

UNIT 1: THEORETICAL CHEMISTRY

Recommended Prior Knowledge: A reasonable standard at IGCSE Science or Chemistry is assumed for this unit.

Context: This unit underpins all succeeding units, so needs to be studied first.

Outline: The unit covers most of the calculations needed for AS (and A2) chemistry, involving the mole and empirical formulae. It also includes atomic structure, bonding, intermolecular forces, and the behaviour of gases.

AO	Learning Outcomes	Suggested Teaching Activities	Learning Resources
1(a) 1(b)	Define the terms <i>relative atomic</i> , <i>isotopic</i> , <i>molecular</i> and <i>formula masses</i> , based on the ^{12}C scale Define the term <i>mole</i> in terms of the Avogadro constant	Definitions of the mole (= an Avogadro number of particles), and molar mass (= the mass of 1 mole of substance). Definition of Avogadro number (L = number of atoms in 12.0g of ^{12}C) Definitions of relative atomic mass (A_r) , isotopic mass , molecular and formula masses (M_r) in terms of 1/12 the mass of 1 mole of ^{12}C atoms.[for isotopes see section 2(e)] Some revision of IGCSE ideas of the mole. Simple determinations of L in the lab could include the oil-drop expt. (If we make assumptions about the density and the M_r of the oil, and the shape of its molecule (cubic), we can calculate the volume of 1 mole, and the volume of 1 molecule. Hence we can calculate L .) A more accurate estimate of L comes from electro-deposition of copper during electrolysis of $\text{CuSO}_4(\text{aq})$, making assumptions about valency and M_r of Cu, and the charge on the electron.	C+H 1.1-1.7 M 37 R+N 2.1, 2.6 site 3 (Avogadro) site 6 (atomic, molecular mass) site 7 (what is a mole?)
1(c) 1(d)	Analyse mass spectra in terms of isotopic abundances [knowledge of the working of the mass spectrometer is not required]. Calculate the relative atomic mass of an element given the relative abundances of its isotopes, or its mass spectrum	Knowledge that a mass spectrum plots relative abundance against mass number. Translating a table of relative abundances and mass numbers into a plotted mass spectrum, and vice versa. Measuring peak heights from a given mass spectrum, and calculating the relative atomic mass from the weighted mean of the peaks [$A_r = \sum a_i m_i$ where a_i = the fractional abundance of isotope of mass m_i] Searching databases and periodic table tabulations will provide a host of examples of elements having several isotopes. Calculating their relative atomic masses is a useful exercise. Whilst the working of the mass spectrometer is not required by the syllabus, the principle of using a magnetic field to separate a beam of ions having a unit positive charge according to their masses could be mentioned. Emphasise also the importance of significant figures in the results of calculations.	C+H 2.5 M 29 R+N 2.2, 2.3, 2.4, 2.5
1(e) 1(f)	Define the terms <i>empirical</i> and <i>molecular formulae</i> . Calculate empirical and molecular formulae, using combustion data or composition by mass	Definitions of empirical (= simplest whole number mole ratio) and molecular (= actual number of atoms of each element in a molecule) formulae. Calculation of empirical formulae using mass data, percentage data or combustion data. Calculation of molecular formula from empirical formula and relative molecular mass. Class sets of experimental data (e.g. on the heating of Mg in air), or sheets showing a series of results, could be analysed using computer spreadsheets or by a graphical method.	C+H 1.8 M 37 R+N 2.7, 2.8 P(AS) 4

