1$

⇒Ga → $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^1$

⇒Ga → $[Ar]4s^2 3d^{10} 4p^1$

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

⇒ $[Xe]6s^2 4f^{14} 5d^6$

- **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]$2s^2 2p^5$; Cl → [Ne]$3s^2 3p^5$; all halogens → $ns^2 np^5$)**

➢**s** and **p** elements → group 1 ns^1, group 2 ns^2, group 13 $ns^2 np^1$, ..., group 18 $ns^2 np^6$

➢**d** elements → group 3 $(n-1)d^1 ns^2$, …, group 12 $(n-1)d^{10} ns^2$

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] $6s^2 4f^{14} 5d^{10} 6p^2$

⇒Valence shell configuration → $6s^2 6p^2$

⇒Valence shell orbital diagram: