

CHEMISTRY NOTES

<http://homepage.mac.com/stray/ib/chem/>

STOICHIOMETRY

1.1 Mole concept & Avogadro's constant

1.1.1 : 1 Mole of something is equivalent to 6.023×10^{23} (<-- Avogadro's constant) units of it...ie lots of atoms, molecules etc...the periodic table gives molar masses...ie the number of grams of a substance required for 1 mol of atoms. This can be extrapolated to molecules of known molecular formula.

1.1.2 : Number of mols = mass / mass per mol (Usually found on periodic table)...The coefficients in chemical equations give the molar ratios of reactants and products...ie $2A + 3B \rightarrow C$. There is $2/3$ as much A as B, and 3 times more B than C involved in the reaction...Assuming the reaction goes to completion, there must be $3/2$ times as much B as A for neither to remain...If this ratio is not followed, one will be a limiting reactant, and so the reaction will have some of the other reactant left over when it completes.

1.2 Formulae

1.2.1 : Atomic mass, Molecular Mass, Formula Mass : All the mass per mol of a particular type of species...atoms, molecules or formula units. These can be found for the periodic table, and will give the mass for 1 mol of the species (or rather the average accounting for different isotopes and their relative abundance). Mr is the ratio between the molar masses of two species. Ar is the ratio of the number of atoms between two species. These two ratios will be equal.

1.2.2 : Moles vs Mass...Moles is a number of something...every mol being 6.023×10^{23} individual elements. Mass is the property which results in 'weight' in the presence of Gravity. Given a molar mass, M a mass m and a number of mols N then $N = m/M$.

1.2.3 : An 'Empirical formula' is the formula describing the different atoms present in a molecules, and their ratios, but not the actual number present. ie $A_xB_yZ_c$ could be an empirical formula if x, y, and z are in lowest common terms. The molar mass can then be used to calculate the actual numbers of each atom present per molecule. The empirical formula can be determined by percentage composition, or anything else which gives the ratios of atoms present.

1.2.4 : A Molecular Formula is similar to an empirical formula except that it includes the the number of atoms present in each molecule, rather than the ratio. It will be an integer multiple of the empirical formula ie $KA_xB_yZ_c$ and can be calculated from the empirical formula and the molar mass of the substance.

1.3 Chemical Equations

1.3.1 : The mole ratio of two species in a chemical equation is the ratio of their coefficients...ie $aX + bY \rightarrow cZ$: The ratio of X/Y is a/b , $Y/Z = b/c$, etc...

1.3.2 : Balancing equations...change only the coefficients, not the subscripts to make sure

all atoms, and charge is conserved (half equations can be balanced by addition of electrons to either side...2 half equations can be added by making the number of electrons equal in each, then vertically adding.)

1.3.3 : State symbols -- (s)-Solid , (l)-liquid, (g)-gas, (aq)-aqueous solution...ie something dissolved in water. Should be included in all chemical reactions (but won't be penalized).

1.4 Mass relationships in chemical reactions

1.4.1 : Mass is conserved throughout reactions. This fact allows masses to be calculated based on other masses in the reaction eg burning Mg in air to produce MgO and so to find the mass of Mg present in the original sample (ie purity)...can be extended to concentrations...ie titration.

1.4.2 : When a reaction contains several reactants, some may be in excess...is more is present that can be used in the reaction. The first reactant to run out is the limiting reagent (or reactant). Knowing the number of mols of the limiting reagent allows all other species to be calculated, and so the yield, and remaining quantities of other reactants.

1.5 Solutions

1.5.1 : Solvent - the stuff you're dissolving in...ie water. Solute - the stuff you're dissolving in it...an ionic compound or something...Solution - the two of them when mixed together. Concentration - the amount of solute per amount of solvent...in mols per dm^3 ...ie mols per liter or grams per liter.

1.5.2 : Apply the equation $\text{concentration} = \frac{\text{number}}{\text{volume}}$...rather obvious from the units of concentration, but remember to convert everything into the same units.

1.5.3 : Use chemical equations to relate the amount of one species to the amounts of others.

ATOMIC THEORY (SL)

2.1 The Nuclear atom

2.1.1 : Protons -- Mass = 1 amu , charge = +1 .. Neutrons -- Mass = 1 amu , charge = 0 ..
Electron -- Mass = $\frac{1}{1840}$ amu (usually insignificant), charge = -1

2.1.2 : Protons and Neutrons form the nucleus of the atom, electrons orbit the nucleus in electron shells.

2.1.3 : Mass number (A) -- Number of protons + neutrons. Atomic number (Z) -- number of proton. Isotope -- atoms with same atomic number but different mass number (ie different numbers of neutrons)

2.1.4 : $A_ZX...$ A = mass number, Z = atomic number, X = atomic symbol.

2.1.5 : Isotopes may differ in physical properties (mass/density) and radioactivity but not generally in chemical properties.

2.1.6 : Atomic masses are the average of the atomic mass of each isotope (isotopic mass) times the isotope's relative abundance. results in non integer atomic masses

2.1.7 : Atomic number = number of protons (or number of electrons - ionic charge) ,
mass number - atomic number = number of neutrons.

2.2 Electron Arrangement

2.2.1 : Continuous spectrum goes continuously through red, orange, yellow, green, blue, indigo, violet. A line spectrum contains only some individual lines from this spectrum.

2.2.2 : Electrons are excited (usually by running an electric current through them). This causes electrons to 'jump' into higher electron shells ($X \rightarrow X^*$) this state is only temporary, however, and the electron falls back to it's ground state. This change decreases the energy of the electron, and this energy is emitted in the form of a photon. If this photon falls into the visible spectrum of light, then it produces a visible spectrum. As electrons move further away from the nucleus, the electron shells become closer together in terms of space and energy, and so lines converge towards the end of the spectrum.

2.2.3 : The main electron levels go : 2, 8, 18 etc... $2^n + 2$ for n_0 , n_1 and n_2 ...

2.2.4 : Electrons are added from the left...after each shell is filled, move to the next...2, 8, 18...only up to Z = 20 is required.

ATOMIC THEORY (HL)

12.1 The mass spectrometer

12.1.1 : Stages of operation : vaporisation, ionisation, acceleration, deflection and detection...Substance to be tested is vaporised (by heat, absence of oxygen) then ionised by electric current. Ions are accelerated through an electric field, then deflected by a magnetic field. Ions are then detected...the angle of deflection reflects their mass to charge ratio.

12.1.2 : The angle of deflection of each fragment is proportional to it's mass, and so it is possible to find the relative atomic mass of each 'spike' the height of the spike represents the frequency, therefore, the abundance can be calculated. The relative atomic mass is the average of the isotope masses times their frequencies.

12.2 Electronic structure of atoms

12.2.1 : Successive electrons can be stripped from an atom until there is only the nucleus left. If the energy required to achieve this for each electron is plotted on a graph (with a log scale) against ionisation number, the 'jumps' in the required energy clearly show the main and sub energy levels.

12.2.2 : $n = (1, s) (2, sp) (3, spd) (4, spdf)$

12.2.3 : Energies of sub-shells : $s < p < d < f$

12.2.4 : Number of orbitals at each level : $s=1, p=3, d=5, f=7$

12.2.5 : Shapes of orbitals : s orbital is a sphere around the nucleus. p orbitals are shaped like a figure 8 (and there are 3 of them at 90 degrees around the nucleus).

1s			
2s	2p		
3s	3p	3d	
4s	4p	4d	4f
5s	5p	5d	5f

12.2.6 : Move diagonally down and left through each diagonal...ie 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d... Pauli's exclusion principle says that there can only be 2 electrons in each orbital (with opposite spins). Hund's rule says that each orbital should be half filled before any is completely filled (since there is less repulsion if all electrons have the same spin). Electrons will therefore fill the lowest energy levels (ie 1 then 2 and so on) with two going in each orbital, but only doubling up when all orbitals in the level are filled.

12.2.7 : Systematically fill the orbitals as shown above up to $Z = 56$. This can be abbreviated by writing [x] where x is a noble gas.

12.2.8 : The small double column on the left is the s shell being filled. The block on the left is the p shell being filled. The d block (in the middle) is (surprisingly) the d shell

being filled. The bits hanging off the bottom are the f shells being filled...forget them, they never matter :)

PERIODICITY (SL)

3.1 The Periodic Table

3.1.1 : Elements increase in atomic number across each period, and down each group. The history is boring and pointless (like all history)...ignore it.

3.1.2 : Group - the columns going down. Period - the rows going across.

3.1.3 : Group = number of valence electrons in the atom. Period = number of main electron shells...s, p, d and f blocks as described above.

3.2 Physical Properties

3.2.1 :

Li->Cs (down the alkali metals) : **Atomic radius** increases due to increased electron shielding. **Ionic radius** increases due to increased electron shielding. **Ionisation energy** decreases due to increased electron shielding. **Melting/boiling point** decreases due to increased electron shielding->decreased forces. **Electronegativity** decreases due to increased shielding -> decreased attraction for outer electrons.

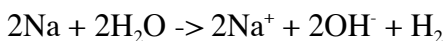
F->I (Down the halogens) : **Atomic radius** increases due to increased electron shielding. **Ionic radius** increases due to increased electron shielding. **Ionisation energy** decreases due to increased electron shielding. **Melting/boiling point** increases due to increased number of electrons->increased London dispersion forces. **Electronegativity** decreases due to increased shielding -> decreased attraction for outer electrons.

Na->Ar (across period 3) : **Atomic radius** decreases due to increased nuclear charge -> greater attraction for electrons. **Ionic radius** decreases Na->Al (due to increased nuclear charge) jumps Al->Si (due to reversal of ionisation direction...increased electron-electron repulsion) decreases Si->Ar (due to increased nuclear charge). **Ionisation energy** increases due to increased nuclear charge. **Melting/boiling point** increases Na->Si (due to stronger metallic bonding - more delocalized electrons than network covalent) drops Si-P (due to network->molecular covalent) increases P->S (due to increased LDF between molecules ie P₄, S₈). Drops to Cl, due to smaller molecules (Cl₂) decreases to Ar (individual atoms->fewer electrons->smaller LDF). **Electronegativity** increases due to increased nuclear charge -> greater attraction for electrons.

3.3 Chemical Properties

3.3.1 : Reactions of elements in the same group are similar because they have identical outer shells (ie same number of valence electrons). Generalized reactions follow :

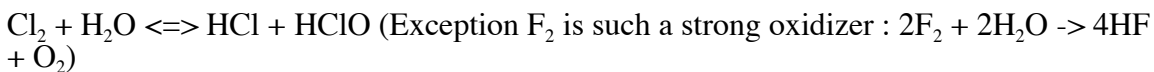
Alkali metal (group 1) with water



Alkali metal (group 1) with Halogen



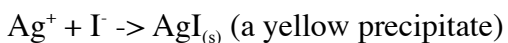
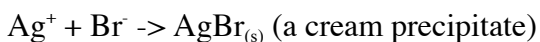
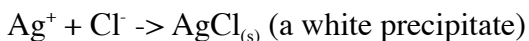
Halogen with water



Halogen + Halide ion

	Cl ⁻	Br ⁻	I ⁻
Cl ₂	Colorless -> Cl ₂	Red -> Br ₂	Violet -> I ₂
Br ₂	Red -> Br ₂	Red -> Br ₂	Violet -> I ₂
I ₂	Violet -> I ₂	Violet -> I ₂	Violet -> I ₂

Halide ion with Silver ion



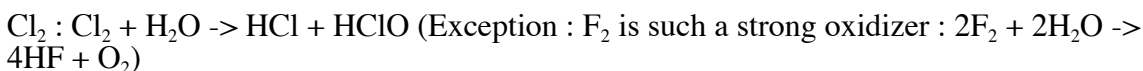
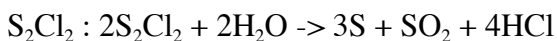
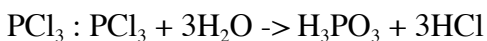
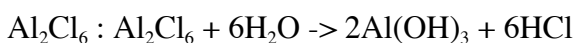
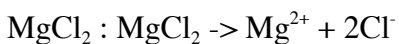
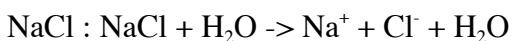
3.3.2 : Elements on the left are metallic...right are non-metals...Al is a metalloid (semi-metal).

Oxides : Non-metals -> Acidic oxides , Metals -> Basic oxides, Metalloids -> Amphoteric (both acidic & basic) oxides.

					P ₄ O ₁₀	SO ₃	
	Na ₂ O	MgO	Al ₂ O ₃	SiO ₂	(or P ₄ O ₆)	(or SO ₂)	Cl ₂ O ₇
Adding H ₂ O	Na ₂ O + H ₂ O -> 2NaOH	MgO + H ₂ O -> Mg(OH) ₂	Insoluble	Insoluble	P ₄ O ₁₀ + 6H ₂ O -> 4H ₃ PO ₄	SO ₃ + H ₂ O -> H ₂ SO ₄	Cl ₂ O ₇ + H ₂ O -> HClO ₄

Reaction with HCl	$\text{Na}_2\text{O} + \text{H}^+ \rightarrow 2\text{Na}^+ + \text{H}_2\text{O}$	$\text{MgO} + 2\text{H}^+ \rightarrow \text{Mg}^{2+} + \text{H}_2\text{O}$	$\text{Al}_2\text{O}_3 + 6\text{H}^+ \rightarrow 2\text{Al}^{3+} + 3\text{H}_2\text{O}$	No reaction	No reaction	No reaction	No reaction
Reaction with NaOH	No reaction	No reaction	$\text{Al}_2\text{O}_3 + 2\text{OH}^- + 3\text{H}_2\text{O} \rightarrow 2\text{Al}(\text{OH})_4^-$	$\text{SiO}_2 + 2\text{OH}^- \rightarrow \text{SiO}_3^{2-} + \text{H}_2\text{O}$	$\text{P}_4\text{O}_{10} + 12\text{OH}^- \rightarrow 4\text{PO}_4^{3-} + 6\text{H}_2\text{O}$	$\text{SO}_3 + \text{OH}^- \rightarrow \text{SO}_4^{2-} + \text{H}_2\text{O}$	$\text{Cl}_2\text{O}_7 + \text{OH}^- \rightarrow 2\text{ClO}_4^- + \text{H}_2\text{O}$
Nature	Basic Oxide	Basic Oxide	Amphoteric Oxide	Acidic Oxide	Acidic Oxide	Acidic Oxide	Acidic Oxide

Halides (assuming Cl...could replace with Br, I, F etc) : Ionic Chlorides \rightarrow dissolved in H_2O with little reaction, Covalent Chlorides \rightarrow dissolve + react to form HCl.



