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# HL CHEMISTRY YEAR 1

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Essential ideas, Understandings, and Applications/Skills



2015-2016

ACADEMY SCHOOL DISTRICT 20

## Year 1

### Semester 1: Essential Ideas

#### Chapter 1: Stoichiometric Relationships

##### 1.1: Physical and chemical properties depend on the way in which different atoms combine

###### Understandings:

1.1.a: Atoms of different elements combine in fixed ratios to form compounds, which have different properties from their component elements

1.1.b: Mixtures contain more than one element and/or compound that are not chemically bonded together so retain their individual properties

1.1.c: Mixtures are either homogeneous or heterogeneous

###### Applications/Skills:

1.1.i: Deduction of chemical equations when reactants and products are specified

1.1.ii: Application of the state symbols (s), (l), (g), and (aq) in equations

1.1.iii: Explanation of observable changes in physical properties and temperature during changes of state

##### 1.2: The mole makes it possible to correlate the number of particles with the mass that can be measured

###### U:

1.2.a: The mole is a fixed number of particles and refers to the amount, **n**, of substance

1.2.b: Masses of atoms are compared on a scale relative to  $^{12}\text{C}$  and are expressed as a relative atomic mass (**A<sub>r</sub>**) and relative formula/molecular mass (**M<sub>r</sub>**)

1.2.c: Molar mass (**M**) has the units  $\text{g mol}^{-1}$

1.2.d: The empirical and molecular formula of a compound give the simplest ratio and the actual number of atoms present in a molecule respectively

###### A/S:

1.2.i: Calculation of the molar masses of atoms, ions, molecules, formula units

1.2.ii: Solution of problems involving the relationship between the number of particles, the amount of substance in moles, and the mass in grams

1.2.iii: Interconversion of the percentage composition by mass and the empirical formula

1.2.iv: Determination of the molecular formula of a compound from its empirical and molecular mass

1.2.v: Obtaining and using experimental data for deriving empirical formulas from reactions involving mass changes

##### 1.3: Mole ratios in chemical equations can be used to calculate reacting ratios by mass and gas volume

###### U:

1.3.a: Reactants can be either limiting or excess

1.3.b: The experimental yield can be different from the theoretical yield

1.3.c: Avogadro's law enables the mole ratio of reacting gases to be determined from volumes of the gases

1.3.d: The molar volume of an ideal gas is a constant at specified temperature and pressure

1.3.e: The molar concentration of a solution is determined by the amount of a solute and the volume of solution

1.3.f: A standard solution is one of known concentration

###### A/S:

1.3.i: Solution of problems relating to reacting quantities, limiting and excess reactants, and theoretical, experimental, and percentage yields

1.3.ii: Calculation of reacting volumes of gases using Avogadro's law

1.3.iii: Solution of problems and analysis of graphs involving the relationship between temperature, pressure and volume for a fixed mass of an ideal gas

1.3.iv: Solution of problems relating to the ideal gas equation

1.3.v: Explanation of the deviation of real gases from ideal behavior at low temperature and high pressure

- 1.3.vi: Obtaining and using experimental values to calculate the molar mass of a gas from the ideal gas equation
- 1.3.vii: Solution of problems involving molar concentration, amount of solute, and volume of solution
- 1.3.viii: Use of the experimental method of titration to calculate the concentration of a solution by reference to a standard solution

## Chapter 11/21: Measurement and Analysis

11.1: All measurement has a limit of precision and accuracy, and this must be taken into account when evaluating experimental results

U:

11.1.a: Qualitative data include all non-numerical information obtained from observations not from measurement

11.1.b: Quantitative data are obtained from measurements, and are always associated with random errors/uncertainties, determined by the apparatus, and by human limitations such as reaction times

11.1.c: Propagation of random errors in data processing shows the impact of the uncertainties on the final result

11.1.d: Experimental design and procedure usually lead to systematic errors in measurement, which cause a deviation in a particular direction

11.1.e: Repeat trials and measurements will reduce random errors but not systematic errors

A/S:

11.1.i: Distinction between random errors and systematic errors

11.1.ii: Record uncertainties in all measurements as a range of (+/-) to an appropriate precision

11.1.iii: Discussion of ways to reduce uncertainties in an experiment

11.1.iv: Propagation of uncertainties in processed data, including the use of percentage uncertainties

11.1.v: Discussion of systematic errors in all experimental work, their impact on the results, and how they can be reduced

11.1.vi: Estimation of whether a particular source of error is likely to have a major or minor effect on the final result

11.1.vii: Calculation of percentage error when the experimental result can be compared with a theoretical or accepted result

11.1.viii: Distinction between accuracy and precision in evaluating results

11.2: Graphs are visual representation of trends in data

U:

11.2.a: Graphical techniques are an effective means of communicating the effect of an independent variable on a dependent variable, and can lead to determination of physical quantities

