CHEMISTRY AT THE UNIVERSITY OF SALFORD

Introduction

Chemistry offers a friendly but challenging learning environment which encourages academic excellence through personal endeavour. The formal part of each course comprises lectures, tutorials and laboratory classes occupying in total about 20 hours per week. Lectures provide the basic introduction to topics, which are explored in greater depth through personal study and in tutorial groups. Each student is allocated specialist tutors for inorganic/analytical, organic and physical chemistry and is actively encouraged to seek their help and advice as a part of their approach to study. Laboratory work is specifically designed to develop practical skills and problem solving abilities, as well as illustrating the chemical principles discussed in lectures and tutorials. Students work both individually and in teams for project activities. The programme also emphasises the benefits of ancillary skills — use of the scientific literature, verbal and written presentations, database management, computing and mathematics. Students are encouraged to be responsible for their own education, plan the effective use of time and develop learning strategies.

A variety of formats are used during our courses to monitor and evaluate progress; self assessment exercises, coursework and regular tests are important. Examinations are held at the end of each semester; most laboratory work is continuously assessed.

We are a working community of undergraduates, postgraduates, and academic staff, plus technical support and secretarial staff. In the research school the main interests include organic synthesis, inorganic synthesis, colloid and interface science, materials science, radiochemistry, molecular structure, combustion chemistry, polymer chemistry and analytical chemistry. Our research programmes receive financial support both from government and industrial sources. Many of the staff have national and international reputations in their individual fields of research, and collaborate with academic and industrial research groups worldwide.

Useful URLs

Homepage: http://www.salford.ac.uk/chemist/homepage.html Qualifications: http://www.salford.ac.uk/chemist/ugindex.html Course Structures: http://www.salford.ac.uk/chemist/ugindex.html Research activities: http://www.salford.ac.uk/chemist/staff.html

SOCRATES coordinator:

Dr Neil Boag Chemistry University of Salford Salford M5 4WT United Kingdom Tel +44 (0) 161 295 5239 Fax +44 (0) 161 295 5111 E-mail N.M.Boag@salford.ac.uk

CHEMISTRY COURSES

Course Codes

The course codes below indicate the level of study and number of ECTS credits associated with each course. The **level of study** is indicated in the first digit (*e.g.* level two course codes start with CH2, *etc.*) and the **number of credits** is indicated at the end of the course code (*e.g.* a code ending in '-05' indicates **five** ECTS credits).

CODE SEMESTER TITLE

-	-	٦
Foundation	and Basic (Chemistry modules (these module will not be offered 2002/2003)
CH101-05	1	Foundation General Chemistry
CH102-05	1	Foundation Organic Chemistry
CH103-05	1	Foundation Analytical Chemistry
CH104-05	2	Basic Inorganic Chemistry
CH105-05	2	Basic Organic Chemistry
CH106-05	2	Basic Physical Chemistry
Core Chemi	stry module	es
CH201-05	1	Core Inorganic Chemistry 1
CH202-05	2	Core Inorganic Chemistry 2
CH203-05	1	Core Organic Chemistry 1
CH204-05	2	Core Organic Chemistry 2
CH205-05	1	Core Physical Chemistry 1
CH206-05	2	Core Physical Chemistry 2
Advanced C	ore and Sp	ecialised modules
CH301-10	1	Advanced Core Chemistry 1
CH302-10	2	Advanced Core Chemistry 2
CH303-10	1	Specialised Lecture Units 1
CH304-10	2	Specialised Lecture Units 2
CH305-05	1	Specialised Lecture Units 1A
CH306-05	2	Specialised Lecture Units 2A
Laboratory	modules	
CH107-05	1	Foundation Chemistry Laboratory
CH108-05	2	Laboratory Skills and Projects (first year)
CH207-10	1 or 2	Laboratory Skills 1
CH208-10	1 or 2	Laboratory Skills 2
CH307-20	1 + 2	Research Project
Other modu	les	
CH109-05	2	Analytical Chemistry B
CH110-05	1	Ancillary Skills 1
CH111-05	2	Ancillary Skills 2
CH112-05	1	Biochemistry (Introduction to)
CH113-05	1	Environmental Chemistry
CH114-05	2	Geochemistry
CH115-05	2	Medicinal Chemistry (Introduction to)
CH209-05	1	Analytical Chemistry C
CH210-05	2	Analytical Chemistry D
CH211-05	1	Medicinal Chemistry 1
CH212-05	2	Medicinal Chemistry 2
CH213-05	2	Chemical Problem Solving Skills

CH214-05	2	Quality Assurance and Quality Control
CH215-05	1	Scientific Communication Skills

FOUNDATION GENERAL CHEMISTRY

ECTS Credits: 5	Level: 1 Semester: 1	Code: CH101-05
Contact Hours:	32 hours comprising: 24 hours lect	ures and 8 hours of tutorials
Pre-requisites:	A-level Chemistry or equivalent	
Assessment:	One written examination (2 hours,	67%) and coursework (33%)

This module will consist of two lecture units, supported by tutorials, and will provide a general introduction to:

- atomic and molecular structure and bonding,
- reaction mechanisms, and the application of thermodynamic and kinetic principles to understanding chemical reactivity.

Atomic and Molecular Structure and Bonding

Academic Objectives

The aim of this unit is to enable the students to develop a qualitative understanding of the structure of the atom, the basis of chemical bonding and reactivity, and to enhance the students' appreciation of the three dimensional character of chemical entities.

- 1. The components of the atom: neutron, proton and electron charge and mass. The relative size of the nucleus and the atom. What holds the atom together? electrostatic attraction and repulsion. Particles and waves how to understand the electron. How much can we know? the Uncertainty Principle, probability and electron density. Orbitals why they are important in chemistry.
- 2. What are quantum numbers and what do they tell us about the energy, shape and orientation of atomic orbitals. Quantum numbers as labels for atomic orbitals relationship to the orbital symbols. The shapes of *s*, *p*, and *d* orbitals. Nodes, lobes and the sign of the wave function.
- 3. Two important concepts which help us understand how atoms and electrons behave shielding and effective nuclear charge. Orbital energies. How to assign electrons to orbitals - electron configuration. Identifying valence electrons. Electron configurations of ions - the problem with the Transition Elements
- 4. How the properties of the elements are determined by their electron configuration. The Periodic Table Blocks, Periods and Groups. Periodic trends: the sizes of atoms and ions. How strongly are electrons held? ionisation energy and electronegativity.
- 5. Predicting the formulae of simple molecules. Electron-pair repulsion: how it determines the shapes of molecules. How to describe the shapes of molecules. Extending the VSEPR approach.
- 6. The advantages and disadvantages of the Molecular Orbital approach. How to construct molecular orbitals from atomic orbitals. Shapes of molecular orbitals. Bonding, antibonding and non-bonding orbitals. Molecular energy level diagrams. Molecular orbitals in homonuclear diatomic molecules: F_2 , C_2 .
- 7. Predicting properties from a molecular orbital diagram bond order, bond strength, bond length, and magnetism. Heteronuclear bonds how are the electrons distributed? HF and CO. Bond polarity from MO theory.

Chemical Changes

Academic Objectives

The aim of this unit is to provide students with an introduction to the concepts of chemical thermodynamics and kinetics in order to appreciate their significance in understanding and describing chemical reactivity.

Detailed Syllabus

Thermochemistry

Standard enthalpy changes. Enthalpies of formation, combustion, reaction, solution. Standard enthalpy of atomisation, ionisation energy, and electron affinity. Hess's Law and its application. Bond dissociation enthalpies.

Thermodynamics

U, q and w. Path-dependent and path-independent functions. Isothermal and adiabatic processes. Work done during reversible and irreversible expansion of a gas. The relationship between enthalpy and internal energy Calorimetry at constant pressure and at constant volume. Molar heat capacities at constant pressure and constant volume. Temperature dependence of reaction enthalpies (Kirchoff's Law).

Kinetics

Reaction rate: definition and calculus notation. The effects of concentration on reaction rate. Orders of reaction, zero, first and second-order reactions. Integrated rate equations, half-lives, rate constants. The temperature dependance of reaction rate. Arrhenius Equation: determination of activation energy. Descriptive approach to the collision theory; activation energy; effective collisions. Techniques for measurement of reaction rate. Homogeneous and heterogeneous catalysis.

FOUNDATION ORGANIC CHEMISTRY

ECTS Credits: 5	Level: 1 Semester: 1	Code: CH102-05
Contact Hours:	32 hours comprising: 24 hours lectures	s and 8 hours of tutorials
Pre-requisites:	A-level Chemistry or equivalent	
Assessment:	One written examination (2 hours, 679	%) and coursework (33%)

Academic Objectives

The academic objective of this course is firstly; to introduce students to important structural, electronic and stereochemical features of organic molecules; then build a framework for understanding the reactivity and properties of some general classes of functionalised hydrocarbons. Some of the main general topics of the course are:

- Atomic and molecular structure and bonding,
- The application of mechanistic, thermodynamic and kinetic principles to understanding and describing chemical reactivity,
- The chemistry of functional aliphatic molecules; emphasis is placed on becoming familiar with methods of naming and preparing such compounds, and their general chemical properties. A series of fundamental reaction mechanisms are analysed at the electronic level to enable the student to develop an understanding of the origins and predictability of reactivity.

- 1. Covalent bonds. Carbon orbitals, hybridisation. The sp³ carbon, methane; sp² carbon, ethene; sp carbon, ethyne (sigma) and (pi) bonds.
- 2. Representations of molecules. Drawing and interpreting structures. Functional groups, Lewis and Kekulé structures.
- 3. Formal charges. Polarisation, electronegativity, inductive (-I and +I) effects in functional groups with a C-X bond.
- 4. Resonance (+R and -R) effects. Radical reactions, homolysis. Polar reactions, heterolysis. Reaction mechanism arrows.
- 5. Reagents and reactions. Reagent types; acids and bases, the pK_a scale; electrophiles and nucleophiles; oxidants and reductants.
- 6. Reaction types; addition, elimination, substitution, rearrangement. Examples of polar reactions. A mechanism for the addition of HBr to simple alkenes.
- 7. The electronic structures of the allyl radical and 1,3-butadiene. Mobility of -electrons, resonance stabilisation. The addition of HBr to 1,3-butadiene.
- 8. Stereochemistry. Definitions of isomer, constitution, configuration, stereoisomer. Chirality, enantiomers. Stereogenic (chiral) centres. Plane of symmetry, nonsuperimposable mirror image criterion. Optical activity as sole difference between enantiomers. Illustration with lactic acid; $[Co(en)_3]^{3+}$; 3-methylcyclohexanone.
- 9. Polarimetry, specific rotation. Dextrorotatory and laevorotatory lactic acids. Optically active natural products. Racemic mixtures. Fischer projections.
- 10. Specification of absolute configuration. The Sequence rule (Cahn-Ingold-Prelog). *R*, *S* nomenclature. *E*, *Z* nomenclature.
- 11. Molecules with more than one chiral centre. Diastereoisomers, meso compounds. Illustration with 2,3-dichloropentane, 2,3-dichlorobutane, tartaric acid.
- 12. Classification of alkanes, isomerism arising from branching of carbon chains. Primary

(1), secondary (2) and tertiary (3) alkyl groups. Systematic nomenclature using the IUPAC rules. Structures of some naturally occurring alkanes.

- 13. Haloalkanes: nomenclature. Preparation from alkanes *via* free-radical halogenation. Chlorination of methane. Bond dissociation energies and heats of formation of reactants and products. Free-radical chain reaction, energetics of the initiation, propagation, and termination steps. Detailed mechanism of the propagation steps. Structure and stability of alkyl radicals.
- 14. Methods for preparing haloalkanes from alkanols via displacement reactions. Reactivity of haloalkanes, electronegativity, polarity of C-X bond, inductive effects. Heterolysis. Formation and use of Grignard and organolithium reagents.
- 15. Nucleophilic substitution general introduction. The SN2 reaction mechanistic evidence from the reaction kinetics and stereochemistry. Detailed reaction mechanism, inversion of configuration. Transition state and energetics of the rate-determining step.
- 16. Nucleophilic substitution of haloalkanes via the S_N^2 mechanism. Factors responsible for high or low reactivity, polarity of C-X bond. Substituent (steric) effects, influence of nucleophile, leaving group, solvent. Synthetic considerations.
- Nucleophilic substitution of haloalkanes via the S_N1 mechanism, molecularity, kinetics, stereochemistry. Substituent (steric) effects, influence of nucleophile, leaving group, solvent. Hyperconjugation, relative stability of 1, 2, and 3 carbenium ions. Resonance in allylic and benzylic cations.
- 18. Elimination reactions of haloalkanes. The E2 and E1 mechanisms, kinetics and stereochemistry. Steric effects, influence of nucleophile, leaving group, solvent.
- 19. Nomenclature when functional groups are present. Preparation of alkenes via elimination, dehydration, reduction of alkynes.
- 20. Reactions of alkenes: addition of X_2 and HX, Markovnikov's rule; addition of HOX, formation of bromohydrins; radical addition of HBr; hydrogenation; oxidation of alkenes with ozone.
- 21. Alkene chemistry; hydroboration. Alkynes; nomenclature, natural occurrence, preparation via elimination reactions.
- 22. Reactions of alkynes, addition of HX and X₂, hydration, hydroboration, keto-enol tautomerism, reduction to alkenes. Relative acidity of terminal alkynes. Alkylation of alkynyl anions.
- 23. Alkanols. Nomenclature. Physical properties, acidity, basicity, nucleophilicity. Preparation of alkanols from alkenes. Preparation from carbonyl compounds via reduction or Grignard addition.
- 24. Nucleophilic displacement of OH, conversion to haloalkanes. Nucleophilic displacement by OH, conversion to tosylates. Oxidation of alkanols to carbonyl compounds using Cr(VI) reagents.

FOUNDATION ANALYTICAL CHEMISTRY

ECTS Credits: 5	Level: 1Semester: 1	Code: CH103-05
Contact Hours:	52 hours comprising: 24 hours lectur hours laboratory work	res, 4 hours tutorials and 24
Pre-requisites:	A-level Chemistry or equivalent	
Assessment:	One written examination (2 hours, 5) continuously assessed laboratory wo	0%), coursework (20%) and rk (30%).

This module will consist of two lecture units, supported by laboratory work and tutorials, and will provide a general introduction to:

- principles of analytical chemistry,
- principles of spectroscopy.

Principles of Analytical Chemistry

Academic Objectives

The aim of this unit is to provide students with an introduction to the principles of analytical chemistry through a study of titrimetric analysis. The unit is designed to be taught in conjunction with a set of practical exercises.

- 1. Definition of qualitative and quantitative analysis. Volumetric apparatus: the burette, pipette and volumetric flask. The grade A and grade B standards. British Standards Institution, International Standards. The need for cleanliness. The use of balances, the weighing bottle, weighing by difference. The use of the taring mechanism on electronic balances.
- 2. The need for standards. The definition of primary standards. Methods of using primary standards, the concept of titrating against a known mass as opposed to making up a standard solution. The provision of secondary standards, the need for these. Elementary statistics: average, mean, standard deviation, confidence limits, percentage error, student's t test. Presentation of analytical results: correlation charts, tables.
- 3. Correlation of results from week 2 practical. The concept of Standard Operating Procedures. The need to check results, the concept of the result as the correct one and that there is no absolute correct answer, the need to report data and to keep a record of the results.
- 4. The fitting of data to a straight line, the regression equation. The problems of using regression in analytical chemistry. The estimation of the quality of the data by use of the correlation coefficient, the standard error and the percentage error. The use of error bars to show errors on a graph.
- 5. The balance: care and standardisation, the need for regular calibration, NAMAS and UKAS. The documentation required for an analytical laboratory. The difference between precision and accuracy. The level of accuracy required for trace and bulk analysis.
- 6. Discussion of results of experiment on standardisation of Mn(VII) solution. More on standards, the use of bought in standard solutions. The validation of standards. Primary redox standards, the problems with standard reducing agents.

- 7. Discussion of results for standardisation of thiosulphate. The contrast between primary and secondary standards, the use of standard solutions as opposed to solids. The chemistry of the thiosulphate-iodine reaction. The application of confidence limits to analysis and the appropriate confidence limits for a given procedure.
- 8. Discussion of results for standardisation of Ce(IV) and determination of nitrite, use of redox indicators. Introduction to practical exercise: distillation, analysis of distillate. The concepts of quality control and the impact of quality control procedures on analytical chemistry.
- 9. Discussion of results from last week's exercise, the use of a liquid as a primary standard. Strong and weak acids and bases, titration curves for various acid-base titrations, the choice of indicators. Instrumental measurement of pH, automatic titrators.
- 10. Further discussion of errors for burettes and pipettes. Accumulation of errors. The calculation of the errors in standardisation using a primary and secondary standard.
- 11. Discussion of results for determination of concentration of hydrochloric acid, choice of an appropriate primary standard. Sampling: what is sampling?
- 12. The need for sampling. The consequences of not sampling properly. Sampling of solids, liquids and gases. The reasons for inhomogeneity in liquids and gases.

Principles of Spectroscopy

Academic Objectives

The aim of this unit is to provide students with an introduction to vibrational, electronic, and nuclear magnetic resonance spectroscopies, and to show their applications in the elucidation of structural information and in qualtitative and quantitative analysis.

- 1. Course objectives. The electromagnetic spectrum: what is electromagnetic radiation? Important regions of the spectrum. Units (and conversion factors).
- 2. Energy levels and Boltzmann distribution (qualitatively). Absorption of electromagnetic radiation: resonance condition, block diagram of a spectrometer, Beer-Lambert Law.
- Infrared spectrometer (block diagram). Origin of vibrational spectra: Hooke's law model of diatomic systems, selection rules, vibrational modes of polyatomic systems (3N-6)/(3N-5) (CO₂, SO₂, *etc.* as examples), effect of variation of mass (e.g., ¹H, ²H, ³H) and force constant (C-C, C=C, CC).
- 4. Group frequencies: types X-H, X=Y/XY, etc., effect of deuteration, examples from organic and inorganic molecules, limitations (conjugation, H-bonding *etc.*). Fingerprint region origin and uses. Examples of structure determination using infrared spectra.
- 5. Uv/visible absorption spectrometer (block diagram). Chromophores. Types of electronic transition in organic and inorganic species, selection rules. Effect of conjugation, substituents, solvents.
- 6. Origin of band breadth: vibrational structure. Examples of structure determination using uv/visible spectra. Analytical applications: environmental, kinetics, *etc*.
- 7. Basis of NMR spectroscopy: nuclear magnetism, nuclei in a magnetic field, resonance condition. NMR spectrometer (block diagram of cw spectrometer). Chemical shift (¹H and ¹³C); shielding and deshielding; tables of examples.
- 8. Chemical equivalence; integration to obtain relative numbers of equivalent nuclei. Spin-spin coupling. Decoupling. Examples of structure determination using NMR spectra: ethyl group, toluene, PH_nF_{3-n}.

- 9. The application of the Beer-Lambert law to measure the concentration of absorbing substances in solution. Methods of measurement.
- 10. The calibration graph. Calculation of errors.
- 11. Deviations from the Beer-Lambert law.
- 12. Basic principles of instrumentation used to measure the absorption of electromagnetic radiation, with particular emphasis on the ultraviolet/visible region of the spectrum.

BASIC INORGANIC CHEMISTRY

ECTS Credits: 5	Level: 1 Semester: 2	Code: CH104-05
Contact Hours:	32 hours comprising: 24 hours lectures and	8 hours tutorials
Pre-requisites:	Foundation General Chemistry	
Assessment:	One written examination (2 hours, 67%), co	oursework (33%)

This half module comprises two units each of 12 lectures, supported by 8 tutorials, and offers an introduction to Transition Metal Chemistry and the Chemistry of Groups 1, 2, 17 and 18.

Introduction to Transition Metal Chemistry

Academic Objectives

The aim of this unit is to provide students with an introduction to the chemistry of the dblock transition elements, concentrating particularly on the first transition series and to provide them with a basic understanding of coordination chemistry.

Detailed Syllabus

Introduction to Transition Metal Elements

1. Definition of transition metals in terms of electron configuration. Occurrence of transition metal elements in the Periodic Table. Trends in physical properties: size of atoms and ions, lanthanide contraction, melting and boiling points, densities, ionisation enthalpies, magnetism. Trends in chemical properties: metallic character, variable oxidation states, electropositive nature.

The Chemistry of the Elements of the First Transition Series

- 2. Scandium to chromium: discovery, occurrence/extraction and uses. Stability of oxidation states. Properties of major compounds: oxides and halides. Aqueous chemistry.
- 3. Manganese and iron: discovery, occurrence/extraction and uses. Stability of oxidation states. Properties of major compounds: oxides and halides. Aqueous chemistry.
- 4. Cobalt to zinc: discovery, occurrence/extraction and uses. Stability of oxidation states. Properties of major compounds: oxides and halides. Aqueous chemistry.