		Various worksheets containing suitable data for simple compounds such as Fe_2O_3 and other oxides, CaCO_3 and other salts, C_2H_6 and other hydrocarbons (mass, % and combustion data), $\text{CH}_3\text{CO}_2\text{H}$ etc Experimental work could include the combustion of Mg in a weighed crucible; passing $\text{H}_2(\text{g})$ or $\text{CH}_4(\text{g})$ over heated CuO; heating $\text{BaCl}_2 \cdot n\text{H}_2\text{O}$ crystals to find n.	
1(g)	Write and/or construct balanced equations	Revise the valencies of ions from IGCSE. Revise the four state symbols. Provide a sheet of essential formulae to learn (e.g. simple covalent compounds, common salts, acids and alkalis). Students should practice both balancing equations where the formulae are given, and also constructing balanced chemical equation, given the word equation.	C+H 1.9 R+N 2.9 site 9 (equations, redox)
1(h)	Perform calculations, including use of the mole concept, involving: (i) reacting masses (from formulae and equations) (ii) volumes of gases (e.g. in the burning of hydrocarbons) (iii) volumes and concentrations of solutions	Use of the equations moles = mass/ M_r or =mass/ A_r moles = gas vol (cm^3)/24000 moles = vol of soln x concentration These equations are used across the syllabus, but initial experiments and/or calculations could include the following: Acid-base and redox titrations etc. e.g. • calculate n in $\text{Na}_2\text{CO}_3 \cdot n\text{H}_2\text{O}$; • $[\text{CH}_3\text{CO}_2\text{H}]$ in vinegar; • % CaCO_3 in limestone (back titration with HCl & NaOH); • % Fe^{2+} in iron pills (& investigation of $\text{Fe}^{2+}/\text{MnO}_4^-$ ratio)	C+H 1.10-1.13 M 39, 40 R+N 2.10 P(AS) 2, 3 site 3 (calculations)
1(i)	Deduce stoichiometric relationships from calculations such as those in (h)		
2(a)	Identify and describe protons, neutrons and electrons in terms of their relative charges and relative masses	Revise IGCSE ideas of the atom. The relative charges (+1, -1, 0) and masses (1, $\frac{1}{1860}$, 1) of the proton, the electron and the neutron. The relationship between proton number, neutron number, atomic number and mass number. The representation of at. no. and mass no. e.g. $^{14}_6\text{C}$.	C+H 2.1-2.2 M 3 R+N 1.1 site 8 (atomic structure)
2(b)	Deduce the behaviour of beams of protons, neutrons and electrons in electric fields	The key points are that neutrons are undeflected; protons are attracted to the negative plate; electrons are attracted to the positive plate, through a much larger angle than protons, due to their much smaller mass.	C+H 2.2 M 3 R+N 1.1
2(c)	Describe the distribution of mass and charges within an atom	The relative sizes of the nucleus and the whole atom. The analogy of a pea in a football stadium (similar analogies could be thought up by students, given the data). Protons and neutrons reside within the nucleus, and electrons are in "orbitals" around the outside.	C+H 2.1 M 3 R+N 1.2
2(d)	Deduce the numbers of protons, neutrons and electrons present in both atoms and ions given proton and nucleon numbers (and charge)	The representation of at. no. and mass no. e.g. $^{14}_6\text{C}$. The appreciation that in ions, the atomic number (and hence the element's symbol) is determined by the number of protons, not the number of electrons. Practice in deducing the numbers of p^+ , e^- and n in an atom or ion given its charge, mass no. etc.	C+H 2.4 M 3 R+N 1.4 site 7 (N-ch1-02)
2(e)	Describe the contribution of protons and neutrons to atomic nuclei in terms of proton number and nucleon number Distinguish between isotopes on the basis of different numbers of neutrons present	Isotopes of the same element differ in both their mass numbers and the number of neutrons present, but they have the same atomic number and contain the same number of protons. Practice in the conversion from the symbol to the atomic structure and vice versa (e.g. ^{31}P has 15 p^+ , 15 e^- , 16 n; the symbol for the species having 16 p^+ , 18 e^- and 17 n is $^{33}\text{S}^{2-}$)	C+H 2.3 M 3 R+N 1.3, 1.6
2(f)	Describe the number and relative energies of the s, p and d orbitals for the	Distinguish between shells (containing a maximum of 2, 8, 18 etc electrons), subshells (s, p, d, containing a maximum of 2, 6, 10 electrons), and orbitals	C+H 2.8 M 12