11.2.b: Sketched graphs have labelled but unscaled axes, and are used to show qualitative trends, such as variables that are proportional or inversely proportional

11.2.c: Drawn graphs have labelled and scaled axes, and are used in quantitative measurements

A/S:

11.2.i: Drawing graphs of experimental results, including the correct choice of axes and scale

11.2.ii: Interpretation of graphs in terms of relationships of dependent and independent variables

11.2.iii: Production and interpretation of best-fit lines or curves through data points, including an assessment of when it can and cannot be considered as a linear function

11.2.iv: Calculation of quantities from graphs by measuring slope (gradient) and intercept, including appropriate units

## Chapter 2/12: Atomic Structure

2.1: The mass of an atom is concentrated in its minute, positively charged nucleus

U:

2.1.a: Atoms contain a positively charged nucleus composed of protons and neutrons (nucleons)

2.1.b: Negatively charged electrons occupy the space outside the nucleus

2.1.c: The mass spectrometer is used to determine the relative atomic mass of an element from its isotopic composition

A/S:

2.1.i: Use of the nuclear symbol notation  ${}^A_ZX$  to deduce the number of protons, neutrons and electrons in atoms and ions

2.1.ii: Calculations involving non-integer relative atomic masses and abundance of isotopes from given data, including mass spectra

2.2: The electron configuration of an atom, which can be deduced from its atomic number, determines the properties of the element

U:

2.2.a: Emission spectra are produced when photons are emitted from atoms as excited electrons return to a lower energy level

2.2.b: The line emission spectrum of hydrogen provides evidence for the existence of electrons in discrete energy levels, which converge at higher energies

2.2.c: The main energy level or shell is given an integer number, **n**, and can hold a maximum number of electrons  $2n^2$

2.2.d: A more detailed model of the atom describes the division of the main energy level into s, p, d, and f sub-levels of successively higher energies

2.2.e: Sub-levels contain a fixed number of orbitals, regions of space where there is a high probability of finding an electron

2.2.f: Each orbital has a defined energy state for a given electron configuration and chemical environment and can hold two electrons of opposite spin

A/S:

2.2.i: Description of the relationship between color, wavelength, frequency, and energy across the electromagnetic spectrum

2.2.ii: Distinction between a continuous spectrum and a line spectrum

2.2.iii: Description of the emission spectrum of the hydrogen atom, including relationships between the lines and the energy transitions to the first, second, and third energy levels

2.2.iv: Recognition of the shape of an s orbital and the  $p_x$ ,  $p_y$ , and  $p_z$  atomic orbitals

2.2.v: Application of the Aufbau principle, Hund's rule and the Pauli exclusion principle to write electron configurations for atoms and ions up to  $Z=36$

12.1: The quantized nature of energy transitions is related to the energy states of electrons in atoms and molecules

U:

12.1.a: In an emission spectrum, the limit of convergence at higher frequency corresponds to the first ionization energy

12.1.b: Trends in the first ionization energy across periods account for the existence of main energy levels and sub-levels in atoms

12.1.c: Successive ionization energy data for an element give information that shows relations to electron configurations

A/S:

12.1.i: Solving problems using  $E=h\nu$

12.1.ii: Calculation of the value of the first ionization energy from spectral data which gives the wavelength or frequency of the convergence limit

12.1.iii: Deduction of the group of an element from its successive ionization energy data

12.1.iv: Explanation of the trends and discontinuities in data on first ionization energy across a period

## Chapter 3/13: Periodicity

3.1: The arrangement of elements in the periodic table reflects their electron configurations

U:

- 3.1.a: The Periodic Table is arranged into four blocks associated with the four sub-levels: s, p, d, and f
- 3.1.b: The Periodic Table consists of groups (vertical columns) and periods (horizontal rows)
- 3.1.c: The period (n) is the outer energy level that is occupied by electrons
- 3.1.d: The number of the principle energy level and the number of the valence electrons in an atom can be deduced from its position on the Periodic Table
- 3.1.e: The Periodic Table shows the positions of metals, non-metals and metalloids
- A/S:
- 3.1.i: Deduction of the electron configuration of an atom from the element's position on the Periodic Table and vice versa
- 3.2: Elements show trends in their physical and chemical properties across periods and down groups
- U:
- 3.2.a: Vertical and horizontal trends in the Periodic Table exist for atomic radius, ionic radius, ionization energy, electron affinity, and electronegativity
- 3.2.b: Trends in metallic and non-metallic behavior are due to the trends above
- 3.2.c: Oxides change from base through amphoteric to acidic across a period
- A/S:
- 3.2.i: Prediction and explanation of the metallic and non-metallic behavior of an element based on its position in the Periodic Table
- 3.2.ii: Discussion of the similarities and differences in the properties of elements in the same group, with reference to alkali metals (Group 1) and halogens (Group 7)
- 3.2.iii: Construction of equations to explain the pH changes for reactions of  $\text{Na}_2\text{O}$ ,  $\text{MgO}$ ,  $\text{P}_4\text{O}_{10}$ , and the oxides of nitrogen and sulfur with water
- 13.1: The transition elements have characteristic properties; these properties are related to their all having incomplete d sublevels
- U:
- 13.1.a: Transition elements have variable oxidation numbers, form complex ions with ligands, have colored compounds, and display catalytic and magnetic properties
- 13.1.b: Zn is not considered to be a transition element as it does not form ions with incomplete d orbitals
- 13.1.c: Transition elements show an oxidation number of +2 when the s electrons are removed
- A/S:
- 13.1.i: Explanation of the ability of transition metals to form variable oxidation states from successive ionization energies
- 13.1.ii: Explanation of the nature of the coordinate bond within a complex ion
- 13.1.iii: Deduction of the total charge given the formula of the ion and ligands present
- 13.1.iv: Explanation of the magnetic properties in transition metals in terms of unpaired electrons
- 13.2: d-orbitals have the same energy in an isolated atom, but split into two sub-levels in a complex ion. The electric field of ligands may cause the d-orbitals in complex ions to split so that the energy of an electron transition between them corresponds to a photon of visible light
- U:
- 13.2.a: The d sub-level splits into two sets of orbitals of different energy in a complex ion
- 13.2.b: Complexes of d-block elements are colored, as light is absorbed when an electron is excited between the d orbitals
- 13.2.c: The color absorbed is complementary to the color observed
- A/S:
- 13.2.i: Explanation of the effect of the identity of the metal ion, the oxidation number of the metal, and the identity of the ligand on the color of transition metal ion complexes
- 13.2.ii: Explanation of the effect of different ligands on the splitting of the d orbitals in transition metal complexes and color observed using the spectrochemical series

## **Year 1**

### **Semester 2: Essential Ideas**

#### Chapter 4/14: Chemical Bonding and Structure

##### 4.1: Ionic compounds form by electron transfer from a metal to a non-metal

U:

4.1.a: Positive ions (cations) form by metals losing valence electrons

4.1.b: Negative ions (anions) form by non-metals gaining electrons

4.1.c: The number of electrons gained or lost is determined by the electron configuration of the atom

4.1.d: The ionic bond is due to electrostatic attraction between oppositely charged ions

4.1.e: Under normal conditions, ionic compounds are usually solids with lattice structures

A/S:

4.1.i: Deduction of the formula and name of an ionic compound from its component ions, including polyatomic ions

4.1.ii: Explanation of the physical properties of ionic compounds (volatility, electrical conductivity, and solubility) in terms of their structure

##### 4.2: Covalent compounds form by electron sharing between two non-metals

U:

4.2.a: A covalent bond is formed by the electrostatic attraction between a shared pair of electrons and the positively charged nuclei

4.2.b: Single, double, and triple covalent bonds involve one, two and three shared pairs of electrons respectively

4.2.c: Bond length decreases and bond strength increases as the number of shared electrons increases

4.2.d: Bond polarity results from the difference in electronegativities of the bonded atoms

A/S:

4.2.i: Deduction of the polar nature of a covalent bond from electronegativity values

##### 4.3: Lewis structures show the electron domains in the valence shell and are used to predict molecular shape

U:

4.3.a: Lewis (electron dot) structures show all the valence electrons in a covalently bonded species

4.3.b: The 'octet rule' refers to the tendency of the atoms to gain a valence shell with a total of 8 electrons

4.3.c: Some atoms, like Be and B, might form stable compounds with incomplete octets of electrons

4.3.d: Resonance structures occur when there is more than one possible position for a double bond in a molecule

4.3.e: Shapes of species are determined by the repulsion of electron pairs according to VSEPR theory

4.3.f: Carbon and silicon form giant covalent/network covalent/macromolecule structures

A/S:

4.3.i: Deduction of Lewis (electron dot) structure of molecules and ions showing all valence electrons for up to four electron pairs on each atom

4.3.ii: The use of VSEPR theory to predict the electron domain geometry and the molecular geometry for species with two, three, and four electron domains

4.3.iii: Prediction of bond angles from molecular geometry and presence of non-bonding pairs of electrons

4.3.iv: Prediction of molecular polarity from bond polarity and molecular geometry

4.3.v: Deduction of resonance structures, including  $C_6H_6$ ,  $CO_3^{2-}$ , and  $O_3$

4.3.vi: Explanation of the properties of giant covalent compounds in terms of their structures

##### 4.4: The physical properties of molecular substances result from different types of forces between their molecules

U:

4.4.a: Intermolecular forces include London (dispersion) forces, dipole-dipole forces, and hydrogen bonding