Coordination Chemistry

- 5. Lewis acids/bases and complexes. Terminology of coordination chemistry. Survey of common ligands. Classification of ligands as pure σ -donors, •-donors and •-acceptors.
- 6. Nomenclature. Coordination number and geometry. Structural isomerism: ionisation, hydrate, coordination, linkage and ligand isomerism.
- 7. Stereoisomerism: Geometrical and optical isomerism.
- 8. Ligand Field Theory. The molecular orbital model for σ -bonded ML₆ complexes. High spin and low spin complexes. Ligand Field Stabilisation Energy.
- 9. Factors affecting the magnitude of \bullet_0 . The Spectrochemical Series. Modification of the MO model for σ -complexes to account for ligands possessing orbitals of \bullet -symmetry.
- 10. Ligand Field Theory and thermochemical correlations. Introduction to the interpretation of the magnetic properties of octahedral complexes.
- 11. Colour and Transition Metal complexes: relation of colour to the absorption of visible light. Explanation of the features of the visible absorption spectra of d¹, d⁹, high spin

 d^4 and d^6 ions. Laporte and spin selection rules. The qualitative interpretation of colour change in terms of the magnitude of \bullet_0 .

12. Hard and Soft Acids and Bases. The Chelate Effect. Stepwise and Overall Stability constants.

Introduction to the Chemistry of Groups 1, 2, 17 and 18

Academic Objectives

The aim of this unit is to provide students with an introduction to the chemistry of Main Group elements, through the consideration of the most important aspects of the chemistry of hydrogen, the alkali metals, the alkaline earth metals and the halogens, and the chemistry of the noble gases.

- 1. Hydrogen: position in the Periodic Table, occurrence, isotopes (protium, deuterium and tritium). Ortho and para hydrogen. Methods of preparation of hydrogen. Uses of hydrogen.
- 2. Hydrides: classification as metallic, ionic and molecular; preparation and properties of hydrides. The ultra-purification of hydrogen.
- 3. Molecular hydrides. Hydrogen bonding: intra and inter-molecular hydrogen bonding, the influence of hydrogen bonding on the properties of compounds. 'The Hydrogen Economy'.
- 4. The alkali metals: discovery, occurrence and isolation. Chemical reactivity. Trends in properties on descending Group I. Caesium ratio.
- 5. The alkali metals: unusual properties of lithium. Oxides, peroxides and superoxides: reactions with water, thermal stabilities.
- 6. The salts of the alkali metals. Solutions of the alkali metals in liquid ammonia. Complexation of the alkali metals with crown ethers and cryptands.
- 7. The alkaline earth metals: occurrence and uses of Group II elements. Trends in properties on descending the Group. Properties of oxides, hydroxides and oxo-salts and how these properties vary down the Group. Unusual properties of beryllium (as first member of the Group) and the Diagonal Relationship. The biological importance of Group II compounds; chlorophyll, hydroxyapatite.
- 8. The halogens: trends in physical and chemical properties on descending Group VII (17). Origins of their names. Chemistry of the synthesis of hydrogen halides from fluorides, chlorides, bromides, and iodides. Occurrence and structure of fluorspar. Isolation of fluorine by electrochemical and chemical methods.
- 9. Preparation of anhydrous HF. Moissan's work on the isolation of fluorine. Industrial production of fluorine. Calculation of the rate of production from Faraday's Laws. Isolation of Cl₂, Br₂, and I₂. Examples illustrating the high reactivity of F₂.
- High reactivity of fluorine examples of and reasons for. Restriction of valency of F to I. Discovery of PTFE and its properties. Uses of fluorine compounds. Halogen oxo-acids.
- 11. History, occurrence and physical properties of the noble gases. Noble gas clathrates. The experiments of Yost and Kaye (1933). The experiment of Bartlett (1962).
- 12. Preparation of XeF_2 , XeF_4 , and XeF_6 especially the photochemical formation of XeF_2 by Streng and Streng. The shapes of the molecules. The special properties of fluorine that facilitate its reaction with xenon. The reaction of xenon fluorides with water. Other reactions of xenon fluorides. Compounds of krypton and radon.

BASIC ORGANIC CHEMISTRY

ECTS Credits: 5	Level: 1 Semester: 2	Code: CH105-05
Contact Hours:	32 hours comprising: 24 hours lectures and 8 hours tutorials	
Pre-requisites:	Foundation Organic Chemistry	
Assessment:	One written examination (2 hours, 67%), c	oursework (33%).

This half module consists of three units: Carbonyl Chemistry (8 lectures); Aromatic Chemistry (10 lectures); Spectroscopic Methods for Structure Determination of Organic Compounds (6 lectures). The lectures are supported by 8 tutorials.

Carbonyl Chemistry

Academic objectives

The aim of this unit is to introduce the basics of carbonyl chemistry.

Detailed syllabus

1. Types of carbonyl compounds

Examples of important C=O containing compounds (retinal, hydrocortisone, PGE₂, dacron, penicillins).

2. Structure and reactivity of the carbonyl group

Bond lengths and angles, electronic structure, -orbital and similarity with C=C, electronegativity of O causes polarisation of C=O group and very different reactivity compared to C=C. Reaction site of nucleophiles, and site of protonation (importance of O lone pairs).

Reactivity of the C=O Group - an overview of the important general types of reactions of C=O compounds. Nucleophilic addition, mechanism and examples of simple nucleophiles (RMgBr + ketone/aldehyde). Addition with loss of water, acid catalysis (imine formation); iminium ions. Nucleophilic acyl substitution, mechanism and examples of simple charged nucleophiles, formation and breakdown of tetrahedral intermediate (*e.g.* PhCOCl + MeONa). Addition of uncharged nucleophiles (*e.g.* PhCOCl + MeNH₂). Acid catalysis for less reactive C=O compounds (e.g. PhCO₂H + MeOH in presence of acid with removal of water); oxonium ions. Alpha-Substitution

Formation of enolates with base; structure and reactivity of enolates. Importance of pK_a of base and C=O compound - exemplified by LDA formation and use for deprotonation of cyclohexane. Reaction of derived enolate with methyl iodide. Acidity of C=O compounds, pK_a of typical bases and carbonyl compounds, and a 1,3-diketone. Keto-enol tautomerism, alpha-bromination of cyclohexane.

3. Aldehydes and ketones. Examples and nomenclature. Preparation of aldehydes and ketones: a) By oxidation of alcohols; b) by ozonolysis of C=C; c) from acid chlorides (formation and use of cuprates for ketone synthesis). Important general reactions of aldehydes and ketones: a) Nucleophilic addition using Nuc⁻ (NaBH₄, LiAlH₄, RLi, RMgBr, HCN/NaOH), Nuc-H and NucH₂ (RNH₂, R₂NH, ROH, RSH). Examples - hydride reduction of a ketone, Grignard addition to an aldehyde, and oxime formation - mechanisms covered previously. Relative reactivity of aldehydes and ketones; reversibility of some additions (HCN addition, example of HCN generation from

cyanohydrin of benzaldehyde as chemical defence in millipedes). Further nucleophilic additions to form enamines and acetals. Reversibility of acetal formation. Thioacetal formation and reduction with Raney Ni (C=O to CH₂). Clemmensen and Wolff-Kishner reactions to achieve (C=O to CH₂) (no mechanism for any of the reduction methods). The Wittig reaction - preparation of phosphoranes, reaction with ketones and aldehydes.

4. Carboxylic acids and derivatives

Examples and nomenclature of carboxylic acids. Structure and properties of carboxylic acids. Acidity, variation with structure (particularly the effect of electron withdrawing groups on pK_a). Preparation of carboxylic acids: a) Oxidation of alkenes; b) Oxidation of alkyl aromatics; c) Oxidation of alcohols and aldehydes; d) Hydrolysis of nitriles; e) Carboxylation of Grignard reagents.

Reactions of carboxylic acids: a) Reaction with bases (salt formation); b) Reduction (LiAlH₄ and BH₃); c) alpha-Substitution (Hell-Volhard-Zelinski reaction); d) Nucleophilic acyl substitution.

Derivatives of carboxylic acids: Examples and nomenclature; acid halides, anhydrides, esters, and amides. Reactions/preparations: a) Relative reactivity of acid chlorides, anhydrides, esters, and amides; b) interconversions between the above groups of compounds; c) Preparation of acid chlorides; d) Hydrolysis of derivatives.

Aromatic Chemistry

Academic Objectives

The aim of this course is to introduce students to the fundamental concept of aromaticity and to examine its consequences on the chemistry of benzenoid compounds. Basic mechanistic concepts are emphasised and reference is made, *inter alia*, to rate data, stable intermediates and kinetic isotope effects to probe the course of the reactions being studied. A combination of resonance bond and molecular orbital treatments are used to develop a theoretical framework for these reactions and so understand the outcome of these reactions and predict the course of reactions on new substrates. Comparisons are made with the chemistry of aliphatic compounds. Finally the various ideas are drawn together in examining the commercial synthesis of the hormone thyroxine.

Detailed Syllabus

1. Aromaticity and the structure of benzene.

Conjugation, delocalisation of electrons, resonance canonicals, the structure of benzene, aromaticity and antiaromaticity, Hückel's rule, Frost-Musulin diagrams - MO treatment of benzene, non-benzenoid aromatic compounds, ¹H NMR, ring currents.

 The four classical methods of substitution at an arene nucleus. Electrophilic aromatic substitution (E.A.S.): (a) Nitration of benzene, energy/reaction coordinate diagrams, σ-complexes (Wheland intermediates), Hammond's postulate, rate laws, kinetic isotope effects, the rate determining step. Sulphonation of benzene, reversibility, nitration vs. sulphonation of naphthalene (kinetic vs. thermodynamic control): (b) The effect of substituents, *o*-, *m*- and *p*- directing effects (resonance, inductive and field effects), partial rate factors, a change in the mechanism of nitration when phenols are the substrate, ipso substitution.

Nucleophilic aromatic substitution (N.A.S.): (a) The addition-elimination mechanism, effect on rate of the leaving group, the rate determining step, Meisenheimer complexes: (b) Diazonium salts, the S_N1 mechanism, ¹⁵N labelling, -deuterium isotope effect. The aryne mechanism: Benzyne, methods of generation, evidence for existence, Cine

substitution. S_{RN}1 mechanism: A brief description.

- 3. The synthesis of aromatic compounds.
- (i) Basic reactions: (a) C-N bond formation and manipulation of nitrogen containing functional groups: Direct and indirect methods of forming C-N bonds to an aromatic nucleus e.g. nitration, addition to diazonium salts, N.A.S. to activated aromatic rings, Hofmann, Lossen, Curtius and Schmidt rearrangements, Beckmann rearrangement. Manipulation of nitrogen functionality e.g. reduction of the nitro group and diazotisation. This part of the course will be illustrated by the application of these reactions to the synthesis of the azo-dye, butter yellow and the analgesic lidocane. In addition we will briefly cover the use of Sanger's reagent. (b) C-halogen bond formation: Direct halogenation using Lewis acid catalysts, -complexes, diazonium salts - the Sandmeyer and Schiemann reactions. Iodination of phenols. (c) C-C bond formation and manipulation of the introduced groups: Direct C-C bond formation, Friedel-Crafts alkylation (thermodynamic vs. kinetic products) and acylation, interconversion of the two types of product. Vilsmeier-Haack, Gatterman-Koch and Kolbe-Schmitt reactions. Indirect C-C bond formation e.g. the Claisen and Fries rearrangements. (d) C-O and C-S bond formation: Oxidation of cumene, the Dakin reaction, sulphonation - the sulphanilamide drugs, diazonium salts - methods of introducing O and S.
- (ii) Designing the synthesis of some simple polysubstituted aromatic compounds: Using the mechanistic principles and basic reactions we have learnt we will design approaches to some polysubstituted aromatic compounds.
- (iii) The total synthesis of thyroxine: Application of basic reactions to the synthesis of the important hormone thyroxine an industrial process.

Spectroscopic Methods for Structure Determination of Organic Compounds

Academic objectives

The objective of this short course is to introduce students to modern spectroscopic methods for structure determination. By the end of the course, students should be able to deduce the structures of simple organic compounds from a range of spectroscopic data; proton NMR, carbon NMR, IR and mass spectrometry.

Detailed syllabus

Building on the material covered in the first semester Principles of Spectroscopy 1. lectures, basic theory will be extended, focusing in particular on applications of IR, NMR, UV and MS to structure determination in organic structures. The position and strength of important organic function group absorptions in IR spectra will be highlighted. The causes of chemical shift in both carbon and proton NMR spectra will be discussed. Correlations will be made between chemical shifts in proton and carbon spectra. Methods for deducing the number of non-equivalent nuclei in carbon and proton spectra will be covered. The use of signal integration in proton NMR will be discussed and the varying strengths of different signals in carbon spectra will be explained. Simple concepts of equivalence and non-equivalence of nuclei will be discussed. Simple splitting patterns in proton and carbon NMR spectra will be explained and the importance of being familiar with common examples will be emphasised. The DEPT technique will be introduced as an alternative for determining the number of protons attached to a carbon nucleus. Mass spectrometry (EI only) will be introduced as a technique used primarily for molecular mass determination, but

some major fragmentation pathways will be observed.

2. A practical strategy for deducing the structure of a compound, using a range of spectroscopic data, will be described. The approach taken will be based on the initial determination of structural elements followed by the construction of a molecular structure which matches all the spectral data. This practical, problem solving approach will be the main part of the course and will be used to reinforce the concepts outlined in 1 above.

BASIC PHYSICAL CHEMISTRY

ECTS Credits: 5	Level: 1Semester: 2	Code: CH106-05
Contact Hours:	32 hours comprising: 24 hours lectures and	8 hours tutorials
Pre-requisites:	Foundation General Chemistry	
Assessment:	One written examination (2 hours, 67%), co	oursework (33%).

This half module comprises two units each of 12 lectures, supported by 8 tutorials, and offers:

- a general introduction to solution chemistry
- a detailed introduction to chemical thermodynamics stressing its pivotal role in providing a theoretical basis for chemical reactivity

Solution Chemistry

Academic Objectives

The aim of this unit is to provide students with an understanding of the physico-chemical properties of aqueous solutions containing ionic species.

- The properties of water as a solvent for ionic species. Meanings of 'strong electrolyte' and 'weak electrolyte'. Ionic equilibria in solution. Definitions of association and dissociation constants. Definition of solubility product. Dissociation of water. Definition of pH in terms of [H⁺] and a_H. Molar and molal definitions of concentration.
- 2. Weak acids and weak bases according to Brønsted and Lowry. Definition of acid and base dissociation constants. Calculation of pH of solutions of weak acids and bases from concentration and dissociation constants.
- 3. Buffer solutions. Titration curves. Dependence of pH of buffers on the base/acid ratio. Determinants of buffer capacity. Indicators.
- 4. Dependence of equilibrium 'constants' on concentration, the introduction of ionic activities. The physical causes of non-ideality in ionic solutions. Definition of mean ionic activity coefficients. Statement of Debye-Hückel limiting law without proof but with comment on its range of applicability. Calculation of ionic activity coefficients.
- 5. Conduction of electric charge by ionic solutions. Definitions in SI units of conductance, conductivity and molar conductivity with explanation of why these quantities are defined in the way that they are. Definition and principles of the measurement of a cell constant.
- 6/7. The variation of conductivity with concentration for strong and weak electrolytes. Molar conductivity at infinite dilution. Ionic molar conductivities. Relationship between ionic molar conductivities of [H⁺] and [OH⁻]. The calculation of the molar conductivity of strong electrolytes from ionic conductivities. The dependence of molar conductivity of weak electrolytes on the degree of dissociation. Calculation of dissociation constants and solubility products from conductivity measurements.
- 8. The measurement of conductivity. The principles of the operation of AC bridges. The dependence of conductivity on temperature and the solvent. Types of conductivity cell.

- 9. Ionic equilibria at the interface of ionic solutions. Definitions of oxidation and reduction. The reasons why an electrode in an ionic solution acquires a charge and a potential. The meaning of the term 'electrical potential' and the necessity of defining a standard against which electrode potentials are measured. The hydrogen electrode standard.
- 10/11.Standard states and standard reduction potentials. The convention adopted in calculating a cell potential from electrode potentials. The derivation of an overall reaction from half cell reactions. The relationship between a cell emf and the direction of spontaneous reaction. The notation used in specifying a cell. Examples of half cell reactions. The relationship between Gibbs free energy for a reaction and the emf of a cell. The Nernst equation. The calculation of cell potentials when components are not in standard states.
- 12. The application of electrode measurements. Glass pH electrodes and ion selective electrodes. The calomel electrode and combination electrodes. The selectivity of ion selective electrodes. Electrochemical cells as devices for the storage of electricity.

Chemical Thermodynamics

Academic Objectives

The aim of this unit is to provide students with an introduction to thermodynamics and its application in chemistry.

Detailed Syllabus

First Law of Thermodynamics

- 1/2. Conservation of energy. Heat and work as forms of energy transfer. Work of expansion. Calorimetry. Heat changes measured at constant volume as the change in internal energy of the system, and heat changes measured at constant pressure as the change in enthalpy of the system. The relationship between enthalpy and internal energy.
- 3. Enthalpies of phase changes (latent heats) vaporisation, sublimation and fusion. Specific heat capacity as the change of enthalpy with temperature. Ionisation enthalpies and electron affinity. Bond enthalpies. Enthalpies of chemical reaction and solution.
- 4. Hess's Law. Standard states and standard reaction enthalpies. Standard enthalpies of formation, combustion. Reaction enthalpies from enthalpies of formation. Temperature dependence of reaction enthalpies and specific heats (Kirchoff's Law).

Second Law of Thermodynamics

- 5/6. The maximisation of total entropy (including both system and surroundings) as the driving force toward equilibrium. Calorimetric measurement of entropy, from specific heats and latent heats. Absolute zero and absolute entropies. Standard entropies of reaction from absolute entropies.
- 7/8. Free-energy as a measure both of the change in total entropy and of available work. The relationship between free-energy, enthalpy and entropy. The concentration dependence of molar free-energy and the activity of chemical components. Reaction quotients and equilibrium constants expressed in terms of activities. Standard freeenergies of reaction, their relationship to equilibrium constants. The temperature dependence of equilibrium constants and its relationship to standard reaction enthalpy (van't Hoff equation).

Phase equilibria

9. Phase diagrams as 'maps' used to describe the occurrence of phases and transitions

between phases. The phase rule. Phase diagrams of pure substances. Phase boundaries, triple points and critical points. Variation of vapour pressure with temperature (Clausius-Clapeyron equation).

10/11.Non-ionic solutions. Raoult's limiting law for the vapour pressure of the solvent. Henry's limiting law for the vapour pressure of the solute. Ideal solutions. Phase diagrams of two-component mixtures. Tie-lines and the lever rule. Liquid-vapour equilibria. Distillation and fractional distillation. The formation of 'constant boiling mixtures' (azeotropes) in non-ideal solutions. Liquid-liquid equilibria and phase separation for partially miscible liquids. Distillation of partially miscible liquids. Liquid-solid equilibria and eutectic formation.

Thermodynamic data of ionic reactions from cell EMFs

12. EMFs and the free-energy of the cell-reaction. Using measurements of the temperature dependence of EMFs to determine the entropy and enthalpy of the cell-reaction.

CORE INORGANIC CHEMISTRY 1

ECTS Credits: 5	Level: 2Semester: 1	Code: CH201-05
Contact Hours:	32 hours comprising: 24 lectures and 8 tutorials	
Pre-requisites:	Basic Inorganic Chemistry	
Assessment:	One written examination (2 hours, 80%) a	and coursework (20%)

This module will consist of two units, one in Main Group Chemistry dealing with Groups 13, 14, 15 and 16, and the other providing an introduction to the use of infrared and NMR spectroscopies in Inorganic Chemistry.

Main Group Chemistry

Detailed Syllabus

Group 13

- 1. Introduction to the natural occurrence of the group 13 elements and their extraction from minerals. Properties, structures, and uses of the elements. Chemical properties and trends in reactivity of the elements.
- 2. The preparation, structure and uses of metal borides. The preparation of bonding in boron hydrides.
- 3. The structures and naming of boron hydrides (closo, nido, arachno, *etc.*). ¹¹B NMR spectroscopy and other methods for the characterisation of boranes. The preparation and properties of carboranes and metalloboranes.
- 4. Boron oxygen compounds: borates, oxides and boric acid. Group 13 halides: preparation, structure and uses *e.g.* in Friedel-Crafts catalysis.
- 5. Oxides and hydrides of the lower group 13 elements. The uses of LiAlH₄ as a reducing agent. Organometallic compounds of the group 13 elements and Ziegler-Natta catalysis.

