CHAPTER 2 ATOMIC STRUCTURE
(IB TOPICS 2 AND 12) SUMMARY

Introduction

- **Relative masses**: p = 1, n = 1, e = 1/1840; *charges*: p = +1, n = 0, e^- = –1.
- Protons and neutrons are present in the nucleus of an atom, electrons are in orbits or shells around the nucleus.
- **Atomic number, Z** = number of protons; the fundamental characteristic of an element.
- **Mass number, A** = number of (protons + neutrons).
- **Isotopes:** same atomic number, different mass number OR same number of protons, different number of neutrons OR atoms of the same element with different masses.
- **Isotopes** differ in physical properties that depend on mass such as density, rate of diffusion etc. Chemical properties are the same because of the same electronic configuration or arrangement.
- **Atomic mass** of an element is the average of the atomic masses of its isotopes; depends on isotopes relative abundance; leads to non-integer atomic masses.

Mass Spectrometer

- Stages of Operation: Vaporization of sample, ionization to produce M^+ ions, acceleration of ions by electric field, deflection of ions by magnetic field, vacuum, detection of ions.
- Degree of deflection:
- Lower the mass, higher the deflection.
- Higher the charge, higher the deflection.
- Deflection reflects mass/charge ratio; for charge of +1, deflection depends on mass.
- For an element, the mass spectrum gives **two** important pieces of information: the number of isotopes, and the abundance of each isotope; thus the relative average atomic mass, A_r can be calculated.
- For a molecule, the highest peak represents the molecular (parent) ion and its mass gives the relative molecular mass, M_r of the compound (and the fragmentation pattern can help determine its structure).
  - A continuous spectrum contains light of all wavelengths in the visible range.
  - A line spectrum consists of a few lines of different wavelengths.
  - When electrons are excited, they jump to higher energy levels.
  - Electrons fall back to lower energy levels, and the energy equivalent to the difference in energy level is emitted in the form of photons.
  - Energy levels come together in terms of energy the farther away they are from the nucleus; this explains the convergence of lines in a line spectrum.
  - The maximum number of electrons in a main energy level n is $2n^2$:

    1st energy level, n = 1; maximum 2 e^-;

    n = 2, maximum 8 e^-;

    n = 3, maximum 18 e^-.

The electron arrangement (or configuration) indicates the number of electrons and their energy distribution. This determines an element's physical and chemical properties.

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- **Main (or principal) energy levels, sub-levels and orbitals:** The main energy levels, n are assigned whole number integers, n = 1, 2, 3, 4… . n = 1 represents the lowest energy level. Each main energy level contains n sub-levels and a total of n^2 orbitals.
  - s, p, d, f etc. is the common notation for sub-levels and orbitals within sub-levels. An orbital is an area of space around the nucleus in which an electron moves.
  - Orbitals have characteristic shapes. There is one *s* orbital which is *spherical* in shape, three *p* orbitals which are *dumbbell* shaped, called p_x, p_y p_z, and arranged in the x, y, and z directions respectively, five *d* orbitals and seven *f* orbitals (both with complex shapes). The relative energies of s, p, d, and f orbitals with in a sub-level are: $s < p < d < f$.
  - Each orbital can have a maximum of 2 electrons. n = 1 has one sub-level which is called an s sub-level and which contains one s orbital. n = 2 has two sub-levels: 2s and 2p; n = 3 has 3 sub-levels: 3s, 3p and 3d; n = 4 has 4 sub-levels:4s, 4p, 4d and 4f, etc.

- **The Aufbau ('building-up') Principle:** Electrons are placed in orbitals in order of increasing energy, starting with the lowest energy level, and in general, filling each sub-level completely before beginning the next. This is due to the fact that systems in nature prefer minimum energy in order to achieve maximum stability.
- **Hund's Rule:** Occupation of sub-levels takes place singly as far as possible before pairing starts.
- **Pauli exclusion principle:** No two electrons in an atom can be in exactly the same state; no two electrons in a given atom can have the same four quantum numbers (that is, these can not be in the same place at the same time)
- $\boldsymbol{nl^x}$ notation is used to describe the electron configuration of an element: $\boldsymbol{n}$ is the main energy level, $\boldsymbol{l}$ the sub-level, and $\boldsymbol{x}$ is the number of electrons in the sub-level.
- The **ionisation energy** of an atom is the minimum amount of energy required to remove a mole of electrons from a mole of gaseous atoms to form a mole of gaseous ions.

(N.B. Shading indicates Topic 12 (AHL) material.)