	principal quantum numbers 1, 2 and 3 and also the 4s and 4p orbitals.	(containing a maximum of 2 electrons each). The number of subshells increases by 1 for each successive shell. The number of orbitals in each subshell is fixed as s=1; p=3; d=5 etc. Within each shell the relative energies are $d > p > s$. The 4s become lower in energy than the 3d from element number 20.	R+N 1.11 site 4 (atomic structure) site 15
2(g)	Describe the shapes of s and p orbitals	Spherical and dumb-bell shaped. the three p orbitals are at right angles to each other.	C+H 2.9 M 11 R+N 1.10
2(h)	State the electronic configuration of atoms and ions given the proton number (and charge)	The aufbau principle. There are various mnemonics for remembering the order in which the orbitals are filled. Use the convention $1s^2 2s^2 2p^3$ etc (for simple atoms this could be extended to include $2p_x^2 2p_y^1$)	C+H 2.13 M 12 R+N 1.12
2(i)	Explain and use the term <i>ionisation energy</i> Explain the factors influencing the ionisation energies of elements Explain the trends in ionisation energies across a period and down a group of the Periodic Table (see also Section 9)	Define I.E. in terms of the energy required to remove 1 mol of electrons from 1 mol of gaseous atoms/ions. Factors include proton number; shielding by inner shells (hence the effective nuclear charge is less than the proton number); distance of outermost electron from the nucleus. I.E. increases across a period and decreases down a group. Slight decreases: from Gp II to Gp III due to p subshell experiencing more shielding than s subshell; and from Gp V to Gp VI due to repulsion between electrons sharing same orbital.	C+H 2.14 M 13 R+N 1.7, 1.8 site 7 (N-ch1-05, 06, 07)
2(j)	Deduce the electronic configurations of elements from successive ionisation energy data.	The jumps in ionisation energies as inner shells begin to be ionised show up better if $\log_{10}(IE)$ is plotted against no. of electrons removed.	C+H 2.14 M 13 R+N 1.9
2(k)	Interpret successive ionisation energy data of an element in terms of the position of that element within the Periodic Table	These data can be plotted using a spreadsheet. Differences in successive ionisation energies should be calculated, and the position of the first large difference noted	
3(a)	Describe ionic (electrovalent) bonding, as in sodium chloride and magnesium oxide, including the use of 'dot-and-cross' diagrams.	Emphasise the electrostatic attraction between two oppositely charged ions; the giant nature of ionic structures (e.g. the cubic lattice of NaCl and MgO). Unless otherwise stated, outer shells only need to be drawn. Usually only the electrons on the product ions need to be shown, but the use of dots and crosses to show which electrons have been transferred from metal to non-metal is recommended. Resultant charges on the ions should be shown. Other examples could include LiF, Li ₂ O, MgF ₂	C+H 4.6-4.8 M 18 R+N 3.1 site 4 (bonding and structure)
3(b)	Describe, including the use of 'dot-and-cross' diagrams, (i) covalent bonding, as in hydrogen; oxygen; chlorine; hydrogen chloride; carbon dioxide; methane; ethene (ii) co-ordinate (dative covalent) bonding, as in the formation of the ammonium ion and in the Al ₂ Cl ₆ molecule.	Dot-and-cross structures for the molecules mentioned (outer shells only). Emphasise that bonds are stable entities, so give out heat when they form. This stability is due to attraction of the bonding electrons to two nuclei rather than just one. The use of two dots (or two crosses) in a dative bond will show which is the donor atom. In "line = bond" diagrams dative bonds can be shown either as a bond with an arrow (e.g. Cl→Al, or (preferably) as a line with charges shown (e.g. Cl ⁺ —Al ⁻). This latter will show that all 4 N-H bonds in NH ₄ ⁺ are equivalent.	C+H 3.2-3.8 M 14 R+N 3.3, 3.4
3(c)	Explain the shapes of, and bond angles in, molecules by using the qualitative model of electron-pair repulsion (including lone pairs), using as simple examples: BF ₃ (trigonal); CO ₂ (linear); CH ₄ (tetrahedral); NH ₃ (pyramidal); H ₂ O (non-	Describe the principles of VSEPR. The bond angle trend in CH ₄ , NH ₃ and H ₂ O ($109\frac{1}{2}^\circ$, 107° , $104\frac{1}{2}^\circ$) should be explained (lone pair repulsion > bond pair repulsion) and learned. The hands-on use of molecular models will help students understand the 3-D shapes of molecules.	C+H 3.9 M 17 R+N 3.8 site 2 (VSEPR) site 7 (N-ch1-15) site 14 (animated molecules)

