3.3 ELECTRON CONFIGURATIONS AND PERIODIC TRENDS

SCH4U  Grade 12 University Chemistry  Ms. Papaiconomou

SINGLE-ELECTRON SYSTEMS (ATOMS WITH ONE ELECTRON)
- All orbitals that have the same value for \( n \) have the same energy
- Ground state (lowest energy & most stable state) when electron in 1s
- Excited state, when electron absorbs energy, electron found in other orbitals

MULTI-ELECTRON SYSTEMS (ATOMS WITH MORE THAN ONE ELECTRON)
- Due to interactions among the additional electrons result orbitals that have the same value for \( n \) have different energies (i.e. 2s has a lower energy than 2p)
- Orbitals within a sublevel have the same energy (3 2p orbitals have same energy)
- Ground state (most stable energy state) when electrons in the lowest possible energy level

Pauli Exclusion Principle
1925 (Wolfgang Pauli) - only two electrons of opposite spin could occupy an orbital
- Orbital may have a maximum of two electrons only, each of which must have the opposite spin direction of the other
- May have only one electron or none at all (empty), but maximum is two electrons (full)
- No two electrons in an atom have the same four quantum numbers; must be unique

Electron Configurations
- Shortcut to represent the number and orbital arrangements of electrons in each atom is intimately connected to the structure and logic of the periodic table
- An atom's chemical properties are mainly associated with its ground state electron configuration

Aufbau Principle
- When writing electron configuration, start with the first element in the periodic table and add an electron to its lowest available energy level
  - Hydrogen 1 e- 1s\(^1\)
  - Helium 2 e-s 1s\(^2\)
  - Lithium 3 e-s 1s\(^2\)2s\(^1\) or [He]2s\(^1\)
**Orbital Diagram**

- plot and keep track of electrons in their orbitals using a box for each orbital in any given principal energy level
  - empty box \( \rightarrow \) orbital with no electrons
  - one arrow box \( \rightarrow \) orbital filled with one electron
  - oppositely pointing arrows \( \rightarrow \) filled orbital

**Guidelines for “Filling” Orbitals**

1. Place electrons into the orbitals in order of increasing energy level.
2. Each set of orbitals of the same energy level must be completely filled before proceeding to the next orbital or series of orbitals.
3. Whenever electrons are added to orbitals of the same energy sub-level, each orbital receives one electron before any pairing occurs.
4. When electrons are added singly to separate orbitals of the same energy, the electrons must all have the same spin.

Guidelines 3 and 4 together comprise what is known as **Hund’s rule**.
If you “obey” Hund’s rule, no two electrons can have the same set of quantum numbers. Thus, this rule follows from Pauli’s exclusion principle.

Orbitals are not filled in order of principal quantum number, but in order of increasing energy.

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

The periodic table provides the pattern for filling the orbitals of elements.

The shape and organization of the periodic table is a direct consequence of the electronic structure of the atoms.

But, some atoms achieve greater stability with electron configurations that do not conform to predicted patterns.

- **Cr** – stable when 4s and 3d orbitals and half-filled
- **Cu** – stable when 4s half-filled and 3d is completely filled

**Main group elements/ Representative elements**

- elements that appear in the s block and the p block
- representative of a wide range of physical and chemical properties
  - metals, non-metals, metalloids; highly reactive, moderately reactive, unreactive; most solid, ¼ gas, l liquid

**Transition elements**

- elements that appear in the d block
- mark the transition from the p orbital filling order to the d orbital filling order

**Inner Transition elements**

- elements that appear in the f block
- mark the transition from the d orbital filling order to the f orbital filling order
**Patterns involving Group Numbers and Period Numbers**

1. For main group elements, the last numeral of the group number is the same as the number of valence electrons.
2. The \( n \) value of the highest occupied energy level is the period number.
3. The square of the \( n \) value \((n^2)\) equals the total number of orbitals in that energy level. Since each orbital may have a maximum of two electrons, the maximum number of electrons in any principle energy level is \(2n^2\).