PERIODICITY (AL)

13.1 Periodic trends Na \rightarrow Ar (the third period)

13.1.1 : (This seems very much like the last bit of SL, but now with explanations :)

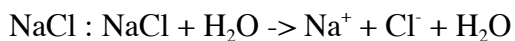
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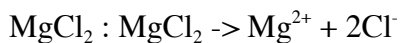
	Na ₂ O	MgO	Al ₂ O ₃	SiO ₂	P ₄ O ₁₀ (or P ₄ O ₆)	SO ₃ (or SO ₂)	Cl ₂ O ₇ Cl ₂ O
Adding H ₂ O	Na ₂ O + H ₂ O -> 2NaOH	MgO + H ₂ O -> Mg(OH) ₂	Insoluble	Insoluble	P ₄ O ₁₀ + 6H ₂ O -> 4H ₃ PO ₄ P ₄ O ₆ + 6H ₂ O -> 4H ₃ PO ₃	SO ₃ + H ₂ O -> H ₂ SO ₄ SO ₂ + H ₂ O -> H ₂ SO ₃	Cl ₂ O ₇ + H ₂ O -> 2HClO ₄ Cl ₂ O + H ₂ O -> 2HOCl
Adding HCl	Na ₂ O + H ⁺ -> 2Na ⁺ + H ₂ O	MgO + 2H ⁺ -> Mg ²⁺ + H ₂ O	Al ₂ O ₃ + 6H ⁺ -> 2Al ³⁺ + 3H ₂ O	No reaction	No reaction	No reaction	No reaction
Adding NaOH	No reaction	No reaction	Al ₂ O ₃ + 2OH ⁻ + 3H ₂ O -> 2Al(OH) ₄ ⁻	SiO ₂ + 2OH ⁻ -> SiO ₃ ²⁻ + H ₂ O	H ₃ PO ₄ + OH ⁻ -> H ₂ PO ₄ ⁻ + H ₂ O	SO ₂ + OH ⁻ -> HSO ₄ ⁻	HClO ₇ + OH ⁻ -> ClO ₇ ²⁻ + H ₂ O

Explaining the physical properties ... Conductivity for ionic solutions (Na₂O->Al₂O₃) is due to ions in solution/molten state. SiO₂ is network covalent...no charges therefore no significant conductivity. Others are covalent molecules therefore no conduction. Melting point...stronger bonds when atoms can be arranged in a simple structure...MgO is highest, then Al₂O₃, Na₂O (the ratio between the two atoms should be as close to 1 as possible). SiO₂ is network covalent -> high melting point (but not as high as ionic bonding). The final 3 decrease in melting point due to decreasing polarity of molecules -> smaller dipole-dipole interactions.

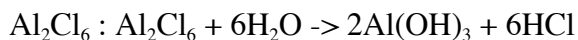
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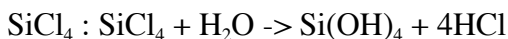
Good conductivity (ionic structure) MP = 801



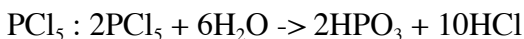
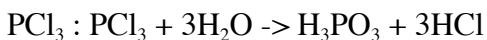
Good conductivity (ionic structure) MP = 714



Poor conductivity (Network covalent) MP = 178

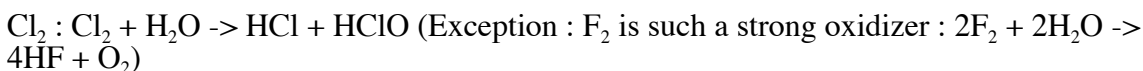


No conductivity (Covalent molecular) MP = -70



No conductivity (Covalent molecular) MP = -112

S_2Cl_2 Not required



No conductivity (Covalent molecular) MP = -101

MP...NaCl and MgCl_2 \rightarrow decreases due to packing (as above), drops to Al_2Cl_6 (network covalent). Others are covalent molecules...decreases due to decreasing polarity (Cl_2 higher due to more electrons...greater LDF ?)

13.2 D-block elements (first row)

13.2.1 : Typical d-block elements are generally those exhibiting multiple oxidation states (in period 4, not Sc or Zn)

13.2.2 : The multiple oxidation states of the d-block (transition metal) elements is due to the proximity between the 4s and 3d sub shells (in terms of energy). All transition metals exhibit a 2+ oxidation state (both electrons being lost from the 4s and all have other oxidation states...ie

V - +4, +5 (apparently we need to know only 2 of these...weird if you ask me...but include Fe...

Cr - +3, +6

Mn - +4, +7

Fe - +3

13.2.3 : Ligands are the molecules which donate an electron pair to form a dative covalent bond with the central atom (thus forming a complex ion).

13.2.4 : Complex ions are molecules which carry a charge. They are formed around a central atom, with other atoms (or molecules) donating an electron pair to form a covalent bond to this central atom. Examples...

$[\text{Fe}(\text{H}_2\text{O})_6]^{3+}$ - Fe is the central atom, H_2O is the ligand

$[\text{Fe}(\text{CN})_6]^{3-}$ - Fe is the central atom, CN is the ligand

$[\text{CuCl}_4]^{3-}$ - Cu is the central atom, Cl is the ligand

$[\text{Cu}(\text{NH}_3)_4]^{2+}$ - Cu is the central atom, NH_3 is the ligand

$[\text{Ag}(\text{NH}_3)_2]^+$ - Ag is central atom, NH_3 is the ligand

13.2.5 : The color in the transition metals (d-block) is predominantly due to the splitting of the d shell orbitals into slightly different energy levels. As a result, certain wavelengths of energy can be absorbed by the d-block elements (with electrons jumping between these slightly different energy levels), resulting in the complement color being visible.

13.2.6 : d-block elements make good catalysts due to their multiple oxidation states (hence their ability to react with different species and produce a path of lower activation energy, and so allow the reaction to proceed at a faster rate). Examples...

MnO_2 in decomposition of hydrogen peroxide

V_2O_5 in the contact process

Fe in Harber process

Ni in conversion of alkenes to alkanes

BONDING (SL)

4.1 Ionic Bond

4.1.1 : Ionic bond - +ve (cations) and -ve (anions) ions are attracted to each other and form a continuous ionic lattice

4.1.2 : Group 1 metals form +1 ions, group 2 metals form +2 ions, metals in group 3 for +3 ions...funny that :) Examples : Li^+ , Mg^{2+} , Al^{3+} ...Greater ease of ionisation Li->Cs is due to the increased electron shielding of the nuclear attraction caused by additional inner shells of electrons. The easier atoms are to ionise, the more reactive they will be because less energy is required to ionise them, and so they react faster.

4.1.3 : Group 6 ions will form 2- ions, Group 7 ions will form - ions. Examples : O^{2-} , Cl^- ...

4.1.4 : The transition metals (elements from Ti to Cu, ignore Sc and Zn) can form multiple ions (ie Fe^{2+} , Fe^{3+}) (due to proximity of 4s and 3d shells)

4.1.5 : The ionic or covalent nature of the bonding in a binary compound is a result in the difference between their electronegativity... $\text{NaCl}_{(s)}$ is ionic, $\text{HCl}_{(g)}$ is (polar) covalent (also, covalent molecules tend to be gases/liquids, ionic tends to be solid...except network covalent which will be solid). In general, if the difference between electronegativities is greater than 1.7, the bond will be more than 50% ionic.

4.1.6 : Take the name of the group 1,2, or 3 metal and add...fluoride, chloride, bromide, iodide etc , oxide, sulfide etc...Nitride and phosphide...how exciting :)

4.2 Covalent Bond

4.2.1 : Covalent bonds are where two atoms each donate 1 electron to form a pair held between the two atoms...Such bonds are generally formed by atoms with little difference in electronegativity...ie C, H and O in organic chemistry.

4.2.2 : All electrons must be paired...Lewis diagrams are the element symbol with the outer (valence) shell of electrons left over and spare electrons pair up...in general C forms 4 bonds, N forms 3, O forms 2, halogens form 1, H forms 1...(Li would form 1, Be 2, and B 3 but they don't usually...metallic or ionic bonding)

4.2.3 : Electronegativity values range from 0.7 to 4...from bottom left to top right respectively (hydrogen falls B and C with a electronegativity of 2.1...

4.2.4 : When covalent molecules have a difference in electronegativity (between the two bonding atoms) then the pair will be held closer to the more electronegative atom...resulting in a small -ve charge on the more electronegative atom, and a small +ve charge on the other...results in polar bonds

4.2.5 : Shape of molecule with 4 electron pairs depends on number of lone pairs.

3 lone pairs -> linear, 2 lone pairs -> bent, 1 lone pair -> trigonal pyramid, No lone pairs -> tetrahedral

4.2.6 : The polarity of a molecule depends on both the shape and the polarity of the bonds...1) if there are no polar bonds, it's not polar. 2) if there are polar bonds, but the shape is symmetrical, it's not polar (think about it like 3D vector addition...if they add to zero, then it's not polar). 3) if there are polar bonds, and it's not symmetric, then the molecule is polar

4.3 Intermolecular forces

4.3.1 : van der Waal's forces -- Electrons will not be evenly spread around an atom/molecule at any given time, meaning the molecule will have a slight +ve charge on one end, and a -ve at the other. this temporary state may cause attraction between two molecules, pulling them together (also known as london dispersion forces). Dipole-dipole forces -- Polar molecules, when properly oriented, will attract each other as a result of this. Stronger than van der Waal's forces. Hydrogen bonding -- When hydrogen is bonded to nitrogen, oxygen or fluorine, a very strong dipole is formed, making the hydrogen very strongly positive. This hydrogen is then attracted to the lone pairs on other similar molecules (nitrogen, oxygen and fluorine all have lone pairs) forming a hydrogen bond, which is stronger than van der Waal's or dipole-dipole, but weaker than covalent bonding.

4.3.2 : Structural features -- Nonpolar molecules...van der Waal's forces only ...also present in all other molecules, though it's strength is insignificant compared to the others. Polar molecules...dipole-dipole forces arise from polar bonds and asymmetry in molecules. Hydrogen bonds result from hydrogen bonded as described above. This results in molecules with hydrogen bonding exhibiting stronger intermolecular forces, ie higher boiling/melting points etc. ie H_2O has a higher bp than H_2S due to hydrogen bonding, and so on down the strength list. (nonpolar molecules don't conduct electricity, polar +hydrogen bonding ones will...I suppose this goes here)

4.4 Metallic bond

4.4.1 : Metallic bonding...the metal atoms lose their outer electrons which then become delocalized, and free to move throughout the entire metal. These -ve delocalized electrons hold the metal cations together strongly. Since these electrons can flow, atoms with metallic bonding exhibit high electrical conductivity. Unlike ionic bonding, distorting the atoms does not cause repulsion so metallic substances are ductile (can be stretched into wires) and malleable (can be made into flat sheets). The free moving electrons also allow for high thermal conductivity, and the electrons can carry the heat energy rather than it being transferred slowly through atoms vibrating.

4.5 Physical Properties

Melting + Boiling point...High with Ionic and metallic bonding (and network covalent), Low with covalent molecular bonding.

Volatility...Covalent molecular substances are volatile, others aren't

Conductivity...Metallic substances conduct. Polar molecular substances conduct, non-polar ones don't. Ionic substances don't conduct when solid, do conduct when molten or dissolved in water.

Solubility...Ionic substances -> generally dissolve in polar solvents (like water). Metallic substances...(Generally not soluble?). Non-polar molecules are generally soluble in non-polar solvents, and polar in polar. Organic molecules with a polar head : Short chain molecules are solubility in polar solvents, long chains can eventually outweigh the polar 'head' and will dissolve in non-polar solvents.

BONDING (HL)

14.1 Shapes of Molecules

14.1.1 : Shapes of molecules...around each atom, there are covalent bonds and lone electron pairs...all of which repel each other (the lone pairs repel a little more, so if possible, they shouldn't be together)...Therefore all the pairs will be as far away from each other as possible. How to work out the shape : 1) decide which atom is at the center...usually the one of which there is only one. 2) find (from the periodic table) the number of electrons on this atom. 3) add an electron if the molecule is negatively charged, subtract one if +ve. 4) Add one electron for each atom joined to the central one. 5) divide this by 2 to get the number of electron pairs...Match up the shape as below.

2 Pairs, bond angle = 180 : 1 bonded atom -> linear, 2 bonded atoms -> linear

3 Pairs, bond angle = 120 : 2 bonded atoms -> bent, 3 bonded atoms -> trigonal planar

(4 Pairs is in SL)

14.1.2 : Continuing on with 5 and 6 pairs...

5 Pairs, bond angles = 120 and 90 : 3 bonded atoms -> T-Shaped, 4 bonded atoms -> distorted tetrahedron, 5 bonded atoms -> trigonal bipyramidal

6 Pairs, bond angle = 90 : 4 bonded atoms -> square planar, 5 bonded atoms -> square pyramid, 6 bonded atoms -> Octahedral

Whenever a molecule can be drawn in multiple structures (eg ClO_2^- can be drawn with 2 double bonds and -ve on Cl or one double, one single, and -ve on either O) the structures differ only in the arrangement of electrons, the positions of nuclei remain constant, and so the above theory can be used to predict the shape (because the actual position is like the average of all the resonance hybrids).

14.2 Multiple bonds

14.2.1 : Sigma bonds -> these are bonds between two atoms where the bond is symmetric around the line between the two nuclei of the atoms. Pi bonds are those which are not symmetric, usually because they fall outside this line. This often occurs after a Sigma bond has formed, when the two atoms p orbitals overlap above and below the sigma bond, forming a new Pi bond. Since Pi bonds are not free to rotate, this allows for cis-trans isomerism etc... Triple bonds, such as those seen in alkynes, are the result of one sigma bond, and two pi bonds.

14.2.2 : In general, more bonds -> stronger, shorter bonds.

14.3 Hybridisation

14.3.1 : The electron structure of carbon is $1s^2 2s^2 2p^2$... so how come it can form 4 identical bonds ? Hybridisation!!!! :) more specifically sp^3 hybridisation. Other times it forms 3 identical sigma bonds, and a pi bond (sp^2 hybridisation) and yet other times, two identical bonds, and two pi bonds (like in ethene), which is sp hybridisation. sp^3 hybridisation occurs when the 2s and 2p orbitals merge to become sp^3 orbitals (all of equal energy, length etc.). sp^2 is the same except only two of the p orbitals are hybridised, leaving one p orbital behind...and the same with sp only two p orbitals are left over.

14.3.2 : sp^3 hybrids have 4 -ve charge centers -> tetrahedral shape. sp^2 has 3 -ve charge centers -> trigonal planar. sp has 2 -ve charge centers -> linear. To work with Lewis structures...find number of identical bonds. 4 identical -> sp^3 , 3 identical -> sp^2 , 2 identical -> sp .

