VC210 Recitation Class 2

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Contents

Degeneracy

What is Degeneracy?
Different wave functions(state) have same energy.

example

(n_x, n_y, n_z)=(2,1,1),(1,2,1),(1,1,2) have same energy for a particle in a box $L_x = L_y = L_z$.

Quantum Number

TABLE 1D.2 Quantum Numbers for Electrons in Atoms

Name	Symbol	Values	Specifies	Indicates
principal	n	$1, 2, \ldots$	shell	size and energy
orbital angular momentum*	l	$0, 1, \ldots, n-1$	subshell: $l = 0, 1, 2, 3, 4, \ldots$ s, p, d, f, g, ...	shape
magnetic	m_l	$l, l-1, \ldots, -l$	orbitals of subshell	orientation
spin magnetic	m_s	$+\frac{1}{2}, -\frac{1}{2}$	spin state	spin direction

Nodes

- total nodes: n-1
- planar nodes: l
- radial nodes: n-l-1

Examples

4d orbital: 3=2+1
6f orbital: 5=3+2

Exercise: write the quantum numbers for 4d.

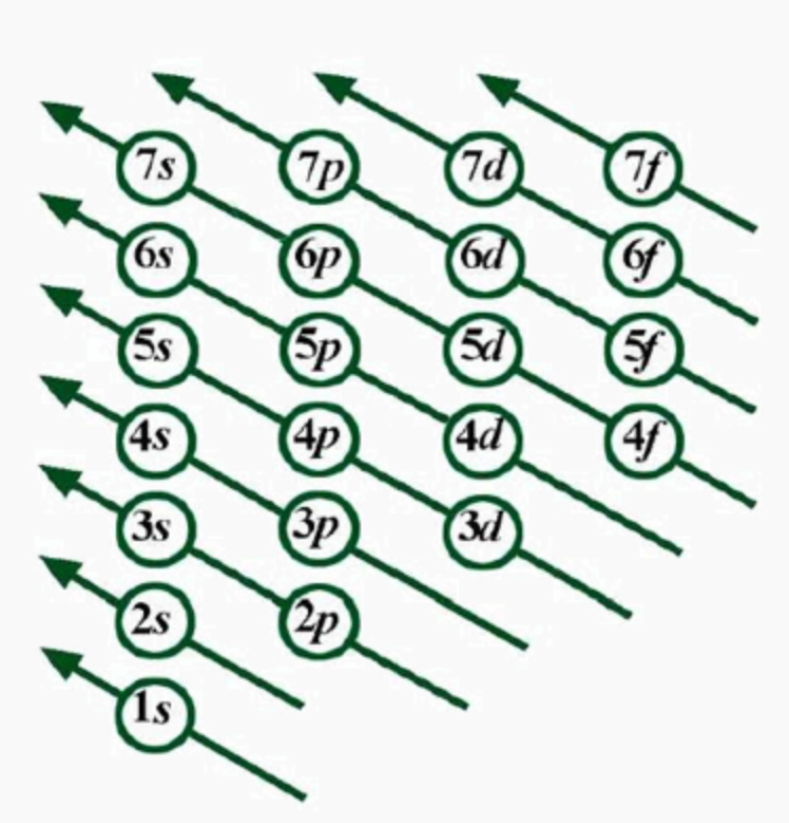
Principles & Rules

Aufbau principle – electron occupies the lowest energy orbital first

Pauli exclusion principle – each orbital may be occupied by two electrons at most. In the case of double occupation, the electron spins are paired.

Hund rule – in degeneracy sub-shell, electrons occupy different subshells in parallel spin states, instead of occupy the same sub-shell with paired spins.

Electron Configuration



Pay attention to s-orbital & d-orbital!!
When you figure out the electron configuration, treat 4s first; but when you **write your answer**, write 4s after 3d.

Exercises

Exercises

Write the electron configuration of Cr(24) and Fe(26).

Special Case for Hund Principle

Cr(24): $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$
Fe(26): $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$

Why?