Group 14

- 1. Introduction to the occurrence, extraction and isolation of the group 14 elements. Group chemical trends in bond strengths, oxidation states (M(II) and M(IV)), and the potential for multiple bond formation.
- 2. Carbon allotropes, graphite, diamond and C_{60} . Oxides and halides of carbon and intercalation compounds *e.g.* C_{60} K. Silicon hydrides and halides. Catenation in group 14 compounds.
- 3. Silicon oxides, silicate structures. Aluminosilicates: the formation and uses of zeolites.
- 4. The direct process for preparing organochlorosilanes, their hydrolysis and the formation and uses of silicones. Preparation and uses of polysilanes and polycarbosilanes. The formation of silicon carbide.
- 5. Hydrides, halides, and oxides of the lower group 14 elements. NMR properties of the group 14 elements.

Groups 15 and 16

- 1. Occurrence and physical properties of the elements. Geochemical, biochemical, atmospheric and industrial reactions of the elements. Trends in radii, ionisation enthalpy, bond energies, and electronegativity. Introduction to oxidation states. Inert Pair Effect. First element anomaly.
- 2. Allotropes and their structures especially those of phosphorus and sulphur.

Polysulphur species and the lability of the S–S bond. The application of VSEPR theory to the compounds of the elements of groups.

- 3. Relation of the chemistry to oxidation states: diversity, and stability. Expression of the stability of oxidation states in terms of electrochemical data. Oxidation-reduction data, Frost and Latimer diagrams.
- 4. Ligand properties of the elements and their compounds. Hydrolysis reactions involving compounds of the elements of groups 15 and 16. Limitations of water as a solvent and the use of group 15 and 16 compounds as non-aqueous solvents.
- 5. Nitrogen: stability, chemical and biochemical reduction to ammonia. Nitrides, hydrides, halides, oxides and oxoacids.
- 6. Phosphorus: the chemistry of the halides, hydrides, oxides and oxoacids of phosphorus. Phosphides. Phosphazenes.
- 7. Oxygen: Structure and bonding of the allotropes of oxygen. Oxidation reactions involving singlet oxygen, atomic oxygen, and peroxo species. Ozone; its production and reactions in the upper atmosphere. Oxides; classification according to bond type and chemical behaviour. Dioxygen as a ligand. Solvent properties of water. Oxidation-reduction properties of hydrogen peroxide.
- 8. Sulphur: Allotropy, S_n rings and chains (polysulphides and polysulphanes), S–S bonding. Sulphides; classification according to bond type and chemical behaviour. Precipitation of metal sulphides from solution as a means of separating metal ions. Chemistry of hydrogen sulphide. Halides, oxohalides, oxides, oxoacids and oxoanions of sulphur. Sulphur-Nitrogen compounds.

The Use of Infrared, Raman and NMR Spectroscopies in Inorganic Chemistry

Academic Objectives

The aim of this unit is to introduce the use of symmetry and point group notation to characterise the structure of molecules and to develop the application of infrared, Raman and NMR spectroscopic methods in the determination of the structures of inorganic molecules.

- 1. Symmetry operations and point groups. Assignment of symmetry point groups, motion of molecules, symmetry and group tables. Determination of stretching modes.
- 2. Identification of bands as infrared/Raman active, identification of specific vibrations, determination of all vibrational modes in a molecule.
- 3. Analysis of ammonia and the ammine ligand, general points concerning infrared/Raman bands arising from metal ammine complexes.
- 4. Practical infrared spectroscopy; metal carbonyl complexes, metal halides, identification of bands using isotopic substitution, general observations concerning (M-X).
- 5. Origins of NMR resonance and spin-spin coupling; CW and FT techniques; proton magnetic resonance, chemical shift ranges for inorganic molecules in ¹H NMR spectroscopy, use of proton-proton coupling constants to determine geometry of molecules; heteronuclear magnetic resonance, general description of problems in observing spectra.
- 6. Chemical shift ranges of ¹⁹F, ³¹P, ⁵⁹Co, ¹¹⁹Sn and ¹⁹⁵Pt, problems solvable from chemical shift data; proton-heteronuclear coupling constants for geometry and connectivity determination; satellite spectra and their use in structure determination.
- 7. NMR spectroscopy of solid samples, MAS and examples of information available from these spectra.

CORE INORGANIC CHEMISTRY 2

ECTS Credits: 5	Level: 2Semester: 2	Code: CH202-05
Contact Hours:	32 hours comprising: 24 lectures and 8 tutorials	
Pre-requisites:	Basic Inorganic Chemistry	
Assessment:	One written examination (2 hours, 80%)	and coursework (20%)

This module will consist of two units both of which are concerned with the chemistry of the transition elements. The first unit is concerned with advanced transition metal chemistry and the second with organometallic chemistry.

Advanced Transition Metal Chemistry

- 1. Introduction and recapitulation of previously taught transition metal chemistry: ligand types, formal oxidation states and valence electron counting, octahedral ligand field splitting, factors affecting the magnitude of \bullet_0 (charge density, position in a group, spectrochemical series and reasons behind the series), high/low spin complexes and identification by magnetic means.
- 2. Review of the basic properties of transition metals: size of M and M²⁺, coordination geometries other than octahedral including tetrahedral, square planar and five coordinate coordination, molecular orbital diagrams for the geometries and their magnetic properties; trends in geometry and the rationale behind them, trends in oxidation state. Application of redox potentials to transition metal chemistry: basic principles, calculation of potentials between oxidation states and for reactions, variation of potential with pH and ligand sphere, stability of species in water as a function of pH, redox potentials of poorly soluble complexes.
- 3. Chemistry of Cr, Mo and W (group 6): topics to be developed include optical and magnetic properties, metal-metal multiple bonds, associative and dissociative substitution at octahedral metal centres; rates of water exchange, charge density arguments, LFSE arguments, prediction of inert configurations, extrapolation to other substitution reactions, identification of reactions as A or D; the dative-conjugate base mechanism.
- 4. Chemistry of Fe, Ru and Os (group 8): topics to be developed include optical and magnetic properties, spin-crossover, high oxidation state metals.
- 5. Chemistry of Ni, Pd and Pt (group 10): topics to be developed include optical and magnetic properties, geometric isomerisation (T_d vs. D_{4h} vs. O_h). Substitution at square planar metal centres, rate law and mechanism, evidence for mechanism, transition state, effect of incoming nucleophile, solvent effects, nature of the incoming nucleophile, discussion of nucleophilicity, adaptation of the Swain-Scott relationship to Pt(II), nature of the leaving group, trans-influence and effect, use of the trans-effect, mechanism of the trans-effect.
- 6. Redox equilibria, outer sphere electron transfer, discussion of important criteria which affect rate, Franck-Condon principle, Marcus theory, examples, inner sphere electron transfer, mechanism and evidence for the mechanism, discussion of important criteria which affect rate, models of biological systems, inner sphere vs. outer sphere.

Organotransition Metal Chemistry

Academic Objectives

The academic objective of this unit is to provide an introduction to the chemistry (including synthesis, reactivity, uses, structure and bonding) of transition metal compounds which contain a metal-carbon bond.

Detailed Syllabus

Metal Carbonyl and Related Complexes

- 1. Full MO description of $M(CO)_6$, M = Cr. Synergic bonding: description, physical consequences, v_{CO} for isoelectronic series and geometrical polycarbonyl isomers, bond length changes. The 18-electron rule: relative energies of 3d, 4s, and 4p orbitals across the series, deviations from the rule. Tolman's rule. Synthesis of binary carbonyls: high pressure *e.g.* Fe(CO)₅, Mo(CO)₆, low pressure by electron transfer *e.g.* V(CO)₆⁻, Ta(CO)₆⁻, Mn₂(CO)₁₀.
- 2. Chemistry of binary carbonyls: thermolysis and photolysis. Dissociative pathways. Preparation of bridging carbonyls: electron counting and the concept of fragments in large cluster building. Supported and unsupported metal-metal bonds in carbonyl clusters. Similarity of synergic bonding for NO, CNR and PR₃ compared to CO. Use of Ru and Rh systems to demonstrate associative and dissociative mechanisms in preparation of complexes of these ligands. The •-bonding ability series for CO, NO, CNR and PR₃.
- 3. Migratory insertion, elimination and addition reactions. Catalytic cycles for hydrogenation, hydroformylation and hydrosilylation [single 2e donor property for olefin assumed at this part]. Use of D_2 to label stereospecificity of above reactions. Monsanto Acetic Acid Process.

Metal Alkene Complexes

- 1. Dewar-Chatt and metallocyclopropane models: effect of dⁿ, structural measures, $v_{C=C}$, X-ray structures $r_{C=C}$, bonding of substituents. Reactivity nucleophilic attack, the Wacker Process.
- 2. Bonding of butadiene, weighting of ψ_1 , ψ_2 and ψ_3 as a function of metal moiety, use of X-ray and ${}^1J_{CH}$ as structural probes. Reactivity comparison between conjugated and non-conjugated dienes.

Organometallic Chemistry

- 1. Classification η number, tautomeric representation, concept of fluxionality in carbocyclic ligands. Odd/even labels, systematic naming of carbocyclic ligands.
- 2. Tolman's rule repeated; 16e/18e fragments and intermediates in synthesis of carbocyclic complexes. Synthesis of $\eta^2 \eta^6$ complexes as a consequence of 2e cycling and 18e rule.
- 3. Consequences of metal basicity: electrophilic attack *e.g.* $(\eta^5-C_5H_5)CoL_2$ to describe full pathway. Rearrangement of carbocyclic ligands on protonation.
- 4. Consequences of ligand charge: nucleophilic attack, Davies, Green, Mingos rules. Synthesis of pheromone using cationic $(\eta^5-C_5Me_5)Mo(CO)_2(\eta^4-diene)$ complexes to illustrate stereocontrol and face selection.

Metal Alkyl and Hydride Complexes

1. Synthesis and stability: revision of earlier material on catalysis. General preparative routes: work of Whitesides (β -elimination), Schrock (α -elimination) and Green (α and

 β elimination). γ and δ elimination (Wilkinson). The molecular hydrogen ligand and its relevance to catalytic cycles seen earlier. Hydrogenation of d⁰ metal alkyls. 2.

CORE ORGANIC CHEMISTRY 1

ECTS Credits: 5	Level: 2Semester: 1	Code: CH203-05
Contact Hours:	32 hours comprising: 24 lectures and 8 tute	orials
Pre-requisites:	Basic Organic Chemistry	
Assessment:	One written examination (2 hours, 80%) as	nd coursework (20%)

This module will consist of three units:

- Spectroscopic Methods for Structure Determination of Organic Compounds, part 2 (4 lectures)
- Heterocyclic Chemistry (10 lectures)
- Carbonyl Chemistry and Reactions at Positions to Carbonyl Groups (10 lectures)

Spectroscopic Methods for Structure Determination of Organic Compounds part 2

Academic Objectives

The aim of this short course is to provide students with further practice of modern spectroscopic methods for structure determination. By the end of the course, students should be able to deduce the structures of simple organic compounds from a range of spectroscopic data, distinguish between diastereotopic protons and groups in NMR spectra, and present spectroscopic data in RSC publication style.

Detailed Syllabus

- 1. Characterisation of organic compounds by spectroscopy: a description of the data required for characterisation and how it should be presented in the style required for RSC publications.
- 2. Some further aspects of mass spectrometry: chemical ionisation; FAB ionisation; electrospray ionisation; simple fragmentation patterns; use of HRMS.
- 3. Proton NMR spectroscopy: chemical shift estimation; determination of proton equivalence; proton coupling patterns; spin-spin decoupling; magnitude of coupling constants.

The aspects listed above will be taught through spectroscopic problem solving exercises.

Heterocyclic Chemistry

Academic Objectives

The aim of this unit is to introduce students to ring-systems containing elements other than carbon, and to show how this heteroatom affects not only the chemistry of the ring but also the chemistry of substituents attached to the ring. Particular emphasis will be given to 5- and 6- membered rings containing one nitrogen atom, *i.e.* pyrrole and pyridine, although 5- membered systems containing an oxygen or sulphur, and systems containing two nitrogen atoms will be included. The importance of naturally occurring and synthetic heterocyclic systems in biological systems and their use as pharmaceuticals will be stressed, *e.g.* quinine.

Detailed Syllabus

1. Brief survey of naturally occurring and synthetic heterocyclic systems and their uses. Saturated and unsaturated systems as exemplified by pyridine and piperidine. Nomenclature of 5- and 6- membered systems containing one or more of the heteroatoms O, N, and S. Aromaticity and basicity of pyridine and its electronic structure. The concept of •-deficiency and the effect of the ring nitrogen on electrophilic and nucleophilic substitution.

- 2. Electronic structure of pyrrole and comparison with that of pyridine. Acidity and basicity of pyrrole. -Excessive nature of pyrrole and the effect of the ring-nitrogen on electrophilic and nucleophilic substitution. The effect of two nitrogens in a five-membered ring *e.g.* imidazole and pyrazole and the concept of tautomerism in these ring-systems, and the different natures of the two nitrogen centres.
- 3. The chemistry of pyridine and its derivatives. Pyridinium ions. Electrophilic substitution at carbon and the effect of ring substituents, *e.g.* amino and hydroxy. N-alkylation and N-acylation. Reduction of the ring Birch reduction. 1,4-dihydropyridines. NADH models. Paraquat. Pyridine N-oxide. Effect of the N-oxide on the electrophilic substitution of the ring. Deoxygenation methods for N-oxides.
- 4. Nucleophilic substitution of pyridine Chichibabin reaction. Metallation. Chemistry of substituents, in particular of 2- and 4- methyl-, chloro-, amino-, and diazonium groups. The pyridone-hydroxypyridine tautomerism. Pyridine carboxylic acids. Pyridinium compounds *e.g.* Mukaiyama's reagent.
- 5. Synthesis of pyridines Hantzsch and Guareschi-Thorpe syntheses. The concept of annulation of a benzene ring to pyridine. Quinoline and isoquinoline: Electrophilic substitution of quinoline and isoquinoline. Explanation of the regiochemistry of these substitutions using transition state theory. Reissert compounds. Abnormal electrophilic substitution *e.g.* 3-bromination.
- 6. The principles of ring-closure reactions to generate quinoline and isoquinoline rings. General methods of synthesis from arylamines, *e.g.* Skraup and related reactions, Knorr and Conrad-Limpach syntheses; Bischler-Napieralski and Pomeranz-Fritsch syntheses. Synthesis from substituted arylamines, *e.g.* Friedlander synthesis.
- 7. Brief introduction to six-membered rings containing two nitrogens in particular pyrimidines and purines and the tautomerism associated with the adenine, cytosine, guanine and tyrosine units in DNA structures.
- 8. The chemistry of five-membered heterocycles. Electrophilic substitution of pyrrole: protonation of the ring and its polymerisation; halogenation, nitration using acetyl nitrate, Vilsmeier reaction, diazonium coupling. Reimer-Tiemann reaction: ring expansion to 3 chloropyridine. Comparison of pyrrole and phenol chemistry. Acidity of pyrrole.
- 9. Effect of acids on furan; Aromaticity *vs.* diene character of furan, pyrrole, thiophene and their derivatives *e.g.* N-acyl pyrroles and thiophene S,S-oxides. Desulphurisation of thiophene derivatives. General synthesis of furans, pyrroles and thiophenes from 1,4-dicarbonyl compounds. Knorr pyrrole synthesis. Introduction to the synthesis of 5-membered rings containing two hetero atoms by ring-closure of 1,3-dicarbonyl compounds. The use of p-toluenesulphonyl isocyanide (TOSMIC).
- 10. The chemistry of indole. Electrophilic substitution. Methods of synthesis: Fischer indole synthesis, Reissert synthesis from o-nitrotoluenes, from o-lithio compounds. Naturally occurring indoles: tryptophan, serotinin, plant hormones. Indoxyl and indigo.
- 11. A brief introduction to the concept of 1,3-dipolar cycloadditions and hetero Diels-Alder cycloadditions for the synthesis of 5- and 6- membered heterocycles. Examples will include nitrones, pyridine N-oxides, N-phenacylpyridinium compounds and Niminopyridines as 1,3-dipolar species; ozonolysis as a 1,3-dipolar reaction. The use of heteromultiple bonds as dienophiles and dipolarophiles. The use of oxazoles as dienes

for the synthesis of pyridines; the diene character of electron-deficient di-, tri-, and tetra-azines.

Carbonyl Chemistry and Reactions at Positions Alpha to Carbonyl Groups

Academic Objectives

The aim of this course is to enable students to understand why and how carbonyl compounds and related systems react with electrophiles at the - position. The principles of designing synthetic routes to organic molecules in a stepwise manner by retrosynthetic analysis will also be introduced. The course should enable students to design simple synthetic sequences involving carbonyl chemistry and basic organic reactions covered in previous courses.

Detailed Syllabus

Carbonyl Chemistry

- 1. Overview and general introduction. Review of First Year carbonyl chemistry, with particular emphasis on general types of reaction, especially nucleophilic addition and alpha-substitution.
- 2. Introduction of 'retrosynthetic analysis': consideration of disconnection approach using the simple nucleophilic additions covered in the general introduction; the synthesis of alcohols.
- 3. Addition-elimination: acetal and thioacetal formation; imines and enamines; Wolff-Kishner reaction; Wittig reaction. Mechansim, synthetic applications, and retrosynthetic analysis involving this chemistry, including C=C formation, reductive amination, reduction of C=O to CH₂.
- 4. Organic synthesis and 'retrosynthetic analysis': some simple examples of multi-step organic synthesis will be analysed and synthesis plans developed based on the chemistry covered in the course and that covered in the First Year.

Reactions at Positions alpha to Carbonyl Groups

Keto-enol tautoerism; important reactions which proceed via the enol form described in retrosynthetic and mechanistic form. Revision of the concept of judging acidity/basicity using the pK_a scale; comparison of common base strengths with acidities of protons in a variety of organic molecules. The general synthetic importance of carbanions; problems associated with carbonyl deprotonation and precise conditions (LDA/THF/-78 • C) for effective enolate formation. Synthetically important reactions involving enolates and their usefulness in terms of retrosynthetic analysis; reaction types to be covered include alkylations, Michael additions and aldol reactions. The selective formation of regioisomeric enolates, from carbonyls, under 'kinetic' and 'thermodynamic' conditions; regiospecific enolate formation from silyl enol ethers and from ,-unsaturated compounds; illustration of synthetic strategies involving such enolates. The use of enamines in synthesis, as mild alternatives to enolates. Explanation of the enhanced acidity of 1,3-dicarbonyl protons; conditions required for enolate formation will be contrasted with those required for enolisation of monocarbonyls; the synthetic utility of 1,3-dicarbonyl reagents. Methods for preparing 1,3-dicarbonyls illustrated in both mechanistic and retrosynthetic form; reaction types covered will include aldol condensations, Knoevangel reactions and Wittig reactions. The mechanism of aldol condensations under protic conditions compared with that of aldol reactions under aprotic conditions. The Robinson annulation method in both

mechanistic and retrosynthetic form; examples showing its synthetic importance. Claisen and Diekmann reactions in mechanistic terms and as methods for preparing 1,3-dicarbonyl compounds.

CORE ORGANIC CHEMISTRY 2

ECTS Credits: 5	Level: 2Semester: 2	Code: CH204-05
Contact Hours:	32 hours comprising: 24 lectures and 8 tutorials	
Pre-requisites:	Basic Organic Chemistry	
Assessment:	One written examination (2 hours, 80%	b) and coursework (20%)

This module will consist of two units, one in Alicyclic Chemistry and the other in Organic Stereochemistry and Conformational Analysis.

Alicyclic Chemistry

Academic Objectives

The aim of this unit is to provide an introduction to the synthesis and chemistry of alicyclic compounds, and to explore their reactivity, structure, and bonding.

