Atomic masses -

Atomic masses are measured using the unified atomic mass unit, u. 1u has a mass of 1.66 x 10⁻²⁷ kg. The mass of a carbon-12 atom is 12u, therefore the mass of 1/12th of a carbon-12 atom is 1u.

Relative isotopic mass -

The mass of an atom of an isotope compared with 1/12th of the mass of an atom of carbon-12.

Relative atomic mass (Ar) -

The weighted mean mass of an atom of an element compared with 1/12th the mass of an atom of carbon-12.

Weighted mean mass is calculated by \sum isotopic masses x percentage abundance 100

Relative molecular mass (Mr) -

The sum of the relative atomic masses of elements in a simple compound (i.e. a molecule). The mass of a molecule is compared to the mass of an atom of carbon-12.

Relative formula mass -

The sum of the relative atomic masses of elements in one formula unit, so is used for giant le.co.uk structures (e.g. ionic compounds, macromolecules)

Mass spectrometry -

A technique used to identify isotopes present in an element one y-axis of a mass spectra shows relative/percentage abundance and the kails shows m/z (mass/charge of ion)

ratio. z is usually 1 for the ion. Relative atomic mass can be determined from the operation by calculating the sum of the relative isotopic mast Cby its abundance and dividing this sum by the sum of the abundances

Formulas of ionic compounds -

lons are formed when electrons are transferred from the outer electron shell of an atom. Elements in the same group react similarly.

[NB: Nobel gases are inert because they have a stable structure]

Atoms of metals (groups 1-13) form positive ions by losing electrons to form the same structure as the previous noble gases in the periodic table.

Atoms of non-metals (groups 15-17) form negative ions by gaining electrons to form the same electron configuration as the next noble gas in the periodic table.

B, Be, C and Si don't usually form ions because it would require too much energy.

Oxidation numbers (written as Roman Numerals) show which ion has been formed when an element can form more than one ion.

e.g. Fe(II): Fe²⁺

Fe(III): Fe³⁺

[NB: number before charge]

Molecular ions -

Molecular ions are groups of covalently bonded ions that have transferred electrons, so have an overall charge.

Key ions include:

 Nitrate - NO3⁻ The dot formula can be found by heating a hydrated salt until its anhydrous and finding the moles of water molecules lost. The ratio of moles of anhydrous salt to water molecules lost is then found. An anhydrous salt doesn't contain water of crystallisation.

When calculating the ratio of water of crystallisation to salt, the following assumptions are made:

- All the water has been lost once the mass of the salt remains constant following continual heating
- No further decomposition of the salt has taken place under heat

Titrations -

Titrations refer to using a known concentration of one solution to find the concentration. purity, molar mass or formula of another solution.

- 1. Use a pipette to add a measured volume of solution (unknown concentration) to a conical flask. Add the other solution to the burette and measure the initial starting point to the nearest 0.05cm³
- 2. Add a suitable indicator
- 3. Add the solution in the burette until the reaction has just completed and the end point is reached. Measure the volume used
- 4. Carry out an accurate titration where solution is added 2cm³ before the end point then added drop by drop
- 5. Repeat until two concordant (agreeing within 0.10cm³) results are achieved and calculate the moles of each reactant used [NB: when calculating the number of moles to neutralise an acid, the number must be doubled if the acid is diprotic]

Indicators -Oxidation numbers -Oxidation numbers tell you the number of electron an element has donated/accepted to form an ions or part of a compound -Traderic accepted by form an ions or part of a compound. They are shown by Frence Numerals when an element has compounds/ions with different oxidative states.