14.4 Delocalisation of electrons

14.4.1 : When a particular molecule can be represented as several different ways (different Lewis structures) it is generally not actually any of these, but a hybrid of all of them. This can be represented either with delocalized electrons, or through resonance (where each possible structure is drawn and the actual state 'resonates' between them). The delocalisation of these pi electrons (which is effectively what happens) makes the molecule more stable (as evidenced by lower energy) and gives the bonds a shorter length than would be expected. Classic example is benzene, but also O_3 etc...

STATES OF MATTER (SL)

5.1.1 : Solids -> molecules/atoms tightly packed. force of attraction between molecules overcomes any translational motion of molecules (they do, however, vibrate in position). Liquids -> particles held close together, but not as strongly as solids in that they are free to move, but not to escape the liquid (except for fast traveling particles -> evaporation). Gas -> particles move independently and randomly, with no significant forces between particles, and a large (comparatively) amount of space between them.

5.1.2 : Ideal gas -> composed of randomly moving point masses occupying no space and with no forces between masses. The average (rms) speed of the movement of particles is proportional to temperature (in K). as a result, the kinetic energy of the particles is also proportional to temperature.

5.1.3 : Solid -> liquid , the rigid structure of the solid is overcome due to increased vibration of particles (due to energy being added in the form of heat). the particles can not escape from the liquid, but can move within it. Liquid to gas -> as energy (in the form of heat) is given to the liquid, the particles gain enough energy to escape the liquid, and become a gas, with particles widely spaced. Gas->liquid...as heat (energy) is removed, the particles slow down to the point where the forces between particles are strong enough to hold them together...a liquid ! Liquid->solid...energy is removed, particles move slower->stronger forces->more rigid structure.

5.1.4 : increase in temp -> larger volume or higher pressure...increase in volume -> decrease in temp or decrease in pressure...increase in pressure -> decrease in volume or increase in temp.

5.1.5 : Since the particles are moving at random, two separated samples of gas will eventually mix causing diffusion. This will occur at a higher rate with higher temperature since the particles are moving faster.

STATES OF MATTER (HL)

15.1 Gases

15.1.1 : $PV = nRT$... P =(pressure in atm) V =(volume in cm^3) n =(number of atoms in mols) R =($82.05 \text{ cm}^3 \text{ atm K}^{-1} \text{ mol}^{-1}$ -- in data book) T =(temperature in K)

15.1.2 : The above equation can be rearranged as $P_1V_1=P_2V_2$ or $V_1/T_1=V_2/T_2$ if temp or pressure are assumed to be constant. Avogadro's law -- equal volumes of gas contain equal numbers of particles (at 273K, 1 atm -> $22.4 \text{ dm}^3 \text{ mol}^{-1}$ -- in data book)

15.1.3 : Dalton's law of partial pressures -> the partial pressure of a gas is the pressure the gas would exert if the gas were alone in its container. ie if there are Gases A, B and C filling a dm^3 , $b \text{ dm}^3$ and $c \text{ dm}^3$ respectively then the partial pressure of a = $\frac{(a)}{(a+b+c)}$ x total pressure.

15.1.4 : $P_p = \frac{\text{(number of molecules in the gas)}}{\text{(total number of molecules)}} \times \text{total pressure ... apply this relationship...}$

Nb -- Apparently, though it's never been in the syllabus, there have been questions on Van Der Waal's equation, which is an extension of $PV=nRT$ for non-ideal gas situations...it is $(P+an^2/V^2)(V-nb)=nRT$ Where a and b are constants for a given gas...which I assume will be given if necessary.

ENERGETICS (SL)

6.1 Exothermic and endothermic reactions

6.1.1 : If the reaction produces heat (increases the temperature of the surroundings) then it's exothermic. If it decreases the temp (ie absorbs heat) then it's endothermic. Also, the yield of an equilibrium reaction which is exothermic will be increased if it occurs at low temps, and so for endothermic reactions at high temps.

6.1.2 : Exothermic -> a reaction which produces heat. Endothermic -> a reaction which absorbs heat. Enthalpy of reaction -> the change in internal energy (H) through a reaction is ΔH .

6.1.3 : ΔH will be -ve for exothermic reactions (because internal heat is being lost) and +ve for endothermic reactions (because internal energy is being gained).

6.1.4 : The most stable state is where all energy has been released...therefore when going to a more stable state, energy will be released, and when going to a less stable state, energy will be gained. On an enthalpy level diagrams, higher positions will be less stable (with more internal energy) therefore, if the product is lower, heat is released (more stable, ΔH is -ve) but if it is higher, heat is gained (less stable, ΔH is +ve).

6.1.5 : Formation of bonds -> release of energy. Breaking of bonds -> gain / absorption of energy.

6.2 Calculation of enthalpy changes

6.2.1 : change in energy = mass x specific heat capacity x change in temperature --> $E = m \times c \times \Delta T$

6.2.2 : Enthalpy changes (ΔH) are related to the number of mols in the reaction...if all the coefficients are doubled, then the value of ΔH will be doubled (attention must be paid to limiting reagents though).

6.2.3 : When a reaction is carried out in water, the water will gain or lose heat from (or to) the reaction, with hopefully little escaping the water. Therefore, the change in energy, and so the ΔH value, can be calculated with $E = m \times c \times \Delta T$ where E is equal to ΔH , m is the mass of water present, and $c = 4.18 \text{ kJ Kg}^{-1} \text{ K}^{-1}$. This ΔH value can then be calculated back to find the enthalpy change for each mol of reactants.

6.2.4 : The solution should be placed in a container as insulated as possible, to keep as much heat as possible from escaping. The temperature should be measured continuously, and the value used in the equation is the maximum change in temp from the initial position.

6.2.5 : The results will be a change in temperature. this can be converted into a change in heat (or energy) by using the above equation and a known mass of water. this can be used

to calculate the delta-H for the amount of reactants present, and then this can be used to calculate for a given number of moles.

6.3 Hess' Law

6.3.1 : Hess' Law states that the total enthalpy change between given reactants and products is that same regardless of any intermediate steps (or the reaction pathway). To calculate...1) reverse any reactions which are going the wrong way and invert the sign of their delta-H values. 2) divide or multiply the reactions until the intermediate products will cancel out when the reactions are vertically added (always multiply/divide the delta-H value by the same number)...3) vertically add them...4) divide or multiply the resulting reaction to the correct coefficients.

6.4 Bond enthalpies

6.4.1 : Bond enthalpy (aka dissociation enthalpy) -- the enthalpy change when one mold of bonds are broken homolitically in the gas phase. ie $X-Y_{(g)} \rightarrow X_{(g)} + Y_{(g)}$: delta- $H_{(dissociation)}$. Molecules such as CH_4 have multiple C-H bonds to be broken, and so the bond enthalpy for C-H is actually an average value. These values can be used to calculate unknown enthalpy changes in reactions where only a few bonds are being formed/broken.

6.4.2 : If the reaction can be expressed in terms of the breaking and formation of bonds in a gaseous state, then by adding (or subtracting when bonds are formed) the delta-H values the total enthalpy of reaction can be found.

ENERGETICS (HL)

16.1 Standard enthalpy changes of reaction

16.1.1 : Standard state -- 101 kPa, 298 K (or 1 atm, 25 degrees celcius).

Standard enthalpy change of formation -- The enthalpy change when 1 mol of a substance is made from its elements in their standard states eg $C_{(graphite)} + 2H_{2(g)} \rightarrow CH_{4(g)}$. (molecules, like H_2 are considered to be 'standard state. Fractions of mols->ie fractions in coefficients, may also be used if necessary as 1 mol must be produced).

16.1.2 : If a reaction can be expressed in terms of changes of formation (and bond enthalpies as in SL) then add up all the delta-H values to get the delta-H for the reaction.

16.2 Lattice enthalpy

16.2.1 : Lattice enthalpy -- the enthalpy change when 1 mol of crystals (ie an ionic lattice) is formed from its component particles at an infinite distance apart. ie $M^+_{(g)} + X^-_{(g)} \rightarrow MX_{(s)}$. The value of lattice enthalpy is assumed to be negative for the separation of the lattice, and positive for the formation of the lattice.

16.2.2 : As above, lattice enthalpies just add another type of reaction to those which can be shown on the Born-Harber cycle.

16.2.3 : lattice enthalpy increases with higher ionic charge and with smaller ionic radius (due to increased attraction).

16.3 Entropy

16.3.1 : Factors which increase disorder in a system : Mixing of particles, change of state to greater distance between particles (solid->liquid or liquid->gas), increased particle movement (temperature), increased number of particles (when more gas particles are produced, this generally outweighs all other factors).

16.3.2 : Predict the sign of ΔS (the change in entropy) for a reaction based on the above factors. ΔS is positive when entropy increases (more disorder) and negative when entropy decreases (less disorder).

16.3.3 : The standard entropy change can be calculated by subtracting the absolute entropy of the reactants from that of the products.

16.4 Spontaneity of a reaction

16.4.1 : Reactions which release heat (and so increase stability) tend to occur. Reactions which increase entropy (ΔS is positive) tend to occur, but neither can be used to accurately predict spontaneity alone.

16.4.2 : when ΔG is negative, the reaction is spontaneous, when it's positive, their reaction is not.

16.4.3 : $\Delta G = \Delta H - \text{Temperature (in kelvin)} \times \Delta S$...spontaneity depends on ΔH , ΔS and the temp at which the reaction takes place (or doesn't as the case may be).

16.4.4 : Yeah...well...stick numbers into that equation above...

16.4.5 : 4 possibilities...

1) ΔG is always negative when ΔH is negative and ΔS is positive.

2) ΔG is negative at high temperatures if ΔH is positive and ΔS is positive (ie an endothermic reaction is spontaneous when $T \times \Delta S$ is greater than ΔH)

3) ΔG is negative at lower temperatures if ΔH is negative and ΔS is negative (exothermic reactions are spontaneous if ΔH is bigger than $T \times \Delta S$)

4) ΔG is never negative if ΔH is positive and ΔS negative.

KINETICS (SL)

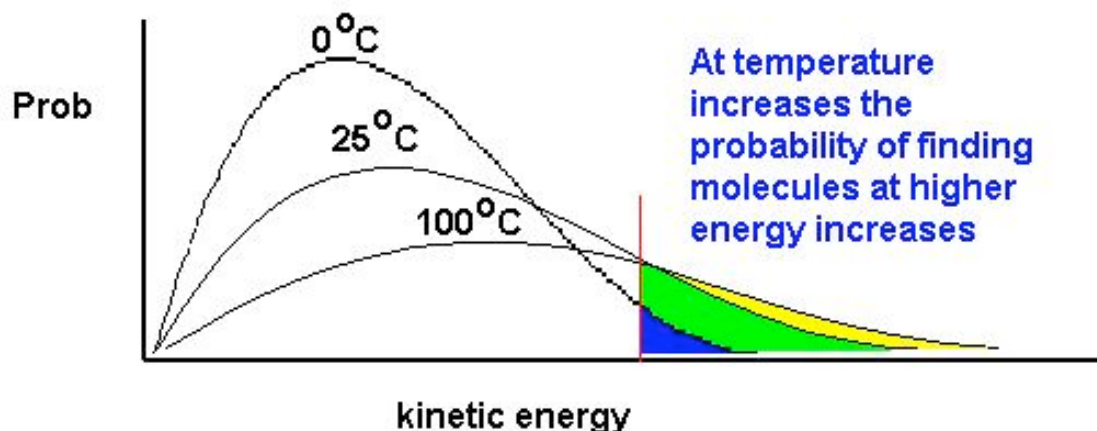
7.1 Rates of reaction

7.1.1 : Rate of reaction is concerned with how quickly a reaction reaches a certain point (not to be confused with how far a reaction goes...ie equilibrium).

7.1.2 : Interpretation of rate graphs. Reaction rate graphs will generally be graphed with time on the x-axis and some measure of how far the reaction has gone (ie concentration, volume, mass loss etc) on the y-axis. This will generally produce a curve with, for example, the concentration of the products approaching zero.

7.2 Collision theory

7.2.1 : Collision theory -- reactions take place as a result of particles (atoms or molecules) colliding and then undergoing a reaction. Not all collisions cause reaction, however, even in a system where the reaction is spontaneous. The particles must have sufficient kinetic energy, and the correct orientation with respect to each other for the two to react.



7.2.2 : Higher temp \rightarrow greater average kE \rightarrow faster reaction. Higher concentration \rightarrow more collisions \rightarrow faster reaction. Catalysts \rightarrow lower activation energy / greater probability of proper orientation \rightarrow faster reaction. In heterogeneous reactions (where the reactants are in different states) the size of the particles of a solid may change reaction rate, since the surface is where the reaction takes place, and the surface area is increased when the particles are more finely divided...(therefore smaller solid particles in a heterogeneous reaction \rightarrow faster reaction).

7.2.3 : Most reactions involve several steps, which can be individually slow or fast, and which, all together, make up the complete reaction. The slowest of these steps is called the rate determining step, as it determines how fast the reaction will go. It is also not necessary that all the reactants are involved in every step, and so the rate determining step may not involve all the reactants. As a result, increasing the concentration (for example) of a reactant which is not involved in the rate determining step will not change the overall

reaction rate.

KINETICS (HL)

17.1 Rate expression

17.1.1 : The rate expression will be of the form -- Rate = $k[A]^m[B]^n$...etc (for each reactant). k is a constant, and m , n etc show the order of the reaction for each reactant.

17.1.2 : Order of reaction is the total of $m+n$ above. k is the rate constant, which will change due to any factor affecting the rate other than concentration (ie temp, catalysts...)

17.2.3 : If temperature increases, then the rate will increase and so the rate constant must increase also to account for this. If the temp decreases, the rate constant will decrease.

17.2.4 : A zero order reaction will be a straight line where the slope gives the rate constant (like $y = mx + c$). A first order reaction will be a curve where the half lives are constant (ie the time taken for the concentration to halve from any given point is constant). A second order reaction is a curve where the half lives are not constant.

17.1.5 : By substituting data into Rate = $k[A]^m[B]^n$, it is possible to solve the resulting simultaneous equations for m and n . for example, if the concentration of A was doubled, B was kept constant and rate doubles as a result, then the reaction would be first order with respect to A (ie $m=1$). If the rate increased by a factor of 4, then the reaction would be second order with respect to a (since $(2a)^2 = 4a^2$ and rate is proportional to a^2). The overall order of the reaction can be calculated from graphical data as above.

