

Unit 1 - Structure and Properties

Quantum Theory

Bohr-Rutherford Model (1913): in this atomic model, presented by Niels Bohr and Ernest Rutherford, electrons orbit around a small, dense nucleus.

Electromagnetic Radiation: perpendicular electric and magnetic fields moving through space as waves.

$$\lambda = \frac{c}{\nu} \text{ and } E = h\nu$$

- λ = wavelength (m)
- ν = frequency (Hz)
- c = speed of light in vacuum ($2.998 \times 10^8 \text{ ms}^{-1}$)
- E = energy of light in Joules (J)
- h = Planck's constant ($6.626 \times 10^{-34} \text{ J} \cdot \text{s}$)

★ The **quantum mechanical model of the atom** treats the electron like a wave.

Atomic Spectra

Photon: a packet of electromagnetic energy.

Quantum: an indivisible packet of energy that must be absorbed or emitted in an “all or none” manner.

Emission Spectrum or Line Spectrum: atoms of a specific element emit a series of separate lines of different colours as their excitation energy decreases.

- atoms emit/absorb particular colours of light
- the frequencies emitted/absorbed are the same
- an emission spectrum is formed when electricity is run through an element in gas form
- an absorption spectrum is formed when light is shone through a gaseous element
- sunlight produces a *continuous spectrum*, which contains all the wavelengths in the visible region of the electromagnetic spectrum

Bohr used the line spectrum of hydrogen when it was “excited” to discover the energies of each energy level in the hydrogen atom.

Electron Transitions

Ground State: the orbit that has the lowest possible energy of the atom.

Excited State: when an atom absorbs energy.

An atom can become excited in one of two ways:

1. collide with a highly energetic particle like an e^- in an electric current passing through a gas.
2. absorb a photon where its energy is equal to the difference between the energy of the orbit it occupies and the energy of a higher orbit.

Used to calculate the potential energy of an electron in a hydrogen atom. Calculating ΔE determines the energy of a photon required to cause a transition.

$$E_n = -\frac{2.18 \times 10^{-18} \text{ J}}{n^2}, \Delta E = E_{\text{higher}} - E_{\text{lower}}$$

The Rydberg formula calculates the wavelength of light emitted from a specific electron transition in hydrogen-like elements (only 1 electron).

$$\frac{1}{\lambda} = RZ^2 \left(\frac{1}{n_l^2} - \frac{1}{n_u^2} \right)$$

- R = Rydberg constant ($1.097 \times 10^7 \text{ m}^{-1}$)
- Z = atomic number and n = energy level

Orbitals

Atomic Orbital: a region in space around the nucleus that is related to a specific wave function.

- they are three-dimensional
- they contain a maximum of two electrons
- shapes are predicted by Schrödinger's equation

The **orbital-shape quantum number, l** , is used to describe an orbital's shape.

Value of l	0	1	2	3	4
Name of orbital	s	p	d	f	g

★ The *overall shape* of an atom is a combination of all its orbitals.

Quantum Numbers

Quantum Numbers: integers that describe specific properties of electrons in atoms, arising from the solutions to the wave equation.

The Principle Quantum Number, n : indicates the energy level and relative size of an atomic orbital.

→ The value of n can range from $n = 1$ to $n = \infty$.

→ The differences between energy levels become smaller as n gets larger.

The Orbital-Shape Quantum Number, l : describes the shape of atomic orbitals within each principle energy level, it refers to energy **sublevels**.

→ The values of l are dependent on the value of the principle quantum number, n .

→ The values of l are positive integers that range in value from 0 to $(n - 1)$.

→ The number of possible values for l in a given energy level is the same as the value of n .

Zeeman effect: the splitting of the spectral lines of an atom in the presence of a strong magnetic field.

The Magnetic Quantum Number, m_l : indicates the orientation of the orbital in the space around the nucleus.

→ The value of m_l depends on the value of l .

e.g. p orbitals have the same shape and energy for a given value of n , but different orientations around the nucleus which are designated p_x , p_y , and p_z .

→ For any given value of l , there are $(2l + 1)$ values for m_l ranging from $-l$ to $+l$.

e.g. If $l = 1$, m_l can be -1 , 0 , or $+1$.

The Spin Quantum Number, m_s : specifies the orientation of the axis on which the electron is spinning.

→ Has only two possible values: $+\frac{1}{2}$ or $-\frac{1}{2}$.

Quantum Numbers for Helium:

Electron	Quantum Numbers
First	$n = 1, l = 0, m_l = 0, m_s = +\frac{1}{2}$
Second	$n = 1, l = 0, m_l = 0, m_s = -\frac{1}{2}$

→ The total number of orbitals for any energy level n is given by n^2 .

→ In general, in any energy level, n , there can be no more than $2n^2$ electrons.

Electron Configurations

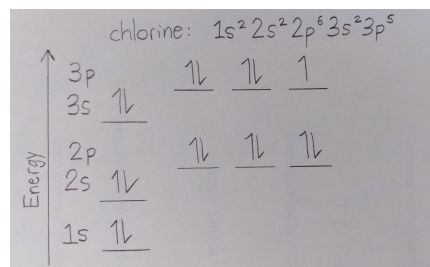
Pauli Exclusion Principle: a maximum of two electrons can occupy an orbital, and the electrons must have opposite spins.