- 1. Introduction to alicyclic compounds. Classification of ring systems. Brief discussion of the shape of cyclic compounds, and the different types of ring strain present (angle strain, non-bonded interactions, torsional strain). How to estimate the ring strain present in cycloalkenes.
- 2. General methods of ring synthesis. Applicability of reversible and non-reversible cyclisation reactions to ring synthesis. General cyclisation methods involving the intramolecular reaction of carbanions with various electrophiles (alkyl halides, carbonyl groups). Intramolecular coupling of radicals (acyloin condensation). Ring expansion methods. Ring contraction methods.
- 3. Structure of cyclopropanes bent bonds, unusual hybridisation of carbon atoms, all consequences of high angle strain. Specific methods for the preparation of cyclopropanes carbene and carbenoid additions to alkenes. Singlet and triplet carbenes and the mechanism of their addition to alkenes. Stereochemical consequences of carbene configuration. Different methods of generating carbenes.
- 4. Chemistry of cyclopropanes. Similarity of the reactions of cyclopropanes with that of alkenes. Reaction with electrophiles, resistance to oxidation, cyclopropyl carbanions (configuration stability), cyclopropyl carbonium ions (spontaneous ring opening), nucleophilic addition to cyclopropyl ketones, electrophilic addition to cyclopropanols.
- 5. Specific methods for the preparation of cyclobutanes [2+2] cycloadditions (including regioselectivity). Specific methods for the preparation of cyclopentanes. General comments regarding the chemistry of these ring systems.
- 6. Specific methods for the preparation of cyclohexanes Diels-Alder reaction (including regioselectivity), reduction of aromatic systems. Robinson annulation. General comments regarding the chemistry of these ring systems.
- 7. Problems in the formation of medium and large ring systems. Cyclisation versus polymerisation. Use of high dilution and template effects to promote cyclisation. Transannular reactions in medium rings.

Organic Stereochemistry and Conformational Analysis

Academic Objectives

The academic objectives are to introduce the student to the fundamental concepts and principles of stereochemistry and conformational analysis and to enable them to understand the basis of stereoselective synthesis, which is an extremely important area of modern organic chemistry.

Detailed Syllabus

Enantiomers

- 1. Chirality; enantiomers, chiral centres, configuration (R/S).
- 2. Properties of isomers; identical in achiral environment, different in chiral environment, *e.g.* biological activity.
- 3. Chiral centres without chirality; compounds with plane of symmetry (meso compounds), centre of symmetry.
- 4. Chirality without chiral centres; atropisomers, allenes, helicenes.
- 5. Heteroatom chiral centres; silanes, amines, amine oxides, ammonium salts, phosphines, phosphates, sulphoxides.

Diastereomers

- 1 Relationships between groups, diastereomers have different properties, 2ⁿ rule, epimers, nomenclature. Resolution and Determination of Enantiomeric Excess.
- 2. Polarimetry, specific rotation measurement of enantiomeric excess.
- 3. Conversion into diastereomers, chiral derivatising agents, resolution, enantiomeric excess by NMR, GC, HPLC.
- 4. Spectroscopy (NMR) in a chiral medium, chiral shift reagents, chiral solvating agents. Chromatography on chiral stationary phases (GC, HPLC).
- 5. Kinetic resolution.

Stereoselectivity

- 1. Control of absolute configuration, strategies; resolution, chiral pool, asymmetric synthesis.
- 2. Using achiral reagents: *e.g.* hydroboration; diastereoselective, enantiomeric transition states, product is racemic.
- 3. Using chiral reagents: *e.g.* hydroboration with a chiral borane; enantioselective and diastereoselective, diastereomeric transition states, prochiral centre, enantiotropic groups and faces, enantioselective epoxidation, *etc*.

Diastereoselectivity: Control of configuration

- 1. Osmylation of an alkene; bishydroxylation, diastereoselectivity arising from mechanism, diastereomeric excess, syn addition, product is racemic; Aldol reaction.
- 2. Osmylation of a chiral alkene; diastereoselectivity relative to existing chiral centres, steric approach control, diastereotopic faces and groups, non-equivalence of diastereotopic protons, geminal/vicinal coupling constants.
- 3. Additions to alkenes; syn/anti addition osmylation, hydroboration, epoxidation, hydrogenation, bromination.
- 4. Eliminations: syn eliminations, selenoxide elimination, anti eliminations, E2.

Reactions at Chiral Centres

- 1. Retention; oxidation of boranes, Baeyer-Villiger, many rearrangements, concerted bond formation/bond breaking.
- 2. Inversion; S_N^2 , concerted bond breaking/formation.

3. Racemisation; non-concerted bond breaking/formation, trigonal intermediates, $S_N 1$: *via* planar carbonium ion.

Conformational Analysis

- 1. Ethane and butane; staggered, eclipsed, antiperiplanar, gauche, synperiplanar conformations. Karplus curve.
- 2. Sources of strain; *e.g.* gauche conformation, bond stretching bond angle, torsional, van der Waals strain, orbital overlap, dipole-dipole interactions. Actual conformations are one in which the total strain is minimised.
- 3. Potential energy curve; butane exists as an equilibrium mixture of isomers.
- 4. Cyclopropane: high angle strain, bent bonds
- 5. Cyclobutane: high angle strain, relief of torsional strain by ring puckering.
- 6. Cyclopentane: little angle strain, considerable torsional strain; puckered: envelope, half-chair, pseudorotation.

Cyclohexane

- 1. Chair, boat, twist-boat forms. Energy profile.
- 2. Monosubstituted cyclohexanes: axial, equatorial groups, chair-chair interconversion, 1,3-diaxial steric interaction, equatorial preference, conformational free energies, variation with size, substitution, and hybridisation.
- 3. Di/poly-substituted cyclohexanes: prediction of more stable chair form, Chirality; ignore puckering, dipolar interactions, coupling constants.
- 4. Cyclohexanone and cyclohexene conformations.
- 5. Heterocycles: chairs, anomeric effect; orbital explanation.
- 6. Decalins: trans; and cis conformations. Medium rings (n = 7-11) and Large rings (n > 11), interpretation of their conformations.

CORE PHYSICAL CHEMISTRY 1

ECTS Credits: 5	Level: 2Semester: 1	Code: CH205-05	
Contact Hours:	32 hours comprising: 24 lectures and 8 tutorials		
Pre-requisites:	Basic Physical Chemistry		
Assessment:	One written examination (2 hours, 80%) and coursework (20%)		

This module will consist of two units each of 12 lectures and will be concerned with Kinetics and Photochemical Kinetics, and Polymers.

Kinetics and Photochemical Kinetics

Academic Objectives

The aim of this unit is to provide the students with an understanding of the basic principles of chemical kinetics and their application to interpret the kinetic behaviour of chemical systems.

Detailed Syllabus

- 1. Derivation of 1st, 2nd and nth order integrated rate equations. Differential rate equations. Calculation of reaction order and rate constants.
- 2. Derivation of integrated rate equations for simultaneous and consecutive reactions.
- 3. Simple Collision Theory. Transition State Theory.
- 4. Significance of activation energy and entropy of activation. Isotope effects.
- 5. Complex reactions: chain reactions; reactive intermediates; steady state treatment.
- 6. Examples of the application of steady state treatment for the kinetic analysis of complex reactions chosen from, for example, (i) H₂/Cl₂ system; (ii) CH₃CHO decomposition; (iii) Enzyme reactions Michaelis-Menten Equation; (iv) Determination of bond strengths.
- 7. Solution reactions: comparison of gas phase and solution reactions; ionic and salt effects.
- 8. Primary kinetic salt effect: Brønsted-Bjerrum Equation.
- 9. Comparison between thermal (Boltzmann) and photochemical (non-Boltzmann) systems. Basic laws of importance to photochemistry: Grotthus-Draper Law; Beer-Lambert Law; Planck's Quantum Theory; Einstein's Law of Photochemical Equivalence.
- Excitation by absorption in UV/visible region. Selection rules for electronic transitions; Franck-Condon Principle. Jablonski diagram - Primary Photochemical Reactions: internal conversion and intersystem crossing; fluorescence and phosphorescence; sensitisation and quenching; chemical reactions; secondary photochemical reactions.
- 11. Quantum Yields: definition and measurement; calculation of kinetic parameters.
- 12. Determination of rate constants for emission and energy transfer processes Stern-Volmer approach. Experimental techniques.

Polymers

Academic Objectives

This unit aims to provide fundamental physicochemical aspects of synthetic macromolecules produced by various mechanistic routes. Kinetics are dealt with in order to afford an appreciation of how long chains are built up. Because the conventional methods of molar mass determination used for simple molecules are inappropriate for macromolecules, the special modern techniques needed are described from both the theoretical and experimental standpoints.

- 1. Concept of macromolecule, repeating unit and chain length. Examples of synthetic and naturally occurring polymers. Nomenclature. Gradation from simple molecules to oligomer to polymer. Bibliography relevant to this unit.
- 2. Synthesis by step growth polymerisation; mechanism and kinetics. Detailed treatment of acid catalysed polyesterification; experimental procedures. Distribution of chain lengths in linear step growth polymers.
- 3. Free radical addition polymerisation; mechanism and kinetics. Experimental procedures for measuring rate. Kinetic chain length and its relation to chain length.
- 4. Cationic polymerisation; mechanism and kinetics. Role of temperature on rate and chain length. Anionic polymerisation; mechanism and simplified treatment of 'living' polymers.
- 5. Reason for heterogeneity in molar mass of polymers. Definitions of molar mass averages.
- 6. Theory and practice of determination of number average molar mass by vapour pressure osmometry, osmotic pressure and end-group analysis. Limitations of methods.
- 7. Theory and practice of determining weight average molar mass by sedimentation equilibrium in the ultracentrifuge.
- 8. Theory and practice of determining weight average molar mass by light scattering from polymer solutions; simultaneous derivation of polymer dimensions.
- 9. Indirect determination of molar mass by solution viscosity; the Mark-Houwink relationship.
- 10. Principles of indirect determination of molar mass by size exclusion chromatography.

CORE PHYSICAL CHEMISTRY 2

ECTS Credits: 5	Level: 2Semester: 2	Code: CH206-05	
Contact Hours:	32 hours comprising: 24 lectures and 8 tutorials		
Pre-requisites:	Basic Physical Chemistry		
Assessment:	One written examination (2 hours, 80%) and coursework (20%)		

Quantum Mechanics and Molecular Spectroscopy

Academic Objectives

The aim of this module is to provide students with an introduction to Quantum Mechanics, an understanding of the theoretical basis of infrared, Raman, microwave and nuclear magnetic resonance spectroscopies and the relation ship between spectra and the properties of molecules.

Detailed Syllabus

Introduction to Quantum Mechanics

The photoelectron effect and its explanation in terms of the photon theory of electromagnetic radiation; the Davisson-Germer experiment and its interpretation using the de Broglie relationship.

Wave description of a particle moving with uniform velocity; the concept of an operator; momentum an kinetic energy operators.

Eigenvalue equations; the Schrödinger equation; properties of a wave function; expectation values.

Application of the Schrö dinger equation to finding the wave functions and energy levels of a particle confined in a one-dimensional box; the uncertainty principle. Electron spin; the symmetry properties of wave functions used to describe Fermi particles; the Pauli exclusion principle; application of the particle in a box model to conjugated •-electron systems.

Particles in 2- and 3- dimensional boxes; the separation of variables; degenerate energy levels.

NMR Spectroscopy

Basic principles: nuclear magnetism, the resonance condition; continuous wave and Fourier transform NMR spectrometers.

Chemical shift: definition and origins.

Spin-spin coupling: origins; spin decoupling.

Chemical and magnetic equivalence; integration.

Spin systems; first order spectra; second order spectra.

Spin relaxation; exchange processes.

Vibrational and Rotational Spectroscopy

Quantisation of vibrational energy; the harmonic oscillator model of a diatomic molecule; selection rules.

Anharmonicity; the Morse potential; fundamentals and overtones; calculation of the dissociation energy of a diatomic molecule.

Polyatomic molecules: infrared and Raman activities; rule of mutual exclusion; group frequencies and the fingerprint region.

Raman spectroscopy: principles; comparison with infrared spectroscopy; the

depolarisation ratio and its relationship to the symmetry of vibrational modes. Quantisation of rotational energy; the rigid rotor model; determination of the bond length of a diatomic molecule from rotational spectra.

Polyatomic molecules: spherical, symmetric and asymmetric tops; rotational spectra; determination of structural parameters by isotopic substitution.

Microwave spectroscopy; the Stark effect.

Vibration-rotation spectra of diatomic molecules; band contours for polyatomic molecules.

Molecular Symmetry

Symmetry operations and symmetry elements; products of symmetry operations; Group Theory; symmetry point groups.

Matrix representations; irreducible representations; group character tables.

Symmetry of normal modes of vibration; prediction of infrared and Raman activities. Applications of symmetry to deduce structures of simple molecules.

ADVANCED CORE CHEMISTRY 1

ECTS Credits: 10	Level: 3	Semester: 1	Code: CH301-10	
Contact Hours:	48 hours of lectures plus 6 tutorials			
Pre-requisites:	Core Inorganic Chemistry 1 and 2, Core Organic Chemistry 1 and 2, Core Physical Chemistry 1 and 2			
Assessment:	One written exa	mination (3 hours)		

The module will comprise lecture units, each of either 8 or 16 lectures, on the following topics :

- The molecular, electronic and magnetic structures of the transition metals, lanthanides and actinides (8 lectures).
- Solid state chemistry (8 lectures).
- Synthesis and biosynthesis of natural products (16 lectures).
- Statistical mechanics (8 lectures).
- Colloid and surface science (8 lectures).

The Molecular, Electronic and Magnetic Structures of the Transition Metals, Lanthanides and Actinides

Academic Objectives

To underpin the observed physical properties of the transition metals, lanthanides and actinides with a basic understanding of the underlying electronic structures.

Detailed Syllabus

Recapitulation of single electron quantum numbers, concept of momentum as applied to quantum chemistry, spin-orbit coupling.

- Multi-electron systems: the Pauli exclusion principle. Quantum numbers for multi-electron systems. Spin orbit coupling schemes, Russell Saunders (RS) and jj coupling. States and microstates of multi-electron systems. Hund's rules. Ordering and energy of spin-orbit states. Configurations and degeneracy. Concept of the hole configuration.
- Energies of states. Slater integrals and Racah parameters. Relationship between λ and ζ . Variation of ζ with oxidation state and metal. Energies of spin orbit states. The Boltzmann distribution revisited, population distributions amongst spin-orbit states.
- The effect of the ligand field. Recapitulation of basic ligand field splitting field splitting patterns with a quantitative explanation. Absorption of radiation. Classification of absorption types. The Laporte rule. Explanation of Perturbation theory. The weak field approach. Derivation of Orgel diagrams. The strong field approach and correlation diagrams. Correlation between the weak and strong field approaches, Tanabe-Sugano diagrams and their use. The nephelauxetic effect. Metal-ligand and ligand metal absorptions. Band broadening factors in transition metal UV/vis spectroscopy.
- Magnetochemistry. Definition of terms. Recapitulation of previous material. First order Zeeman splitting. Boltzmann distributions as a function of temperature. Saturation. Curie and Curie-Weiss laws. Neel temperature. Second order Zeeman splitting. Quenching and mixing. Magnetic properties of various states, A, E and T. Explanation of the Van Vleck relationship using simple examples, Magnetic properties
of second and third row elements. Magnetic cooperativity. Dinuclear systems. Lanthanide and actinide chemistry. Magnetic and electronic properties. Stability and uses.

Separation of the elements using ion exchange. Basic descriptive chemistry.

Solid State Chemistry

Academic Objectives

This unit will provide a general introduction to the study of the solid state. The main academic objectives of the course are:

- to consider the subject from the standpoint of the chemist
- to show the relationship between crystal and electronic structure and the properties of solids
- to outline how the properties of solids can be utilised both to construct useful devices and to facilitate chemical reactions

Detailed Syllabus

- 1. Lattices, unit cells, crystal systems, Bravais lattices. Close packed systems, hexagonal and cubic close packing, tetrahedral and octahedral sites in close packed arrangements.
- 2. The crystal structures of metals.
- 3. The crystal structure of ionic materials: Rock Salt NaCl; Niccolite/Nickel Arsenide NiAs; Zinc Blende/Sphalerite ZnS; Wurtzite ZnS; Caesium Chloride CsCl; Fluorite CaF₂; Antifluorite Li₂O; Rutile TiO₂; Cadmium Iodide CdI₂; Cadmium Chloride CdCl₂; Bismuth Triiodide BiI₃; ReO₃ (Rhenium trioxide); Al₂O₃ (corundum); CaTiO₃ (perovskite); FeTiO₃ (ilmenite); MgAl₂O₄ (spinel); NiFe₂O₄ (inverse spinel).
- 4. Radius ratio. Prediction of normal and inverse spinel structures based on Ligand Field Stabilisation Energy.
- 5. The crystal structures of molecular crystals. Simple rules for packing together diatomic molecules, chains and sheets. The effect of hydrogen bonding on crystal structures.
- 6. Silicate structures: A brief introduction to silicate structures, discrete, chain and layer silicates.
- 7. Superconductivity: introduction to the terms critical temperature, Meissener effect, critical field strength, critical current, Silsbee effect, Josephson Effect, type I and II superconductors, ferro- and antiferromagnetism.
- 8. Cooper Pairs and BCS theory.
- 9. The structures of high temperature superconductors and their relationship to the perovskite structure. The potential uses and drawbacks of high temperature superconductors.
- 10. Band Theory of bonding in metals. Semiconductor and insulator properties. Photocopying and solar cells.
- Defects in crystals: Schottky and Frenkel Defects. Use of density measurements to infer type of defect present. F-centres. Mechanisms for ionic conduction in solids. Fast ion conductors. Lithium iodide and Sodium/Sulphur batteries. Oxygen sensors/meters. The photographic process.
- 12. Zeolites: the structures of zeolites, sodalite unit etc. Internal dimensions of cavities in zeolites. The significance of the Si/Al ratio. Cation sites and the use of zeolites as molecular sieves and catalysts. Fibrous, lamellar zeolites, ZSM-5 and ZSM-11.
- 13. Synthesis of zeolites. Uses of zeolites as ion-exchangers, separating agents, desiccants and catalysts. Shape selectivity: reactant selective, product selective, transition-state selective catalysis.

- 14. Low Dimensional Solids: Polyacetylene, platinum chain compounds, tetrathiafulvalene-tetracyanoquinonedimethane (TTF/TCNQ), graphite, intercalation compounds.
- 15. Optical Properties of Solids: Lasers (ruby and gallium arsenide), phosphors and optical fibres and optical switches.

Synthesis and Biosynthesis of Natural Products

Academic Objectives

The course falls into two parts, one concerned with the biosynthesis of natural products and the other the synthesis of selected natural products.

• The aim of the biosynthesis part of the course is to provide the student with an overview of various types of natural products, the main biosynthetic pathways to such compounds, and some of the methods which are used to establish these. The main areas will include the biosynthesis of terpenes, steroids, and polyketides. For these classes of natural products their classification will be outlined, and the details of the biosynthetic pathways will be presented. The various elements of course will be bought together in the final section which is designed to introduce standard rules for prediction of biosynthetic pathways and to allow the student to make reasonable proposals for the biosynthetic pathway in an 'unknown' case.

• The synthesis element of the course will involve the study of methods which have been used for the laboratory synthesis of natural products. The examples will be taken from various selected areas such as steroids, terpenes, and polyketides (to build on the preceding biosynthetic lectures), and prostaglandins and morphine derivatives. Selected examples from this list will be used to illustrate the various different approaches which have been used for the synthesis of a particular compound or group of compounds. Emphasis will be laid on the role of stereochemistry in the synthesis design and in the subsequent synthesis.

Detailed Syllabus

Biosynthesis

- 1-3. Classification of natural products. Enzymes. General biosynthetic reactions. Coenzymes. Overview of main biosynthetic pathways. Establishment of biosynthetic pathways.
- 4-5. Classification and structure of terpenes and steroids. Isoprene rule. Biosynthesis of acyclic precursors to the terpenes geranyl pyrophosphate, farnesyl pyrophosphate and geranyl geranyl pyrophosphate. Cyclisation of acyclic precursors to give monoterpenes and sesquiterpenes. Biosynthesis of acyclic precursors to the steroids squalene. Cyclisation of squalene to give lanosterol.
- 6-7. Classification and structure of polyketides. Polymerisation of acetate to give acyclic precursors to the polyketides. Cyclisation of acyclic precursors to give tetraketides, pentaketides, heptaketides, and nonaketides.
- 8. Rules for the prediction of biosynthetic pathways towards terpenes and polyketides. Synthesis
- 9-10.The concept and methods of 'retrosynthetic analysis', introduced in the previous year ion the context of carbonyl chemistry, will be broadened to include other important disconnections and functional group interconversions, with particular emphasis on stereochemical aspects. These will be illustrated by examples selected from the synthesis of natural products such as terpenes, steroids, and polyketides.

- 11-12. The diversity of synthetic approaches to a given natural product class will be introduced by considering some of the most successful approaches to the synthesis of prostaglandins and related compounds.
- 13-14. The synthesis of one group of natural products with interesting biological activity will be investigated in detail. The group will be chosen from the following list of compound types: some of the individual examples used in the biosynthesis part of the course; the morphine group of alkaloids; the gibberellins; enediyne anti-tumour natural products.
- 15-16.'Biomimetic', or 'biogenetically patterned' synthesis of steroids, terpenes, and polyketides, examples based on the preceding biosynthesis course.