	linear); SF ₆ (octahedral)		
3(d)	Describe covalent bonding in terms of orbital overlap, giving σ and π bonds	σ bonds are formed by the overlap of an s orbital with another s orbital (e.g. in H ₂); overlap of an s orbital with a p orbital (e.g. CH ₄ – there is no need to introduce the idea of hybridisation); or end-on overlap of two p-type orbitals (e.g. F ₂ or C ₂ H ₆). π bonds are formed by the sideways overlap of two p orbitals (e.g. C ₂ H ₄). Explain that this results in restricted rotation around the C=C bond.	C+H 3.13 M 15 site 14 (double bond formation) site 4 (bonding and structure)
3(e)	Explain the shape of, and bond angles in, the ethane and ethene molecules in terms of σ and π bonds (see also Section 10.1)	Assume all bond angles are 109½° in ethane and 120° in ethene. The bonding in ethene considered as a planar framework of five σ bonds, on which is superimposed a π bond. See also 10.1(d).	C+H 3.13, 22.3
3(f)	Predict the shapes of, and bond angles in, molecules analogous to those specified in (c) and (e)	For example, AlCl ₃ , CH ₂ O, SiCl ₄ , PCl ₃ , C ₂ Cl ₄ . Further examples could include BeF ₂ , SF ₂ , SO ₃ , HOCl, and, for the advanced student, ClF ₃ , ClF ₅ and XeF ₄ .	site 7 (N-ch1-14)
3(g)	Describe hydrogen bonding, using ammonia and water as simple examples of molecules containing N-H and O-H groups.	Represent the hydrogen bond as a dotted line. Include the lone pair and the partial charges on diagrams thus: O ^{δ-} ...H ^{δ+} — . Mention the lack of hydrogen bonding in HCl, H ₂ S etc	C+H 3.15 M 21 R+N 3.12, 3.13 site 7 (N-ch1-09)
3(h)	Explain the terms <i>bond energy</i> , <i>bond length</i> and <i>bond polarity</i> and use them to compare the reactivities of covalent bonds (see also 5b(ii))	Bond energy in terms of the breaking of 1 mole of bonds in the gas phase (i.e. the endothermic change); bond length as the distance between the centres of adjacent atoms; bond polarity in terms of differing electronegativities of the two bonded atoms. Reactivity is associated with weak or long bonds (e.g. F-F, or O-O in H ₂ O ₂ compared to C-C in ethane; C-I compared to C-Cl). See also 10.3(c) and (d).	C+H 3.10, 5.5 M 19, 42 R+N 3.7
3(i)	Describe intermolecular forces (van der Waals' forces), based on permanent and induced dipoles, as in CHCl ₃ (l); Br ₂ (l) and the liquid noble gases	Distinguish between polar bonds and polar molecules (e.g. the molecules of CO ₂ and CCl ₄ are not polar, although they contain polar bonds). Induced dipole forces are experienced by all molecules, and their strength depends on total number of electrons. The additional attraction of permanent dipoles is usually weaker. See also 9.4(b)	C+H 3.11, 3.13 M 20 R+N 3.10 site 3 (intermolecular forces)
3(j)	Describe metallic bonding in terms of a lattice of positive ions surrounded by mobile electrons.	Point out that the more outer-shell electrons, the more the electrons are delocalised and the stronger is the attraction (e.g. m.pt. Al > Mg > Na).	C+H 4.11 M 22 R+N 3.9
3(k)	Describe, interpret and/or predict the effect of different types of bonding (ionic bonding; covalent bonding; hydrogen bonding; other intermolecular interactions; metallic bonding) on the physical properties of substances	See also 4(e). Distinguish between giant structures (diamond, metals, salts) that have high melting points, and simple molecular structures (water, CO ₂ etc) that have low melting points. The increase of induced dipole forces (and hence the increased m.pt. and b.pt.) with no. of electrons. A plot of the trends in b.pt.s down Groups 4, 5, 6 and 7 against group number shows this, and also the effect of H-bonding in NH ₃ , H ₂ O and HF. The enhanced b. pts. and solubility in water of hydrogen-bonded compounds. The conductivity of metals and molten/dissolved salts.	C+H 4.4, 4.5, 4.10, 4.11, 4.12 R+N 3.14
3(l)	Deduce the type of bonding present from given information	See 3(k). Such information might be m.pt. or b.pt., solubilities, conductivities.	C+H 4.4, 4.5, 4.9 R+N 3.15
3(m)	Show understanding of chemical reactions in terms of energy transfers associated with the breaking and making	See 5(b). Bond-breaking being an endothermic process, and bond-making an exothermic process. Reactions that break weak bonds or make strong bonds are favoured.	C+H 5.1, 5.5 M 42