4.4.b: The relative strengths of these interactions are London (dispersion) forces < dipole-dipole forces < hydrogen bonds

A/S:

4.4.i: Deduction of the types of intermolecular force present in substances, based on their structure and chemical formula

4.4.ii: Explanation of the physical properties of covalent compounds (volatility, electrical conductivity, and solubility) in terms of their structure and intermolecular forces

4.5: Metallic bonds involve a lattice of cations and delocalized electrons

U:

4.5.a: A metallic bond is the electrostatic attraction between a lattice of positive ions and delocalized electrons

4.5.b: The strength of the metallic bond depends on the charge of the ions and the radius of the metal ion

4.5.c: Alloys usually contain more than one metal and have enhanced properties

A/S:

4.5.i: Explanation of electrical conductivity and malleability in metals

4.5.ii: Explanation of trends in melting points of metals

4.5.iii: Explanation of the properties of alloys in terms of non-directional bonding

14.1: Larger structures and more in-depth explanations of bonding systems often require more sophisticated concepts and theories of bonding

U:

14.1.a: Covalent bonds result from the overlap of atomic orbitals. A sigma bond ( $\sigma$ ) is formed by the direct head-on/end-to-end overlap of atomic orbitals, resulting in electron density concentrated between the nuclei of the bonding atoms. A pi bond ( $\pi$ ) is formed by the sideways overlap of atomic orbitals, resulting in electron density above and below the plane of the nuclei of the bonding atoms

14.1.b: Formal charge (FC) can be used to decide which Lewis (electron dot) structure is preferred from several. The FC is the charge an atom would have if all atoms in the molecule had the same electronegativity.  $FC = (\text{number of valence electrons} - \frac{1}{2}(\text{number of bonding electrons}) - (\text{number of non-bonding electrons}))$ . The Lewis (electron dot) structure with the atoms having FC values closest to zero is preferred

14.1.c: Exceptions to the octet rule include some species having incomplete octets and expanded octets

14.1.d: Delocalization involves electrons that are shared by/between all atoms in a molecule or ion as opposed to being localized between a pair of atoms

14.1.e: Resonance involves using two or more Lewis structures to represent a particular molecule or ion. A resonance structure is one of two or more alternative Lewis structures for a molecule or ion that cannot be described fully with one Lewis structure alone

A/S:

14.1.i: Prediction whether sigma ( $\sigma$ ) or pi ( $\pi$ ) bonds are formed from the linear combination of atomic orbitals

14.1.ii: Deduction of the Lewis structures of molecules and ions showing all valence electrons for up to six electron pairs on each atom

14.1.iii: Application of FC to ascertain which Lewis structure is preferred from different Lewis structures

14.1.iv: Deduction using VSEPR theory of the electron domain geometry and molecular geometry with five and six electron domains and associated bond angles

14.1.v: Explanation of the wavelength of light required to dissociate oxygen and ozone

14.1.vi: Description of the mechanism of the catalysis of ozone depletion when catalyzed by CFCs and  $\text{NO}_x$

14.2: Hybridization results from the mixing of atomic orbitals to form the same number of new equivalent hybrid orbitals that can have the same mean energy as the contributing atomic orbitals

U:

14.2.a: A hybrid orbital results from the mixing of different types of atomic orbitals on the same atom

A/S:

14.1.i: Explanation of the formation of  $sp^3$ ,  $sp^2$  and  $sp$  hybrid orbitals in methane, ethane, and ethyne

14.1.ii: Identification and explanation of the relationships between Lewis structures, electron domains, molecular geometries, and the types of hybridization

## Chapter 10/20: Organic Chemistry

10.1: Organic chemistry focuses on the chemistry of compounds containing carbon

U:

10.1.a: A homologous series is a series of compounds of the same family, with the same general formula which differ from each other by a common structural unit

10.1.b: Structural formulas can be represented in full and condensed format

10.1.c: Structural isomers are compounds with the same molecular formula but different arrangements of atoms

10.1.d: Functional groups are the reactive parts of molecules

10.1.e: Saturated compounds contain single bonds only and unsaturated compounds contain double or triple bonds

10.1.f: Benzene is an aromatic, unsaturated hydrocarbon

A/S:

10.1.i: Explanation of the trends in boiling points of members of a homologous series

10.1.ii: Distinction between empirical, molecular, and structural formulas

10.1.iii: Identification of different classes: alkenes, alkynes, halogenoalkanes (or haloalkanes), alcohols, ethers, aldehydes, ketones, esters, carboxylic acids, amines, amides, nitriles, and arenes

10.1.iv: Identification of typical functional groups in molecules, e.g. phenyl, hydroxyl, carbonyl, carboxyl, carboxamide, aldehyde, ester, ether, amine, nitrile, alkyl, alkenyl, and alkynyl