7.1.6 : The rate constant can be found from a graph by taking a point, finding it's concentration, then finding a point on the graph which corresponds to half this concentration. The half life is the time between thee two points. The half life is also equal to $\frac{\ln 2}{k}$ where k is the rate constant (equation given in data book).

17.2 Reaction mechanism

17.2.1 : Rate determining step -- the slowest step in a reaction which determines the rate for the overall reaction. Molecularity -- The number of molecules reacting in an elementary step of a reaction. Activated complex -- as two particles collide (with sufficient energy to react and in the correct orientation) they form an intermediate called the activated complex...not literally a chemical substance, but an intermediate in which the bonds are in the process of being broken and formed.

17.2.2 : The order of the reaction is defined by the particles involved in the rate determining step (which is one step in the mechanism). For example, if two of one type of particle are colliding, the order with respect to that particle will be 2 (and zero to any others). The activated complex is formed by (in this example) the two colliding molecules, weakening the bonds, which then break and form to create the new

molecule(s).

17.3 Collision theory

17.3.1 : Maxwell-Boltzmann energy distribution curve...sometime I'll actually draw a picture of it, but for now...The curve is on a graph of kinetic energy (x-axis) against fraction of molecules with this KE (y-axis). The curve rises sharply to a peak, then falls off with the x-axis as an asymptote (ie it is possible, though statistically unlikely, for a molecule in any gas to be traveling at very high speed).

17.3.2 : At higher temperatures, the peak of the curve is lower, and further to the right. The graph is overall 'flatter' resulting in a greater proportion being above any given temperature...and so whatever the required activation energy, a greater proportion of the particles will have sufficient activation energy for the reaction to proceed...thus making the reaction occur faster.

17.4 Activation energy

17.4.1 : Arrhenius equation : $k = Ae^{(-E_a/RT)}$ (equation in data book)...The A in this equation is a constant related to the number and frequency of collisions occurring between the reactants.

17.4.2 : Enthalpy level diagrams showing a curve demonstrating the path between the reactants and products on the graph. Energy is shown on the y-axis, and presumably the reactants and products are of different energies...the curve goes between the two levels (the reactants and products) peaking above both between them (with the distance between the highest point and the reactants being the activation energy). A catalysed reaction graph is the same, only the curve peaks lower, representing a lower activation energy requirement.

17.4.3 : Reactions only occur when the reacting particles have energy greater than the activation energy.

17.4.4 : Homogeneous catalysts -- catalysts in the same state (phase -- ie solid, liquid or gas) as the reactants. Heterogeneous catalysts -- catalysts in a different phase (usually a solid) from the reactants.

17.4.5 : Homogeneous catalysts operate by reacting with the reactants and eventually producing a reaction pathway of lower activation energy (and also being regenerated at the end of this process). Heterogeneous catalysts provide a reactive site on which an activated complex forms, weakening the bonds and increasing the rate of collisions thus increasing the rate of reaction.

EQUILIBRIUM (SL)

8.1 Dynamic equilibrium

8.1.1 : In all reactions, there are in fact two reactions occurring, one where the reactants produce the products, and the other where the products react to form the reactants. In some reactions, this second reaction is insignificant, but in others there comes a point where the two reactions exactly cancel each other out...thus the reactants and products remain in equal proportions, though both are continually being used up and produced at the same time.

8.2 The position of equilibrium

8.2.1 : The equilibrium constant K_c is a constant which represents how far the reaction will proceed at a given temperature.

8.2.2 : When K_c is greater than 1, products exceed reactants (at equilibrium). When much greater than 1, the reaction goes almost to completion. When K_c is less than 1, reactants exceed products. When much less than 1 (K_c can never be negative...so when it is close to zero) the reaction hardly occurs at all.

8.2.3 : The only thing which can change the value of K_c for a given reaction is a change in temperature. The position of equilibrium, however, can change without a change in the value of K_c .

Effect of Temperature : The effect of a change of temperature on a reaction will depend on whether the reaction is exothermic or endothermic. When the temperature increases, Le Chatelier's principle says the reaction will proceed in such a way as to counteract this change, ie lower the temperature. Therefore, endothermic reactions will move forward, and exothermic reactions will move backwards (thus becoming endothermic). The reverse is true for a lowering of temperature.

Effect of Concentration : When the concentration of a product is increased, the reaction proceeds in reverse to decrease the concentration of the products. When the concentration of a reactant is increased, the reaction proceeds forward to decrease the concentration of reactants.

Effect of Pressure : In reactions where gases are produced (or there are more mols of gas on the left), and increase in pressure will force the reaction to move to the left (in reverse). If pressure is decreased, the reaction will proceed forward to increase pressure. If there are more mols of gas on the left of the equation, this is all reversed.

8.2.4 : Yeah...well...based on the previous section, you should be able to predict what's going to happen given a reaction if the temp, pressure or concentration is changed.

8.2.5 : A catalyst does not effect either K_c or the position of equilibrium, it only effects the rate of reaction.

8.2.6 : $\text{N}_{2(\text{g})} + 3\text{H}_{2(\text{g})} \rightleftharpoons 2\text{NH}_{3(\text{g})}$: $\Delta\text{-H} = -92.4 \text{ kJ mol}^{-1}$...as can be seen, there are more mols of gas on the left than the right, so a greater yield will be produced at high pressure. The reaction is exothermic, therefore it will give a greater yield at low temperatures, however this is not possible as the rate of reaction becomes too low, and the temperature must actually be increased. A catalyst of finely divided iron is also used to help speed the reaction (finely divided to maximize the surface area).

EQUILIBRIUM (HL)

18.1 Phase equilibrium

18.1.1 : A liquid in an enclosed chamber will form an equilibrium with its own vapor. Fast moving particle in the liquid will escape from the surface and become part of the vapor, but slow moving particles in the vapor will be 'captured' by the liquid and become part of it. At a certain vapor pressure, the number of particles escaping (or evaporating) from the liquid will exactly equal the number being captured by it, and so a dynamic equilibrium is formed between the two.

18.1.2 : As the temperature increases, the average speed of particles is higher. As a result, more particles will have sufficient speed to escape the liquid, and fewer will be slow enough to be recaptured by the liquid. This means that as temperature increases, the equilibrium vapor pressure will also increase. This can be shown graphically with a graph of pressure against temperature, where, as temperature increases, so does pressure.

18.1.3 : Liquids with a high boiling point will have high intermolecular forces. Enthalpy of vaporisation is a measure of the energy change when 1 mol of liquid is converted to gas at standard pressure. As a result a lower enthalpy of vaporisation implies that less energy is required to break the intermolecular bonds, and so a lower enthalpy of vaporisation will result in a higher vapor pressure.

18.1.4 : When two liquids are in a mixture, particles from both liquids escape, forming a partial pressure for each above the mixture. The partial pressure of each liquid will be directly related to its volatility and to the mole fraction of it compared to the total number of mols in the liquid.

18.1.5 : When it is necessary to separate the components of a mixture in which there is more than one volatile component, fractional distillation must be used. (simple distillation is when there is only one volatile fraction, and it is boiled off and the condensed). Fractional distillation is achieved by continuous boiling of the two liquids while they are being condensed (like in reflux)...the more volatile liquid will escape from the top of the fractionating column (the condenser type bit with the water running through it), while the less volatile component will be condensed and returned to the boiling flask. In this way, it is possible to (in theory) completely separate the two components of the mixture.

18.2 The equilibrium law

18.2.1 : The value of K_c can be expressed for a general reaction $\text{A} + 2\text{B} \rightleftharpoons 3\text{C} + \text{D}$ as $K_c = \frac{[\text{C}]^3[\text{D}]}{[\text{A}][\text{B}]^2}$ ie the concentrations of the products (each to the power of their

coefficient) over the concentrations of the reactants (each to the power of their coefficient). All concentrations are taken when the system has reached equilibrium, and so given all concentrations, K_c can be calculated, or given K_c and all but one of the concentrations, the final concentration can be calculated. (It should be noted, however, that concentrations are linked, and so it may not always be necessary to have all the concentrations, or in the second case all but one...but the quadratic formula is not required...so I guess they have to be simple.) The units for K_c can also be calculated by replacing each concentration with mols dm^{-3} (remembering to take exponents into account) and canceling out.)

ACIDS AND BASIS (SL)

9.1 Properties of acids and bases

9.1.1 : Properties of acids and bases in aqueous solutions on stuff...nb...the term alkali refers to a base dissolved in water.

Indicators...they change color depending on whether they're in acidic or basic conditions...each one's different, so I suppose I'd better list some common ones...

	Methyl orange	Bromophenol blue	Methyl red	Bromothymol blue	Phenolphthalein
Acid	red	yellow	red	yellow	colorless
Base	yellow	blue	yellow	blue	red

Each one change color as a different pH, and so there will be cases where one is useful and others are not. (not really necessary is SL?)

Reaction of acids with bases...They will often produce water, and the remaining components will combine to form a salt...ie $\text{HCl} + \text{NaOH} \rightarrow \text{H}_2\text{O} + \text{NaCl}$.

Acids with metals...will produce hydrogen ie $2\text{HCl} + \text{Mg} \rightarrow \text{MgCl}_2 + \text{H}_2$.

Acids with carbonates...will produce water and CO_2 ie $2\text{HCl} + \text{CaCO}_3 \rightarrow \text{CO}_2 + \text{H}_2\text{O} + \text{CaCl}_2$.

9.1.2 : Experimental properties of acids and bases...when acids and bases neutralize, the reaction is noticeably exothermic (ie heat can be felt coming from the reaction). Obviously, they will have an effect on the color of indicators as described above. The hydrogen produced in the reaction of acids with metal will produce a 'pop' sound if a match is held to it, and the CO_2 from the carbonate reaction will turn limewater a milky white when bubbled through it.

Examples of some acids : HCl , CH_3COOH , H_2SO_4 , NH_4^+ .

Examples of bases : NaOH , NH_3 , CH_3COO^- .

9.2 Bronsted-Lowry acids and bases

9.2.1 : According to the bronsted-lowry theory acids are defined as proton (H^+ ion) donators and bases are defined as proton acceptors.

9.2.2 : For a compound to act as a BL acid, it must have a hydrogen atom in it, which it is capable of losing while remaining fairly stable. A BL base must be capable of accepting a hydrogen ion while remaining relatively stable (or reacting to form a stable compound...ie water and a salt). Some compounds (such as water) may act as both ie ($H_2O \rightarrow OH^-$ or H_3O^+)

9.2.3 : Acid base reactions always involve an acid-base conjugate pair...one is an acid, one is its conjugate base...ie HCl/Cl^- , CH_3COOH/CH_3COO^- , NH_4^+/NH_3 .

9.2.4 : The conjugate base will always have one less H atom than the acid (or the acid one more than the base). In compounds where there are many hydrogen atoms, the one which is held the weakest is generally the one which is lost, and this must be reflected in the writing of the compound...as in the CH_3COOH example above.

9.3 Strong and weak acids and bases

9.3.1 : Strong and weak acids are defined by their ease of losing (or donating) a proton. A strong acid, when placed in water, will almost fully ionise/dissociate straight away, producing H_3O^+ ions from water. a weak acid will, however, only partially do this, leaving some unreacted acid remaining. This is set up as an equilibrium, and so when some of the H_3O^+ ions produced by a weak acid are reacted, LCP means that more of the acid will react to form H_3O^+ ions. This means that, given an equal number of mols of acid, they will be neutralized by the same amount of strong base, but their solutions will have different pH values. A weak base is the same as this, only it accepts protons and so produces OH^- ions from water rather than H_3O^+ . Any solution's ability to conduct electricity is defined by its charged ions in it. As a result, a strong acid will produce more charged ions than a weak one, and so its solution will be a better electrical conductor than a weak acid. The same goes for strong/weak bases.

9.3.2 : Strong acids : HCl , HNO_3 , H_2SO_4 . Weak acids : CH_3COOH , H_2CO_3 . Strong bases : group 1 hydroxides (ie $NaOH$ etc), $BaOH$. Weak bases : NH_3 , $CH_3CH_2NH_2$.

9.3.3 : The strength of an acid or base can obviously be measured with an indicator (universal) or a pH meter. also the rate of reaction...hydrogen production with metals or CO_2 with $CaCO_3$ will reveal the strength of an acid. The relative acidities (I'm assuming that means diprotic or whatever) can also be found by neutralizing two acids with a strong base in the presence of an indicator.

9.4 The pH scale

9.4.1 : pH values range up and down from 7 (being the neutral value of pure water at 20°C and 1 atm). Lower pH values are acidic, higher values are basic. pH can be measured with a pH meter, or with pH paper (paper containing a mixture of indicators to cause a continuous color change). pH is a measure of the dissociation of an acid or base, and also of the concentration of that acid / base (actually it's related to the concentration of H_3O^+ ions).

9.4.2 : If we have two solutions with their pH values, the lower one will be more acidic and the higher one will be more basic (though they could both still be basic/acidic with respect to water -- pH 7).

9.4.3 : a change of 1 in the pH scale represents a 10 times change in the acidity or basicity of the solution (because it's a log scale). Concentration is proportional to 10^{pH} .

ACIDS AND BASES (HL)

19.1 Lewis theory

19.1.1 : A Lewis acid is defined as a species which accepts an electron pair to form a dative/coordinate covalent bond. A Lewis base is a species which donates an electron pair to form such a bond. This is a special type of covalent bond because the bond is formed by two electrons from one species and none from the other. This often occurs in the formation of complex ions (or in BL acid/base reactions because the H^+ ion has no electrons, and so must accept a pair to bond with anything...Lewis theory is more general than BL).

19.2 Calculations involving acids and bases

19.2.1 : $H_2O_{(l)} \rightleftharpoons H^+_{(aq)} + OH^-_{(aq)}$. $K_w = [H^+][OH^-]$ The value of K_w is 1×10^{-14} at 25°C but varies with temperature.

19.2.2 : $pH = -\log[H^+]$ (pH is the negative log of the concentration of H^+ ions), $pOH = -\log[OH^-]$, $pK_w = -\log([H^+][OH^-])$ (is equal to 14 at 25°C)

19.2.3 : Use the above equations to calculate other values. Nb... $[H^+]$ or $[OH^-]$ are directly related to the concentration of the acid/base....therefore doubling the concentration of the acid will double $[H^+]$ and halve $[OH^-]$ (and the reverse is true for bases).

19.2.4 : in general $HA_{(aq)} \rightleftharpoons H^+_{(aq)} + A^-_{(aq)}$ -- or -- $B_{(aq)} + H_2O_{(l)} \rightleftharpoons BH^+ + OH^-_{(aq)}$.

therefore $K_a = ([H^+][A^-] / [HA])$ and $K_b = ([BH^+][OH^-] / [B])$

19.2.5 : K_a is a constant which describes the ionisation of an acid (ie how strong it is) and K_b does the same for bases. pK_a is the log for of K_a , defined as $pK_a = -\log(K_a)$ and pK_b

= $-\log(K_b)$. Like previously with the pH scale, a 1 fold change in pK_a will signify a ten fold change in K_a and the same for K_b .

