Chemistry with Chloe

AQA A Level Chemistry — 3.1 Physical Chemistry

3.1.1 Atomic Structure

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3.1.1.1 *Fundamental particles: protons, neutrons and electrons – relative charge and relative mass.*

Proton: relative mass = 1, relative charge = +1. Found in the nucleus.

Neutron: relative mass = 1, relative charge = 0. Found in the nucleus.

Electron: relative mass = 1/1836 (≈0), relative charge = –1. Found in shells/orbitals around the nucleus.

The nucleus is small, dense and positively charged. Most of the atom is empty space.

3.1.1.2a *Mass number (A) and atomic (proton) number (Z). Determine fundamental particles in atoms and ions. Explain the existence of isotopes.*

Atomic number (Z): number of protons. Defines the element.

Mass number (A): total protons + neutrons.

Neutrons = A – Z. Electrons = Z for a neutral atom; for ions, adjust by the charge.

Isotopes: atoms of the same element (same Z) with different numbers of neutrons (different A). Same chemical properties, different physical properties.

3.1.1.2b *Principles of a simple time of flight (TOF) mass spectrometer: ionisation, acceleration, ion drift, ion detection, data analysis.*

1. Ionisation: sample ionised (electron impact or electrospray) to form positive ions.

2. Acceleration: ions accelerated by electric field — all given the same kinetic energy (KE = ½mv²).

3. Ion drift: ions travel through a field-free region. Lighter ions travel faster and arrive first. Time depends on m/z.

4. Detection: ions hit detector — signal proportional to abundance.

5. Data analysis: m/z and abundance give mass spectrum. Used to find isotopic masses and Ar.

Ar = Σ(isotopic mass × abundance) / Σ(abundances)

3.1.1.3 *Electron configurations of atoms and ions up to Z = 36. First and successive ionisation energies.*

Fill order: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6$

Anomalies: Cr = [Ar] $3d^5\ 4s^1$, Cu = [Ar] $3d^{10}\ 4s^1$

For ions: remove 4s electrons before 3d.

First IE: $X(g) \rightarrow X^+(g) + e^-$ — energy to remove one mole of electrons from one mole of gaseous atoms.

Trend in Period 3 (Na→Ar): generally increases. Drop at Al (3p easier than 3s) and S (paired 3p repulsion).

Trend in Group 2 (Be→Ba): decreases — more shells, greater shielding, electron further from nucleus.

Successive IEs: large jump = electron removed from new inner shell = evidence for shell structure.