Statistical Mechanics

Academic Objectives

To introduce the concepts of statistical mechanics and to demonstrate the link between the molecular energy levels, which can be measured spectroscopically, and the bulk thermodynamic properties of a substance.

Detailed Syllabus

- 1-2. Microscopic *versus* macroscopic states of a system; Bose-Einstein and Fermi-Dirac statistics; the Maxwell-Boltzmann distribution; evaluation of β .
- 3. The molecular partition function; thermodynamic properties expressed in terms of the partition function for a system of independent particles.
- 4-6. The molecular partition function for an ideal gas and calculation of thermodynamic properties; translational contribution; rotational contribution; symmetry numbers; vibrational contribution; electronic contribution.
- 7. Equipartition; calculation of equilibrium constants for reactions of ideal gases.
- 8. Non-ideal gases; heat capacities of solids.

Colloid and Surface Science

Academic Objectives

The aim of this unit is to examine the fundamental principles of colloid and surface science and to show how they assist in understanding processes occurring in chemistry.

Detailed Syllabus

- Introduction: Definitions of colloidal dimensions, surface area, nomenclature, classification. Natural and synthetic examples will be given.
- Particle size and morphology: Particle size distributions and monodisperse colloids. Nucleation and growth. Particle sizing techniques. Purification. Static and dynamic light scattering. Optical and electron microscopy.
- Colloid stability: Mechanisms. Charge stabilisation. Gouy-Chapman theory. DLVO theory. Schulz-Hardy rule. Steric stabilisation.
- The gas/solid interface: Chemical and physical adsorption. Langmuir and BET isotherms. Applications in catalysis. Surface area measurements.
- Liquid/gas interface: Surface tension. Kelvin equation. Ostwald ripening.
- Liquid/liquid interface: Miscibility of liquids. Spreading of oil on water.

Solid/liquid interface: Spreading and wetting. Contact angles and surface energy.

Surfactants and adsorption at liquid interfaces.

- Air/water interface. Gibbs surface excess equation. Effects of addition of electrolyte and surfactant on surface tension.
- Micelle formation. Micelle size and shape (spheres, discs, rods). Critical micelle concentration (CMC). Factors affecting the CMC. What is detergency? Krafft temperature. Liquid/liquid colloids. Emulsions. Micro-emulsions.

ADVANCED CORE CHEMISTRY 2

ECTS Credits: 10	Level: 3	Semester: 2	Code: CH302-10
Contact Hours:	48 hours of lectures plus 6 tutorials		
Pre-requisites:	Core Inorganic Chemistry 1 and 2, Core Organic Chemistry 1 and 2, Core Physical Chemistry 1 and 2		
Assessment:	One written example	mination (3 hours)	

The module will comprise lecture units, each of either 8 or 16 lectures, on the following topics :

- Clusters in inorganic chemistry (8 lectures).
- Organometallic reaction mechanisms (8 lectures).
- Pericyclic reactions (16 lectures).
- Electrode processes (8 lectures).
- Chemical dynamics and photochemistry (8 lectures).

Clusters in Inorganic Chemistry

Academic objectives

This unit aims to develop a knowledge and understanding of inorganic clusters in terms of their structure, bonding, and reactivity. There is no universally-agreed definition of a cluster, but for the purposes of this unit it may be defined as a *polyhedral molecule or ion in which the atoms constituting the vertices of the polyhedron are bonded directly to the atoms at neighbouring vertices*. Although formerly regarded as rather rare and exotic species, it is now recognised that cluster compounds are widely distributed across the Periodic Table, a point highlighted by the recent discovery of the carbon clusters (C₆₀, C₇₀ *etc.)* known as fullerenes.

Detailed Syllabus

- 1. Introduction to cluster-chemistry an exemplified by the polyhedral boranes and transition metal carbonyl clusters. Recognition of non-classical bonding patterns and 'electron-deficient' structures.
- 2. The isolobal principle, electron counting, and the Wade-Mingos rules for predicting the structures of cluster compounds. The MO basis of electron counting. Unification of organometallic and cluster chemistry. Interpreting •-complexes as cluster compounds.
- 3/4. Synthesis, structures, and chemistry of boranes and carbaboranes. Substitution of heteroatom (both main group and transition metal) for boron in cluster compounds. Structure and bonding of heteroboranes, metallaboranes and metallocarbaboranes. The chemistry of boron sub-halide clusters.
- 5/6. Transition metal carbonyl clusters. Structural patterns in low and high-nuclearity clusters. The capping principle. Closed and capped polyhedra. Large, close-packed arrays (*cf.* bulk metals), stacked triangular structures, and planar arrays. Transition metal halide and chalcogenide clusters.
- Cluster compounds of gold. Failure of conventional electron counting schemes in gold clusters. Development of alternative bonding theory. Synthesis and structure of 'naked' polyhedral clusters (based an low-valent main group elements) such as [Sb₇]³⁻ and [Sn₉]⁴⁻, the so-called Zintl anions.

8. Carbon clusters - the fullerenes. Development of carbon-cluster chemistry. Identification of C_{60} in the mass spectrometer. The polyhedral hypothesis. Assignment to C_{60} of IR and UV bands in evaporated carbon-soot. Synthesis, isolation, characterisation, and chemistry of C_{60} and C_{70} . Higher and *lower* fullerenes.

Organometallic Reaction Mechanisms

Academic Objectives

The aim of this unit is to acquaint students with the application of basic thermodynamic and kinetic principles to the elucidation of mechanism and reactivity in organometallic systems.

Detailed Syllabus

Review of basic kinetic and thermodynamic principles

Rates of reaction, first and second order, determination of reaction order, pseudo first order reactions, Arrhenius relationship, Eyring relationship, volume of activation, reaction profiles, experimental determination of rate and thermodynamic data.

Review of experimental techniques

Relaxation methods: T-jump, P-jump, E-jump and examples. Standard spectroscopic techniques: UV/visible, IR, NMR, polarimetry, fluorescence, etc. and examples. Flow methods: stopped flow, continuous flow.

Review of organometallic chemistry

Electron counting, oxidation states, common and uncommon ligands.

Substitution chemistry

Mechanisms of substitution, dissociative and associative, disubstitution, *cis* labilisation and its mechanism, isomerisation, Bailar twist, substitution as a function of ligand size, substitution of complexes containing carbocyclic ligands, hapticity changes.

Oxidative addition

Review of fundamental principles incl. 3 main classes; addition of alkyl halides, brief discussion of radical pathways, polar 2 step pathways, kinetic *vs.* thermodynamic control of products, rates as a function of metal, incoming group, solvent, *etc.*; protonation, kinetic *vs.* thermodynamic control of products, rates as a function of metal, incoming group, solvent, *etc.*, weak organic acids; addition of dihydrogen, mechanism, dihydrogen complexes; one electron addition over one and two metal centres.

Reductive elimination

Review of fundamental principles; elimination from mononuclear centres, factors favouring elimination, C-C elimination, C-H elimination; dinuclear elimination, Norton's rules for elimination from dinuclear centres.

Nucleophilic attack at coordinated ligands

Review of fundamental principles; attack of CO by a variety of nucleophiles, use of amine oxides to oxidise CO, Fischer carbenes.

Migratory insertion

Review of fundamental principles; rationalisation of the variation of kinetics of migratory insertion, rate enhancement by solvent and Lewis acids.

Putting it all together: Some case studies

Substitution of $M_2(CO)_{10}$ (M = Mn, Re), C-H activation, determination of catalytic cycles such as the Monsanto Acetic acid process.

Pericyclic Reactions

The course falls into two parts, the first covers the general principles and 'all carbon' examples of pericyclic reactions. The second is concerned with 1,3-dipolar cycloadditions.

The first part of the course is designed to enable students to understand the principles which lie behind the operation of the main types of pericyclic reaction, recognise the different types of pericyclic processes and predict the outcome of pericyclic reactions. The course should enable students to understand why and how both relative and absolute stereochemistry is governed during the pericyclic process. The second part of the course introduces the concept of pericyclic reactions involving 1,3-dipolar cycloadditions. It is designed to provide an overview of various types of 1,3-dipoles and their cycloaddition reactions, with particular reference to understanding the mechanistic, synthetic, regiochemical, and stereochemical aspects of these reactions.

Detailed Syllabus

Pericyclic Reactions (12 lectures)

In the introduction to the course some relevant mechanistic principles will be reviewed including definitions and explanations of: transition state theory; concerted reactions; pericyclic reactions. Common methods for determining whether or not a concerted transition state will have a low energy will be reviewed including the FMO method which will be used throughout the course.

Basic LCAO MO theory will be revised and an empirical method for drawing orbital sets/MO energy levels for conjugated polyenes will be presented. Thus, the HOMO and LUMO orbitals for any conjugated • system will be identified.

Electrocyclic reactions will be defined and the stereochemical consequences of conrotatory *versus* disrotatory cyclisation will be illustrated. By superimposing frontier molecular orbital diagrams on the alternative cyclisation diagrams the Woodward-Hoffmann rules for electrocyclic reactions will be deduced. Methods for drawing ring opening/cyclisation reactions will be presented which allow the outcome of such reactions to be determined easily.

Various types of sigmatropic rearrangements and the terminology used to describe them will be described. An FMO method for judging whether or not a sigmatropic rearrangement will proceed *via* a low energy transition state will be presented. Sigmatropic hydrogen migrations will be considered to define which reactions proceed, and what the stereochemical consequences are.

[3.3] Sigmatropic rearrangements will be considered in FMO terms and empirical stereochemical evidence will be used to show that chair-like transition states are generally favoured over boat-like transition states. Types of [3.3] sigmatropic rearrangements covered will be Cope, Oxy-Cope, Claisen, Orthoester-Claisen and Enolate-Claisen rearrangements. Simple practical methods for determining the products from both cyclic and acyclic [3.3] sigmatropic rearrangement will be presented. Examples of how these rearrangements can be used in synthesis will be given.

An FMO method for determining which cycloaddition reactions will proceed under thermal and photochemical conditions will be described.

The Diels-Alder reaction will be reviewed in detail. Electronic and steric effects which affect the reactivity of the diene and dienophile components will be discussed. Hetero Diels-Alder reactions will be described briefly. Factors that influence the relative stereochemistry generated during Diels-Alder (and other cycloadditions) will be described in detail and a wide variety of examples will be used to reinforce the

principles. Empirical rules and an FMO explanation will be presented that allow the regioselectivity of most Diels-Alder reactions to be predicted easily. A very simple method will be outlined which allows the major product of most Diels-Alder reactions (including stereochemistry and regiochemistry) to be determined very quickly. Intramolecular reactions will be exemplified and the influence of geometric as well as electronic factors in controlling their stereoselectivity will be discussed. The effects of Lewis acid catalysts on Diels-Alder reactions will be explained and exemplified for intramolecular processes.

Ways for determining how Diels-Alder reactions can be identified in retrosynthetic analysis will be illustrated.

Methods for controlling the absolute asymmetric outcome of Diels-Alder reactions will be described. The alternative modes of reaction which lead to enantiomers, when the component parts of the reaction are achiral, will first of all be illustrated. The principles involved in allowing facial selectivity to occur will be considered. Methods that employ a chiral auxiliary as the controlling element will be reviewed, followed by selected catalytic methods.

Numerous problems will be provided for each element of the course and the problem solving element will be stressed, not only for its innate usefulness, but as a means to a fundamental understanding of the reactions.

1,3-Dipolar Cycloadditions (4 lectures)

Types of 1,3-dipoles; Allyl anion as a model for FMO treatment of 1,3-dipolar systems; The ambivalent nature of the dipole system; Control of the regiochemistry of cycloaddition.

Generation of nitrile oxides from oximes and from nitroalkanes, and their dimerisation to furoxazans; Their use in the synthesis of 1,2-oxazoles and 1,2-oxazolines;

Generation of nitrile sulphides from oxathiazolones, and the synthesis of 1,2-thiazoles; Generation of nitrile sulphides from oxathiazolones, and the synthesis of 1,2-thiazoles; Generation of nitrilimines by thermolysis of tetrazoles, from acylhydrazines, from aldehyde hydrazones; The synthesis of pyrazoles; Generation of nitrile ylides from Nacyl-4-nitrobenzylamines, by photolysis of 2H azirines; Synthesis of pyrroles. Preparation of nitrones and their 1,3-dipolar character; Pyridine N-oxide as a 1,3dipole; Preparation of azomethine imines from N-iminopyridines and their use in synthesis of fused ring systems; Azomethine ylides; Generation from aziridines; Stereochemistry of ring-openings - conrotatory vs. disrotatory control; Generation by the Grigg method; Non-stabilised azomethine ylides by desilylation of Ntrimethylsilyl anils.

Heterocycles as 1,3-dipoles; Sydnones and Mü nchones; 3-Oxidopyridiniums; Ozonolysis as an example of a double 1,3-dipolar cycloaddition process; Carbonyl oxides and ylides; Examples of intramolecular 1,3-dipolar cycloadditions.

Electrode Processes

Academic Objectives

The aim of this unit is to enable a student to appreciate the relationship between a detailed understanding of the kinetic processes at a metal/solution interface and their application in practical electrochemical energy storage devices.

Detailed Syllabus

1. Revision of the definitions of fundamental electrical quantities: The definition of electric field strength; the relationship between electric field strength and electrical potential; the relationship between electrical potential and charge distribution; the

Poisson equation; electric current and current density; Ohm's law; the measurement of potential difference; the reason for using high impedance instruments.

- 2. The double layer at the interface between a metal and an ionic solution at equilibrium: The Gouy-Chapman theory of the double layer; the Poisson-Boltzmann equation and the nature of its solution; the structure of the diffuse part of the double layer.
- 3. Charge transfer at the metal-solution interface: The kinetics of charge transfer across a metal-solution interface; the Butler-Volmer equation, limiting forms at low and high values of the overpotential; Tafel plots, measurement of overpotential and determination of the exchange current density.
- 4. Role of diffusion at high current densities: limiting current density; the measurement of limiting current density by polarography; the rotating disc electrode as a method of making measurements under well-defined diffusion conditions.
- 5. Electrochemical cells: current/voltage characteristics: the Tafel equation; internal resistance; relationships between power output and EMF; effect of temperature on cell output; capacity (amp.hour) of cells.
- 6. Primary cells: Zn/MnO₂ (Leclanché); Zn/MnO₂ (alkaline); Zn/HgO; Lithium cell.
- 7. Secondary cells: Lead/acid; Cd/NiO.
- 8. Fuel cells: Hydrogen/oxygen fuel cell efficiency of fuel cells.

Chemical Dynamics and Photochemistry

Academic Objectives

In contrast to previous lectures given on the topic of chemical reaction kinetics these eight lectures will focus not on the behaviour of macroscopic systems but on microscopic systems in which we follow chemical kinetics at the molecular level. At this level the calculation of rate constants from the properties of individual molecules or atoms is complex because reaction probability will depend upon energies, angle of approach and the states of reactants and products.

Detailed Syllabus

- 1. Simple collision theory of bimolecular reactions.
- 2. Potential energy eurfaces.
- 3. Theoretical calculation of rate constants.
- 4. Transition state theory on the microscopic level.
- 5. Transition state theory and thermodynamics.
- 6. Use of molecular beams.
- 7. Microscopic principles of photochemical reactions.
- 8. Intramolecular processes.
- 9. Quenching mechanisms.
- 10. Intermolecular processes.
- 11. Applications, *e.g.* stratospheric ozone, transition state spectroscopy with lasers, photosynthesis.

SPECIALISED LECTURE UNITS 1 SPECIALISED LECTURE UNITS 2

ECTS Credits: 10 ECTS Credits: 10	Level: 3 Level: 3	Semester: 1 Semester: 2	Code: CH303-10 Code: CH304-10
Contact Hours:	Minimum of 40	hours lectures/tutorials	8
Pre-requisites:	Vary according	to lecture unit	
Assessment:	One written exa	mination (3 hours)	

In each of the Specialised Lecture Unit modules, up to 12 units (drawn from the following lists of Inorganic/Analytical Chemistry, Organic Chemistry and Physical Chemistry units), each comprising 10 lectures/tutorials, will be offered. Students must attend a minimum of **four lecture units in each module** and may not answer more than **three questions** from any one section (Inorganic/Analytical Chemistry, Organic Chemistry or Physical Chemistry), except for students on the Chemistry with Medicinal Chemistry course who must answer at least three questions from the Organic Chemistry section.

SPECIALISED LECTURE UNITS 1A SPECIALISED LECTURE UNITS 2A

ECTS Credits: 5 ECTS Credits: 5	Level: 3Semester: 1 Level: 3Semester: 2	Code: CH305-05 Code: CH306-05
Contact Hours:	Minimum of 20 hours lectures/tutorials	
Pre-requisites:	Vary according to lecture unit	
Assessment:	One written examination (1.5 hours)	

In each of the Specialised Lecture Unit A modules, up to 12 units (drawn from the following lists of Inorganic/Analytical, Organic and Physical Chemistry units), each comprising 10 lectures/tutorials, will be offered. Students must attend a minimum of **two lecture units in each module**.

IMPORTANT NOTE ON TIMETABLING OF SPECIALISED LECTURE UNITS

The Specialised Lecture Units listed below are distributed between Semester 1 (September to January) and Semester 2 (February to June). This distribution may vary from year to year, and students wishing to attend for only one semester are advised to consider several alternative units and contact the Chemistry SOCRATES Coordinator in order to determine whether the timetable will permit their attendance at their preferred choices.

INORGANIC/ANALYTICAL CHEMISTRY SPECIALISED LECTURE UNITS

- I.11 Modern NMR Techniques for Problem Solving (S.J. Simpson)
- I.12 Applications of Organotransition Metal Chemistry to Organic Synthesis (S.J. Simpson)
- I.15 Geochemistry (R. Blackburn)
- **I.16** Radioactivity, its Measurement and Analytical Applications (R. Blackburn)
- **I.19** Organometallic Chemistry of Nickel, Palladium and Platinum (N.M. Boag)
- **I.23** Application of Spectroscopic Techniques to Inorganic Problems (N.M. Boag, S.J. Simpson)
- I.24 Principles of Photochemistry (A.K. Davies)
- I.25 Advanced Chromatography Techniques for Target Compound Analysis (P.J. Baugh)
- **I.28** Techniques and Methodology in Transition Metal Biochemistry (N.M. Boag)
- **I.29** Modern Electroanalysis: Stripping and Sensing (D.W.M. Arrigan)
- **I.30** Chemistry and Biochemistry of Nitrogen Fixation (H.M. Colquhoun)

I.11 Modern NMR Techniques for Problem Solving (S.J. Simpson)

This unit builds on a short course given in Year 2, and is designed to be taken prior to taking Unit I.23. The unit will consist of eight lectures, one tutorial and one workshop.

The basic proton and multinuclear magnetic resonance techniques required to look at structural and synthetic problems in inorganic chemistry (particularly organometallic and transition metal) will be outlined. Emphasis will be placed on application rather than theory of the technique discussed.

The following areas of pulse methods are to be covered: Fourier Transform Spectrometry *vs.* Continuous Wave Spectrometry; one dimensional experiments, NOE measurements, relaxation methods, spin-spin decoupling for absolute sign determination, structural information from coupling constants and chemical shifts, fluxional systems; two dimensional experiments, ¹H-¹H correlation spectroscopy, ¹³C-¹H correlation spectroscopy, ¹³C-¹³C connectivity determination, exchange processes (fluxional processes) by 2-D techniques; heteronuclear spectroscopy, ¹⁵N, ¹⁷O, ¹⁹⁵Pt, ³¹P, ¹⁰³Rh and others, problems of spectral acquisition for these nuclei, physical properties of non-spin = 1/2 nuclei and special pulse techniques; reverse correlation spectroscopy to overcome sensitivity and relaxation problems associated with these nuclei.

I.12 Applications of Organotransition Metal Chemistry to Organic Synthesis (S.J. Simpson)

The unit will consist of eight lectures and two tutorials. The principles to be emphasised include the use of metal complexes to control regioselectivity and stereoselectivity of addition of nucleophiles and electrophiles to organic substrates. Elements will include the following: complexation and decomplexation of organic substrates to metal complexes, stereochemical consequences of complexation of achiral substrates; protecting organic functionalities by use of metal moieties; redox reaction; cyclisation, coupling and carbon-carbon bond forming reactions; isomerisation and rearrangements mediated by metal complexes; carbonylation reactions and utilisation of metal acyl complexes as organic synthons; trapping and stabilisation of organic species by metal centres.

I.15 Geochemistry (R. Blackburn)

The Earth is the chemist's only store of chemicals. Geochemistry concerns itself with how the elements were formed, why they have the relative abundances they do, how they were distributed when the planet was born, how they are differently distributed now (and why).