In some special shell, electrons tend to form a structure of **full, half-full, empty**.
e.g. Cu(29)

Atomic Radius

Two determinants:

- Number of valence shells: number of shells↑, radius ↑.
- Effective nuclear charge: effective nuclear charge ↑, radius ↓.
  Effective nuclear charge:
  - Atom (non-charged): proton number ↑, effective nuclear charge ↑.
  - Ions (charged): charge number ↑, effective nuclear charge ↑.

Atomic Radius

- When proton numbers are equal…

  The more the electron numbers, the bigger the radius.

  e.g. Cs- > Cs > Cs+

- When two atoms have the same principal quantum number…

  The more the proton numbers, the smaller the radius.

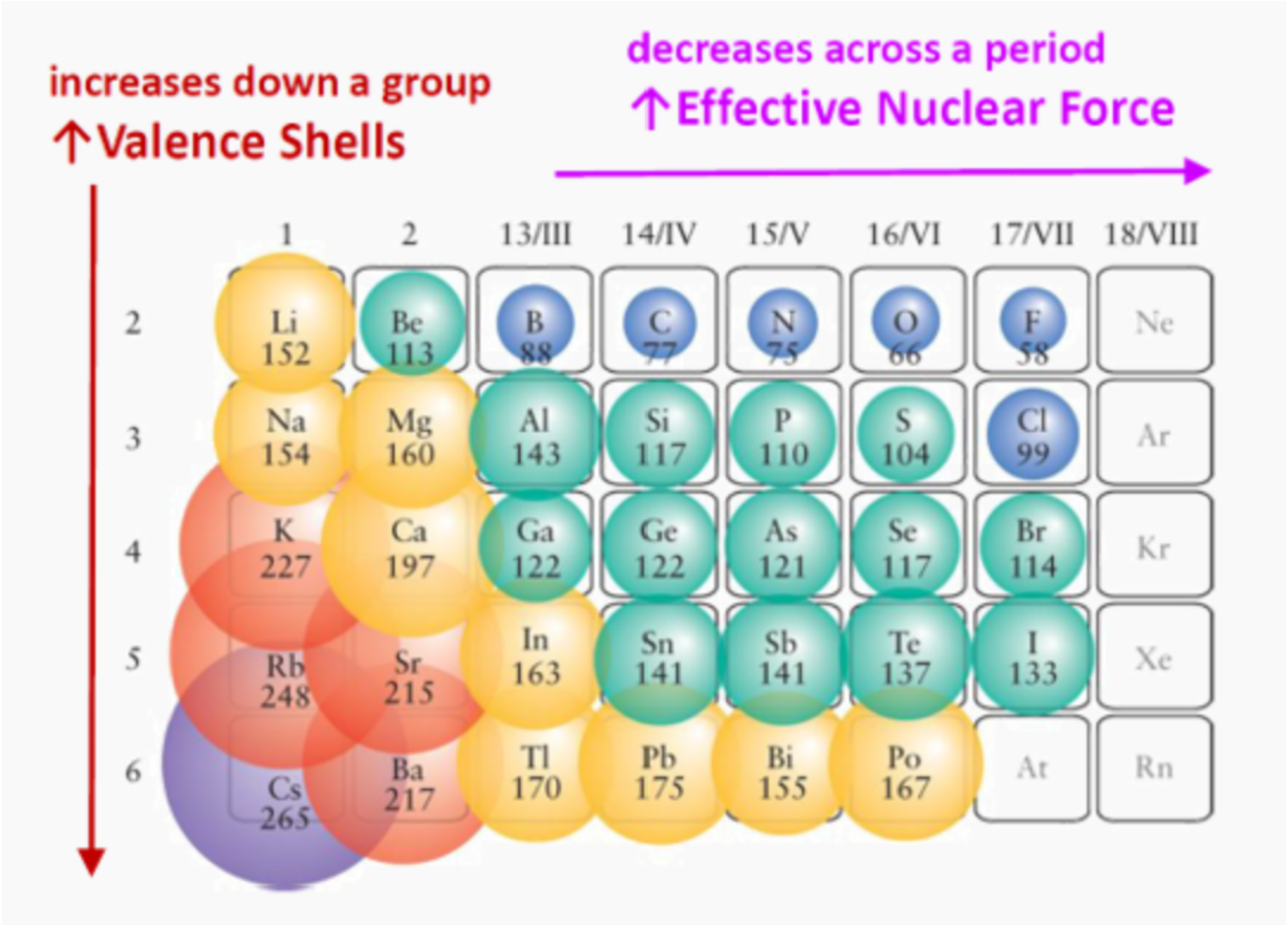
  e.g. Na > Mg > Al

- When two ions have the same electron numbers…

  The more the proton numbers, the smaller the radius.

  e.g. $O^{2-} > F^{-} > Na^{+} > Mg^{2+} > Al^{3+}$

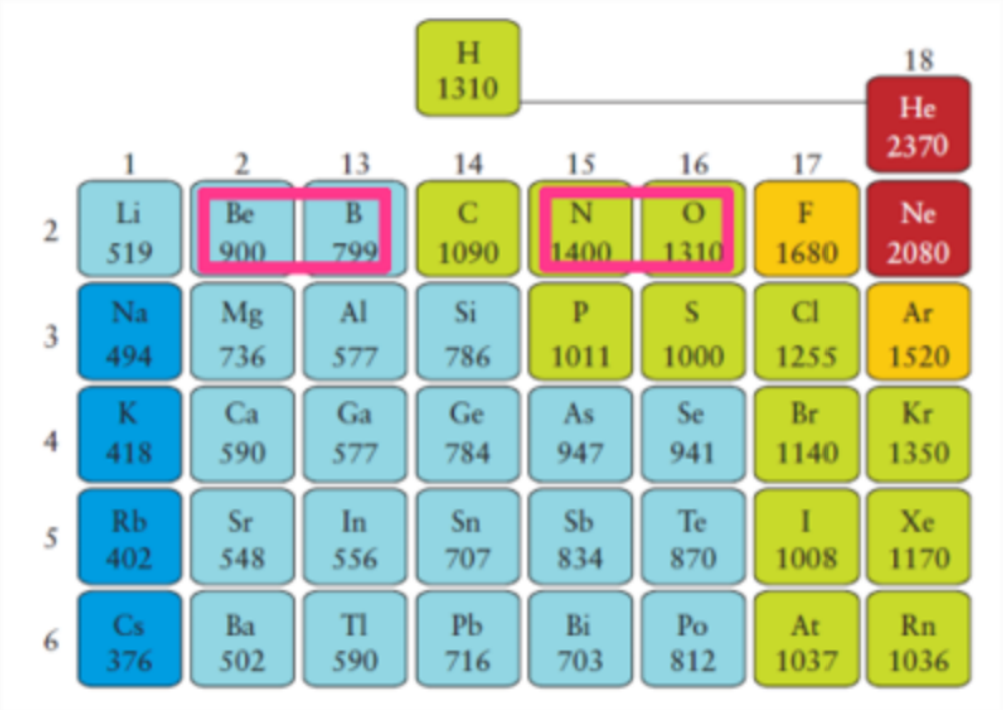
Atomic Radius



Ionization Energy

- Definition: the minimum energy needed to remove 1 electron from a **gas** atom.
- Unit:**kJ/mol**
- Trend of the first ionization energy:
  - Valence shells $\uparrow$, I_1 $\downarrow$.
  - Effective nuclear charge $\uparrow$, I_1 $\uparrow$.

