Physical Chemistry

Atomic Structure

Structure of an Atom
- An atom is the smallest particle of an element that can exist independently
- an atom consists of a nucleus with protons and neutrons, electrons orbit around the nucleus
- protons are positively charged, neutrons have no charge, electrons are negatively charged
- the nucleus has an overall positive charge
- an atom has an overall neutral charge

Subatomic particles
- The protons, neutrons, and electrons in an atom are subatomic particles
- their masses and charges are measured in relation to each other
- Such as Relative Atomic Mass and Relative Atomic Charge

Subatomic Particle	Relative Atomic Charge	Relative Atomic Mass
Proton	+1	1
Neutron	0	1
Electron	-1	1/1836

Atomic Number and Mass Number
- *Atomic Number/Proton Number* is the number of protons in the nucleus of an atom
- The atomic number is equal to the number of electrons in a neutral atom
- The *Mass Number/Nucleon Number* is the total number of protons and neutrons in an atom
- The number of neutrons can be calculated by *Mass Number - Atomic Number*

Atomic Radius
- The atomic radius of an element is half the distance between the two nuclei of covalently bonded atoms of the same type
- The atomic radius generally decreases across a period and increases down a group
- The atomic radius decreases across the period because with higher proton number there is higher nuclear charge and more electrons are added in the same quantum shell with approximately constant shielding, resulting in greater attraction between nucleus and electrons, pulling them closer.
- Down the group, the quantum shells increase and there is increased shielding, resulting in greater atomic radius.

Ionic Radius

- Size of cation is always smaller than that of its parent atom
- Size of anion is always greater than that of its parent atom
- Size of cation is always lesser than the size of anion provided they are in the same period.

Ionisation Energy

- Ionisation energy is the amount of energy required to remove one mole of electrons from one mole of gaseous atoms of an element to form one mole of gaseous ions
- Ionisation energy is measured under standard conditions of temperature and pressure
- The unit of I.E is Kilo joule per mole ($KJmol^{-1}$)
- Ionisation energy is always endothermic as we are breaking the electrostatic force between proton and electron
- The first ionisation energy is the amount of energy required to remove one mole of electrons from one mole of isolated gaseous atoms to form one mole of 1+ ions

The first I.E of an element X can be represented by the equation:

$$\mathbf{X_{(g)} \rightarrow X^{+}_{(g)} + e^{-}}$$

- Second I.E is always larger than the first I.E as upon removing electrons radius will become smaller, and there will be less repulsion, and greater nuclear force of attraction thus we need more I.E for the removal of second electron

Factors affecting Ionisation Energy

- The ionisation energy increases across a period and decreases down the group
- The I.E depends on factors of atomic radius, nuclear charge, shielding effect, and spin-pair repulsion

Atomic Radius: As the electrons get further from the nucleus, they experience lesser attraction from the nucleus and are easier to remove

Nuclear Charge: As the nuclear charge increases, the electrons experience greater force of attraction and are more difficult to remove

Shielding Effect: Electrons repel each other so the inner quantum shell electrons pushes the outer quantum shells away from the nucleus, reducing the nuclear attraction and making the electrons easier to remove

Spin pair repulsion: it occurs when two electrons are paired in the same orbital, they repel each other making one electron easier to remove

- Across a period, the nuclear charge increases, which results in stronger attraction between the nucleus and electrons, pulling the electrons closer and decreasing the atomic radius, the shielding effect remains constant as the electron shell is the same. This requires more energy to remove an electron, increasing the I.E
- Down the group, the atomic radius and shielding effect increases, which decreases the I.E

Ionisation Energy trends (Exceptions)
- An increase in subshell will decrease the I.E as outer subshell electrons are further away from the nucleus such as between Beryllium and Boron
- Another example would be Magnesium and Aluminium
- There is a decrease in I.E when a second electron enters the px subshell as it experiences spin-spin repulsion make it easier to remove an electron such between Nitrogen and Oxygen
- Another example would be Phosphorus and Sulfur
- There is a large decrease in ionisation energy between the last element in a period and the first element of the next to the change in quantum shell

Successive Ionisation Energies of an Element
- The successive ionisation energies of an element increases
- it is harder to remove an electron from an ion as compared to its neutral atom
- this is due to the decreased shielding effect and increased nuclear attraction
- A change in quantum shell causes a large increase in successive ionisation energy
- The large jump can be used to deduce the group number of an element
- For example, a large increase between the third and fourth I.E indicates that the element belongs to group 3

