Chemistry Level 3: Thermochemistry

Chem 3.4 Electron configuration

Summary – what you need to know!
Electrons are around the nucleus in orbitals, in electron subshells. Each electron shell contains subshells.

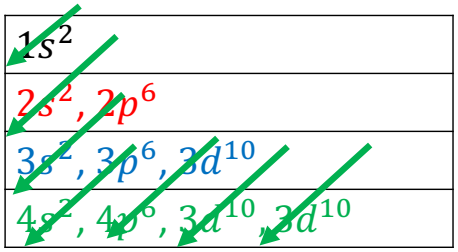
s	p	d	f
2	6	10	14

Energy level	Orbitals
1	1s
2	2s, 2p
3	3s, 3p, 3d
4	4s, 4p, 4d, 4f

We can use **shorthand**
$Iron = 1s^2, 2s^2, 2p^6, 3s^{2,}, 3p^6, 3d^6, 4s^2$
$Iron = [Ar]3d^6, 4s^2$

Ions
$Phosporous \rightarrow K^{3-}$
$1s^2, 2s^2, 2p^6, 3s^2, 3p^3 \rightarrow 1s^2, 2s^2, 2p^6, 3p^6$

Aufbau principle
Electrons always fill orbitals with the lowest energy first



$1s^2, 2s^2, 2p^6, 3s^{2,}, 3p^6, 3d^6, 4s^2, 3d^{10}, 4p^6$

4s has a lower energy than 3d, thus the 4s orbital fills **before** the 3d orbital

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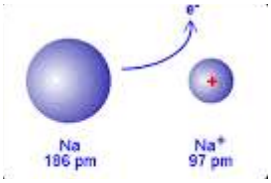
Chem 3.4 Periodic Table Trends

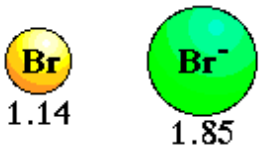
Summary – what you need to know!

Electronegativity – measure of the attraction between a nucleus and a pair of bonded electrons.
First ionisation energy – amount of energy required to remove one valence electron from a mole of atoms when they are in a gas state. Unit $kJ\ mol^{-1}$

Across group	Electrostatic attraction increases	Number of protons increases. No change in shielding or distance.
Down group	Electrostatic attraction decreases	Number of protons increases, but distance from nucleus increases and shielding increases.

	Across rows	Down groups
Electronegativity	↑	↓
Ionisation energy	↑	↓
Atomic radius	↓	↑





Positive ions – smaller than atom
Negative ions –larger than atom

Chem 3.4 Lewis diagrams

Lewis diagrams – what you need to know

1. Count the total number of valence electrons.
2. Connect the atoms with single bonds.
3. Place electrons in pairs around atoms.
4. Octet rule – check all valence shells are full. If not, move non-bonding pairs to form double or triple bonds.
5. Ions – enclose in [ ] and show charge.

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Molecular Shape and Polarity

What you need to know – compare/ contrast/ explain

Molecular shape

1. There are _____ electron pairs around the central atom _____.
2. There are _____ bonding pairs and _____ non bonding pairs.
3. The electron pairs repel each other so get as far away from each other as possible.
4. So they form a molecule with a _____ shape (OR if there were no non-bonding pairs the shape would be _____ but since the

Polarity

1. The A—B **bond** is polar /non polar because there is no /a difference in electronegativity between A and B (A is more/less δ^- thai

No polar bonds - because there are no polar bonds the molecule is non polar.

2. The **shape** of the molecule is _____.

As this shape is / is not symmetrical the dipoles do /don't cancel out so ABC is non polar / polar.

Molecular Shape and Polarity

1. Draw Lewis diagram ✅
2. Count total number of electron pairs around central atom
3. Count number of bonding pairs
4. Work out shape

				4	5	6
				90° Square planar FS_4	90° Square pyramid ICl_5	90° Octahedral PCl_6
5				90° T shaped ICl_3	90° 120° Distorted tetrahedron (or see saw) SF_4	90° 120° Trigonal bipyramid PCl_5
4	Bromine 109.5° Br–Br Linear	Water 109.5° Bent	Phosphine 109.5° Trigonal Pyramidal	Methane 109.5° Tetrahedral		
3	Oxygen 120° O=O Linear	Nitroxyl 120° Bent	Formaldehyde 120° Trigonal Planar			
2	Nitrogen 180° N≡N	Carbon Dioxide 180° O=C=O				

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Enthalpy

Summary – what you need to know!