### s block
- H, He, Groups 1 (IA) & 2(IIA)
- valence electrons occupy only the \(ns\) orbitals
- H & Group 1 \(ns^1\)
- He & Group 2 \(ns^2\)

### p block
- Groups 13(IIIA) to 18(VIIIA)
- three \(p\) orbitals can hold a max of six electrons, and so span six groups
- \(ns^2 np^a\) \(a = 1\) to \(6\)
- Noble gases \((ns^2 np^6)\) have full \(s\) and \(p\) orbitals that is very stable

### d block
- transition elements
- filled \(ns\) orbitals and partially filled \((n-1)d\) orbitals
- five \(d\) orbitals can hold a maximum of 10 electrons, so span 10 groups
- there are exceptions because these two sublevels \([ns \text{ and } (n-1)d]\) are very close in energy

### f block
- inner transition elements
- filled \(ns\) orbitals and partially filled \((n-2)f\) orbitals
- seven \(f\) orbitals can hold a maximum of 14 electrons, so span 14 groups
- there are MANY exceptions, so difficult to predict electron configurations

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**Periodic Trends in... ATOMIC RADIUS**

- Atomic radius = the distance between nuclei of bonded, neighbouring atoms
- Atomic radius generally (1) decreases across a period, (2) increases down a group
- Factors:
  - (A) Changing \(n\) – with higher \(n\), higher probability of finding electrons farther from the nucleus
  - Governs the trend of increasing atomic radius down a group
  - (B) Effective nuclear charge (net force of attraction between electrons and the nucleus they surround)
    - Hydrogen’s electron experiences the full positive charge of its nucleus, a nuclear charge of \(Z\)
    - All other atoms, nuclear charge is offset by other electrons and is \(Z_{\text{eff}}\) (may be small or large)
    - Inner electrons shield valence electrons from the attractive force of the nucleus, and experience a lesser \(Z_{\text{eff}}\)
  - Governs the trend of decreasing atomic radius across a period
- Transition elements do not display the same pattern as main group elements due to the \(d\) orbital which maintains the atomic size fairly constant

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**Periodic Trends in... IONIZATION ENERGY**

- Ionization energy = energy needed to completely remove one electron from a ground state gaseous atom
- Multi-electron atoms have 2 or more electrons, and so have more than one ionization energy
  - Need to add energy to remove an electron in order to overcome the force of attraction exerted on the electron by the nucleus
  - First IE \((IE_1)\) is least energy required to remove electron from outermost occupied energy level
  - Second IE \((IE_2)\) is always greater than the first IE because electrons removed from positively charged ion, etc.
- Ionization Energy generally (1) decreases down a group, (2) increases across a period
  - Variations:
    - 1 electrons in higher energy sublevels are easily removed (B & Al)
      - half-filled orbitals are more stable than over half-filled orbitals due to electron repulsion (O & S)
    - Linked to reactivity of metals
**Periodic Trends in… ELECTRON AFFINITY**

- Electron Affinity = change in energy that occurs when an electron is added to a gaseous atom
- Multi-electron atoms have more than one electron affinity
  - First EA results in a negatively charged atom of charge 1-
  - Second EA results in a negatively charged atom of charge 2-
- Electron Affinity can be positive (need to add energy), negative (energy given off when electron added)
  - High electron affinity = High negative number
  - Low electron affinity = Low negative number or positive number
- Irregular trend seen, but significant when consider ionization energy as well
  - Group 17 (VIIA) and to lesser degree Group 16 (VIA) have high IE and high EA
    → a lot of energy to remove electrons from these, so attract electrons and form negative ions
  - Group 1 (IA) & Group 2 (IIA) have low IE and low EA
    → give up electrons easily, but attract them poorly, so form positive ions
  - Group 18 (VIIIA) have very high IE and very low EA
    → do not gain, give up or share electrons at all

**HOMEWORK**

- Please re-read Section 3.3 (pp.139-158) and answer:
  - p.145-6 Q.6-9
  - p.150 Q.10-13
  - pp.157-8 Q.1-8