[NB: they are written as charge then number] Oxidation rules -

- 1. Uncombined elements have an oxidation number of 0
- 2. Combined oxygen has an oxidation number of -2
- 3. Combined oxygen in peroxides has an oxidation number of -1
- 4. Combined hydrogen has an oxidation number of +1
- 5. Combined hydrogen in hydrides has an oxidation number of -1
- 6. Simple ions have the same oxidation number as their charge
- 7. Combined fluorine has an oxidation number of -1
- 8. Oxygen has an oxidation number of +2 when combined with fluorine
- 9. Compounds have an oxidation number of 0
- 10. Molecular ions have the same oxidation number as their charge

Oxyanions -

Oxyanions are negative ions containing oxygen. As with transition elements, an element may form oxyanions where is has different oxidation numbers.

e.g. NO₂ \rightarrow Nitrate (III) \rightarrow N: +3

 $NO_{3^{-}} \rightarrow Nitrate (V) \rightarrow N: +5$

Redox reactions -

Redox reactions occur when both a reduction and oxidation reaction happen simultaneously. An oxidising agent is reduced (gains an electron) and a reducing agent is oxidised (losses electrons). Reduction leads to a decrease in oxidation number, whereas oxidation leads to an increase in oxidation number. Metals generally lose electrons and non-metals tend to gain electrons. In the reaction of metals and dilute acids, the metal is oxidised and the hydrogen is reduced.

Electronic structure -

Electrons orbit the nucleus in fixed energy shells. A shell is a group of atomic orbitals with the same principal quantum number, n.

The larger the value of n, the further the energy level is from the nucleus and the higher the energy level. When electrons move energy levels they emit or absorb radiation. Energy levels are divided into sub-shells, each of which contains a different number of orbitals. An orbital is a region of space where electrons may be found. Each orbital can hold two electrons. Orbitals within the same sub-shell have the same energy. An orbital with two electrons exhibits spin-pairing, because both electrons have a negative charge and repel.



Sub-shell notation -

This involves writing all of the electrons present in an atom. Electron energy level diagrams show the different energy levels of sub-shells within a shell. e.g. Vanadium (Z=23)

Rules for drawing electron energy level diagrams -

- 1. Electrons fill lower energy sub-shells first [NB: 3d has a higher energy level than 4s]
- 2. Electrons fill the same energy level singly before they pair
- 3. Paired electrons have opposite spins; the arrows are written so that they face opposite directions

lonic bonding -

lonic bonding describes strong electrostatic attraction between oppositely charged ions. It occurs between metals and non-metals; the metal transfers electrons to become a positive ion and the non-metal is reduced to a negative ion.



and difficult to control due to the reactivity of the intermediates formed, therefore creating a mix of products which need to later be separated (e.g. by fractional distillation or chromatography)

Alkenes -

Alkenes are unsaturated hydrocarbons containing a carbon-carbon double bond. As with alkenes, the bonding between carbons and hydrogens involves single covalent sigma bonds. However, the carbon-carbon double bond is made up of a sigma bond and a pi bond, which involves the sideways overlap of adjacent carbons p-orbitals above and below the plane of the carbon atoms. The pi bond holds the atoms in position, thus restricting rotation and giving alkenes a planar, flat shape. The double bond has the same effect on shape as a single pair covalent bond in terms of electron repulsion, giving alkenes a trigonal planar shape.

The pi bond has a high election density, so is very reactive. This attracts electrophiles (species that are electron-pair acceptors, such as cations). Also, the pi bond has a low bond enthalpy, so is easily overcome.

Alkenes take part in electrophilic addition reactions;

- Hydrogenation to form alkanes at a temperature of 150 degrees Celsius and in the presence of a nickel catalyst
- Halogenation to form dihaloalkanes (e.g. bromine water, which decolourises in the presence of an alkene because the month the alkene) P
- Chis can form a mixture of Halogenation using hydrogen halides to form halogenetics products if the alkene is unsymmetrical. Then a product can be decided using Markownikoff's principle, where moteo the most ñ O stable carbonation (i.e. has the most alkyl groups attached, so a secondary carbocation rather than a primal Dark gradion for example, vil be formed Starting the
- Hydration using gaseous alkenes and steam at 300 degrees Celsius and 65 atmospheres in the presence of a phosphoric acid catalyst to form alcohols

Electrophilic addition reaction mechanism -

- 1) The high electron density of the pi bond attracts electrophiles, breaking the pi bond and causing heterolytic fission of the bond within the electrophiles molecule (if present)
- 2) This forms a positive carbonation intermediate, which is extremely reactive, and an anion
- The carbonation bonds to the negative ion that has been formed via heterolytic fission

Polymerisation -

Alkenes can also take part in addition polymerisation reactions. Polymers are macromolecules made from small repeating units of monomers. A repeating unit is a specific arrangement of atoms that occurs in a structure over and over again. During the reaction the pi bond is broken



monomer - any alkene



bonds to



and the electrons are used to form sigma bonds between adjacent monomer molecules. The repeating unit can be generated by drawing the carbon-carbon double bond with square brackets around it. The atoms surrounding the double bond can be deduced and added to the diagram using their structural formula.