10.1.v: Construction of 3D models (real or virtual) of organic molecules

10.1.vi: Application of IUPAC rules in the nomenclature of straight-chain and branched-chain isomers

10.1.vii: Identification of primary, secondary, and tertiary carbon atoms in halogenoalkanes and alcohols and primary, secondary, and tertiary nitrogen atoms in amines

10.1.viii: Discussion of the structure of benzene using physical and chemical evidence

10.2: Structure, bonding and chemical reactions involving functional group interconversions are key strands in organic chemistry

U:

10.2.a: Alkanes – have a low reactivity and undergo free radical substitution reactions

10.2.b: Alkenes – are more reactive than alkanes and undergo addition reactions. Bromine water can be used to distinguish between alkenes and alkanes

10.2.c: Alcohols – undergo nucleophilic substitution reactions with acids (also called esterification or condensation) and some undergo oxidation reactions

10.2.d: Halogenoalkanes – are more reactive than alkanes. They can undergo (nucleophilic) substitution reactions. A nucleophile is an electron-rich species containing a lone pair that it donates to an electron-deficient carbon

10.2.e: Polymers – addition polymers consist of a wide range of monomers and form the basis of the plastics industry

10.2.f: Benzene – does not readily undergo addition reactions but does undergo electrophilic substitution reactions

A/S:

10.2.i: Alkanes

- Writing equations for the complete and incomplete combustion of hydrocarbons

- Explanation of the reaction of methane and ethane with halogens in terms of a free radical substitution mechanism involving photochemical homolytic fission

10.2.ii: Alkenes



- Writing equations for the reactions of alkenes with hydrogen and halogens and of symmetrical alkenes with hydrogen halides and water
- Outline the addition polymerization of alkenes
- Relationship between the structure of the monomer to the polymer and repeating unit

#### 10.2.iii: Alcohols

- Writing equations for the complete combustion of alcohols
- Writing equations for the oxidation reactions of primary and secondary alcohols (using acidified potassium dichromate(VI) or potassium manganate(VII) as oxidizing agents). Explanation of distillation and reflux in the isolation of the aldehyde and carboxylic acid products
- Writing the equation for the condensation reaction of an alcohol with a carboxylic acid, in the presence of a catalyst (e.g. concentrated sulfuric acid) to form an ester

#### 10.2.iv: Halogenoalkanes

- Writing the equation for the substitution reactions of halogenoalkanes with aqueous sodium hydroxide

20.1: Key organic reaction types include nucleophilic substitution, electrophilic addition, electrophilic substitution and redox reactions. Reaction mechanisms vary and help in understanding the different types of reactions taking place

U:

#### 20.1.a: Nucleophilic substitution reactions

- $S_N1$  represents a nucleophilic unimolecular substitution reaction and  $S_N2$  represents a nucleophilic bimolecular substitution reaction.  $S_N1$  involves a carbocation intermediate.  $S_N2$  involves a concerted reaction with a transition state
- For tertiary halogenoalkanes the predominate mechanism is  $S_N1$  and for primary halogenoalkanes it is  $S_N2$ . Both mechanisms occur for secondary halogenoalkanes
- The rate-determining step (slow step) in an  $S_N1$  reaction depends only on the concentration of the halogenoalkanes, rate =  $k[\text{halogenoalkanes}]$ . For  $S_N2$ , rate =  $k[\text{halogenoalkanes}][\text{nucleophile}]$ .  $S_N2$  is stereospecific with an inversion of configuration at the carbon
- $S_N2$  reactions are best conducted using aprotic, polar solvents and  $S_N1$  reactions are best conducted using protic, polar solvents

#### 20.1.b: Electrophilic addition reactions

- An electrophile is an electron-deficient species that can accept electron pairs from a nucleophile. Electrophiles are Lewis acids
- Markovnikov's rule can be applied to predict the major product in electrophilic addition reactions of unsymmetrical alkenes with hydrogen halides and interhalogens. The formation of the major product can be explained in terms of the relative stability of possible carbocations in the reaction mechanism

#### 20.1.c: Electrophilic substitution reaction

- Benzene is the simplest aromatic hydrocarbon compound (or arene) and has a delocalized structure of  $\pi$  bonds around its ring. Each carbon to carbon bond has a bond order of 1.5. Benzene is susceptible to attack by electrophiles

#### 20.1.d: Reduction reactions

- Carboxylic acids can be reduced to primary alcohols (via the aldehyde). Ketones can be reduced to secondary alcohols. Typical reducing agents are lithium aluminium hydride and sodium borohydride

A/S:

#### 20.1.i: Nucleophilic substitution reactions

- Explanation of why hydroxide is a better nucleophile than water
- Deduction of the mechanism of the nucleophilic substitution reactions with halogenoalkanes with aqueous sodium hydroxide in terms of  $S_N1$  and  $S_N2$  mechanisms.