Special Cases



But there are special cases…

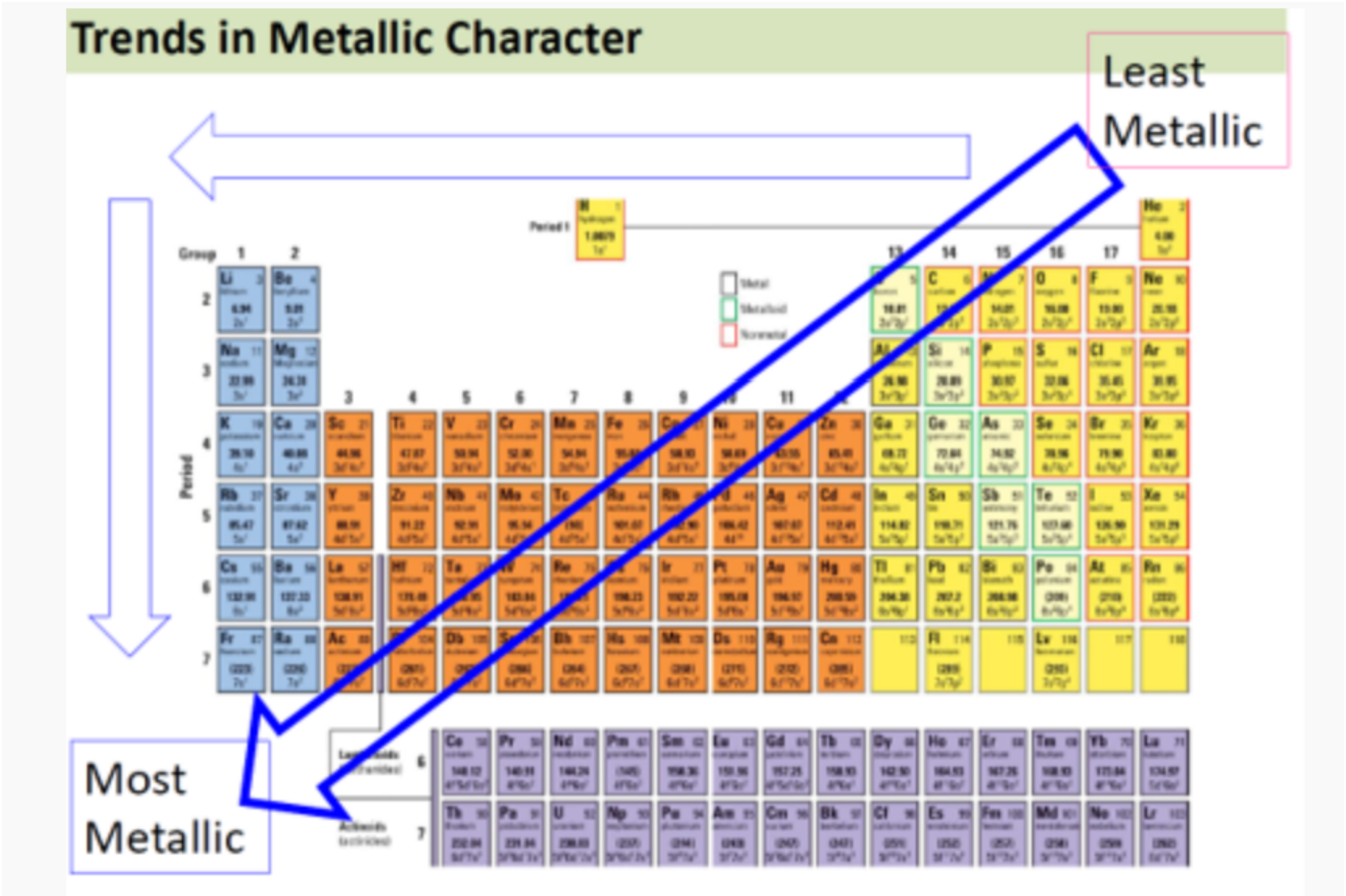
How could this happen?

Half-shell or full shell are more stable, so that the additional electron is less stable

Electron Affinity

- Definition: the energy released when 1 electron is added to a neutral atom in **gaseous** state to form a negative ion.
  - Positive: energy released
  - Negative: energy absorbed
- Contrast to ionization energy.

Metallic Character



Comparison between metal & nonmetal

Metals:

Malleable (bend) and ductile (make a wire).
Shiny so reflect light (mirrors).
Electrical and thermal conduct.
Basic.
Lose electrons—**oxidized**.

Nonmetals:

Brittle.
Dull.
Electrical and thermal insulators.
Acidic.
Gain electrons—**reduced**.

The End

Thanks for attendance. Q& A