Essentially the Earth is a giant chemical reactor in which two main types of process are taking place. One process occurs in molten silicates, the other involves aqueous solutions. In both cases, the behaviour of individual elements is determined by a variety of physico-chemical factors and their fate is of prime importance to the prospector and miner looking for economically important minerals. The unit will examine the physical and chemical processes which lead to the formation of rock and minerals of both the major and minor elements, whether or not they are of economic value. Radioactivity in Nature, Geochronology. This unit should appeal to inorganic/physical chemists, environmentalists and anyone with a geological background or interest (there will not be time to deal with organic geochemistry).

I.16 Radioactivity, its Measurement and Analytical Applications (R. Blackburn) Radiation types. Measurement systems: gamma counting; gamma spectroscopy (low resolution); gamma spectroscopy (high resolution); liquid scintillation counting - cocktails, quenching and spectral matching. Cerenkov phenomenon and Cerenkov counting. Simple statistical considerations. Labelled compound; preparation; nomenclature; self-radiolysis. Isotopic dilution analysis. Activation analysis.

I.19 Organometallic Chemistry of Nickel, Palladium and Platinum (N.M. Boag) The first organometallic complex described, $K[PtCl_3(\eta^2-CH_2=CH_2)]$. H₂O was prepared in the 1820's by the Danish pharmacist Zeise. Since that time, platinum has been an important element in organometallic chemistry because it forms a wide range of compounds that are sufficiently kinetically inert to enable them to be isolated and characterised. Recent advances in multinuclear NMR have supported studies as the spin active nucleus of platinum, ¹⁹⁵Pt, is by far the easiest of the transition elements to observe directly at natural abundance. In contrast, it was not until the discovery of the catalytic activity of nickel complexes by Reppe in the 1930s and 40s that the organometallic chemistry of nickel began to flourish. In the 1960s and 70s, work at Mulheim laid the foundations of organonickel chemistry with their discovery of the 'naked' nickel complexes, zerovalent nickel complexes containing only olefins as ligands. Nickel's catalytic activity stems from its high kinetic lability. By contrast, the kinetic inertness of platinum allows the isolation of intermediates which have only a fleeting existence on nickel. The chemistry of palladium resembles that of palladium, however, it is more labile and also has found use in catalytic processes, e.g. the Wacker Process. This unit will be concerned with the detailed organometallic chemistry of these three elements

I.23 Application of Spectroscopic Techniques to Inorganic Problems (N.M. Boag, S.J. Simpson)

This unit will discuss the use of spectroscopic techniques (primarily NMR and infrared) to solve problems in inorganic and organometallic chemistry. The emphasis will be on practical application of these techniques and will make extensive use of examples from the literature. Topics that will be explored include:

- Second order NMR spin systems. When do you expect them? How do you recognise them? What information can be derived from them?
- Fluxional molecules and exchange processes. Designing experiments to measure fluxional and exchange processes.
- What is meant by timescale and can we make use of it?
- Isotopic labelling. Use of labelling for characterisation and mechanistic uses.
- Transient species. How can you identify something that only lasts for a fraction of a second?

Attendance at Unit I.11 is a pre-requisite for taking this Unit.

I.24 Principles of Photochemistry (A.K. Davies)

Excitation of molecules by absorption of radiation. Fates of electronically excited states. Quantum yield. Kinetics of photochemical reactions. Photodissociation. Jablonski diagrams. Luminescence-fluorescence and phosphorescence. Chemiluminescence. Energy transfer processes. Excimers and exciplexes. Photochemical reactions. Experimental techniques *e.g.* flash photolysis. Applications and examples of photochemistry *e.g.* atmospheric photochemistry, photosynthesis, photoimaging, photochromism, photomedicine.

I.25 Advanced Chromatographic Techniques for Target Compound Analysis (P.J.

Baugh)

Keywords: Separation, chromatography, GLC, HPLC, SFC, detection systems, GC/MS, LC/MS, target organic molecules, sample preparation, detection, characterisation, identification, analytical method development and validation.

Chromatographic separation techniques and instrumentation are widely employed by chemical industry and analytical laboratories in general for determining target compound for quality and environmental monitoring purposes. A range of chromatographies is available to the analyst in an industrial, consultant analytical, water company and regulatory laboratories of which gas/liquid and high performance (pressure) liquid chromatographies are the most prominent using conventional (GC-FID) and sophisticated (GC-MS) detection systems.

This module provides and overview of the fundamentals and principles of chromatographic separations and instrumental techniques involved to identify, characterise and quantify target compounds with a consideration of analytical methodology - method development and validation and the requirements for sample preparation and presentation for instrumental analysis.

I.28 Techniques and Methodology in Transition Metal Biochemistry (N.M. Boag)

The aim of this unit is to familiarise the student with the techniques used to characterise and identify active transition metal sites in biological molecule and apply these techniques to an understanding of the functionality of iron and copper in living systems.

Mössbauer, ESR, CRD and ORD spectroscopies

- Mössbauer: The Mössbauer experiment (source, Doppler shift/broadening, recoil problems, the spectrometer, isotope shift of Fe and Sn, dependence on electron density at nucleus, quadrupolar splitting, models for quadrupolar splitting, Zeeman splitting.
- ESR: The ESR experiment, X-band, Q-band, appearance of spectra, determination of the g-value, hyperfine coupling for I = 1/2 and I > 1/2 nuclei including ratios, metals and non-100% spin active isotope abundance, isotropic *vs.* non-isotropic, square planar geometry.

Iron in biological systems

- A review of the essential chemistry of Fe²⁺ and Fe³⁺. Iron as an oxygen carrier in biological systems. The identity and chemistry of the prosthetic centre in haem proteins, the porphyrins. The significance of high and low spin states and their effect upon the iron-porphyrin complex and the molecular mechanism for the reversible binding of oxygen to haem proteins. The evolution of synthetic model structures of the haem complex (*e.g.* 'picket fence' model) and their importance to our understanding of the biological processes. A survey of the potential for exploiting this chemistry.
- Iron haem proteins and electron transfer; a review of the essential molecular mechanisms with reference to cytochrome c.

Copper chemistry and the role of Cu(I)/Cu(II) in biological systems

- Electron transfer and the copper blue proteins. Categorisation of types I, II & III according to their coordination environment and geometry. The consequences of this diversity in their biochemical roles.
- Oxygen transport and hemocyanin; a review of the chemistry and structure of the binuclear copper binding pocket. The mechanism of reversible oxygen binding.

I.29 Modern Electronalyis: Stripping and Sensing (D.W.M. Arrigan)

This unit will review recent advances in electroanalytical chemistry in the areas of stripping voltammetry and electrochemical sensors.

Stripping voltammetry is the most sensitive of the electoanalytical techniques available and consists of accumulation of the analyte onto/into the working electrode of the electrochemical cell, followed by voltammetric determination of the accumulated analyte. The accumulation step provides stripping voltammetry with its ultra-trace capabilities, allowing sub-nanomolecular determinations on a routine basis. The various chemistries employed in the accumulation and stripping steps of these procedures will be presented along with the various voltammetric techniques employed in detection.

Electrochemical sensors, simple-to-use portable devices which provide chemical information in a rapid and unambiguous manner, continue to revolutionise the practice of analytical chemistry. Such sensors consist of a recognition component immobilised onto a transducer (electrode) surface. The recognition chemistries and biochemistries employed in electrochemical sensors will be presented and case studies of practical, real-world chemical sensing undertaken.

I.30 Chemistry and Biochemistry of Nitrogen Fixation (H.M. Colquhoun)

This unit aims to develop a knowledge and understanding of the chemistry and (so far as it is known) the biochemistry of elemental dinitrogen.

- Introduction to dinitrogen. Electronic structure and reasons for its 'inert' character. Importance of biological and industrial nitrogen fixation processes. Non-catalytic chemistry: cyanamide formation, nitriding of metals and metalloids, oxidation of N₂.
- Coordination chemistry of N_2 . Modes of binding. Complexes formed and electronic consequences for reactivity of N_2 .
- Reactions of coordinated N_2 . Electrophilic, nucleophilic and free radical pathways. Electrocatalytic processes. Synthesis of organonitrogen compounds from N_2 .
- Surface chemistry of N₂. Heterogeneous catalysis and the indsutrial synthesis of ammonia (Haber process).
- Nitrogen in the biosphere. Bacterial and algal sources of nitrogen fixation. Identification and isolation of nitrogenase enzymes. Sources of reducing power and electron transfer pathways within the cell. Crystallographic studies of nitrogenase and the structure of the active site. Proposed models for the operation of nitrogenase.

ORGANIC CHEMISTRY SPECIALISED LECTURE UNITS

- **O.03** Alkaloid Chemistry (J. Leonard)
- **0.05** Aspects of Asymmetric Synthesis (G. Procter)
- **O.06** Advanced Organic Synthesis (G. Procter)
- **0.07** Transition Metals in Organic Synthesis (A.T. Russell)
- **0.10** Antibiotics (T.W. Wallace)
- 0.15 Techniques for Structure Determination in Organic Chemistry (J. Leonard)
- 0.18 Process Chemistry in the Pharmaceutical Industry (B. Lygo, J. Leonard)
- **0.19** Anticancer Compounds and Chemotherapy (A.T. Russell)

O.03 Alkaloid Chemistry (J. Leonard)

Alkaloids are a diverse range of nitrogen containing organic molecules which are mainly extracted from plants and are perhaps the most important group of natural medicines. The diverse range of structures which alkaloids possess will be illustrated and a general classification will be given which unifies compounds according to their biogenetic origins. As drugs, alkaloids are used and abused for a wide range of purposes, from anti-cancer chemotherapy to hallucinogenic tripping, and these biological properties will be described. For selected groups of alkaloids, biosynthetic pathways and synthetic routes will be discussed.

O.05 Aspects of Asymmetric Synthesis (G. Procter)

The synthesis of enantiomerically pure organic compounds ('optically active' compounds) is of great current interest from the academic and industrial point of view. For example, the useful biological properties of drugs are usually exhibited by only one enantiomer. As a consequence of this, and of other matters, many new pharmaceuticals, agrochemicals, and other industrially important classes of organic compounds are required to be synthesised as the enantiomer that possesses the desired properties, and this will become of even greater importance in the future. In this unit some of the most effective and practically useful modern general methods for the synthesis of enantiomerically pure compounds, 'Asymmetric Synthesis,' will be discussed. Methods which are currently finding application in both academic and industrial research laboratories will be emphasised. Together with simpler examples of this methodology, one example of a 'state of the art' synthesis, usually a natural product, is used to demonstrate the power of this new synthetic chemistry. Topics covered: Asymmetric alkylation and aldol reactions (concentrating on Evans' methodology); Asymmetric Diels Alder reactions (briefly); Sharpless asymmetric epoxidation and kinetic resolution. Concepts covered include 'chiral auxiliaries' (why and how they work), and asymmetric catalysis. Examples of all these synthetic reactions, and one 'state of the art' synthesis of a complex molecule.

O.06 Advanced Organic Synthesis (G. Procter)

This unit will provide an overview of key areas of modern organic synthesis. It will begin with a survey of the strategies for planning the synthesis of complex molecules, focusing particularly on carbon-carbon bond forming reactions of carbonyl compounds. Three fundamentally important reaction types, additions to carbonyls, reactions of enolates, and conjugate additions to α , β -unsaturated carbonyl compounds, will then be discussed in more detail. The emphasis throughout will be on problems of selectivity, the general strategies for tackling these problems, and the best currently available solutions. Important methods for selective functional group interconversions, such as oxidations and reductions, will also be described. Topical examples of total syntheses of natural and unnatural products will be used throughout the unit to illustrate the methods and reagents under discussion. This unit offers a good background to the units on synthesis, natural products, and biologically active molecules.

0.07 Transition Metals in Organic Synthesis (A.T. Russell)

This unit will attempt to cover the use of the more important transition metals in organic synthesis over the last fifteen years. Metals covered will include:

• Palladium: Pd⁰ catalysed cross coupling reactions. Pd⁰ catalysed additions to multiple

bonds. Pd^{II} catalysed cyclisation-carbonylation reactions. • -allyl Pd complexes in synthesis. Pd^0 catalysed cycloaddition reactions.

- Nickel: Ni⁰ catalysed [4+2] and [4+4] cycloaddition reactions.
- Cobalt: Co⁰ the Pauson-Khand reaction. Co¹ catalysed trimerisation of alkynes.
- Copper: The use of organocopper and lower and higher order cuprates in synthesis.

O.10 Antibiotics (T.W. Wallace)

The aim of this course is to familiarise the student with some of the fundamental principles involved in the discovery, production, and development of antibiotics. Particular emphasis is placed on the molecular aspects of antibiotic chemistry (structure, mode of action, modification, total synthesis), and illustrative examples are selected on the basis of their historical and clinical significance. These include the sulphanilamides; chemical modifications with enhanced properties. Penicillins (penams). Cephalosporins (cephams), discovery and structural relationship to penams. Complementary action against Gram (–) and Gram (+) bacteria, SARs of analogues. Synthesis of cephems from penams. The problem of resistance, the development of new β -lactams. Clavulanic acid; discovery, synthesis, mode of action as β -lactamase inhibitor. Combination antibacterials (augmentin, timentin, zosyn). The anthracycline anticancer agents. The discovery and mode of action of the enediyne DNA-cleaving agents.

O.15 Techniques for Structure Determination in Organic Chemistry (J. Leonard) Modern techniques used for determining the structures of complex organic molecules will be described and recent research examples will be used to show how various techniques can be used practically. Proton NMR techniques covered will include spin-spin decoupling and the use of nuclear Overhauser effects. ¹³C NMR, mass spectrometry, infrared, X-ray and other techniques will also be covered and an emphasis will be placed on using a combination of techniques to determine structures.

O.18 Process Chemistry in the Pharmaceutical Industry (B. Lygo, J. Leonard) New drugs are initially produced on a tiny scale, sometimes as little as 20 mg, by medicinal chemists. Once a useful biological property has been established, larger quantities are required for further biological and toxicological evaluation but a laboratory scale preparation is normally sufficient. There is very little restriction on the methods used to synthesise such materials and the economic cost of the materials is of no consequence. Once a compound becomes a development drug the situation is quite different and chemists must develop a robust route, which is technically and economically viable and can be used on a manufacturing scale. This is the work of process research chemists. In this unit, real case examples of the development of manufacturing routes to drugs will be examined. By studying these examples students will gain an insight into the challenges involved when complex structures have to be manufactured on a large scale by multi-step synthetic techniques. A visiting lecturer from a major pharmaceutical company will deliver an example of a contemporary piece of process chemistry.

0.19 Anticancer Compounds and Chemotherapy (A.T. Russell)

This unit will examine various anticancer agents from both a medicinal and synthetic perspective. We will examine their modes of action and in so doing build up a picture of the

strategies open to the medicinal chemist in this area. Consideration of synthetic approaches will allow us to learn some more about synthetic chemistry and to evaluate the limits of chemical synthesis as a means of accessing compounds for testing and producing commercial quantities of substances of proven clinical worth.

PHYSICAL CHEMISTRY SPECIALISED LECTURE UNITS

- P.04 Surfactants, Liquid Crystals and Colloids (T.L. Crowley)
- P.05 Modern Spectroscopy (A.J. Barnes)
- P.07 Lasers and their Application in Chemistry (J. Gormally)
- P.15 The Chemistry of Fire and its Prevention (D. Price, W.D. Woolley)
- P.22 Atmospheric Pollution (A.J. Barnes)
- P.24 Applications of Neutron, X-ray and Light Scattering Techniques (T.L. Crowley)
- P.25 Atmospheric Chemistry (A.J. Barnes)
- P.31 Mass Spectrometry (J. Gormally)
- P.32 Introduction to Surface Science (M.E. Pemble)
- P.33 Bonds to Bands: Chemical and Electronic Properties of Solids (M. E. Pemble)

P.04 Surfactants, Liquid Crystals and Colloids (T.L. Crowley)

Surfactants and micellisation. Chemical structure and general properties; critical micelle concentration (cmc), measurement techniques. The structure, thermodynamics and kinetics of micelles; their dependence on chemical structure, additives and mixed surfactants; biological surfactants. Liquid crystals: thermotropic and lyotropic (surfactant) liquid crystal structures and chemical structure, measurement techniques. Micro-emulsions and emulsions, foams, latex based paints. Applications, stabilisation by surfactants.

P.05 Modern Spectroscopy (A.J. Barnes)

Spectroscopy is a very extensive subject, covering a wide range of methods, which has increased considerably since the mid-1960s because of the development of lasers and various types of electron microscopy. This unit will concentrate on these newer spectroscopic techniques. In particular, it will cover some of the uses of lasers in spectroscopy (for example, non-linear Raman effects) as well as photoelectron spectroscopy and related techniques (such as Auger electron spectroscopy). Illustrative examples of the information that can be derived from these techniques will be discussed. Note: Some previous knowledge of lasers would be helpful (*e.g.* Unit P.07).

P.07 Lasers and their Application in Chemistry (J. Gormally)

The high intensity of light emitted by laser sources is one of their better known characteristics. Pulsed lasers can generate peak powers exceeding a gigawatt and are the most powerful instrumental probes that can be found in a laboratory. In addition, lasers emit radiation with higher spectral purity than any other source and this has led to a wide range of applications in spectroscopy. Also the short pulse durations (less than a picosecond) that can be generated by laser techniques has found applications in the study of the fastest chemical processes. This unit will be concerned with the principles of laser action and the mode of operation of particular types of laser. The factors that influence laser power, pulse duration, spectral purity and coherence will be discussed in the context of their relevance to chemistry.

P.15 The Chemistry of Fire and its Prevention (D. Price, W.D. Woolley)

Modern plastics and textiles make major contributions to the quality of every day life. Unfortunately, with few exceptions they are flammable and thus a fire hazard. The cost, both in human lives and in financial terms, of fire has resulted in pressure on the polymer and textile industries to develop flame resistant products that meet legislative safety standards. The plastics and textile industries are thus actively seeking to extend their knowledge of fire chemistry to enable them to develop new and better flame retardant products. This unit will give an insight into these developments by providing a background knowledge of the chemistry or fire and its prevention. The topics to be covered are: fire science and combustion chemistry; diffusion and pre-mixed flames; ignitions and flame spread; spontaneous ignition and smouldering; polymer/textile combustion; flame retardant plastics and textiles; smoke and toxic gas evolution; safety standards. This unit is presented jointly by Professor Dennis Price and Professor Dave Woolley, formerly of the Fire Research Station.

P.22 Atmospheric Pollution (A.J. Barnes)

This unit will discuss the most significant atmospheric pollutants and their effects on critical atmospheric properties such as acidity of precipitation ('acid rain'), radiation trapping (the 'greenhouse effect'), ultraviolet radiation blocking (the 'ozone hole'), *etc.* The topics covered will include: the existence of legal limits for emission of gaseous and particulate pollutants; the sources of the most commonly occurring pollutants and their effect on humans and

animal and plant life; techniques of sampling and analysis of gaseous and particulate pollutants; the practice of pollution control; economic and political aspects of atmospheric pollution.

P.24 Applications of Neutron, X-ray and Light Scattering Techniques (T.L. Crowley) Scattering techniques find a wide range of application in studying the structure and dynamics of macromolecular and colloidal systems, *e.g.* the measurement of molecular weight, size, shapes and interactions of polymers, surfactants, colloids and biological systems; the measurement of surface structure from reflectivity measurements (*e.g.* surfactants at surfaces); the measurement of diffusion and molecular motion.

P.25 Atmospheric Chemistry (A.J. Barnes)

Widely debated environmental issues, such as the 'ozone hole,' are related to the properties of molecules present at low concentrations in the upper atmosphere. The processes leading to the formation of the ozone hole over the Antarctic are not yet fully understood, but certainly involve a complex cycle of chemical and photochemical reactions including heterogeneous chemistry on the particles constituting polar stratospheric clouds. This unit will explore the present state of knowledge on this topic and describe some of the methods used to study the concentrations of molecules and the processes occurring in the stratosphere. A brief outline of the origin of the earth's atmosphere, together with an account of the chemistry of significant tropospheric pollutants will also be given.

P.31 Mass Spectrometry (J. Gormally)

This unit will deal with the principles of the determination of molecular mass by mass spectrometry and their application in chemical analysis. Mass spectrometry is a precise and versatile instrumental technique that has been extensively developed to allow the accurate determination of the molecular mass of a wide variety of compounds. Recently, the incorporation of laser methods has extended the accessible mass range to over 100,000 mass units and has opened the way to the mass analysis of large biological molecules. Mass spectrometry is an essential facility in many chemical laboratories. The unit will cover widely used conventional instrument techniques including methods of sample introduction together with the more recent developments such as fast atom bombardment, secondary ion mass spectrometry, laser desorption/ionisation and Fourier transform mass spectrometry.