19.2.6 : $K_a \times K_b = K_w$ (ie they equal 1×10^{-14} at 25c) and $pK_a + pK_b = pK_w$ (ie 14 at 25c)

19.2.7 : Strong acids have weak conjugate bases. Strong bases have weak conjugate acids...A strong acid has a large K_a value (or a small pK_a value). A strong base, likewise, has a large K_b value and a small pK_b value.

19.2.8 : All the above equations need to be applied as appropriate given the required input data. The quadratic formula will not be required (but it is often easier than messing around with assumptions etc...especially when your calculator can solve it in a second :)

19.3 Buffer solutions

19.3.1 : A buffer solution is composed of a weak acid/base and its conjugate base/acid. (assuming weak acid for what follows, reverse for base). A solution of weak acid is made, and this forms an equilibrium with the water as follows $HA + H_2O \rightleftharpoons A^- + H_3O^+$. To this solution, some of the acid's conjugate added (A^-), resulting in an increase in the concentration of A^- , some of which reacts with the H_3O^+ . The result of this is, when equilibrium is reestablished, there is a considerable amount of both HA and A^- present in the solution, in a dynamic equilibrium. If some other acid is added, this will react with the A^- , but this causes the equilibrium to shift to the right, almost completely counteracting any pH change. The addition of a base, which reacts with the HA, cause the equilibrium to be shifted to the left, again resulting in very little pH change. This continues until one of the two components, either HA or A^- are completely used up, at which time the pH then changes normally.

19.3.2 : The pH of a buffer solution can be found from the expression for K_a ($K_a = \frac{[H^+][A^-]}{[HA]}$). this can be rearranged to $[H^+] = K_a \times \frac{[HA]}{[A^-]}$. Given the concentration of both the Acid and its conjugate base, and the K_a value of the acid, the $[H^+]$ can be calculated and this can then be converted into a value for pH.

19.4 Salt solutions

19.4.1 : for cations... $2A^+ + H_2O \rightarrow A_2O + 2H^+$, $A^{2+} + H_2O \rightarrow AO + 2H^+$ etc...for anions... $A^- + H_2O \rightarrow AH + OH^-$, $A^{2-} + 2H_2O \rightarrow AH_2 + 2OH^-$ etc...

19.4.2 : Cations (positive ions) will be acidic, Anions (negative) will be basic in water...with the following exceptions

Neutral cations ... Group 1, Be and Mg

Neutral Anions ... Cl^- , Br^- , I^- , SO_4^{2-} , NO_3^- , ClO_4^- .

19.5 Acid-base titrations

19.5.1 : Titration curves... (see page 57-58 of Advanced chemistry by Michael Lewis)

Strong acid, strong base...The curve starting off very low is initially very flat until at equivalence it is almost vertical then very flat again (starting and finishing very low and high respectively on the graph due to low and high pH of strong acid and base respectively).

Weak acid, strong base...The curve begins comparatively high on the graph, and rises sharply initially. After a period it reaches a region where the solution acts as a buffer, still rising continually, but not as steep. The curve then turns up sharply at equivalence and then tapers off to the strong base's pH value.

Strong acid, weak base...identical to the strong acid strong base curve only the eventual point is lower since the weak base will have a lower pH.

Weak acid, weak base... the graph starts sharply up, but then tapers off, reaching only a somewhat steep section in center, before flattening off to the weak base pH. There is no steep section and so it is not possible to find a suitable indicator.

(One other thing...at the point halfway to equivalence $\text{pH}=\text{pK}_a$ or $\text{pOH}=\text{pK}_b$...and $\text{pH}+\text{pOH} = 14$...so you can find pK_a or pK_b from the curve...it can be derived, but it's easier to remember it)

19.6 Indicators

19.6.1 : Indicators work by setting up a weak acid/base equilibrium where the acid and its conjugate base have different colors... $\text{HIn}_{(\text{aq})} \rightleftharpoons \text{H}^+_{(\text{aq})} + \text{In}^-_{(\text{aq})}$. Where HIn is one color and In is the other. This equilibrium can be adjusted by the concentration of H^+ being through the addition of acids or bases.

19.6.2 : The pH range of the indicator falls around its pK_a value, and so to be useful, the pK_a must fall within the inflection of the titration curve.

19.6.3 : the value of pK_a for the indicator must fall around the equivalence point of the titration to work effectively.

OXIDATION AND REDUCTION (SL)

10.1 Oxidation and reduction

10.1.1 : Oxidation is the loss of electrons, reduction is the gain of electrons...ie Oxidation half equation... $\text{Mg} \rightarrow \text{Mg}^{2+} + 2\text{e}^-$. Reduction half equation... $\text{O} + 2\text{e}^- \rightarrow \text{O}^{2-}$.

10.1.2 : The oxidation number of an element is zero. The oxidation number of an ion is equal to the charge of the ion. In compounds, Hydrogen has an oxidation number of +1. In compounds, Oxygen (usually...except in peroxides) has an oxidation number of -2 ... that should be enough information to deduce the oxidation numbers of every element in any IB reaction. The oxidation numbers of ions will be related to the group of the element (ie group 1 elements will be +1...up to group seven elements which will be -1). The elements in the d block will have multiple oxidation states.

10.1.3 : If an element is oxidized, its oxidation number will go up. If an element is reduced, its oxidation number will go down. To find out, simply write down the oxidation numbers for each element as explained previously.

10.1.4 : An oxidizing agent is an element which causes oxidation (and is reduced as a result). A reducing agent is an element which causes reduction (and is oxidized as a result).

10.1.5 : Iron Oxide, for example, come in two forms...FeO and Fe₂O₃. Iron (II) oxide and Iron (III) oxide respectively. The number after the Iron is determined by the oxidation number of the iron in the compound. This convention (including the use of roman numerals) is followed for all compounds in which there is some ambiguity as to the oxidation states of elements (generally d-block elements).

10.2 Electrolysis of a molten salt

10.2.1 : a diagram of an electrolytic cell should include a positive and negative electrode, a current source and the molten salt being electrolysed.

10.2.2 : Current is carried as in a normal circuit for the circuitry, and through the reaction occurring below. At the cathode positively charged ions gain electrons...ie $\text{X}^+ + \text{e}^- \rightarrow \text{X}$ (the cathode must therefore be connected to the -ve pole of the source to supply electrons. At the anode negatively charged ions lose electrons...ie $\text{Y}^{2-} \rightarrow \text{Y} + 2\text{e}^-$. the circuit is completed by the two oxidation and reduction half equations creating an effectively complete circuit.

10.2.3 : In the above example, X will be produced at the cathode, and Y at the anode. Since only two species are present in a molten salt, there is no possibility for any other chemicals to be produced (ie water can not be involved etc...)

10.3 Reactivity

10.3.1 : A more reactive metal will displace a less reactive one from a compound and a more reactive halogen will displace a weaker one from a compound. This can be generalized to say a stronger reducing agent will displace a weaker one from a compound, and a stronger oxidizing agent will displace a weaker one from a compound. Thus, if a metal displaces another, we know it must be more reactive and ditto for halogens (which are the given examples).

10.3.2 : Based on the information in the IB data book...Add the two half equations in question together (one will have to be reversed, invert the sign of the E-zero value also) If the total E-zero value is positive, the reaction is possible. If not, it isn't. (This can be done based on their position in the table, but it makes more sense to use E-zero values, even if SL doesn't need to know them).

OXIDATION AND REDUCTION (SL)

20.1 Redox equations

20.1.1 : Balancing...Copy down both complete half equations, reversing one so the electrons are on opposite sides and so the reactants for both are on the left, and the products on the right. Multiply the equations by the appropriate factors so the number of electrons in each equation is the same. Vertically add the equations, and cancel out any molecules which appear on both sides.

20.2 Standard electrode potentials

20.2.1 : Standard electrode potential --> The potential difference between a given half cell (at 1 mol dm⁻³ conc) and the standard hydrogen electrode

20.2.2 : The standard hydrogen electrode consists of a solution of H₃O⁺ ions at 1 mol dm⁻³ in a beaker. Placed into this is a platinum electrode surrounded by a gas tube submerged in the solution, with hydrogen at 1 atm inside. The circuit to the other half cell is then attached to the platinum electrode, and a salt bridge saturated in potassium chloride. The entire process should take place at 298K and 1 atm pressure.

20.2.3 : The potential difference between half cells is a relative value, dependent on both half cells, and so a standard is required...the standard hydrogen electrode (why they didn't use a nice simple metal one escapes me...perhaps this is more accurate of something :)

20.2.4 : Cell potential --> the potential difference between two half cells (if one half equation is reversed and the two equations are added, the cell potential will be given...it should be positive if you reversed the right one, if it's negative the reaction occurs in the opposite direction to the one you're writing).

Super-secret-bonus stuff they just slipped in without a sub-topic number...

Be able to draw a labeled diag of a half cell and how to link them together...which is basically described above. Cells should also be written in the form $\text{Cu}_{(s)}/\text{Cu}^{2+}_{(aq)}||\text{Zn}^{2+}_{(aq)}/\text{Zn}_{(s)}$, which describes both half cells involved. also, the direction of current flow should also be deduced based of the standard cell potentials, as should the actual reaction occurring. The anode will lose electrons, and so the electrons must flow towards the cathode...that should allow everything else to be worked out.

20.2.5 : The cell potential will be the potential difference between two half cells (and will be positive, unless the reaction occurs backwards). The magnitude is defined by the difference between the E-zero values of each half cell. One of the half equations will have to be reversed (the one which makes the total positive) and adding these two half equations will give you the overall reaction occurring.

20.2.6 : Most reactions with positive E-zero values will occur, however it is possible that at non-standard conditions reactions may not occur, or that some reaction may have very high activation energy, and so will no occur at any reasonable rate.

20.3 Electrolysis

20.3.1 : Electrolysis is where the above cells are forced to run in reverse by attaching an electricity source to overcome the potential difference. In aqueous solutions, however, water is also present, and will sometimes be oxidized/reduced in preference to the dissolved salts (or whatever). It is possible to use the standard electrode potentials to predict this, in that species above water (when it is on the left) will not be oxidized, and species below water (on the right) will not be reduced in an aqueous solution. If necessary, this can be checked by working out the cell potential for all possible combinations (involving the, presumably, two elements and water)...the reaction with the smallest negative potential difference will be the one which occurs. Highly concentrated solutions may overcome this to some degree however...ie it is possible for Cl_2 to be oxidized in a concentrated solution.

20.3.2 : The faraday constant is the charge (in magnitude because it should really be negative) of 1 mole of electrons.

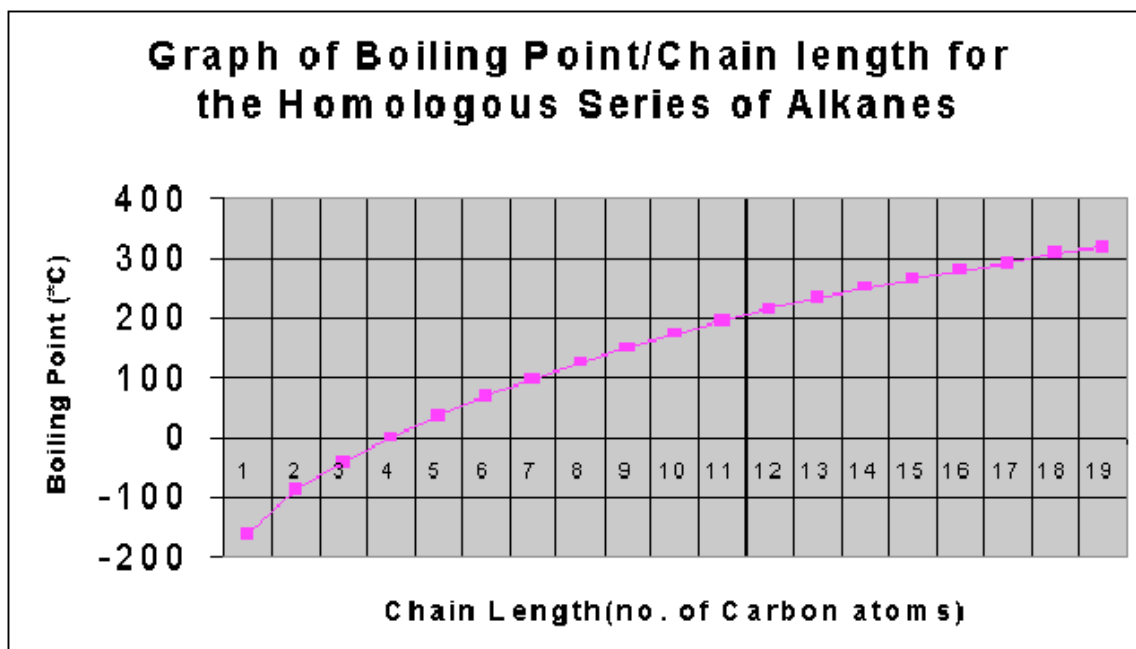
20.3.3 : Faraday's law states that the mass of product produced will be proportional to the charge passed. (Nb...the equation charge = current x time , or $q=It$ may be necessary). Farady's law may also be restated as...the number of faradays required to discharge 1 mol of an ion at an electrode equals the number of charges on that ion.

ORGANIC CHEMISTRY (SL)

11.1 Homologous series

11.1.1 : A homologous series is a set of compounds whose components differ by a single repeating functional group...in the case of (straight chain) alkanes, CH_2 ...and their general formula is $\text{C}_n\text{H}_{2n+2}$.

11.1.2 : The boiling points of alkanes increase as the chains get longer (increased number of electrons \rightarrow increased van de Waal's forces), increasing rapidly initially but flattening off (since the number of additional CH_2 units required to double the chain length increases rapidly...so it flattens of...or you could just believe it)

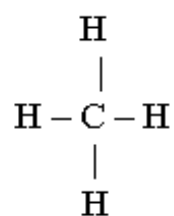


11.2 Hydrocarbons

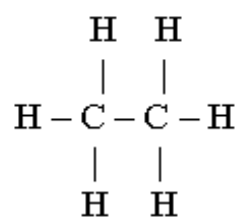
11.2.1 : Basically, each will have a CH_3 group at either end (except methane has only one CH_3) and fill out the required number of CH_2 groups.

