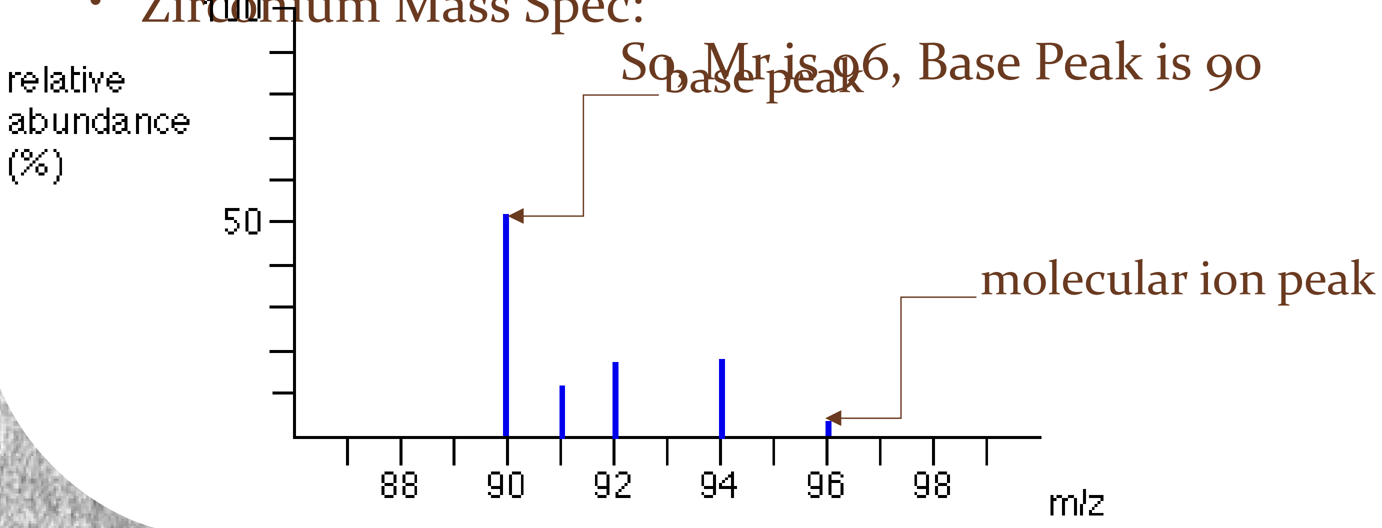
Atomic Structure – Additional Mass Spectrometry

- Working out Atomic Mass from Isotopes
  - Ar of X = [sum of (m/z * relative abundance)] / (sum of relative abundance)
  - Ar of Mg = [(24*79.0)+(25*10.0) +(26*11.0)] / (79.0 + 10.0 + 11.0) = 24.3
- Relative Molecular Mass (Mr)
  - “the mean mass of a molecule compared to one-twelfth of a 12C atom”
  - Zirconium Mass Spec:

So, Mr is 96, Base Peak is 90



Atomic Structure – Electron Configurations of Ions

- The S and P Blocks
  - For +1 Ions
    - Calcium (11) = 1s2 2s2 2p6 3s1
    - Calcium+ (10) = 1s2 2s2 2p6
  - For +2 Ions
    - Magnesium (12) = 1s2 2s2 2p6 3s2
    - Magnesium2+ (10) = 1s2 2s2 2p6
  - For +3 Ions
    - Aluminium (13) = 1s2 2s2 2p6 3s2 3p1
    - Aluminium3+ (10) = 1s2 2s2 2p6
  - They have all become **isoelectronic** with Neon (10) = 1s2 2s2 2p6
- The D Block
  - We take from the 4s first
    - Chromium (24) = [Ar] 3d5 4s1
    - Chromium3+ (21) = [Ar] 3d3
    - Iron (26) = [Ar] 3d6 4s2
    - Iron2+ (24) = [Ar] 3d6
- Non metal Ions
  - We give to the highest energy level first
    - Phosphorous (15) = 1s2 2s2 2p6 3s2 3p3
    - Phosphorous3- (18) = 1s2 2s2 2p6 3s2 3p6
  - Phosphorous as become **isoelectronic** with Argon (18) = 1s2 2s2 2p6 3s6