	of chemical bonds		
4(a)	State the basic assumptions of the kinetic theory as applied to an ideal gas	Molecules have zero volume (N.B., NOT mass); zero intermolecular forces; constant random motion; elastic collisions.	C+H 4.13-4.14 M 35 R+N 4.2 site 6 (behaviour of gases; Maxwell-Boltzmann)
4(b)	Explain qualitatively in terms of intermolecular forces and molecular size: (i) the conditions necessary for a gas to approach ideal behaviour (ii) the limitations of ideality at very high pressures and very low temperatures	At low pressure the molecules are far apart, so their volumes are negligible. At high temperatures molecules have sufficient excess kinetic energy to make intermolecular forces insignificant. Both the sizes of, and the interactions between, molecules become significant at high pressures and low temperatures.	C+H 4.14 M 34 R+N 4.3
4(c)	State and use the general gas equation $pV = nRT$ in calculations, including the determination of M_r	$M_r = mRT/pV$ [m in grams; T in Kelvins; p in Pascals and V in m ³] Experiments weighing known volumes of gases in gas syringes (the use of a gently heated oven extends this to volatile liquids) can be used here. Plugging results into a spreadsheet allows the effects of experimental error to be seen clearly.	C+H 4.13 M 34 R+N 4.4 P(AS) 5, 6
4(d)	Describe, using a kinetic-molecular model, the liquid state; melting; vaporisation and vapour pressure.	The random nature of molecular movement in liquids, despite molecules touching each other. The dynamic equilibria between solid-liquid and liquid-gas. Vapour pressure as the result of molecules colliding with the sides of the vessel.	C+H 4.1 M 23 R+N 4.1
4(e)	describe, in simple terms, the lattice structure of a crystalline solid which is: (i) ionic, as in sodium chloride, magnesium oxide (ii) simple molecular, as in iodine (iii) giant molecular, as in graphite; diamond; silicon(IV) oxide (iv) hydrogen-bonded, as in ice (v) metallic, as in copper	The alternating oppositely charged ions in 3 dimensions in ionic solids allows a strong attraction between them. The continuous, 3-dimensional, tetrahedral, strongly-bonded covalent structures of diamond and silicon(IV) oxide also result in strong attractions and hence high m.pt. The layer nature of graphite (briefly mention the "2-dimensional metal" nature of the electron delocalisation within each layer being responsible for its electrical conductivity, but no detail is required, since delocalisation in benzene is not covered until A2). The close packing of metal atoms ("ions") in their sea of delocalised electrons. The regular zig-zag array of I ₂ molecules with weak induced dipole forces causes the m.pt. to be low. The directional hydrogen bonding in ice causes an open structure (hence less dense than water) with a comparatively high m.pt. The use of molecular model kits is helpful, as are some interactive cd-roms.	C+H 4.4, 4.5, 4.9, 4.11 M 18, 32 R+N 3.2, 3.11, 4.5 P(AS) 7
4(f)	Explain the strength, high melting point, electrical insulating properties of ceramics in terms of their giant molecular structure.	Localised electrons in the solid lattice causes insulating properties. Strong covalent or ionic bonds between the atoms/ions causes high strength (although some brittleness) and high m.pt.	C+H 4.5 R+N 4.7
4(g)	Relate the uses of ceramics, based on magnesium oxide, aluminium oxide and silicon(IV) oxide, to their properties (suitable examples include furnace linings; electrical insulators; glass; crockery)	Students could be encouraged to perform an internet search of materials used for furnace linings and electrical insulators.	
4(h)	Describe and interpret the uses of the metals aluminium, including its alloys, and copper, including brass, in terms of their physical properties	Relevant properties of aluminium are: low density (due to low A_r); high conductivity (Group III). For copper: high conductivity (lots of 3d and 4s electrons to delocalise); malleability and colour. Mention that the alloying with different metals usually	C+H 4.11, 19.2 M 22 R+N 4.8

		makes the metal harder, since the sliding of one layer of atoms over another is hampered by an atom of a different size. Internet searches on the uses of Al and Cu and their alloys, and discussion as to why these particular metals/alloys are used for these purposes.	
4(i)	Understand that materials are a finite resource and the importance of recycling processes	Examples are: metals such as Al, Cu, scrap steel; glass;, plastics. Recycling not only conserves material and energy resources, but also minimises pollution.	R+N 4.9
4(j)	Outline the importance of hydrogen bonding to the physical properties of substances, including ice and water	Apart from those mentioned in 4(e), others include high viscosity, high thermal capacity (specific heat), high surface tension.	C+H 3.15 M 21 R+N 3.13, 4.6
4(k)	Suggest from quoted physical data the type of structure and bonding present in a substance.	See also 3(l) above. Applications of the chemistry in sections 4(e). For example, BeCl_2 (simple covalent); GeO_2 (giant molecular); GaF_3 (ionic) – based on given m.pts. etc.	C+H 4.2 R+N 3.15, 4.10