11.2.1 :

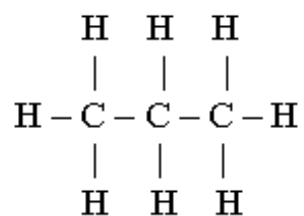
Methane:



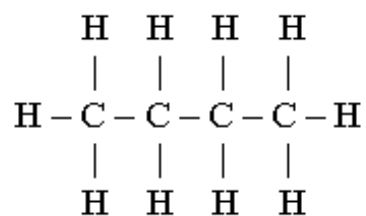
Ethane:



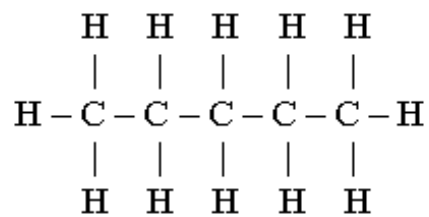
Propane:



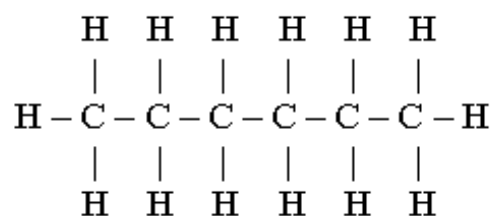
Butane:



Pentane:



Hexane:

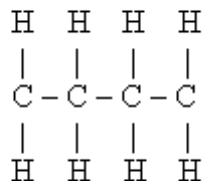


11.2.2 : Names...Methane, ethane, propane, butane, pentane, hexane.

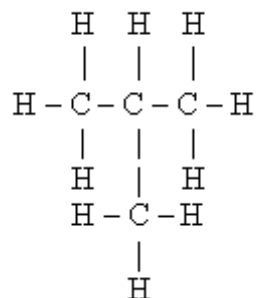
11.2.3 : Basically, move the groups around to make branches, C₁ should have 1, C₂ has 1, C₃ has 1, C₄ has 2, C₅ has 3.

ISOMERS OF THE ALKANES:

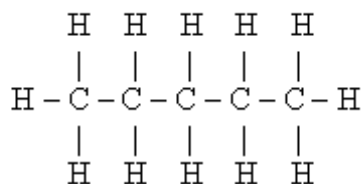
BUTANE:



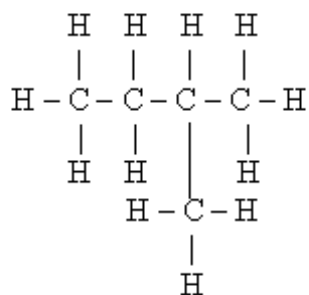
ISOBUTANE or METHYLPROPANE



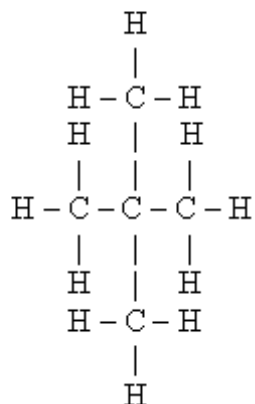
PENTANE :



2-METHYLBUTANE:



2, 2-DIMETHYLPROPANE:

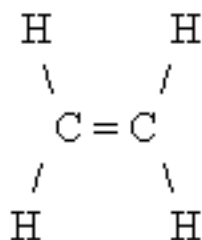


11.2.4 : These structures will be the same as 11.2.1, except two hydrogens on adjacent carbons are replaced by a double bond between those hydrogens.

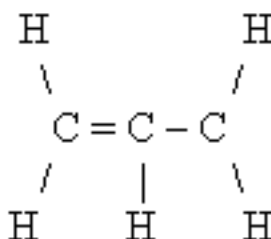
11.2.4

ALKENES:

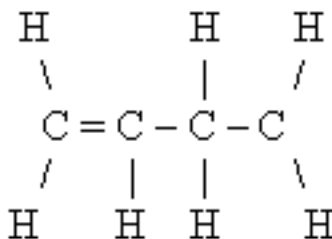
ETHENE:



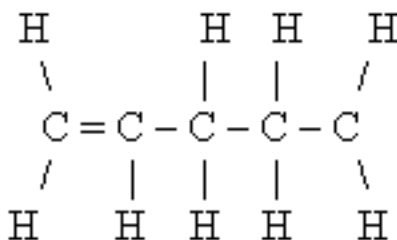
PROPENE:



BUTENE:



PENTENE:



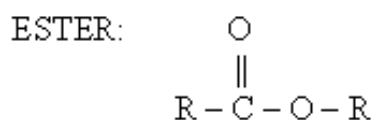
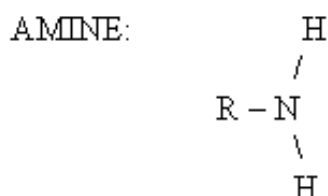
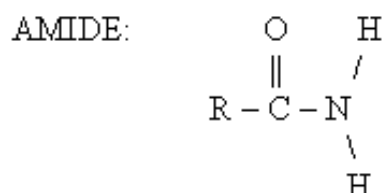
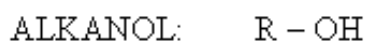
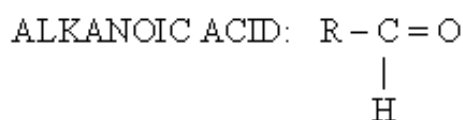
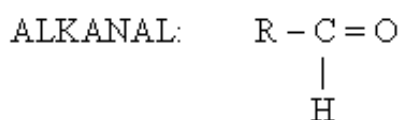
11.2.5 : Complete combustion produces CO_2 and H_2O , incomplete combustion produces CO , C and H_2O (usually occurs with saturated alkanes, where there is a lot of hydrogen, or where there is a limited supply of oxygen). C produces a 'dirty' flame leaving carbon deposits on everything, CO is toxic and CO_2 is a greenhouse gas. Incomplete combustion is where the carbon is not completely oxidised.

11.2.6 : The combustion of hydrocarbons is an exothermic process (otherwise there wouldn't be much point in burning them would there...). This is a result of the fact that the O-H bond is stronger than the C-H bond, and the C=O bond is stronger than the C-C . This means that, the C-C and C-H bonds breaking requires energy, but this is more than made up for by the energy released by the formation of the C=O and O-H bonds.

11.3 Other functional groups

11.3.1 : Functional groups

11.3.1 7 MAIN FUNCTIONAL GROUPS



Alkanal... RCHO (with a double bonded O coming off the C (aldehyde)...but it can be moved along the chain \rightarrow ketone). Naming...(aldehyde) end in al - ie ethanal. (ketone) end in one - ie ethanone.

Alkanoic acid... R-COOH Naming...end in oic acid - ie ethanoic acid (commonly called carboxylic acid)

Alkanol... R-OH . Naming...end in ol - ie ethanol.

Amide... RCONH_2 Naming...end in amide - ie ethylamide.

Amine...R-NH₂ (The two hydrogens on the N can be replaced by R groups to give primary, secondary and tertiary structures). Naming...end in amine - ie ethylamine.

Ester...R-COO-OR. Naming...Think of it like an alkanic acid with a carbon chain rather than a H...the alkanic acid type bit is ...oate this is preceded by the stem of the other half - ie Ethyl ethanoate.

Halogenoalkane...R-X. Naming...Name of halogen (fluro, chloro, bromo, iodo) followed by R name - ie Chloroethane.

11.3.2 : Functional groups can actually be isomers (though their properties are not generally similar). For example ethanoic acid and methyl methanoate are isomers (CH₃COOH vs HCOOCH₃).

11.3.2 ISOMERS OF FUNCTIONAL GROUPS

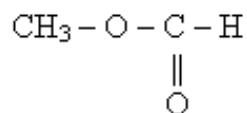
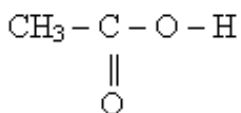
ETHANOIC ACID

CH₃COOH

vs

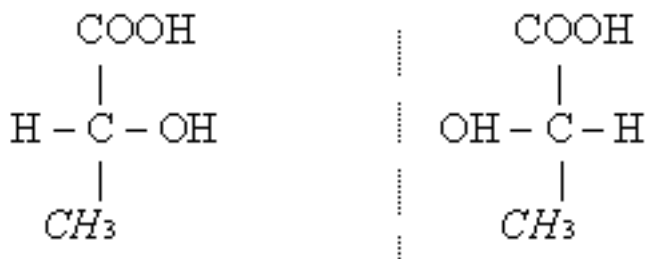
METHYLMETHANOATE

HCOOCH₃



11.3.3 : Optical isomers result if a carbon atom has 4 different groups on each bond. If this is the case, the compound exists in 2 enantiomeric forms (ie optical isomers). In general they react very similarly except in the presence of other optical isomers (also known as chiral molecules -- the chiral center is the carbon atom with 4 different groups). The two enantiomers are mirror images of each other which cannot be superimposed on each other. Biological systems commonly have a strong preference for one enantiomer over the other (one can be bitter, the other sweet for example). The isomers can be identified by their effect on polarised light (by a polarimeter)...when polarised light passes through one isomer it will be rotated to the left, while the other will rotate to the right.

11.3.3 OPTICAL ISOMERS



LACTIC ACID

11.3.4 : O-H groups create hydrogen bonding (alcohols, alkanolic acids) -> less volatile and also solubility (long chain molecules become less soluble since the non-polar chain dominates the molecule).

C=O bonds in Alkanolic acids, Alkanals -> polar bond...dipole forces...higher bp (more significant in small molecules). Small molecules are soluble due to polarity (effect decreases with long chains).

Esters...no Hydrogen bonding -> very volatile, low BP. Polar molecules, therefore short are soluble in water.

Amides...N-H bond is polar with extensive hydrogen bonding -> highly soluble and all molecules have higher BP than alkanes.

Amines...Hydrogen bonding present in Primary and secondary -> soluble (when short) and higher than alkane boiling points. Tertiary amines are very similar to alkanals (but branched -> less dense packing etc).

Halogenoalkanes...short molecules will be soluble due to polar bonds, BP will be somewhat higher

Acid Base properties...Alkanolic (carboxylic) acids are, obviously, acidic. Alcohols are generally not due to the donating effect of the R group. Amines are derivatives of ammonia, and so are basic (though stronger due to the donating effect of the R groups). Amides are not due to withdrawing effect of the C=O group. The others, in general, are neutral (however alkanols can, in acidic conditions act as a base and accept a proton, though the electron donating effect of the alkyl groups generally stop any acidic action).

11.3.5 : Reactions of alkenes with stuff...hydrogen, bromine, hydrogen halides and water.

Before we begin : The C=C bond is not twice as strong as a C-C bond...the second is weaker making it easier to break, and thus a reactive site...this reactivity makes alkenes important starting molecules in the production of other organic molecules.

$\text{RCH}=\text{CHR} + \text{H}_2 \rightarrow \text{RCH}_2\text{-CH}_2\text{R}$... Hydrogen adds to the double bond

$\text{RCH}=\text{CHR} + \text{Br}_2 \rightarrow \text{RCHBr-CHBrR}$... bromine adds onto the double bond

$\text{RCH}=\text{CHR} + \text{HBr} \rightarrow \text{RCH}_2\text{-CHBrR}$... HBr adds across the double bond

$\text{RCH}=\text{CHR} + \text{H}_2\text{O}$ -- With H_3PO_4 + water + 300c + 70 atm --> $\text{RC(OH)H-CH}_2\text{R}$.

11.3.6 : (addition) Polymerisation of alkenes (by a free radical mechanism)...

Initiation ... $2\text{R}^\bullet \rightarrow 2\text{R}^\bullet$ (R^\bullet is a free radical with a lone electron)

$\text{R}^\bullet + \text{CH}_2=\text{CH}_2 \rightarrow \text{R-CH}_2\text{-CH}_2^\bullet$

Propagation ... $\text{R}\sim\sim\sim^\bullet + \text{CH}_2=\text{CH}_2 \rightarrow \text{R}\sim\sim\sim^\bullet$.

Termination ... $\text{R}\sim\sim\sim^\bullet + \sim\sim\sim\text{R}^\bullet \rightarrow \text{R}\sim\sim\sim\sim\sim\sim\text{R}$.

Polythene ... Monomer is $\text{CH}_2=\text{CH}_2$... General polymer is $[-\text{CH}_2\text{-CH}_2-]_n$

Polyvinyl chloride ... Monomer is $\text{CClH}=\text{CH}_2$ (chloroethene) ... General polymer is $[-\text{CH}_2\text{-CHCl-}]_n$

11.3.7 : Production of an ester from an alkanol and alcanoic acid...this is an addition elimination reaction (or addition-dehydration, since we're eliminating water)

$\text{CH}_3\text{CH}_2\text{OH} + \text{HOOCCH}_3$ -- H_2SO_4 and warming --> $\text{CH}_3\text{CH}_2\text{OOCCH}_3 + \text{H}_2\text{O}$

Esters are commonly used as artificial flavoring agents ... Mmmmmm ... Ester ...

11.3.8 : Oxidation of Ethanol to ethanoic acid...

This process requires a primary alcohol (which ethanol is) otherwise the reaction is stopped because the intermediate formed is a ketone rather than an aldehyde.

$\text{CH}_3\text{CH}_2\text{OH}$ -- oxidized by $\text{K}_2\text{Cr}_2\text{O}_7/\text{H}^+$ --> CH_3CHO -- oxidized by $\text{K}_2\text{Cr}_2\text{O}_7/\text{H}^+$ --> CH_3COOH

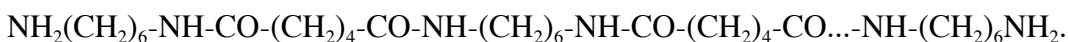
Ethanal is an intermediate which is intentionally not isolated so it can be oxidized again.

11.3.9 : The reaction is between ethanoic acid and ethanamide to form N-ethyl ethanamide (the N means the ethyl group is connected to the N atom. It is also a dehydration reaction (ie water is eliminated).

$\text{CH}_3\text{-CO-OH} + \text{C}_2\text{H}_5\text{NH}_2 \rightarrow \text{CH}_3\text{-CO-NH-C}_2\text{H}_5 + \text{H}_2\text{O}$

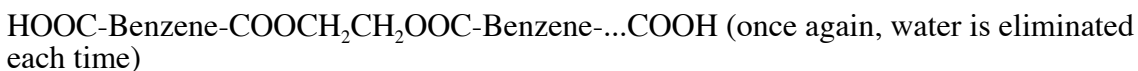
11.3.10 : Condensation polymers

Nylon ... hexane -1,6-diamine + hexanedioic acid



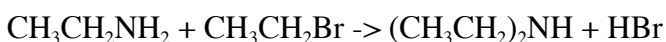
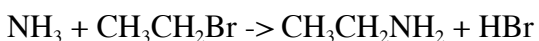
As each new group is created, a water molecule is eliminated...