- Explanation of how the rate depends on the identity of the halogen (i.e. the leaving group), whether the halogenoalkane is primary, secondary, or tertiary and the choice of solvent
- Outline of the difference between protic and aprotic solvents
- 20.1.ii: Electrophilic addition reactions
- Deduction of the mechanism of the electrophilic addition reactions of alkenes with halogens/interhalogens and hydrogen halides
- 20.1.iii: Electrophilic substitution reactions
- Deduction of the mechanism of the nitration (electrophilic substitution) reactions of benzene (using a mixture of concentrated nitric acid and sulfuric acid)
- 20.1.iv: Reduction reactions
- Writing reduction reactions of carbonyl-containing compounds: aldehydes and ketones to primary and secondary alcohols and carboxylic acids to aldehydes, using suitable reducing agents
  - Conversion of nitrobenzene to aniline via a two-state reaction
- 20.2: Organic synthesis is the systematic preparation of a compound from a widely available starting material or the synthesis of a compound via a synthetic route that often can involve a series of different steps
- U:
- 20.2.a: The synthesis of an organic compound stems from a readily available starting material via a series of discrete steps. Functional group interconversions are the basis of such synthetic routes
- 20.2.b: Retro-synthesis of organic compounds
- A/S:
- 20.2.i: Deduction of multi-step synthetic routes given starting reagents and the product(s)
- 20.3: Stereoisomerism involves isomers which have different arrangements of atoms in space but do not differ in connectivity or bond multiplicity (ie whether single, double or triple) between the isomers themselves
- U:
- 20.3.a: Stereoisomers are sub-divided into two classes: conformational isomers, which interconvert by rotation about an  $\sigma$  bond, and configurational isomers, which interconvert only by breaking and reforming a bond
- 20.3.b: Configurational isomers are further sub-divided into *cis-trans* and E/Z isomers and optical isomers
- 20.3.c: *Cis-trans* isomers can occur in alkenes or cycloalkanes (or hetero-analogues) and differ in the position of atoms (or groups) relative to a reference plane. According to IUPAC, E/Z isomers refer to alkenes of the form  $R_1R_2C=CR_3R_4$  ( $R_1 \neq R_2$ ,  $R_3 \neq R_4$ ) where neither  $R_1$  nor  $R_2$  need be different from  $R_3$  or  $R_4$
- 20.3.d: A chiral carbon is a carbon joined to four different atoms or groups
- 20.3.e: An optically active compound can rotate the plane of polarized light as it passes through a solution of the compound. Optical isomers are enantiomers
- 20.3.f: Enantiomers are non-superimposable mirror images of each other. Diastereomers are not mirror images of each other
- 20.3.g: A racemic mixture (or racemate) is a mixture of two enantiomers in equal amounts and is optically inactive
- A/S:
- 20.3.i: Construction of 3-D models (real or virtual) of a wide range of stereoisomers
- 20.3.ii: Explanation of stereoisomerism in non-cyclic alkenes and C<sub>3</sub> and C<sub>4</sub> cycloalkanes
- 20.3.iii: Comparison between the physical and chemical properties of enantiomers
- 20.3.iv: Description and explanation of optical isomers in simple organic molecules
- 20.3.v: Distinction between optical isomers using a polarimeter

11.3: Analytical techniques can be used to determine the structure of a compound, analyze the composition of a substance or determine the purity of a compound. Spectroscopic techniques are used in the structural identification of organic and inorganic compounds

U:

11.3.a: The degree of unsaturation or index of hydrogen deficiency (IHD) can be used to determine from a molecular formula the number of rings or multiple bonds in a molecule

11.3.b: Mass spectroscopy (MS), proton nuclear magnetic resonance spectroscopy ( $^1\text{H}$  NMR), and infrared spectroscopy (IR) are techniques that can be used to help identify and to determine the structure of compounds

A/S:

11.3.i: Determination of the IHD from a molecular formula

11.3.ii: Deduction of information about the structural features of a compound from percentage composition data, MS,  $^1\text{H}$  NMR, or IR

21.1: Although spectroscopic characterization techniques from the backbone of structural identification of compounds, typically no one technique results in a full structural identification of a molecule

U:

21.1.a: Structural identification of compounds involves several different analytical techniques, including IR,  $^1\text{H}$  NMR, and MS

21.1.b: In a high-resolution  $^1\text{H}$  NMR spectrum, single peaks present in low resolution can split into further clusters of peaks

21.1.c: The structural technique of single crystal X-ray crystallography can be used to identify the bond lengths and bond angles of crystalline compounds

A/S:

21.1.i: Explanation of the use of tetramethylsilane (TMS) as the reference standard

21.1.ii: Deduction of the structure of a compound given information from a range of analytical characterization techniques (X-ray crystallography, IR,  $^1\text{H}$  NMR, and MS)

## Chapter D/15: Medicinal Chemistry

D.1: Medicines and drugs have a variety of different effects on the functioning of the body.