Polymers are extremely stable and thus non-biodegradable in landfill sites. They are also made using non-renewable fossil fuels, decreasing their sustainability.

Polymer waste can be dealt with by combusting waste products for energy reusing them (e.g. as organic feedstock for the production of plastics and other organic chemicals) and recycling. When polymers are burnt however, they release toxic and acidic gases (e.g. HCl gas), which must be removed using basic gas scrubbers, such as calcium oxide

scrubbers. Recycling is a laborious process and only a degree of the polymers can be used again. Feedstock recycling is a mechanism that tries to combat this.

Bioplastics are biodegradable polymers that contain plant starch molecules.

Photodegradable polymers are also being produced, which are chemically broken down by the wavelengths of light. The bonds within the structure are weakened by the absorption of these wavelengths, initiating an irreversible degradation of the polymer.

Alcohols -

Alcohols form a homologous series that is saturated and has the general formula C_nH_{2n} +1OH. This makes them polar molecules that can dissolve in polar substances.

The position of the -OH functional groups determine the type of alcohol.

A primary alcohol has the alcohol group attached to an end of a chain.

A secondary alcohol has the alcohol group attached to a carbon attached to two alkyl groups.

A tertiary alcohol has the alcohol group attached to a carbon at check o three alkyl groups.

As the chain length of the alcohol increases to coes the boiling point, as there are stronger induced dipole-dipole interaction, between motec the OThe boiling point of alcohols are higher than that or corresponding a kan subcause there are also hydrogen bonds between the OC goods. For this passes they are also less volatile than corresponding a kan substance evaporates and increases when boiling point decreases.

As the chain length of an alcohol increases solubility decreases because the longer chains cannot form hydrogen bonds with the water molecules like the -OH functional groups can. The miscibility of the alcohol therefore declines.

Reactions of alcohols -

- Combustion

When alcohols undergo complete combustion they form carbon dioxide and water. They transfer stored chemical energy in their bonds into thermal energy

- Oxidation

Primary and secondary alcohols can be oxidised using the oxidising agent potassium dichromate and a strong acidic catalyst (e.g. dilute sulphuric acid).

Primary alcohols can be partially oxidised then distilled to form aldehydes under gentle heating. They can also be oxidised into carboxylic acids under reflux conditions, where the reagents are heated strongly with excess potassium dichromate and the product is not distilled immediately (as distillation prevents any further reaction from occurring); reflux is the constant boiling and condensing of a reaction mixture. Secondary alcohols can be oxidised to ketones under reflux. Tertiary alcohols cannot be oxidised. When an alcohol is oxidised, the potassium dichromate changes from organ to green. If there is no colour change the alcohol is tertiary.

transfer of protons. Conjugate acid-base pairs are two species related to each other by the loss or gain of a proton (i.e. they only have a H ion difference).

Models for acids and bases over time:

- 1778; Lavoisier
 Proposed that oxygen was the source of acidity, because it was important in rusting
- 1815; Davy
 - Showed some acidic substances (e.g. HCl) did not contain oxygen
- 1832; Leibig
- Defined an acid as a substance containing hydrogen that could be replaced by a metal 1880s; Arrhenius

Proposed acids dissociated in water to for hydrogen ions and bases dissociated to for hydroxide ions. This is the definition for Arrhenius acids and bases, but cannot be used for non-aqueous solutions and non-soluble bases

- 1916; Lewis
 Described a (Lewis) acid as an electron-pair acceptor and a (Lewis) base as an electron-pair donor
- 1929; Bronsted-Lowry

Proposed that acids were proton donors and bases were proton acceptors. It still cannot be used for some solvents

A monobasic acid is an acid that releases one proton. A dibasic acid can release two protons at different stages and a tribasic acid can release three protons at different stages. A strong acid full dissociates in solution, where as a weak acid partially in sociates in solution. Strong acids include hydrochloric acid, nitric acid, suppletic acid, hydrobromic

acid, hydroiodic acid and chloric(VII) acid. When acids release protons in water, they are to be by water for form the bydronium/eventile form.

by water for form the hydronium/oxenium on. This involves a dative covalent bond between the proton in a water molecule, giving the overall ion a positive charge. An alkalitis a warel soluble bare that is eases hydroxide ions.