Polyester ... benzene-1,4-dicarboxylic acid + ethane-1,2-diol



Notice the fact that two functional groups are required on each monomer...Otherwise the reaction would stop without producing a long chain.

11.3.11 : This reaction produces a series of stronger and stronger nucleophiles until a complex ion, $(\text{CH}_3\text{CH}_2)_4\text{N}^+$ is produced.



11.3.12 : Formation of peptides and proteins to form 2-amino acids

Amino Acids ... $\text{H}_2\text{N}-\text{CHR}-\text{CO}-\text{H}$... carbon atom (asymmetric) is connected to 4 different species \rightarrow optically active (except glycine).



$-\text{NH}-\text{CHX}-\text{CO}-\text{NH}-\text{CHY}-\text{CO}-\text{NH}-\text{CHZ}-\text{CO}-$ (poly peptide) This group can join to other peptides to form a protein.

ORGANIC CHEMISTRY (HL)

21.1 Determination of structure

21.1.1 : The structure of a chemical compound can usually not be determine accurately with information form only one source. This stems firstly form the great number of possible organic compounds possible, many of which have very similar chemical properties but different physical properties, similar physical properties but different chemical properties or very similar properties in both categories. There are a variety possible techniques which go beyond both chemical and physical properties, and by combining the information form all these sources it is generally possible to deduce the structure of a compound through the individual pieces of evidence given by each of the sources.

21.1.2 : Covalent bonds are not generally of a static length, but rather they resonate in and out rapidly. This effect allows such bonds to absorb electro-magnetic energy if it is of a certain wavelength (equivalent to a certain energy). The wavelength corresponding to many organic molecules just happens to be within the infrared spectrum. as a result, bonds can be identified in a compound by the wavelengths they absorb. This, however, is usually insufficient as it does not offer enough information about the relative placement of the bonds, or their quantity. The spectrum information is given in the data book and can be matched to any given data.

21.1.3 : We already did how it works...so skipping on...There will usually be a peak in the spectrum at the mass of the entire molecule. There may also be, if present, a peak at Mr-15 representing the loss of a CH₃ fragment (so there must be one in the molecule). Mr-18 represents the loss of water, Mr-31 represents CH₃O and Mr-45 is COOH. Various other fragments could be lost, but the IB only seems to be worried about those listed here.

21.1.4 : H NMR spectrum are based on some complex nuclear magnetic resonance stuff, but basically it gives information about what atoms H atoms are bonded to (though other nearby functional groups have an effect, so really it identifies 'bits' of the molecule), and how many bonds of each type there are. The information is in the data book.

21.2 Hydrocarbons

21.2.1 : The C-C and C-H bonds are very unreactive due to their lack of significant polarity and the high bond energy.

21.2.2 : Homolytic (the same) fission ... A° °B ... each atoms remains with one lone electron -> highly reactive. Hetrolytic (different) fission ... A :B ... One atom gets a lone pair of electron, the other gets none.

Reaction of alkanes with halogens (ie Cl-Cl)...(Initiation) In the presence of UV light, the Cl-Cl bond breaks homolytically resulting in two Cl° free radicals ie Cl₂ -- UV light --> 2Cl°. (Propagation) These radicals then react with alkane (ie CH₄) to form HCl and CH₃°

ie $\text{Cl}^\circ + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3^\circ$. This CH_3° free radical can then react with a chlorine molecule to form another chlorine free radical ie $\text{CH}_3^\circ + \text{Cl}-\text{Cl} \rightarrow \text{CH}_3\text{Cl} + \text{Cl}^\circ$. (Termination) This reaction is continued until two free radicals react to form a single molecule ie $\text{Cl}^\circ + \text{Cl}^\circ \rightarrow \text{Cl}_2$ or $\text{Cl}^\circ + \text{CH}_3^\circ \rightarrow \text{CH}_3\text{Cl}$ or $\text{CH}_3^\circ + \text{CH}_3^\circ \rightarrow \text{C}_2\text{H}_6$.

21.2.3 : The structure of Benzene was originally thought to be a ring of alternating double and single bonds, however this does not fit for several reasons. Firstly, there the enthalpy of combustion of Benzene as compared with this model (an unstable compound called cyclohexatriene). The enthalpy of combustion can be projected from the enthalpies of cyclohexadiene and cyclohexene, but benzene is significantly lower (and therefore more stable) than this projected value. Also significant are the reactions which benzene undergoes. Double bonds, as seen with alkenes tend to undergo addition reactions, where a double bond breaks forming a single bond between the carbons and two new bonds. Benzene, however, does not undergo such reactions, but rather has substitution where the hydrogens are replaced by other electrophiles.

21.2.4 : Octane rating is a scaled devised to measure how smoothly a fuel burns in a combustion engine. The scale is bases around two measuring points, heptane which has an octane rating of 0, and 2,2,4-trimethylpentane which has an octane rating of 100. A fuel with an octane rating of 60, for example, would be the same as a mixture of 60% 2,2,4-trimethylpentane and 40% heptane. In the past, tetraethyl lead (IV) was added to fuels to retard it's ignition and make the fuel burn more smoothly, however this has caused significant problems with lead concentrations in the atmosphere. The other way to increase octane rating is by using highly branched chains, or aromatic compounds (benzene rings) which also burn more smoothly, thus producing high octane, lead free fuels.

21.3 Halogenoalkanes

21.3.1 : Nucleophilic substitution by $\text{S}_\text{N}1$ and $\text{S}_\text{N}2$ mechanisms

$\text{S}_\text{N}1$ mechanism ... First, due to the electron donating effect of the alkyl groups, the carbon-halogen bond breaks heterolytically, resulting in (using CH_3Cl as an example) CH_3^+ and Cl^- produced. This is the rate determining step (hence the 1st order reaction). The nucleophile then attacks the positive carbon atom and forms CH_3N .

$\text{S}_\text{N}2$ mechanism ... Rather than completely breaking the bond, a polar bond is formed between the halogen and carbon, producing a delta+ve charge on the carbon. This is enough to attract the nucleophile to form an intermediate with carbon forming an intermediate with effectively 5 bonds...one to the nucleophile, one with the halogen and 3 others. This is the rate determining step, hence the second order reaction. The halide ion then breaks off heterolytically forming again $\text{CH}_3\text{N} + \text{Cl}^-$, but by a different mechanism ... Some good nucleophiles are ROH , CN^- , OH^- , and RNH_2 .

I think Markovnikov's rule fits in here...In this example...When HX adds across an asymmetrical double bond, the major product formed is the molecule where the less electronegative atom adds to the carbon with the most hydrogens already on it (this is since hydrogen adds on, and produces a carbocation intermediate...the intermediate where the C^+ has the most electron donating groups around it will be most common...ie the most alkyl groups.)

21.3.2 : S_N1 reactions tend to occur with tertiary carbon (ie with 3 alkyl groups off the carbon connected to the halogen) for two reasons. Firstly, there is not room for a nucleophile to attack due to the steric hindrance caused by the bulky alkyl groups, and secondly the inductive electron donating effect of these groups mean it is much more likely that the C-X bond will break, rather than just becoming highly polar. S_N2 reactions, however, occur on primary carbons since there is plenty of space between small hydrogen atoms for the nucleophile to attack, and it is unlikely that the C-X bond will break on its own.

21.3.3 : Different halogens will obviously have different bond strengths. the F-H bond is strongest (and shortest) while I-H is the longest (and weakest). As a result, the H-I bond is easiest to break, and does so most easily therefore has the highest rate, while H-F is the slowest.

21.4 Alkanols

21.4.1 : Dehydration to form alkenes and alkoxyalkanes

Alkenes ... In the presence of H₂SO₄ and the proper temperature (hot for primary, warm for secondary and cool for tertiary) alcohols can lose a water molecule and form an alkene. ie - CH₂H-CH₂OH -- H₂SO₄ and heat --> CH₂CH₂ + H₂O.

Alkoxyalkanes ... In acidic conditions alcohols act as a base, and accepts a proton. This produces a positive charge on the oxygen (and inductively a delta+ve on the carbon). The spare pair of electrons on the oxygen atom of another alcohol are attracted to the delta+ve carbon making it act like a nucleophile, and so it attacks the carbon atom (this assumes an S_N2 reaction though S_N1 is possible under other conditions...ie tertiary alcohols). Water and a proton are then split off producing an ether (alkoxyalkane) and water (and regenerating the acid as a catalyst). ie CH₂OH + H⁺ -> CH₂OHH⁺. then CH₂OHH⁺ + CH₂OH -> CH₂OCH₂ + H₂O + H⁺.

21.4.2 : Oxidation of alkanols is different depending on whether they are primary, secondary or tertiary. For primary and secondary, a C=O bond replaces the C-OH, but this bond will either be on the end (an aldehyde) or in the middle (a ketone). Aldehydes can be reoxidized to form carboxylic acid. Tertiary alcohols will not oxidize.

Primary ... CH₃CH₂OH --Cr₂O₇²⁻--> CH₃CHO (aldehyde/alkanal) + H₂O --Cr₂O₇²⁻--> CH₃COOH (alkanoic acid)

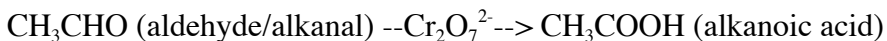
Secondary ... CH₃-CH(OH)CH₃ --Cr₂O₇²⁻--> CH₃-CO-CH₃ (ketone/alkanone)

21.5 Alkanals and alkanones

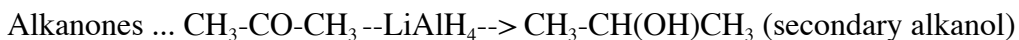
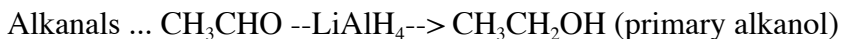
21.5.1 : Carbonyl compounds are reactive because they contain a delta+ve carbon atom, and are unsaturated (both due to the C=O bond). Thus, the Pi electrons can be relatively easily shifted to form a new bond on both the carbon and oxygen atoms, and since nucleophiles are attracted to the carbon atom, the happens relatively quickly.

21.5.2 : This is the same as with the alcohols alkanals will react to form carboxylic acid as

follows.

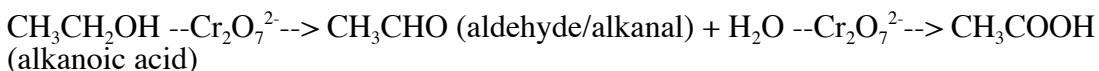


21.5.3 : This is the reverse of the process shown in the alcohols above...alkanals will be reduced to primary alkanols, alkanones will be reduced to secondary alkanols by LiAlH_4 .



21.6 Alkanoic acids

21.6.1 : Alkanoic acids can be formed by oxidizing primary alkanols with acidified dichromate (IV) as follows.



21.6.2 : The OH group in alkanols doesn't act as an acid, but that is alkanoic acids do...why ? ... This is a result of the inductive effect of the C=O group. In alkanols, the R groups are electron donating, resulting in a negative charge being inductively pushed along the chain, creating a large -ve charge on the oxygen atom. The C=O bond, however, is electron withdrawing which results in a delta+ve carbon atom. This inductively increase the polarity of the O-H bond, and also produces a more stable anion when the proton is lost (because electron density is being pulled away creating a smaller negative charge on the oxygen).

21.6.3 : Soaps are formed basically of a long hydrocarbon chain ending in a COO^-Na^+ , or similar, head -- ie $\text{CH}_3\text{CH}_2\text{--}[\text{--CH}_2\text{--}]_n\text{--COO}^-\text{Na}^+$. They work because the head is hydrophilic (dissolves in water) while the tail is hydrophobic (doesn't dissolve in water, but does in fats, non-polar dirt etc). this means the molecules position themselves around small 'blobs' of non-polar dirt (called micelles). these are pulled out of the fabric etc by these molecules and are then held in suspension in the water and eventually washed away.

CHEMICAL INDUSTRIES

E.1 Initial overview

E.1.1 : Sources of materials

Raw materials -- Natural substances which can be converted by chemical processes into useful products.

By-Products -- Substances produced as a result of a chemical process, but not the major (or important) product.

Waste products -- Substances produced that have no value/are dangerous and must be disposed of.

Minerals -- Naturally occurring inorganic substances ... metals and their ores.

Air -- O₂, N₂, Ar

Petroleum -- Coal, Oil etc...

E.1.2 : Factors influencing positions for chemical industry establishment.

Must comply with regulations (ie environmental restrictions), good transport access to market and raw materials, availability and cost of labour, land, plant, equipment and energy source (electricity). Availability and cost of raw materials.

E.1.3 : Specialty vs Bulk chemicals...

Specialty ... Drugs, Many organic substances (w/ specific uses)

Bulk ... Sulphuric acid, Nitrogen, Oxygen, Ammonia, Sodium hydroxide, Chlorine

E.2 Principles of extraction and production

E.2.1 : Metals are rarely found free in nature, and have to be extracted and processed before they can be used ... with the exception of Gold and some other stuff like that.

E.2.2 : Physical separation and purification from ores...

Concentration of ores ... Froth, flotation etc

Separation ... Filtration, Centrifuge type stuff, magnetic properties, chromatography

Purification ... Zone refining (explained later)

E.2.3 : Chemical principles in the extraction of useful substance from raw materials ...

Changing into suitable form for oxidation ... $\text{ZnS} + \text{O}_2 \rightarrow \text{ZnO} + \text{SO}_2$.

Reduction to metal, by electrolysis or chemical reaction (blast furnace)

Also consider ... Reduction (Iron), electrolysis (Al₂, Al), equilibrium (Contact and Harber), energy requirements (electrolysis...lots of energy and heat), catalysts (rate of reaction)

E.3 Metals - iron and aluminum

E.3.1 : Main sources of iron are iron ores and scrap iron...not much else to say.

E.3.2 : Reactions which occur in a blast furnace (to produce iron)

$\text{C}(\text{s}) + \text{O}_{2(\text{g})} \rightarrow \text{CO}_{2(\text{g})}$... Carbon is partially oxidized to CO₂.

$\text{CO}_{2(\text{g})} + \text{C}(\text{s}) \rightarrow 2\text{CO}(\text{g})$... The carbon in CO₂ is reduced to CO.

$3\text{CO}(\text{s}) + \text{Fe}_2\text{O}_{3(\text{s})} \rightarrow 2\text{Fe}(\text{s}) + 3\text{CO}_{2(\text{g})}$... Iron (III) oxide is reduced to Fe by the CO.