U:

D.1.a: In animal studies, the therapeutic index is the lethal dose of a drug for 50% of the population ( $\text{LD}_{50}$ ) divided by the minimum effective dose for 50% of the population ( $\text{ED}_{50}$ )

D.1.b: In humans, the therapeutic index is the toxic dose of a drug for 50% of the population ( $\text{TD}_{50}$ ) divided by the minimum effective dose for 50% of the population ( $\text{ED}_{50}$ )

D.1.c: For ethical and economic reasons, animal and human tests of drugs (for  $\text{LD}_{50}/\text{ED}_{50}$  and  $\text{TD}_{50}/\text{ED}_{50}$  respectively) should be kept to a minimum

D.1.d: The therapeutic window is the range of dosages between the minimum amount of the drug that produce the desired effect and a medically unacceptable adverse effect

D.1.e: Dosage, tolerance, addiction, and side-effects are considerations of drug administration

D.1.f: Bioavailability is the fraction of the administered dosage that reaches the target part of the human body

D.1.g: The main steps in the development of synthetic drugs include identifying the need and structure, synthesis, yield, and extraction

D.1.h: Drug-receptor interactions are based on the structure of the drug and the site of activity

A/S:

D.1.i: Discussion of experimental foundations for therapeutic index and therapeutic window through both animal and human studies

D.1.ii: Discussion of drug administration methods

D.1.iii: Comparison of how functional groups, polarity, and medicinal administration can affect bioavailability

D.2: Natural products with useful medicinal properties can be chemically altered to produce more potent and safe medicines.

U: Aspirin

D.2.a: Mild analgesics function by intercepting the pain stimulus at the source, often by interfering with the production of substances that cause pain, swelling, or fever

D.2.b: Aspirin is prepared from salicylic acid

D.2.c: Aspirin can be used as an anticoagulant, in prevention of the recurrence of heart attacks and strokes, and as a prophylactic

U: Penicillin

D.2.d: Penicillins are antibiotics produced by fungi

D.2.e: A beta-lactam ring is a part of the core structure of penicillins

D.2.f: Some antibiotics work by preventing cross-linking of the bacterial cell walls

D.2.g: Modifying the side-chain results in penicillins that are more resistant to the penicillinase enzyme

A/S: Aspirin

D.2.i: Description of the use of salicylic acid and its derivatives as mild analgesics

D.2.ii: Explanation of the synthesis of aspirin from salicylic acid, including yield, purity by recrystallization, and characterization using IR and melting point

D.2.iii: Discussion of the synergistic effects of aspirin with alcohol

D.2.iv: Discussion of how aspirin can be chemically modified into a salt to increase its aqueous solubility and how this facilitates its bioavailability

A/S: Penicillin

D.2.v: Discussion of the effects of chemically modifying the side-chain of penicillins

D.2.vi: Discussion of the importance of patient compliance and the effects of the over-prescription of penicillin

D.2.vii: Explanation of the importance of the beta-lactam ring on the action of penicillin

D.3: Potent medical drugs prepared by chemical modification of natural products can be addictive and become substances of abuse.

U: Opiates

D.3.a: The ability of a drug to cross the blood-brain barrier depends on its chemical structure and solubility in water and lipids

D.3.b: Opiates are natural narcotic analgesics that are derived from the opium poppy

D.3.c: Morphine and codeine are used as strong analgesics. Strong analgesics work by temporarily bonding to receptor sites in the brain, preventing the transmission of pain impulses without depressing the central nervous system

D.3.d: Medical use and addictive properties of opiate compounds are related to the presence of opioid receptors in the brain

A/S:

D.3.i: Explanation of the synthesis of codeine and diamorphine from morphine

D.3.ii: Description and explanation of the use of strong analgesics

D.3.iii: Comparison of the structures of morphine, codeine and diamorphine (heroin)

D.3.iv: Discussion of the advantages and disadvantages of using morphine and its derivatives as strong analgesics

D.3.v: Discussion of the side-effects and addiction to opiate compounds

D.3.vi: Explanation of the increased potency of diamorphine compared to morphine based on their chemical structure and solubility

D.4: Excess stomach acid is a common problem that can be alleviated by compounds that increase stomach pH by neutralizing or reducing its secretion.