P.32 Introduction to Surface Science (M.E. Pemble)

Over the past two decades enormous advances have been made in our ability to understand and control surface processes such as corrosion, heterogeneous catalysis and materials deposition. In part these advances have been brought about by developments in both technology, *e.g.* the ability to create an ultra-high vacuum environment and instrumentation, and the scanning tunnelling microscope which can image individual atoms and molecules on surfaces. This unit sets out to describe from first principles the 'surface science' approach. It will deal explicitly with adsorption and desorption phenomena, adsorption isotherms and the measurement of heat of adsorption/desorption. It will also describe some of the novel techniques which enable the modern surface scientist to completely characterise the structure of an adsorbed species. Finally, the unit will deal with the rudiments of simple catalytic processes that occur on surfaces.

P.33 Bonds to Bands: Chemical and Electronic Properties of Solids (M.E. Pemble) How does the laser in a CD player work? Where does the light come from in a light-emitting diode (LED)? How is sunlight converted to electricity by a solar cell? All of these questions may be answered by considering the way in which certain solids respond to optical or electrical input, which in turn depends critically upon their structure and the nature of the bonding within the solid. This unit will describe in simple terms the origins of band theory, beginning with a review of simple bonding models and then will extend these concepts to cover factors influenced directly by the choice of synthesis technique, *i.e.* where the solid state chemist may play a role in designing novel 'electronic' materials.

FOUNDATION CHEMISTRY LABORATORY

ECTS Credits: 5	Level: 1 Semester: 1	Code: CH107-05
Contact Hours:	72 hours laboratory-based work	
Pre-requisites:	A-level Chemistry or equivalent	
Assessment:	The practicals are continuously assessed.	

Academic Objectives

The aim of the laboratory course is to provide training in basic laboratory skills and, where possible, to complement the first year Chemistry lecture courses. The specific skills which the students should acquire are:

the manipulation of laboratory equipment the preparation and purification of compounds making accurate measurements the calculation of values for parameters derived from the measurements laboratory notebook maintenance

Detailed Syllabus

The experiments are changed as new and appropriate ones are developed. Current examples:

- 1. Determination of the solubility product of $Ca(OH)_2$ by multiple titration.
- 2. Preparation and analysis of ammonium copper(II) sulphate.
- 3. Chemistry of the halogens synthesis.
- 4. Chemistry of the halogens characterisation.
- 5. Purification of acetanilide by crystallisation.
- 6. Distillation and GLC analysis of a mixture.
- 7. Separation of a mixture by liquid-liquid extraction.
- 8. Preparation of 4-nitroacetanilide.
- 9. Determination of the kinetic rate constant for the acid hydrolysis of an ester.
- 10. Determination of the activation energy of an ionic reaction.
- 11. The absorption of light.
- 12. The measurement of atomic spacings in graphite by electron diffraction.
- 13. Infra-red spectroscopy of a liquid sample.
- 14. Reactivity of transition metals.
- 15. Preparation, analysis and properties of potassium trioxalatoferrate(III). Absorption spectra of Cu(II) complexes
- 16. Separation of a mixture by column chromatography and quantitative determination of chromium by colorimetry.
- 17. TLC of aromatic compounds.
- 18. Reduction of benzophenone.
- 19. Preparation of phenyl acetate.
- 20. Bromination of stilbene.
- 21. Determination of the degree of hydrolysis of a salt from conductance measurements.
- 22. Determination of the dissociation constant of a weak acid by potentiometric titration.
- 23. Application of the Nernst equation to a redox titration.
- 24. Determination of the dissociation constant of a weak acid by pH measurements using (a) an indicator and (b) a pH meter.

LABORATORY SKILLS AND PROJECTS

ECTS Credits: 5	Level: 1 Semester: 2	Code: CH108-05	
Contact Hours:	72 hours laboratory-based work		
Pre-requisites:	Foundation Chemistry Laboratory		
Assessment:	The set practicals are continuously assessed. The project is assessed on the basis of the final report and the poster presentation. The students are asked to assess the contribution made by their co- workers in the project and the final team mark is apportioned in lir with the students' assessment.		

Academic Objectives

The aim of this module is to consolidate and extend the training in basic laboratory skills received in the pre-requisite laboratory programme and to provide the student with the opportunity to contribute towards a team project which will allow the inculcation of Enterprise skills.

Detailed Syllabus

The first half of the module may require students to undertake a variety of experiments. Amongst those currently on offer are:

- 1. Reactivity of Transition Metals.
- 2. Preparation, analysis & properties of potassium trioxalatoferrate(III).
- 3. Absorption spectra of Cu(II) complexes.
- 4. The n–Bottle Experiment.
- 5. The Kinetics of the Acid Hydrolysis of an Ester (Word Processed Report required)
- 6. The Extraction of Caffeine from Tea.
- 7 Preparation of and Dye Formation from Benzenediazonium Chloride.
- 8. The Identification of an Unknown Organic Compound.
- 9. Determination of the dissociation constant of a weak acid by potentiometric titration.
- 10. Determination of the dissociation constant of a weak acid by pH measurements using (a) an indicator and (b) a pH meter.
- 11. Application of the Nernst equation to a redox titration.
- 12. Determination of the degree of dissociation of a weak acid from conductance measurements.
- Team Project. The second half of the module is devoted to a team project. The students work in teams based upon their tutorial groups. The project is in analytical, environmental, inorganic, organic or physical chemistry. The aim is to give the students more practice in the skills which they have obtained in their first year laboratory classes and also to enable them to gain an introductory experience in the areas of research and information retrieval. A member of staff is allocated to each group in order that advice might be given concerning the progress of the project, and the advisability of any proposed experiments. Students are required to hold regular team meetings in order to organise their work. The meetings must be reported in their log book and tasks must be provided for each member of the team. The final report is word processed, and each team is required to present a poster containing their results and these are judged by Chemistry staff. Selected teams are chosen to make an oral

presentation of their results to the rest of the year group.

LABORATORY SKILLS 1 LABORATORY SKILLS 2

ECTS Credits: 10 ECTS Credits: 10	Level: 2 Level: 2	Semester: 1 or 2 Semester: 1 or 2	Code: CH207-05 Code: CH208-05
Contact Hours:	108 hours labora	tory-based work	
Pre-requisites:	Foundation Chemistry Laboratory or equivalent		
Assessment:	The practical work is continuously assessed		

Academic Objectives

The aims of these modules are to provide the student with a thorough grounding in the methodology and techniques employed in modern synthetic inorganic and organic chemistry, and to underpin the modules in inorganic, organic and physical chemistry with laboratory illustrations. In addition, the requirements to maintain a thorough and accurate laboratory notebook, and to be aware of and able to deal with hazards implicit in working in a chemical laboratory are emphasised and enforced.

Detailed Syllabus

Examples of the many experiments currently offered in these modules are given below. Inorganic Chemistry

t-Butylamine-borane adduct, preparation and characterisation. Synthesis and reactivity of tertiary phosphines. Synthesis of bis(triphenylphosphine)copper(I) tetrahydroborate(III). Synthesis and resolution of tris(1,10-phenanthroline)nickel(II) ion. Preparation of a cobalt 'dioxygen carrier.' Determination of \bullet_0 for ligands in Cr(III) complexes. Allyl complexes and fluxional behaviour:synthesis of $[Pd(\eta^3-C_3H_5)(\mu-Cl)]_2$ Synthesis and structural investigation of cyclopentadienyliron dicarbonyl complexes. Transition metal catalysis.

Organic Chemistry

Structure determination of organic compounds by spectroscopy.

Separation of a mixture by flash chromatography.

Functional group transformations; aromatic substitution reactions.

Preparations involving enolate anions, Grignard reactions, pericyclic reactions.

Preparations of heteroaromatic compounds.

Reactions of alkenes.

Preparation of important optically active compounds.

Reactions involving carbanions.

NMR experiments.

Physical Chemistry

An investigation of the kinetics of bromination of an aromatic amine.

Dissociation constant by conductivity.

Selectivity ratios of ion selective electrodes.

Viscosity of liquid mixtures.

Adsorption of surfactants.

Molar mass of a polymer.

Primary kinetic salt effect.

Infrared spectra of CO and SO₂. Refractometry.

RESEARCH PROJECT

ECTS Credits: 20	Level: 3	Semester: 1 and 2	Code: CH307-20
Contact Hours:	240 hours labora	tory-based work	
Pre-requisites:	Laboratory Skills 1 and 2		
Assessment:	Assessment of experimental work (45%), by the supervisor, assessment of the dissertation (45%) and an oral examination (10% by the supervisor and an independent second marker.		

Academic Objectives

The purpose of the Research Project is to introduce into the assessment of a student's ability a test of individual progress in problem solving, on an original topic, and of the character requirements necessary for a professional career. Important among the latter is the development of initiative and also the capacity for reliable hard work, whether the circumstances are good or bad. Additionally, there is the experience of carrying out a literature survey, training in the techniques inherent in research, and making a critical appraisal, in the dissertation, of the results obtained.

Detailed Syllabus

Descriptions of the Research Projects offered vary from year to year and are available separately from the SOCRATES coordinator. Information on the research interests and activities of individual members of staff can be obtained from their Internet entries (http://www.salford.ac.uk/chemist/staff.html).

Assessment

The assessment of the experimental work carried out during the project takes account of a variety of aspects, including practical ability, the time spent in the laboratory, organisation of the laboratory programme, persistence in overcoming difficulties, contributions to the development of the project, *etc.* Above all, the assessment measures the value of the student's attempts in a problem-solving situation taking into account, as far as possible, that different students may be involved in widely different projects. The dissertation is assessed on the basis of the thoroughness of the literature search, the physical presentation of the dissertation (the care given to and accuracy of the text, diagrams, tables, equations, *etc.*), the quality of the discussion and interpretation of the experimental data, and evidence of scientific method in tackling the project. The oral presentation is assessed on the quality of the presentation, how well the project was summarised, and the ability to answer relevant questions.

Time Schedule for the Research Project

- Experimental work: Two days per week (Monday and Tuesday) are allocated during Semester 1 and the first half of Semester 2 for the experimental work on the project, which has to be completed by no later than the end of the Easter Term.
- Oral Presentation: As part of the assessment process (and also as a preparation for a possible viva by the External Examiners), each student is required to give an oral presentation of 10-15 minutes duration on their project work to their supervisor and a second marker. Students should be prepared to answer questions following their presentation. **The presentations will normally take place during the first week of**

the Summer Term; students will be informed by their supervisor of the date/time of the oral presentation.

• Project Dissertation: A typed dissertation has to be presented, double spaced, on A4 paper (210 x 297 mm), with a sufficient (32 mm) left-hand margin to allow for binding. The project dissertation should include in sequence: a title page, acknowledgements, a summary, an introductory chapter, chapters describing experimental procedures and presenting results, a discussion chapter, a statement of conclusions and suggestions for further work, and a list of references. Two bound copies (binding is done by Chemistry) of the dissertation are required, one for Chemistry and one for the academic supervisor. In addition, students are advised to prepare a permanent copy for their personal reference and a student sponsored by another institution must provide a copy for that institution. The dissertation (2 unbound copies) has to be handed in to the Chemistry Office by **no later than 12 noon on the Friday of the penultimate week of teaching in Semester 2**. There is a penalty of 2% of the project mark per day for late submission of the dissertation.

ANALYTICAL CHEMISTRY B

ECTS Credits: 5	Level: 1Semester: 2	Code: CH109-05
Contact Hours:	24 hours comprising: 16 hours lectures and 8 hours laboratory we	
Pre-requisites:	Foundation Analytical Chemistry	
Assessment:	One written examination (2 hours, continuously assessed laboratory w	50%), coursework (25%) and ork (25%).

Academic Objectives

This module introduces the principles of liquid phase chromatography, gas liquid chromatography and quantitative infrared spectroscopy, incorporating complementary practical exercises.

Detailed syllabus

Liquid phase chromatography

- Adsorption and partition
- Application to paper, thin layer and liquid column techniques; one way, two way, normal and reverse phase, zone spreading and tailing
- Ion exchange techniques
- Gas liquid chromatography (glc)
- Basic instrumentation: Schematic diagram
- Mobile phase partition
- Packed column, open tubular columns
- Isothermal operation and temperature programming
- Detectors, resolution, retention time
- Use of internal standards and method of standard additions

Quantitative infrared spectroscopy

• A and %T, Beer-Lambert law, apparent deviations, applications Practical exercises. Selection from:

- Separation of a dyestuff mixture by column chromatography
- Identification of acid dyestuffs by paper chromatography
- Identification of drugs by thin layer chromatography
- Identification of alcohols by gas liquid chromatography
- Quantitative determination of ethanol using internal standardisation
- Quantitative determination of naphthalene by infrared spectroscopy
- Separation of cobalt and nickel by ion exchange

ANCILLARY SKILLS 1

ECTS Credits: 5	Level: 1 Semester: 1	Code: CH110-05
Contact Hours:	Maximum 36 hours	
Pre-requisites:	None	
Assessment:	By coursework.	

This module will consist of two units which will enable the students to learn and practice skill in:

- Information Technology
- Basic Mathematical Methods: students should attend *either* unit A *or* unit C according to their prior knowledge of mathematics

Information Technology

Contact Hours:	12 hours
Course Delivery:	All classes take place in the teaching room in the library and are organised as practical exercises using the University network of PCs. Supervision by Chemistry staff.

Academic Objectives

This course will enable the students to become familiar with the Information Technology facilities at Salford and gain practice at accessing and using the facilities provided on the network.

Detailed Syllabus

- 1. Description of network and log-in procedure, including password changing. Tour of network menus including the specialised Chemistry menu system.
- 2. Description of CALCHEM computer assisted learning tutorial package and details of usage, production and collection of printed output.
- 3. Introduction to use of floppy discs. Instruction on formatting of floppy discs. Introduction to Word Perfect followed by a simple exercise in typing in a document and saving to network and to floppy disc.
- 4. Further practice using Word Perfect involving formatting of text, moving and copying blocks of information, spell-checking and importing of graphs and diagrams into a document. Instruction on printing of documents produced using Word Perfect on the network.
- 5. Introduction to Quattro Pro spreadsheet and exercises illustrating the input of text, data and formulae into the spreadsheet. Solution of a problem to find the turning points of a cubic equation arithmetically. Practice in saving the spreadsheet to the network and to floppy disc.
- 6. Exercise using Quattro Pro to examine kinetic data graphically and to determine the order of reaction. Instruction and practice in printing out the spreadsheet on the network printer.
- 7. Exercise using Quattro Pro illustrating the use of a spreadsheet, to import data already held in a file, to convert the data to linear form and to carry out a linear regression

analysis producing the equation of the best straight line

- 8. Instruction and practice in obtaining a high quality graph plot on the network plotter.
- 9. Use of the spreadsheet for the sorting of information using primary and secondary keys. Calculation of distribution pattern of set of data and presentation graphically.
- 10. Introduction to the drawing of molecular structures using an animated demonstration of a molecular drawing package followed by a tutorial and an exercise in molecular drawing.
- 11. Use of Word Perfect to construct a simple report based on the data processed in Quattro Pro in 6, illustrating the incorporation into the report of the spreadsheet data and the graphs produced in the original exercise.
- 12. Exercise using Word Perfect for the production of a CV to a standard format. Instruction on the production of the final document to a high quality on the network Laser printer.

Basic Mathematical Methods for Chemists A

Contact Hours: 12 lectures and 12 tutorials

Academic Objectives

This component of the half module is intended to introduce and reinforce the mathematical techniques used in the study of chemistry; to develop the confidence of students by giving them experience of the application of the techniques specifically in the context of the theory of Chemistry and in the manipulation and analysis of experimental data. All students will be required to demonstrate the necessary competencies and the teaching time will concentrate on the needs of those students who need to develop the required skills. The programme is supervised by Physical Chemistry staff.

Detailed Syllabus

Manipulation of numbers. Balancing a chemical equation. Precision of a number; significant figures. Accuracy in calculations; rounding errors. Priority order of operations. Meaning of symbols, SI units and prefixes. Elementary algebra. Indices and logarithms; application to pH. Solution of linear equations. Graphs of linear functions. Elementary trigonometry: Definition of the basic trigonometric functions. Simple formulae for the solution of triangles (without proof).

Basic Mathematical Methods for Chemists C

Contact Hours: 12 lectures and 12 tutorials

Academic Objectives

This component of the half module is intended to introduce and reinforce the mathematical techniques used in the study of chemistry; to develop the confidence of students by giving them experience of the application of the techniques specifically in the context of the theory of Chemistry and in the manipulation and analysis of experimental data. All students will be required to demonstrate their competence and the teaching will focus on the needs of students with particular requirements. The course is supervised by Physical Chemistry staff.

Detailed Syllabus

Solution of linear and quadratic equations. Solution of simultaneous equations. Graphs of linear and quadratic functions. Reduction of non-linear functions to linear form; log-linear and log-log plots. Mathematical series. Binomial theorem. Arithmetic and geometric series. Trigonometry: graphs and simple identities. Radian measure; polar co-ordinates. Statistical techniques for error analysis of experimental data. Mean and standard deviation. Precision of results. Regression.

ANCILLARY SKILLS 2

ECTS Credits: 5	Level: 1 Semester: 2	Code: CH111-05
Contact Hours:	Maximum 36 hours	
Pre-requisites:	Ancillary Skills 1	
Assessment:	By coursework.	

This module will consist of two units which will enable the students to learn and practice skills in:

- Written Communication
- Basic Mathematical Methods: students should attend *either* unit B *or* unit D according to their prior knowledge of mathematics

Written Communication

Contact Hours: 6 tutorials

Course Delivery: The course will operate as a supported self study activity. Reading sources and tutorial support will be provided. Chemistry staff with a proven record as scientific authors will be involved.

Academic Objectives

To equip students with the skills required to communicate successfully both within and outside the scientific community.

Detailed Syllabus

Students will be required to present:

- 1. A précis of a piece of non technical writing.
- 2. A précis of a piece of technical writing, for example, a section of a text book.
- 3. A summary of a restricted literature review.
- 4. An essay on a topic of general interest which may have a scientific context.
- 5. A word-processed report on a piece of experimental work.
- 6. A word-processed Curriculum Vitae.

Basic Mathematical Methods for Chemists B

Contact Hours: 12 lectures and 12 tutorials

Academic Objectives

This component of the half-module is intended to introduce and reinforce the mathematical techniques used in the study of chemistry; to develop the confidence of students by giving them experience of the application of the techniques specifically in the context of the theory of Chemistry and in the manipulation and analysis of experimental data. All students will be required to demonstrate the necessary competencies and the teaching time will concentrate on the needs of those students who need to develop the required skills. The programme will

be supervised by Physical Chemistry staff.

Detailed Syllabus

Differential Calculus

- The idea of a limit and the meaning of a derivative.
- Derivatives of the elementary functions.
- Simple techniques of differentiation: products, quotients.
- Simple applications of derivatives: small changes.
- Maxima and minima and points of inflexion.

Integral Calculus

- Integration as the limit of a summation and as the reverse of a derivative.
- Indefinite and definite integrals.
- Elementary standard integrals.
- Simple applications of integration.

Basic Mathematical Methods for Chemists D

Contact Hours: 12 lectures and 12 tutorials

Academic Objectives

This component of the half-module is intended to introduce and reinforce the mathematical techniques used in the study of chemistry; to develop the confidence of students by giving them experience of the application of the techniques specifically in the context of the theory of Chemistry and in the manipulation and analysis of experimental data. All students will be required to demonstrate the necessary competencies and the teaching time will concentrate on the needs of those students who need to develop the required skills. The programme will be supervised by Physical Chemistry staff.

Detailed Syllabus

Differential Calculus

- Simple techniques of differentiation: products, quotients.
- Chain rule differentiation, implicit differentiation.
- Maclaurin expansions of exp(x), 1n(1+x), $\cos x$ and $\sin x$.
- Simple operations with power series.
- Taylor's expansion (without proof).

Integral Calculus

- Simple techniques of integration: substitution, by parts.
- Use of partial fractions.
- Integration of particular functions which occur in Chemistry.
- Simple applications of integration, in particular to the calculation of mean and root mean square values and the solution of first order differential equations with separable variables.

Numerical methods

• Newton's method for the solution of non-linear equations.
BIOCHEMISTRY (Introduction to)

ECTS Credits: 5	Level: 1 Semester: 1	Code: CH112-05
Contact Hours:	12 lectures, 8 tutorials, 12 hours prac assignment	tical work and a written
Pre-requisites:	None	
Assessment:	One written examination (2 hours) ar	nd coursework.