Neutralisation is the chemical reaction in which an acid and base react to produce a salt and water.



Types of neutralisation reactions:

- Acids and carbonates to form salt, carbon dioxide and water
- Acids and bases to form salt and water
- Aqueous acids and alkalis to form salt and water

When an acid reacts with a metal, a redox reaction occurs to form salt and hydrogen.

The acid dissociation constant -

The acid dissociation constant (Ka) can be used to measure the extent to which an acid dissociates.

$$HA(aq) \Longrightarrow H^+(aq) + A^-(aq)$$

$$K_a = \frac{[H^+(aq)] [A^-(aq)]}{[HA(aq)]}$$

A large Ka value indicates a large extent of dissociation, suggesting the acid is strong. A small Ka value indicates little dissociation,

 $pK_a = -\log_{10} K_a$ $K_a = 10^{-pK_a}$



The human blood contains buffers where carbonic acid is the weak acid and the hydrogen carbonate ion acts as the conjugate base in order to maintain blood pH between 7.2 and 7.6.

Excess carbonic acid are removed by being converted into aqueous carbon dioxide by enzymes and then expelled via expiration.

Redox titrations -



When the arc equal amount of the yeak acid and conjugate base, the indicator is at its end point. The colour at the end point is midway between the colours of the weak acid and conjugate base.

An indicator that has an end point which is as close to the pH of the equivalence point of an acid-base titration can be used for said titration.

points.

More exothermic lattice association enthalpy values mean there are stronger ionic bonds within the ionic substance, so more energy is needed to overcome these bonds and the melting/boiling point are higher.

The smaller the radius of the ion, the greater the ionic bond strength and the larger the charge of ions, the greater the magnitude of the lattice enthalpy. Smaller ions with a smaller radius can align more closely together, increasing their charge density and thus

the attraction between them. lons with larger charges also have greater attraction. Overall this increases the electrostatic attraction and ionic bond strength, making the lattice enthalpy more exothermic.

Likewise, with enthalpy changes of hydration, smaller ions with larger charges can interact more with the water molecules, so the enthalpy change of hydration is more exothermic. If the sum of the hydration



enthalpies is larger than the magnitude of the attic enthalpy, the overall enthalpy change will be exothermic and the substance should dissolve. This is not always the calc due to

Entropy -Entropy, S - A quantitative measure of the days of the system; the more disordered the system, the higher the fit hopy System - The actual particles involved in a reaction/process Surroundings - The to Pamer in which the system takes place Standard And The entrop of the of one mole of a substance under standard condition. Above 0K entropy is always a positive number because they are thermodynamic and in constant motion. At 0K, perfect crystals have no entropy. The total entropy of a reaction is the sum of the entropy of the system and the surroundings Standard entropy change of reaction - The entropy change that accompanies a reaction in the molar quantities expressed in a chemical equation under standard conditions, all reactants and products being in their standard states. There is a higher tendency for entropy to increase (second law of thermodynamics), but entropy can decrease (e.g. during freezing). It is measured by the sum of the entropy of the products minus the sum of the entropy of the reactants

Free energy change - The balance between enthalpy, entropy and temperature for a process; it is equal to the enthalpy change minus the product of temperature and entropy change. A process can only take place spontaneously if the free energy change is less than zero

Entropy (per K) of pure substances increases with an increase in temperature, because particles have higher energy and therefore more kinetic energy. Their arrangement thus becomes more random. Solids have the lowest entropy, then liquids and finally gases. Examples of entropy increasing include water evaporating to water vapour and ionic substances dissolving in water.