U:

D.4.a: Non-specific reactions, such as the use of antacids, are those that work to reduce excess stomach acid

D.4.b: Active metabolites are the active forms of a drug after it has been processed by the body  
A/S:

D.4.i: Explanation of how excess acidity in the stomach can be reduced by the use of different bases

D.4.ii: Construction and balancing equations for neutralization reactions and the stoichiometric application of these equations

D.4.iii: Solving buffer problems using the Henderson-Hasselbach equation

D.4.iv: Explanation of how compounds such as ranitidine (Zantac) can be used to inhibit stomach acid production

D.4.v: Explanation of how compounds such as omeprazole (Prilosec) and esomeprazole (Nexium) can be used to suppress acid secretion in the stomach

D.5: Antiviral medications have recently been developed for some viral infections while others are still being researched.

U:

D.5.a: Viruses lack a cell structure and so are more difficult to target with drugs than bacteria

D.5.b: Antiviral drugs may work by altering the cell's genetic material so that the virus cannot use it to multiply. Alternatively, they may prevent the viruses from multiplying by blocking enzyme activity within the host cell

A/S:

D.5.i: Explanation of the different ways in which antiviral medications work

D.5.ii: Description of how viruses differ from bacteria

D.5.iii: Explanation of how oseltamivir (Tamiflu) and zanamivir (Relenza) work as preventative agents against flu viruses

D.5.iv: Comparison of the structures of oseltamivir and zanamivir

D.5.v: Discussion of the difficulties associated with solving the AIDS problem

D.7: Chiral auxiliaries allow the production of individual enantiomers of chiral molecules.

U:

D.7.a: Taxol is a drug that is commonly used to treat several different forms of cancer

D.7.b: Taxol naturally occurs in yew trees but is not commonly synthetically produced

D.7.c: A chiral auxiliary is an optically active substance that is temporarily incorporated into an organic synthesis so that it can be carried out asymmetrically with the selective formation of a single enantiomer

A/S:

D.7.i: Explanation of how Taxol (Paclitaxel) is obtained and used as a chemotherapeutic agent

D.7.ii: Description of the use of chiral auxiliaries to form the desired enantiomer

D.7.iii: Explanation of the use of a polarimeter to identify enantiomers

D.8: Nuclear radiation, whilst dangerous owing its ability to damage cells and cause mutations, can also be used to both diagnose and cure disease.

U:

D.8.a: Alpha, beta, gamma, proton, neutron, and positron emissions are all used for medical treatment

D.8.b: Magnetic resonance imaging (MRI) is an application of NMR technology

D.8.c: Radiotherapy can be internal and/or external

D.8.d: Targeted alpha therapy (TAT) and boron neutron capture therapy (BNCT) are two methods which are used in cancer treatment

A/S:

D.8.i: Discussion of common side-effects from radiotherapy

D.8.ii: Explanation of why technetium-99m is the most common radio isotope used in nuclear medicine based on its half-life, emission type, and chemistry

D.8.iii: Explanation of why lutetium-177 and yttrium-90 are common isotopes used for radiotherapy based on the type of radiation emitted

D.8.iv: Balancing nuclear equations involving alpha and beta particles

- D.8.v: Calculation of the percentage and amount of radioactive material decayed and remaining after a certain period of time using the nuclear half-life equation
- D.8.vi: Explanation of TAT and how it might be used to treat diseases that have spread throughout the body
- D.9: A variety of analytical techniques is used for detection, identification, isolation, and analysis of medicines and drugs.
- U:
- D.9.a: Organic structures can be analyzed and identified through the use of infrared spectroscopy, mass spectroscopy, and proton NMR
- D.9.b: The presence of alcohol in a sample of breath can be detected through the use of either a redox reaction or a fuel cell type breathalyzer
- A/S:
- D.9.i: Interpretation of a variety of analytical spectra to determine an organic structure including infrared spectroscopy, mass spectroscopy, and proton NMR
- D.4.ii: Description of the process of extraction and purification of an organic product. Consider the use of fractional distillation, Raoult's law, the properties on which extractions are based and explaining the relationship between organic structure and solubility
- D.4.iii: Description of the process of steroid detection in sport utilizing chromatography and mass spectroscopy
- D.4.iv: Explanation of how alcohol can be detected with the use of a breathalyzer
- D.6: The synthesis, isolation, and administration of medications can have an effect on the environment.
- U:
- D.6.a: High-level waste (HLW) is waste that gives off large amounts of ionizing radiation for a long time
- D.6.b: Low-level waste (LLW) is waste that gives off small amounts of ionizing radiation for a short time
- D.6.c: Antibiotic resistance occurs when microorganisms become resistant to antibacterials
- A/S:
- D.6.i: Description of the environmental impact of medical nuclear waste disposal
- D.6.ii: Discussion of environmental issues related to left-over solvents
- D.6.iii: Explanation of the dangers of antibiotic waste, from improper drug disposal and animal waste, and the development of antibiotic resistance
- D.6.iv: Discussion of the basics of Green Chemistry (sustainable chemistry) processes
- D.6.v: Explanation of how Green Chemistry was used to develop the precursor for Tamiflu (oseltamivir)