Isotopes
- Isotopes are atoms of the same element that contain the same number of protons but different number of neutrons
- An Isotope is represented by the name of the element followed by dash and mass number
- For example Carbon-12
- Isotopes have similar chemical properties but different physical properties
- Due to the same number of electrons, isotopes react in the same manner
- Due to the different number of neutrons, isotopes have differences in mass and density

Electron Shells
- Electronic configuration is the arrangement of electrons in an atom
- Electrons are arranged around the nucleus in principal energy levels or principal quantum shells
- The energy level or quantum shell is represented by the Principal Quantum Number (n)
- A higher principal quantum number means the shell is further from the nucleus
- Each quantum shell can hold a fixed number of electrons

Subshells
- The principal quantum shells are split into subshells
- Subshells are represented by s, p and d
- The energy of the subshells increases in the order s<p<d
- s subshell contains 2 electrons
- p subshell contains 6 electrons
- d subshell contains 10 electrons

Orbitals

- Subshells contain one or more atomic orbitals
- Orbitals exist at specific energy levels and electrons can only be found at these specific levels
- Each orbital can have a maximum of 2 electrons
- Hence, s subshell has 1 orbital, p subshell has 3, and d subshell has 5
- Each orbital has a specific shape
- the three orbitals of p subshell are px, py and pz

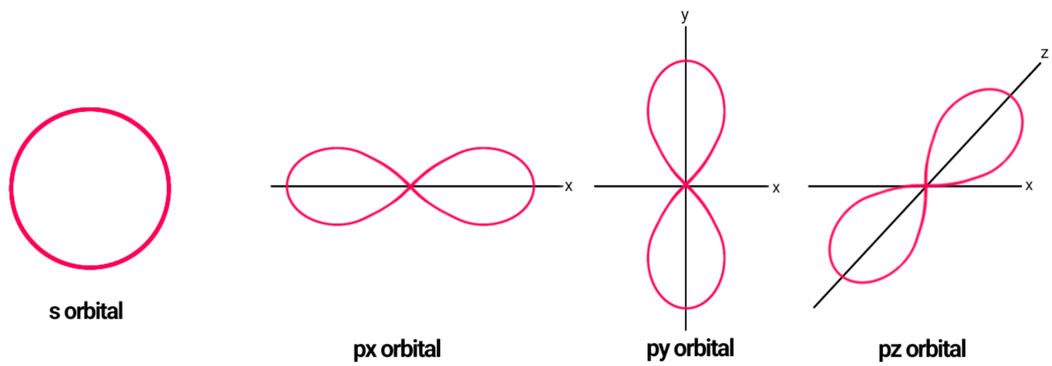
n	Electrons ($2n^2$)	Subshells
1	2	$1s^2$
2	8	$2s^2,2p^6$
3	18	$3s^2,3p^6,3d^{10}$
4	32	$4s^2,4p^6,4d^{10},4f^{14}$

Ground State

- The Ground state is the most stable electronic configuration of an atom which has the lowest amount of energy
- The subshells with lower energy levels are filled first
- The pattern is disrupted at quantum shells n=3 and above
- 4s has a lower energy level than 3d and hence is filled first

- Orbitals in the same subshell have the same energy and are known as degenerate
- px, py and pz all have the same energy levels

S & p orbitals
- s orbitals are spherical in shape
- the s orbitals are bigger at a higher principal quantum number
- p orbitals are dumbbell shaped
- every p subshell has 3 orbitals except for when n=1
- the p orbitals become larger and longer with increasing quantum number



Electronic Configuration
- subshells are filled in increasing order of energy levels
- electrons are spinning charges rotating clockwise or anticlockwise about their own axis
- electrons with similar spin repel each other, causing spin-pair repulsion
- electrons occupy different orbitals in the same subshell first to avoid spin-pair repulsion
- they are paired when there are no more empty orbitals
- the paired electrons spin in opposite directions to minimise repulsion
- if there are three electrons in the p subshell, all three orbitals will have one electron each
- a fourth electron in the p subshell will pair in px subshell

Periodic Table Blocks
- Group 1 and 2 elements are known as s block elements
- s block elements have their electrons in an s subshell
- Group 13 to 18 elements are p block elements
- their valence electrons are located in the p subshell
- Transition block elements are d block elements
- Their valence electrons are in the d subshell

Exceptions
- Copper has configuration $3d^5$,$4s^1$ instead of $3d^4$,$4s^2$
- Chromium has configuration $3d^{10}$,$4s^1$ instead of $3d^9$, $4s^2$
- This is because the configuration is more stable when the d subshell is half full or full as compared to having one lesser, so one electron moves from 4s subshell to 3d subshell