Amount of Substance – Amount of Substance

- The Mole (the Avogadro Constant)
  - "the number of atoms in 1 gram of any given substance relative to 1/12 of 12C"
  - 6.023 * 1023
- n (mol) = mass (g) / amu
  - What is the mass of 3 mol of Helium atoms?
  - *mass = amu * n*
  - *mass = 4.0 * 3*
  - *mass = <u>12 grams</u>*

Amount of Substance – Acid-Base Titrations

- How to do Acid-Base Titration Questions:

1. Write the Balanced Equation
2. Underline the (two) substances involved in the question
3. Write down the information of each substance beneath it
4. Use the information to find the number of moles
5. Use the ratio in the equation to find the number of moles for the other underlined substance
6. Then find the mass with the answer to (5.)

<u>Acid-Base Titration Example:</u>

25.0 cm3 of NaOH is neutralised by 22.5 cm3 of HCl at 0.10 mol dm-3.

What was the concentration of NaOH?

1. HCl + NaOH → NaCl + H2O
2. <u>HCl</u> + <u>NaOH</u> → NaCl + H2O
3. <u>HCl</u> + <u>NaOH</u> →
   22.5 cm3 25.0 cm3
   0.10 mol dm-3
4. 0.10 * (22.5/1000) = 2.24 * 10-3
5. 1:1, so no change

Bonding and Periodicity – Permanent Dipole

- Dipole Attraction
  - When two atoms in a covalent bond have different electronegativities
- Hydrogen Bonds
  - Will happen if:
    - A molecule contains a hydrogen atom covalently bonded to F, O or N
    - There is also a lone pair on the FON atom
- The Structure of Ice
  - Ice has a regular open lattice
  - Further apart in solid than liquid so it expands
  - This is because the water forms hydrogen bonds

Energetics – Calculating Enthalpy Changes

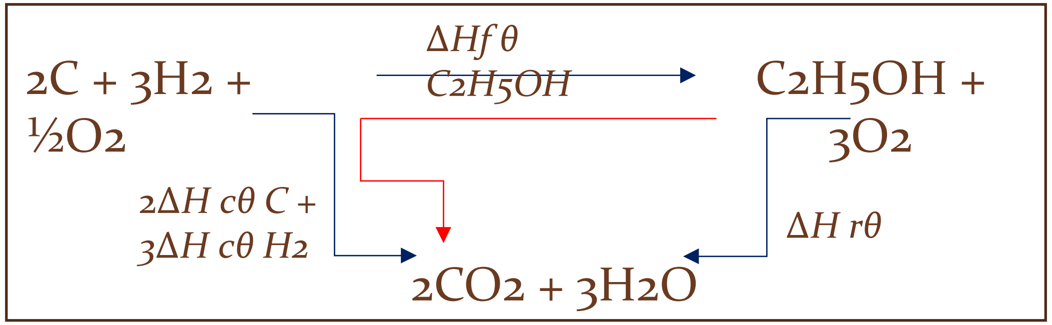
Calculating Enthalpy Changes Example:

- Calculate the enthalpy change for the reaction below using the data given.

$$C_2H_5OH + 3O_2 \rightarrow 2CO_2 + 3H_2O$$

$\Delta H c\theta\ C$: $C + O_2 \rightarrow CO_2$ (-394 kJ mol-1)
$\Delta H c\theta\ H_2$: $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$ (-286 kJ mol-1)
$\Delta H f\,\theta\ C_2H_5OH$: $2C + 3H_2 + \frac{1}{2}O_2 \rightarrow CO_2$ (-278 kJ mol-1)