When a reaction leads to an increase in gas molecules, there is an increase in entropy. If it leads to a decrease in gas molecules, there is a decrease in entropy. In short, if the



Phenols -

Phenols are a class of aromatic compounds where a hydroxyl group is directly attached to the aromatic ring. Phenol is the first member of the group. An aromatic ring attached to an alkyl chain attached to a hydroxyl group is an aromatic alcohol.

Phenol is a weak acid, as it partially dissociates in water. It reacts with strong bases to form salt and water. It does not react with carbonates and weak bases.

Phenol is more reactive than benzene as the nonbonding pair of p-orbital electrons from the oxygen of the hydroxyl group donate electrons into the ring of delocalised electrons. This increases the electron density of the aromatic ring, making it more susceptible to electrophilic attack as it can induce dipoles in non-polar molecules more easily. As a result, phenols can undergo direct halogenation.

$C_6H_5OH + H_2O \implies H_3O^+ + C_6H_5O^-$

 $C_6H_5OH + NaOH \rightarrow C_6H_5O^-Na^+ + H_2O$

Phenol will undergo a triple substitution with bromine $\mathbf{D} \in \mathbf{C}^{\mathbf{O}}$ room temperature, resulting in a white precipitate of 2.4.6-tribromonbane in a white precipitate of 2,4,6-tribromophend

However, phenol only undergoes a eingle substitution with the nitric acid at room temperature, to form a mixture of 2 mitrophenol and entrophenol. Unlike nitration with benzene, this does no require a $L_5OH + 3Br_2 \rightarrow C_6H_2Br_3OH + 3HBr_3OH$ concentration and catalyst. If concentrated nitric acid is $C_6H_5OH + HNO_3 \rightarrow C_6H_4(NO_2)OH + H_2O$

used 2,4,6-trinitrophenol is formed.

In phenol, the additional electrons from the oxygen into the pi-electron system make the reactions occur on the 2 and 4 positions of the aromatic ring. This is known as the directing effect; how a functional group attached directly to the aromatic ring affects which carbon atoms are more likely to undergo substitution. Other electron-donating groups such as amine groups also have 2- and 4-directing effects. As a result they 'activate' the benzene ring. Electron withdrawing groups such as nitro groups have a 3-directing effect. They 'deactivate' the benzene ring by making it less susceptible to electrophilic attack. This is important as it can be used to create a

reaction pathway that maximises the yield of a desired product.

2-and 4-directing (<i>ortho</i> -and- <i>para</i> directing)	3-directing (<i>meta</i> directing)
-NH ₂ or -NHR	RCOR
-0H	-C00R
-0R	-S0 ₃ H
$-R \text{ or } -C_6H_5$	-CHO
−F, −CI, −Br, −I	-COOH
	-CN
	-N0 ₂
	-NR3+

Carbonyls -

A carbonyl functional contains a carbon to oxygen double bond; this includes the functional groups aldehydes (-CHO) and ketones (-CO).

Aldehydes undergo oxidation using potassium dichromate and sulfuric acid under reflux to form carboxylic acids.

A nucelophile is a species attracted to an



electron-deficient part of a molecule, where it donates a pair of electrons to make a new covalent bond. Carbonyls have a dipole in the carbon to oxygen double bond, making them susceptible to nucleophilic attack on the delta positive carbon atom. This breaks the pi-bond to form a reactive intermediate, followed by a nucleophilic addition reaction.



<u>Esters -</u>

Esters contain the functional group R-COO-R'. They are carboxylic acid derivatives, where the H has been replaced by an alkyl chain. The first part of the name is the alkyl chain bonded to one oxygen and the second is the alkyl chain containing the carbon to oxygen double bond, followed by the suffix -oate (e.g. methyl ethanoate).



Esterification can occur by;

 Reacting a carboxylic acid with an alcohol by heating gently in the presence of a sulphuric acid catalyst. It is a slow, reversible reaction. The ester can be separated quickly using distillation to prevent the reverse reaction from occurring. Larger esters can be made under reflux until equilibrium is achieved, then removed using fractional distillation.



Esters can also be hydrolysed. Depending on the acidity of the conditions in which hydrolysis (breaking down by adding water) takes place, the products vary.