$\text{CaCO}_{3(\text{s})} \rightarrow \text{CaO}(\text{s}) + \text{CO}_{2(\text{g})}$... This bit is about the production of slag, which is going to sit on top of the iron.

$\text{CaO}(\text{s}) + \text{SiO}_2 \rightarrow \text{CaSiO}_{3(\text{l})}$... CaSiO₃ is the slag.

E.3.3 : Conversion of iron to steel in oxygen converter (steel is iron with a low proportion of carbon)

First, the converter is charged with about 25% scrap steel. In the bottom of the converter is also calcium oxide (lime) which reacts with impurities to form slag. Molten iron is then poured into the converter. In the converter there is also a tube blowing super heated oxygen into the molten iron. This will react with the carbon in the steel to produce CO₂, which then escapes. When The steel has been produced, the converter is tipped and the steel is tapped off through an outlet pipe.

E.3.4 : Different forms of iron...

Cast iron -- same as pig iron, high carbon content -> relatively brittle, but also harder

Wrought iron -- more malleable (due to lower carbon content). Hammering/rolling removes impurities.

Carbon steel -- Small (>1%) carbon content + Iron ... thus it's very malleable, but not

very hard.

Alloy Steels -- The addition of other elements can change the physical properties of the alloy. eg Tool steels have to be strong, corrosion resistant and heat resistant. Stainless steel (18% chromium, 8% nickel) is resistant to corrosion, used in cutlery and surgical instruments.

E.3.5 : The principle uses of steel is in construction, and as reinforcement. Plus the ones given above...tools, cutlery, surgical instruments and so on.

E.3.6 : Production of Alumina from bauxite (aka Aluminum oxide, Al_2O_3)...

Al_2O_3 will eventually be electrolysed, but first it must be purified...

$\text{Al}_2\text{O}_{3(s)} + 2\text{NaOH} + 3\text{H}_2\text{O} \rightarrow 2\text{NaAl}(\text{OH})_{4(aq)}$... Aluminum oxide produces sodium aluminate (and dissolves out any soluble impurities)

$\text{NaAl}(\text{OH})_{4(aq)}$ -- dilution --> $\text{Al}(\text{OH})_{3(s)} + \text{NaOH}_{(aq)}$... This occurs when the solution is diluted with water, producing aluminum hydroxide...which is a solid precipitate, and can be removed (leaving impurities behind)

$2\text{Al}(\text{OH})_{3(s)} \xrightarrow{\text{heat}} \text{Al}_2\text{O}_{3(s)} + 3\text{H}_2\text{O}_{(g)}$... after heating, Pure anhydrous aluminum oxide is produced.

E.3.7 : The aluminum oxide is then dissolved in molten cryolyte (Na_3AlF_6)...requiring the temperature to be kept above 850°C ... and then electrolysed...

Cathode ... $\text{Al}^{3+} + 3\text{e}^- \rightarrow \text{Al}$

Anode ... $2\text{O}^{2-} \rightarrow \text{O}_2 + 4\text{e}^-$ followed by $\text{C} + \text{O}_{2(g)} \rightarrow \text{CO}_{2(g)}$... because the anode is made of carbon.

The molten aluminum is then tapped off from the bottom of the container, since it is more dense than the cryolyte.

Cryolyte is used because it greatly reduces the amount of energy to keep the aluminum oxide in a molten state. The cell is generally produced as a large 'vat' ... The cryolyte is in this, which is lined with carbon to be used as the cathode. Carbon anodes are dipped at intervals along it, and are slowly lowered as are eaten away (by the production of CO_2).

E.3.8 : Properties of aluminum ... Aluminum is resistant to corrosion (because it naturally forms a protective coating on Al_2O_3). it is also very lightweight, and inexpensive compared to some alloys (stainless steel). It can not be made hard by the addition of carbon like iron.

E.3.9 : Aluminum is widely used due to its resistance to corrosion. Common uses are cans, construction (roofing, fences) and its lightweight nature also makes it useful in cars and airplanes. Aluminum can not be made hard and so it is not very useful for tools, but doesn't corrode, making it useful in areas such as roofing, where steel would corrode, and

stainless steel is too expensive.

E.3.10 : Environmental impacts of Aluminum production...

Mining -- Destruction of land ... may require rehabilitation

Siting -- some effluent and waste gases are inevitable, and so the plant would be best situated away from population centers.

Recycling -- Avoids above problems, and may be less expensive than the production from bauxite. Also, bauxite is a non renewable resource.

E.4 Air

E.4.1 : Gases (oxygen, nitrogen and argon) are obtained by cooling air to below the boiling point of the gas wanted ... $O_2 \rightarrow 183^\circ\text{C}$, $N_2 \rightarrow 196^\circ\text{C}$, but I don't think these will be necessary.

E.4.2 : Uses...

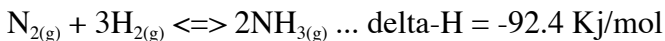
N_2 ... Producing NH_3 , HNO_3 , Inert gas in incandescent light bulbs (and as an inert atmosphere in general). Also, as a liquid coolant for freezing food etc.

O_2 ... Respiration (to air, eg oxygen rich air), production of steel, fuel ($O_2 + C_2H_2$ or $O_2 + H_2 \rightarrow$ welding) oxidizer in rocket propellant as liquid with reducer.

Ar ... Inert gas \rightarrow fluorescent tubes, thermometers (above Hg), where an inert gas is needed but N_2 can't be used.

E.5 Equilibrium processes - The Harber and contact processes

E.5.1 : Many industrial processes depend on the manipulation of equilibria. (because the expensive products are usually those which are hard to make ;) ... the ones we're going to see here are the harber and contact processes ... First the harber process (this is sort of a recap from Topic 8...)



Considerations ... LCP predicts that the best yield will occur with low temperature and high pressure. Rate requires high temp for fast reaction. Equipment to maintain high pressure is expensive.

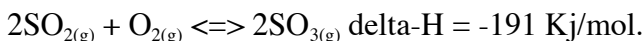
Generally used ... 450°C , 250 atm and a catalyst (finely divided iron)

\Rightarrow about 30% yield ... NH_3 is separated by liquifying (NH_3 melts at about 20°C) ... other gases are returned to the reaction.

E.5.2 : Uses of ammonia ... Essential nutrient for healthy plant growth ... Problem

(nitrogen fixation) . It is difficult to use $N_{2(g)}$ from the atmosphere, thus nitrogen based fertilizers are used. Used to make nitric acid (HNO_3), for the nitration of benzene. Also, for production of TNT (trinitrotoluene ... methyl benzene with 3 substituted NO_2 groups...at 2,4,6). and it's used to make dyes.

E.5.3 : Contact process ... This is the production of H_2SO_4 .



LCP suggests low temperature and high pressure. (other considerations as above)

Generally used ... 450°C, 1 atm and vanadium (v) oxide catalyst ... this produces about a 97% yield...high pressure not really necessary.

$SO_{3(g)} + H_2O \rightarrow H_2SO_4$... when this is diluted in H_2O , H_2SO_4 will be produced.

E.5.4 : Uses of sulphuric acid ... Making fertilizers, explosives, dyes, production of other acids, detergents, catalyst for making esters, producing nitrating mixture and as a dehydrating mixture. It's the most important industrial acid...understand that ;)

E.6 The oil industry

E.6.1 : Importance of oil as a chemical feedstock.

About 90% of the crude oil products from fractional distillation is used in transport, heating fuels and electricity production. The other 10% is used as a feedstock for the production of other organic chemicals, but it is still the most significant source of organic chemicals.

E.6.2 : Cracking ... three types ... catalytic cracking, thermal cracking and hydrocracking.

Catalytic cracking ... Superior to thermal cracking. Occurs at a lower temp (250°C) 1 atm pressure and a catalyst. Produces high quality gasoline ... less CH_4 , more useful C_3 and C_4 molecules and many alkenes rather than alkanes.

Thermal cracking ... 500°C, 50 atm pressure (older and possibly out of date).

Hydrocracking ... variation of thermal cracking using sodium aluminosilicate where some Na^+ is replaced by Pt. Performed in the presence of H_2 , so products are saturated (alkanes not alkenes).

E.6.3 : Reforming...a bunch of types...

Catalytic reforming -- Produces branched carbon chains, which have a higher octane number. This is done at 500°C in an atmosphere of hydrogen.

Aromatisation -- The production of aromatic molecules (benzene rings) (usually 500°C and H_2 atmosphere like catalytic)

Cyclisation -- The production of cyclic molecules ... again at 500°C and in atmosphere of H₂.

Alyklation -- the reaction of alkanes and alkenes to form branched alkanes.

In all of these, hydrogen will be produced, which is commonly used in the Haber process.

E.6.4 : Removal of sulphur from crude oil.

S in crude oil, when heated or burned forms SO₂ (and some SO₃), which can dissolve in water and form acid rain...Removal...

SO₂ formed in fractional distillation can be removed by reaction with MgO or NaOH., both of which react with SO₂/SO₃ to form a salt and water. The SO₂/SO₃ can then be used in the production of H₂SO₄.

E.6.5 : Refinery products as feedstock.

Can produce from spare fractions of crude oil -- solvents, plastics, pesticides, food additives, pharmaceuticals, detergents, cosmetics, dyes.

E.6.6 : Properties and uses of polymers ...

Polythene -- Long branched molecules produce a soft, malleable substance, useful in packaging.

Polyvinyl Chloride -- Considerably more rigid, and this stronger due to polar C-Cl bonds. Useful for glue and as a sealant.

Nylon -- Strong, long fibers, commonly used in tights or stockings, but also to as strength to other fibers (ie carpets are a combination of wool and nylon).

Polyester -- Long chain fabrics with great strength and do not rot. Commonly used in sails, ropes and other fibers which must be strong and not rot.

E.6.7 : These polymers will not break down naturally and can not be burnt without the production of toxic gases. They are also produced from oil non-renewable resource (but can sometimes come from agricultural products).

E.7 Other chemical industries

E.7.1 : Other chemical industries include the production of --

alloys, cement, ceramics, glasses, paper, silicones and natural products.

E.7.2 : Biotechnology is also an important source of some chemicals, such as ethanol, insulin and biopolymers (such as starch, rubber, proteins, wool, cotton, paper).

E.8 The chlor-alkali industry

E.8.1 : Chlorine is produced by the electrolysis of sodium chloride, because it is not easy to chemically separate them. This is, today, done in a diaphragm cell...

The diaphragm cell is basically a container separated down the center with a porous (commonly asbestos) diaphragm. The container has brine (NaCl in water) pumped into the left hand side. Above is a Ti anode where Chlorine is produced, and piped off. Spent brine flows through and at the steel cathode on this side, water is reduced to form H₂ (and OH which forms NaOH with the sodium left over from before). This sodium hydroxide solution is then piped out from the bottom, while the H₂ is piped off the top. The two gases must be separated because they would react explosively if they came into contact.

E.8.2 : The fact that the above cell produces Cl₂, H₂ and NaOH is very convenient, since all three are useful products, and the cell uses comparatively little energy...uses

Chlorine -- Dry cleaning solvents, refrigerants, PVC, disinfectant

Hydrogen -- Ammonium production, fuel cells, reducing agent.

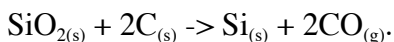
NaOH -- Neutralizing acids, producing soap, aluminum production

E.8.3 : The diaphragm cell above has replaced a similar one using a flowing mercury cathode due to concerns about mercury poisoning. Also, many problems with Chlorine containing solvents have been found (specifically the ozone layer) which makes this process somewhat less favorable.

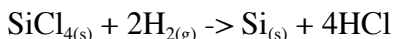
E.9 Silicon

E.9.1 : Silicon is the second most abundant element in the earth's crust (28%)

Extraction -- Reduction of silica (sand) by coke in an electric furnace



More pure Si can be obtained from SiCl₄ by reduction in H₂.



Very pure silicon can be produced by zone refining the silicon above. Long rods of impure silicon are passed through a heating element, which melts the silicon as it passes through. Impurities dissolve in this molten portion, and so as the Silicon passes through, the impurities are left behind, and eventually the end is cut off. (Silicon does have a high melting point however, so this is expensive).

E.9.2 : Semiconductors ...

In its natural state, silicon is a large covalent lattice of silicon molecules. Semiconductors

are created by doping (or adding one to about every million) the silicon with either Phosphorus (P) or Boron (B). Because Phosphorus has one extra valence electron, it can be removed and effectively carry a voltage through the lattice. Boron, on the other hand, has one less, and so it is possible to excite a valence electron from an Si atom into the gap...this allows a positive charge to be carried by the hole. Phosphorus is an n-type semiconductor (n for negative) while boron is p-type (positive).

E.10 Ellingham diagrams

There is an ellingham diagram in the data book, it works like this...The graph shows gibbs free energies at various temperatures. If you want one reaction to force the other to occur in reverse, then it's line must be below the other for the given temperature (because the second will be reversed, and -ve will become +ve). In general, it is used to see if reaction can be used to reduce another.

E.11

E.11.1 : Thermal cracking vs Catalytic ...

Thermal cracking uses homolytic breaking of bonds, creating free radical carbon chains. These, therefore act with a free radical mechanism.

Catalytic cracking breaks the bonds homolytically, producing complex ions, and thus an ionic mechanism.

E.11.2 : LDPE vs HDPE polythene mechanisms.

LDPE (Low density polythene) -- this is produced by the polymerisation of ethene of 200°C and 1200 atm, with trace amounts of O_2 present. This produces highly branched chains, and so is soft, malleable etc.

Mechanism ...

Initiator ... Benzene(=O)-O-O-(O=)Benzene ... the central peroxide link breaks, and $2\text{Benzene}^\circ + 2\text{CO}_2$ is produced. These benzene radicals react with ethene, forming a Benzene- $\text{CH}_2\text{-CH}_2^\circ$ free radical, and so on until it terminates with two free radicals meeting.

HDPE (high density polythene) is produced at 60°C and 1 atm using a ziegler catalyst, and an ionic mechanism. It has fewer branched chains, and so is less malleable and has a higher melting point...and obviously it's higher density.

E.11.3 : Principles of condensation polymers.

-- The forming of monomers with the expulsion of a small group (H_2O or H_2) to form a polymer.

-- The monomers must have two functional groups to react and form a continual chain with other monomers.

Nylons (1,6-hexanedioic acid + 1,6-hexanedamide, expelling water) and Polyesters (1,4-Benzenediol and ethanedioic acid, expelling water)

Polyurethanes -- I'll come back to this (probably never)...it's hard to describe without a diagram.

Silicones ... Monomer is HO-(R)Si(R)-OH and produces ---O-(R)Si(R)-O-(R)Si(R)-O-(R)Si(R)-O-...Expelling water each time.