$\Delta H\ r\theta = -[\Delta H c\theta\ C_2H_5OH] + [2\Delta H\ c\theta\ C + 3\Delta H\ c\theta\ H_2]$
$\Delta H\ r\theta = -[-278] + [2(-394) + 3(-286)]$
$\Delta H\ r\theta = -[-278] + [-1646]$
$\underline{\Delta H\ r\theta = -1368 \text{ kJ mol-1}}$



Kinetics – Catalysis

- Catalyst
  - "Provides an alternate pathway of lower activation energy"
- Heterogeneous Catalyst
  - In a different phase from the reactants
  - E.g. Hardening of Vegetable Oils (Nickel Catalyst)
- Homogenous Catalyst
  - In the same phase as the reactants
  - E.g. The Ozone (Cl•)
    - $Cl\bullet + O_3 \rightarrow ClO\bullet + O_2$
    - $ClO\bullet + O_3 \rightarrow Cl\bullet + 2O_2$
    - The Cl• is reproduced again and goes on to destroy more Ozone

Redox Reactions – Combining Half-Equation

- How to combine Half equations
  1. Write out the two half-equations
  2. Note the number of electrons each half equation gains or loses
  3. Multiply the half equations to get the electrons to equal values
  4. Combine the equations by putting all the reactants on one side and all the products on the other
  5. Cancel the electrons to get the final equation
- (A) $Fe^{3+} + e^- \rightarrow Fe^{2+}$, (B) $Zn \rightarrow Zn^{2+} + 2e^-$
  1. Done
  2. We need to multiple A by 2
  3. (A) $2Fe^{3+} + 2e^- \rightarrow 2Fe^{2+}$
  4. $2Fe^{3+} + 2e^- + Zn \rightarrow 2Fe^{2+} + Zn^{2+} + 2e^-$
  5. $2Fe^{3+} + Zn \rightarrow 2Fe^{2+} + Zn^{2+}$

Group 2 – Sulphates

- Solubility **decreases** as you go down
- Barium Sulphate
  - Barium Sulphate is very insoluble in water (as it's at the bottom of gp. 2)
  - It is also opaque to X-rays and so can be used as a contrast medium in scans of the digestive system
  - Is also used in rat poison
    - $BaCO_3(s) + 2HCl(aq) \rightarrow BaCl_2(aq) + H_2O(l) + CO_2(g)$

- Testing for sulphates
  - Because Barium Sulphate is insoluble it has become the basis for a laboratory test
  - If an unknown solution contains sulphate ions then when its added to Barium Chloride/Nitrate, a white precipitate forms
    - $BaCl_2(aq) + Na_2SO_4(aq) \rightarrow BaSO_4(s) + 2NaCl(aq)$
  - This can be simplified to the ionic equation:
    - $Ba^{2+}(aq) + SO_4^{2-}(aq) \rightarrow BaSO_4(aq)$
  - We must first acidify the test sample with Hydrochloric acid or Nitric Acid
    - This is to prevent the false detection of sulphite

Metal Extraction – Acid Mine Drainage

- Acid Mine Drainage
  - Pumps are needed to stop underground mines from flooding
  - When the mine is used and finished with the pumps are taken away
  - The mine floods, oxidising sulphides to H_2SO_4 which dissolves potentially toxic metals, e.g. iron
  - This produces Fe^{2+} and Fe^{3+} which ruins rivers and coats fish gills
  - It can be stopped with:
    - Calcium Carbonate – to neutralise the acid
    - Reed beds – to reduce the H_2SO_4 to **Hydrogen Sulphide** (with its bacteria)
  - This reacts with the metals ions to form **insoluble sulphide** minerals again