↔ No two electrons in an atom can have the same four quantum numbers.

Aufbau Principle: each electron occupies the lowest energy orbital available.

$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < \dots$

Hund's Rule: single electrons with the same spin must occupy each equal-energy orbital before additional electrons with opposite spins can occupy the same orbitals.



Anomalous Electron Configurations

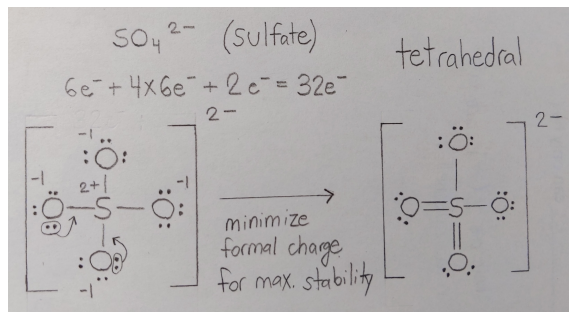
chromium: $[\text{Ar}]4s^1 3d^5$, copper: $[\text{Ar}]4s^1 3d^{10}$

- they are more stable when all of the d orbitals are half-filled, than if the s orbitals were filled
- s orbitals overlap in space with nearby d orbitals
- repulsion between electrons is minimized when electrons are removed from the s orbitals first

Lewis Structures

S , P , Si , Cl , and Xe can have expanded octets.

F.C. = # of valence e^- - # of dots - # of lines



Ionization Energy

Ionization Energy: the energy required to remove an electron from a ground-state gaseous atom.

The *second ionization energy* is always greater than the first ionization energy.

→ Within a group, first ionization energies generally decrease as you move down a group.

↔ Atomic radii increases, the distance of valence e^- from the nucleus increases.

→ Within a period, first ionization energies generally increase from left to right.

↔ Atomic radii decreases because Z_{eff} increases.

$Z_{\text{eff}} = \# \text{ of } p^+ \text{ in the nucleus} - \# \text{ of inner-shell } e^-$
★ The repulsion of electrons in an orbital decreases the amount of energy needed to remove the electron.

Magnetism

Paramagnetism: certain materials can become magnetic when in the presence of a magnetic field.

e.g. L , O , Na , Al

A material is magnetic when:

- unpaired electrons are present in its valence shell
- magnetic dipole moments of atoms are aligned with one another

When there is no external magnetic field, the magnetic fields of atoms are misaligned and cancel.

Ferromagnetism: when tightly-packed atoms cannot misalign when the external field is taken away.

e.g. Fe , Ni , Co , and their alloys

VSEPR Theory

Valence-Shell Electron-Pair Repulsion Theory: electron groups around an atom are positioned as far as possible from the others to minimize repulsions.

An *electron group* is a single bond, double bond, triple bond, or lone pair.

AX	linear	H_2	s	180°
AX ₂	linear	CO_2	sp	180°
AX ₃	trigonal planar	BF_3	sp^2	120°
AX ₄	tetrahedral	CH_4	sp^3	109.5°
AX ₅	trigonal bipyramidal	PCl_5	sp^3d	90° and 120°
AX ₆	octahedral	SF_6	sp^3d^2	90°

Quantum Mechanics and Bonding

Valence Bond Theory: a covalent bond forms when the atomic orbitals of two atoms overlap to share a common region in space and a pair of electrons occupies that region of overlap.

e.g. HF , the half-filled $2p$ orbital in fluorine overlaps with the half-filled $1s$ orbital in hydrogen (σ bond).

Molecular Orbital Theory: when atomic orbitals overlap, they combine to form new orbitals called molecular orbitals.

e.g. CH_4 , each of the 4 sp^3 hybrid orbitals that carbon forms, bonds with a hydrogen atom.

Sigma Bond (σ): The first bond made with any other atom and made from hybridized orbitals.

↔ Occurs when there is head-on-head overlap.

Pi Bond (π): Any 2nd or 3rd bond made with any other atom and made from left over p orbitals.

↔ Formed from side-by-side overlap of p orbitals.

Hybrid Orbital: an orbital that is formed by the combination of two or more orbitals in the valence shell of an atom.

★ A sigma (σ) bond is stronger than a pi (π) bond.

Intermolecular Forces

Factors affecting melting points of ionic compounds:

- ionic radii: the smaller the ionic radius, stronger the electrostatic attraction is between the ions.
- charge of ions: the larger the charge an ion has, the stronger the attraction is between the ions.

Strength of London Dispersion forces is affected by:

- area of contact between molecules: the more contacting area, the more attractions can be formed.
- polarizability: the more electrons (or shells), the easier it is for an electron cloud to become polar.

Solid types:

- ionic crystals: very high boiling points
- molecular crystals: relatively low boiling points
- metallic bonding: electron-sea model of free e^-
- covalent networks: large # of atoms are bonded