	Standard enthalpy of	Energy change when 1 mole converts
$\Delta_{fus}H°$	Fusion	Solid → liquid (at mp)
$\Delta_{vap}H°$	Vapourisation	Liquid → gas (at bp)
$\Delta_{sub}H°$	Sublimation	Solid → gas
$\Delta_c H°$	Combustion	Undergoes complete combustion in oxygen
$\Delta_f H°$	Formation	Is formed from constituent elements

Exothermic reactions – give off heat
Endothermic reactions – require heat

$\Delta\ H°$= standard enthalpy change (kJ mol^{-1})

-Exothermic reactions

+ Endothermic reactions

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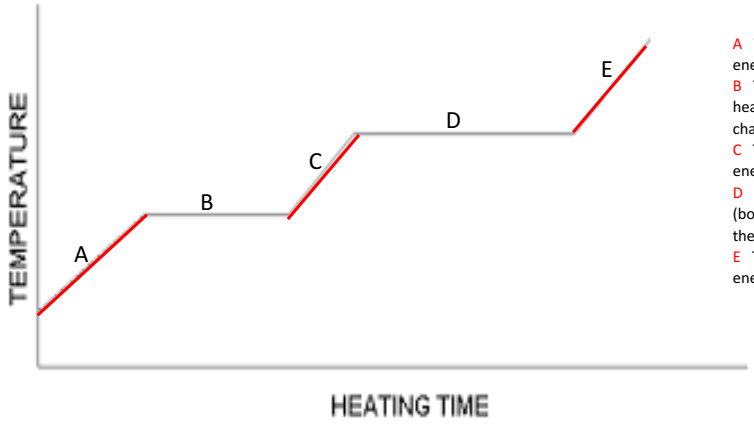
Graphing State Changes

Summary – what you need to know!
Stronger attractive forces between particles means higher $\Delta_{fus}H°$ and $\Delta_{fus}H$ °



A The substance is a solid. Heat energy is being used to increase the kinetic energy of the solid so its temperature increases
B The substance reaches melting point and is undergoing fusion (melting). The heat energy is being used to overcome the attractive forces so the solid changes into a liquid
C The substance is a liquid. Heat energy is being used to increase the kinetic energy of the liquid so its temperature increases
D The substance reaches boiling point and is undergoing vaporisation (boiling). The heat energy is being used to overcome the attractive forces so the liquid changes into a gas
E The substance is a gas. Heat energy is being used to increase the kinetic energy of the gas so its temperature increases

Enthalpy Calculations – Part 1

What you need to know

Enthalpy changes can be measured experimentally

$$q(j) = m \times c \times \Delta T$$

$m = mass\ of\ water\ (grams)$
$c = specific\ heat\ capacity\ of\ water\ = 4.8\ Jg^{-1\circ-1}$
$\Delta T = change\ in\ temperature(°C)$

$$\Delta_r H = \frac{-q}{n}$$

$n = number\ of\ moles$

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Enthalpy Calculations – Part 2

What you need to know!

Hess's Law: enthalpy change due to a chemical reaction is independent of the route taken.

Use known $\Delta_r H^\circ$ of given reactions to calculate the unknown $\Delta_r H^\circ$ of a reaction

1. Manipulate the given equations to match equation of interest
   - Flip
   - Multiply
2. Add equations together (products, reactants, enthalpies)
3. Cancel
4. Check

NB: you need to balance the equation in terms of moles

$$\Delta_r H^\circ = \Sigma \Delta_f H^\circ(\text{products}) - \Sigma \Delta_f H^\circ(\text{reactants})$$

Entropy

Entropy (S) is a measure of the disorder of a system
Spontaneity of a chemical reaction: determined by the change in both the enthalpy and entropy of the reaction.

Factors affecting entropy:

	Particle movement	Random motion	Disorder	Entropy
Physical state S→L→G	Increases	Increases	Increases	Increases
Increase in volume (gas)	Increases	Increases	Increases	Increases
Increase in temperature	Increases	Increases	Increases	Increases
Increase in number of particles	Increases	Increases	Increases	Increases
Surroundings (exothermic reaction)	Increases (temp increases)	Increases	Increases	Increases
Surroundings (endothermic reaction)	Decreases (temp decreases)	Decreases	Decreases	Decreases