Haloalkanes – The Ozone Layer

- Ozone, O_3 is an allotrope of Carbon
- Reactions in the Ozone Layer
  - With UV light: $O_2 \rightarrow \bullet O \bullet + \bullet O \bullet$
  - They can react with oxygen: $\bullet O \bullet + O_2 \rightarrow O_3$
  - Ozone can dissociate with UV: $O_3 \rightarrow O_2 + \bullet O \bullet$
  - (Decomposition = Production) of Ozone
- CFC's and the Ozone Layer
  - Each chlorine molecule can decompose 1000's
  - $CCl_3F \rightarrow \bullet CCl_2F + \bullet Cl$
  - $\bullet Cl + O_3 \rightarrow ClO\bullet + O_2$
  - $ClO\bullet + O_3 \rightarrow 2O_2 + \bullet Cl$
- Repairing the Ozone Layer
  - Nitrogen Monoxide catalyses Ozone Decomp.
    - $NO + O_3 \rightarrow: NO_2 + O_2$
    - $NO_2 + O \rightarrow NO + O_2$
  - CFC's have been banned as of 1987 in most countries
  - Alternatives
    - Hydrochlorofluorocarbons (HCFC's)
    - Hydrofluorocarbons are chlorine free

Haloalkanes – OH- with Bromoethane

- OH- with Bromoethane (Substitution):

Haloalkanes – CN- with Bromoethane

- CN- with Bromoethane (Substitution):

Alkenes – Haloalkanes from Alkenes

- Electrophiles
  - Accept pairs of electrons
  - Positively charged ions (e.g. H+)
  - Atoms that have a partial positive charge (attached to a largely electronegative atom)
- Electrophilic Addition Reactions
  - Hydrogen Bromide (HBr)
    - $CH_2{=}CH_2 + HBr \rightarrow CH_3CH_2Br$
  - Bromine (Br_2)
    - $CH_2{=}CH_2 + Br_2 \rightarrow BrCH_3CHBr$
  - Sulphuric Acid
    - $CH_2{=}CH_2 + H_2SO_4 \rightarrow CH_3CH_2OSO_3H$
- (see mechanisms)

Alcohols – Oxidising Alcohols

- Primary Alcohols
  - Primary Alcohols → *Oxi.* → Aldehydes
    - Ethanol → Ethanal
    - $CH_3CH_2OH + [O] \rightarrow CH_3CHO + H_2O$
  - If the Acidified Potassium Dichromate is in excess then it further oxidises to Carboxylic Acid
    - Ethanal → Ethanoic Acid
    - $CH_3CHO + [O] \rightarrow CH_3COOH + H_2O$
  - We prevent further oxidation by distilling the aldehyde as the reaction proceeds (removing the aldehyde from the oxidising agent)
- Secondary Alcohols
  - Secondary Alcohols → *Oxi.* → Ketones
    - Propan-2-ol → Propanone
    - $CH_3CH(OH)CH_3 + [O] \rightarrow CH_3COCH_3 + H_2O$
- Tertiary Alcohols
  - Tertiary Alcohols → *Oxi.* → No change
  - It can't oxidise because the R group has no Hydrogen and Oxygen to be taken, only Oxygen

Alcohols – Distinguishing the Three Types of Alcohols

Alcohol	Acidified Potassium Dichromate (VI)	Product of Reaction with APD(VI)	Result of testing Product with:	
Primary	Orange → Green	Aldehyde	Silver Mirror Forms	Brick-Red Ppt
Secondary	Orange → Green	Ketone	No Change	No Change
Tertiary	No Change	None	No Change	No Change

Analytical Techniques – Using Infrared Spectroscopy

- Identifying Functional Groups

- Alkanes
  - C-H bonds
  - C-C bonds
- Alkenes
  - C-H bonds
  - C-C bonds
  - C=C bonds
- Carboxylic Acids
  - C=O
  - O-H
- Aldehyde
  - C=O
- Impurities
  - Can be identified due to absorption bands that should not be there

Bond	Wavenumber (cm-1)
C-H	2850 – 3300
C-C	750 – 1100
C=C	1620 – 1680
C=O	1680 – 1750
C-O	1000 – 1300
O-H (alco)	3230 – 3550
O-H (acid)	2500 - 3000

- Ethers
  - C-O
- Alcohols
  - O-H bonds
  - H bonds cause the trough to be deep and wide