Academic Objectives

There is a close relationship between the disciplines of biological and chemical science. The aim of this course is to introduce the student to the elements of biochemistry and to highlight the links between chemical processes and biological function. Although not a comprehensive summary of the subject, the course is designed to provide chemists with a stimulating window to the living organic world.

- 1. Cell biology: A primer of the essential elements of cellular biology and a review of the role of specific organelles in cell function.
- 2. Biological molecules: The chemistry and biology of vital biological macromolecules, including proteins (with special emphasis on enzymes), polysaccharides, nucleic acids and lipids.
- 3. Biosynthesis: A review of the common themes and principles which unify the array of biochemicals and reaction pathways adopted in the biosynthetic strategies for the fabrication of complex macromolecules.
- 4. Bioenergetics: The generation of biologically useful energy by oxidative processes in living organisms. The occurrence and significance of specific bioenergetic relationships will be discussed.
- 5. Molecular biology and biotechnology: An introduction to the nature and behaviour of genetic material.

ENVIRONMENTAL CHEMISTRY

ECTS Credits: 5	Level: 1 Semester: 1	Code: CH113-05
Contact Hours:	24 hours lectures and 12 hours practi	cal work
Pre-requisites:	None	
Assessment:	One written examination (2 hours, 50 and coursework (25%)	0%), assessed practicals (25%)

Academic Objectives

This module is designed to give students an appreciation of those aspects of chemistry which are important in an environmental context. It will enable students to appreciate the ways in which their analytical skills can be applied to environmental monitoring and control and to be aware of the basic features of environmental processes.

- Air. Sulphur dioxide; hydrocarbons; carbon monoxide; nitrogen oxides; ozone; the atmospheric aerosol.
- Water. The water cycle; treatment of waste waters; specific water pollutants; nutrient removal; synthetic detergents; industrial effluents; effects of pollution on natural waters.
- Land. The chemistry of waste treatments; hazardous wastes; incineration; landfill gas generation.
- Control procedures currently in operation. Brief outline of legislative control; examples of emission control of both moving and stationary sources; catalytic converters; lean burn engines; flue gas desulphurisation; low NO_x burners.
- Sampling techniques. Water; land, soil, sediments; air.
- Analytical techniques used to monitor pollutants in the environment. Spectrophotometric; chromatographic; ion-selective electrodes; titrimetric.

GEOCHEMISTRY

ECTS Credits: 5	Level: 1 Semester: 2	Code: CH114-05
Contact Hours:	24 lectures and 6 practical tutorials	
Pre-requisites:	None	
Assessment:	One written examination (2 hours)	

Academic Objectives

To provide the students with an introduction to geochemistry, its contribution to the study of chemistry, and its importance in economic and environmental studies.

Detailed Syllabus

There is a close relationship between the disciplines of geochemistry and chemistry which dates back to the quest for new elements in rare minerals. Many of the concepts that are thought of as chemical, *e.g.* ionic radius and radius ratio, were developed with geochemical problems in mind. The only source of chemicals available to the chemist is the Earth, and the abundance and distribution of the chemical elements are essentially determined by geochemical considerations. Recent concern with carbon dioxide imbalances and acid rain serve as a reminder that geochemical processes continue and are a proper subject of study for chemists.

This course will be a survey of the field of geochemistry. Emphasis will be on the applications of chemical principles to large scale Earth processes. Factual detail will be minimised. Hopefully it will be a window onto the chemistry occurring outside the laboratory and the factory.

- 1. Definition of geochemistry and cosmochemistry. Relationship with chemistry, physics and geology. The Earth as a chemical storehouse. Rocks and minerals. Igneous and sedimentary rocks.
- 2. The origin of the chemical elements. Cosmic, solar and terrestrial elemental abundances. Methods of extra-terrestrial analysis. Importance of elements Z = 1,2 and the cosmic insignificance of the rest. Big Bang, nuclear fusion, r and s processes.
- 3. The shell structure of the Earth. Seismic and other evidence. Measured crystal and internal mantle/core compositions.
- 4. Primitive Earth as a molten chemical system. Primary geochemical differentiation of the Earth, and its consequences. Geochemical classification of the elements. Secondary differentiation, one formation, diagenesis
- 5. 'Clarke' and 'Clarke of Concentration.' The pre-geological history of the Earth. The development of an oxidising atmosphere.
- 6. The crystalline state. Radius ratio and structure. The SiO_4^{4-} tetrahedron and its polymeric forms
- 7. Composition and structure. Substitution and the myth of solid solutions. Diadochy, aluminosilicates. Significance of the latter in mineralogy and soils.
- 8. The basic rock-forming silicates (olivine, pyroxene, amphiboles, quartz, feldspar and micas). Bowen's Series and the development of igneous rocks from the same type of 'basic' magma. Magmas. Basic and acid rocks.
- 9. Igneous rocks. Extrusive (lavas, basalts).and intrusive (batholyths, dykes, sills). Volume mineralogical composition of igneous rocks.
- 10. Basic crystallography. Elements of symmetry. Systems, classes, habit. Like and

unlike faces, interfacial angle. Weathering processes, transport process.

- 11. Sedimentary minerals and rocks. Evaporites, sandstones, shales. Biological processes in rock formation (coral, limestone, chalk, coal, oil, peat).
- 12. Role of solubility, ionic size, ionic charge, pH, E^o, and the colloidal state, in sedimentary processes. Buffer systems and geochemical fences. The aqueous environment and its composition; ocean and river water.
- 13. The oceans and the atmosphere. CO_2 and the greenhouse effect. The Earth as a store of fuels: a) fossil b) nuclear
- 14. The radioactivity of the Earth. The geological time-scale. Historical, geological evidence, use of fossils, absolute methods of dating.

Practical work

Extensive practical work will not be possible but it is proposed to include 'practical tutorials' on the following topics:

- 1. Recognition of crystal form in models.
- 2. Recognition of common minerals in hand specimens.
- 3. Simple chemical tests.
- 4. Streak, hardness, lustre.
- 5. Petrological examination of some thin sections (this will involve some discussion of the Petrological Microscope).

MEDICINAL CHEMISTRY (Introduction to)

ECTS Credits: 5	Level: 1 Semester: 2	Code: CH115-05
Contact Hours:	24 lectures and 12 hours laboratory work	
Pre-requisites:	Analytical Chemistry	
Assessment:	One written examination (2 hours, 80%) a	nd coursework (20%)

Academic Objectives

This is the foundation course in a series of Medicinal Chemistry courses available here. It provides a general background to the activities of chemists in the pharmaceutical industry; it is a prerequisite for other Medicinal Chemistry options and is compulsory for students taking the MChem Chemistry with Medicinal Chemistry degree programme.

Detailed Syllabus

This module consists of two units:

- Introduction to Medicinal Chemistry (12 lectures).
- Analytical Chemistry in Pharmaceutical Research, Development and Manufacture (12 lectures + 12 hours laboratory work).

Introduction to Medicinal Chemistry

The aim of this part of the course is to provide a general introduction to the area of Medicinal Chemistry. In particular we will be concerned with the various stages that lead to the development of a new pharmaceutical agent and the role that chemists play in this process.

- 1. Historical Perspective. A brief outline of the development of the modern pharmaceutical industry.
- 2. Drug Discovery. 'Folk' medicine; drug discovery without a lead compound; drug discovery with a lead compound.
- 3. Drug Development. Pharmacophore identification; functional group modification; structure activity relationships; 'rational' drug design; drug trials.
- 4. Drug targets. Receptors; enzymes; DNA.

Analytical Chemistry in Pharmaceutical Research, Development and Manufacture

The aim of this part of the course is to provide an overview of areas where analytical chemistry plays a role in the pharmaceutical industry. It is divided into two sections: Reasons and Requirements for Drug Analysis; Instruments and Techniques.

- Reasons and Requirements for Drug Analysis. This section will highlight the different roles which analytical chemistry plays at different stages of drug development and manufacture. It will provide an introduction to the methods and techniques that are used to characterise, analyse the purity, and assure the quality of organic compounds produced in the pharmaceutical industry. It will also introduce students to regulatory aspects of drug manufacture and quality assurance.
- 1. Structure of a typical pharmaceutical company.
- 2. The role of analytical chemistry in drug discovery.
- 3. The role of analytical chemistry in drug development.
- 4. Drug manufacture, synthesis, formulation and analysis.
- 5. Analytical Chemistry in Quality Assurance. Drug licensing agencies. GMP, GLP and

GCLP. Standard Operating Procedures (SOPs) and Standard Operating Methods (SOMs). The role of the Qualified Person (QP).

- 6. Work of the QA Laboratories. General types of chemical tests carried out. Testing of simple raw materials and purchased drug additives. Testing of purchased organic drug precursors and intermediates. Testing of in-house intermediates. Testing of the final bulk drug. Testing of formulated products.
- 7. QA methods of analysis and specifications. Standards for patented drugs. Pharmacopoeia standards.
- 8. Examples of analytical methods for particular compounds. Lanolin, Atenolol (Tenormin).

Instruments and Techniques. This section of the course will provide an introduction to the principles and application of chromatographic techniques for quantitative analysis of organic compounds.

- 1. General principles of solid/ liquid chromatography (on silica). The structure of silica. Relative polarity of different types of organic compounds and solvents. Mechanism of chromatographic separation of compounds on silica. Reverse phase chromatography.
- 2. Thin layer chromatography (TLC). Method for running TLCs.
- 3. High performance liquid chromatography (HPLC). Typical HPLC instrumentation. Procedure for running HPLC. Features of good chromatography. HPLC columns and solvent systems. Reverse phase chromatography. Types of reverse phase column. Solvents and additives for reverse phase HPLC. Chiral modified stationary phases.
- 4. Gas chromatography (GC). General principles of GC. Typical GC system and procedure for operation. GC using packed columns. GC using capillary columns. Capillary column stationary phases. Injector design for capillary GC.
- 5. Quantitative chromatographic analysis. Instrument validation and calibration. Identification of individual components and method checks. Quantification of individual components. Quantification using an external standard (HPLC). Quantification using an internal standard (Capillary GC).
- 6. Laboratory Work. HPLC Quantification of an impurity using an external standard. Capillary GC Quantification of an impurity using an internal standard.

ANALYTICAL CHEMISTRY C

ECTS Credits: 5	Level: 2Semester: 1	Code: CH209-05
Contact Hours:	24 hours comprising: 16 hours lectu	rres and 8 hours laboratory work
Pre-requisites:	Foundation Analytical Chemistry	
Assessment:	One written examination (2 hours, 5 continuously assessed laboratory we	50%), coursework (25%) and ork (25%).

Academic Objectives

This module introduces the principles of sample preparation, atomic spectroscopy and electroanalytical chemistry, incorporating complementary practical exercises.

- Sample preparation. An introduction to methods of sample preparation for instrumental analysis: classical (wet digestion, fluxes, dry ashing), microwave digestion, liquid-liquid extraction, solid phase extraction, accelerated solvent extraction.
- Atomic spectroscopy. Principles of atomic emission, absorption and fluorescence spectrophotometries; flame atomisation, electrothermal atomisation, hydride generation methodology; instrumentation for atomic spectrometry; interferences (spectral and chemical) and their correction; inductively coupled plasma spectrometry; detection limits and calibration; applications.
- Electroanalytical chemistry. Potentiometry: electrode potentials and their application, membrane potentials and electrodes, pH and fluoride ion selective electrodes as case studies. Polarography: the dropping mercury electrode (DME), currents at the DME, the Ilkovic equation, the equation of the polarographic wave, pulsed potential techniques at the DME. Applications of polarography and potentiometry.
- Practical exercises: Sample preparation for atomic absorption spectrometry; investigation of interferences in flame atomic absorption spectrometry; operation of ion selective electrodes (determination of fluoride in toothpaste and/or measurement of the pH of beverages); polarographic analysis of a mixture of metal ions

ANALYTICAL CHEMISTRY D

ECTS Credits: 5	Level: 2Semester: 2	Code: CH210-05
Contact Hours:	24 hours comprising: 16 hours lectu	rres and 8 hours laboratory work
Pre-requisites:	Foundation Analytical Chemistry	
Assessment:	One written examination (2 hours, 5 continuously assessed laboratory we	50%), coursework (25%) and ork (25%).

Academic Objectives

This module introduces high performance liquid chromatography and advanced molecular spectroscopic methods, incorporating complementary practical exercises.

- High performance liquid chromatography (HPLC). Definitions and modes of operation. Instrumental layout and components: solvent reservoirs, pumps, injectors, columns, detectors. Column efficiency in liquid chromatography. Reversed phase hplc: column materials, method development and applications. Ion pair and ion exchange HPLC, applications. Introductory capillary electrophoresis.
- Advanced molecular spectroscopic methods. Uv/visible absorption spectrophotometry instrumentation; electronic transitions in inorganic and organic analytes; chromophores, auxochromes, solvent effects; Beer-Lambert law, analysis of mixtures; applications.
- Molecular luminescence. Fluorescence and phosphorescence, deactivation processes; transition types, structural and solution effects; instrumentation; applications; chemiluminescence.
- Mass spectrometry. General description and instrument components; ion sources, sample inlet, mass analysers; mass spectra of organic and biological molecules, identification and molecular mass measurement; introduction to hyphenated techniques (GC/MS, MS/MS, LC/MS).
- Practical exercises: Determination of analgesics in a mixture by HPLC; evaluation of efficiency and solvent optimisation (two week practical); fluorescence spectrometric determination of vitamins in biological and food samples; mass spectrometric identification of biological molecules (*e.g.* demonstration of MALDI-MS).

MEDICINAL CHEMISTRY 1

ECTS Credits: 5	Level: 2Semester: 1	Code: CH211-05
Contact Hours:	24 lectures	
Pre-requisites:	Medicinal Chemistry (Introduction to)	
Assessment:	One written examination (2 hours)	

Academic Objectives

The aim of the module is to reinforce the general principles of drug discovery and drug modes of action which were introduced in the Introduction to Medicinal Chemistry module. The application of these principles will be presented in the context of drug classes used to combat particular disease types.

Detailed Syllabus

The module consists of two units, each of 12 lectures: antiviral drugs and heart drugs. Antiviral Drugs

- 1. Introduction to viruses. Discovery of viruses, vaccination, antiviral chemotherapy. Structure of viruses, DNA and RNA viruses. Viruses as antigens; vaccines; resistance. Main groups of viruses affecting man.
- 2. Carbohydrate chemistry, DNA and RNA. Properties and structure of pyranose and furanose sugars. Glucose, ribose, 2-deoxyribose; nucleosides; structure of DNA and RNA.
- 3. Biochemical targets for chemotherapy. The stages of viral replication: opportunities for chemotherapy.
- 4. Nucleoside Analogues as Antivirals. Nucleoside structure, phosphorylation and delivery. Design of nucleoside analogues as antivirals. Isosteres and prodrugs for nucleoside phosphates.
- 5. Herpes viruses. HSV and treatments. Cytomegalovirus and treatments.
- 6. HIV and AIDS. Retroviruses. Reverse Transcriptase (RT). Course of HIV. AIDS chemotherapy: RT inhibitors and HIV protease inhibitors. Other biochemical targets.

Heart Drugs

- 1. The cardiovascular system. Basic physiology how the heart works. Biochemical control of the cardiovascular system.
- 2. Types and causes of heart disease. Different types of heart disease will be identified. Their causes, physiology and biochemical progress will be examined. Topic will include: Congenital heart disease; arrhythmias; atherosclerosis; congestive heart failure.
- 3. Drugs to relieve heart disease. The design and synthesis of drugs used to tackle various types of heart disease will be studied. Biochemical modes of action of individual drug types will be identified. The design of drugs with selective receptor interactions will be highlighted. The challenges involved in developing second and third generation drugs for improved treatment of individual diseases will be studied. Some of the main classes of drugs which will be examined are: Beta-blockers; ACE inhibitors; cholesterol lowering drugs; anti-arrhythmics; calcium channel blockers.

MEDICINAL CHEMISTRY 2

ECTS Credits: 5	Level: 2Semester: 2	Code: CH212-05
Contact Hours:	24 lectures	
Pre-requisites:	Medicinal Chemistry (Introduction to)	
Assessment:	One written examination (2 hours)	

Academic Objectives

The aim of the module is to reinforce the general principles of drug discovery and drug modes of action which were introduced in the Introduction to Medicinal Chemistry module. The application of these principles will be presented in the context of drug classes used to combat particular disease types.

Detailed Syllabus

The module consists of two units, each of 12 lectures: antibacterial drugs and biopolymers. • Antibacterial Drugs. The aim of this part of the module is to provide an introduction to the area of antibacterial chemotherapy. A brief historical introduction will lead to a discussion of bacteria, and the main ways in which they can be attacked by drug treatment. Examples of each of these classes of drugs will be dealt with in detail, discussing where appropriate their structure, stereochemistry, reactivity, preparation, activity, and mode of action.

- 1. Historical perspectives.
- 2. Bacteria: Cell structure, function of component parts.
- 3. General mechanism of action of antibacterial drugs.
- 4. Antimetabolites: The sulfonamides.
- 5. Cell wall synthesis inhibitors: Penicillins and related b-lactam antibiotics.
- 6. Ion conducting antibiotics: Valinomycin and related compounds.
- 7. Protein synthesis inhibitors: Rifamycins, aminoglycosides, tetracyclines, chloramphenicol, macrolides.
- 8. DNA transcription and replication inhibitors: Quinolones, aminoacridines.
- 9. Resistance: origins, strategies to combat resistance.
- Biopolymers: Amino acids, peptides, proteins, and nucleic acids
- 1. Introduction, L-configuration. Classification as neutral, acidic, or basic. Physical properties, amphoteric nature, dipolar form. Titration curve for glycine, isoelectric points, pK_a values.
- 2. Reactions of amino acids: Esterification, amide formation, ninhydrin, oxidation of cystine units. Separation and analysis of amino acid mixtures; chromatography, ion exchange, electrophoresis. Peptides, nomenclature, covalent bonding, physical properties. Examples, methionine enkephalin, insulin.
- 3. Peptide structure determination: Amino acid analysis, end group analysis (Edman, Sanger, dansyl, carboxypeptidase), sequencing.
- 4. Synthesis of polypeptides: Protection of amino and carboxyl functions; solid phase (Merrifield) method.
- 5. Proteins, classification according to structure and function. Examples of conjugated proteins. Bonding types; disulphide, hydrogen, polar-ionic, van der Waals. Fibrous and globular types, occurrence and properties. Primary and secondary structure; amide geometry, H-bonds.
- 6. Random coil, helix, and pleated sheet structures. Role of proline. Tertiary structure,

myoglobin. Quaternary structure, haemoglobin. Enzymes.

- 7. Polysaccharides. Brief review of monosaccharide chemistry. Glycosides. Disaccharide (lactose, sucrose) and polysaccharide structures. Starch and glycogen. Glycoproteins.
- 7. Nucleic acids. Hydrolysis to monomeric components. Pyrimidines and purines. Nucleosides, nucleotides. The structure of DNA. Base-pairing (Watson-Crick).
- 8. The chemical basis of heredity, DNA replication. Structure and synthesis of RNA, transcription, protein biosynthesis.
- 9. Sequencing DNA. The Maxam-Gilbert reactions.
- 10. Polysaccharides. Overview of monosaccharide chemistry. Glycosides.
- 11. Disaccharide (lactose, sucrose) and polysaccharide structures. Starch and glycogen.
- 12. Blood group determinants, glycoproteins.

CHEMICAL PROBLEM SOLVING SKILLS

ECTS Credits: 5	Level: 2Semester: 2	Code: CH213-05
Contact Hours:	6 problem solving workshops	
Pre-requisites:	None	
Assessment:	One written examination (2 hours, 50%) a	and coursework (50%)

Academic Objectives

The aim of the module is to enable the student to:

- Develop a better understanding of fundamental principles and concepts of chemistry.
- Be able to solve chemical problems using fundamental chemical principles.
- Be able to solve chemical problems by applying their chemical knowledge.
- Develop their independent study skills.

Detailed Syllabus

In each branch of Chemistry, students will be given group tuition in solving general problems through workshop classes. However, the most important mode of learning will be the work students undertake individually on problems which they will be given each week. Examples of areas in which problems will be set and reviewed include:

- General methods of structure determination using a combination of spectroscopic techniques NMR, MS, IR, UV, *etc*.
- Synthetic organic chemistry tuition will be given in applying logical principles to devising synthetic routes to simple organic molecules, using reactions and principles already covered in previous Organic Chemistry courses.
- Mechanistic chemistry problems will be set which illustrate and reinforce an understanding of common general principles which apply to the way in which organic reactions proceed, emphasising kinetic and thermodynamic principles.

QUALITY ASSURANCE AND QUALITY CONTROL

ECTS Credits: 5	Level: 2Semester: 2	Code: CH214-05
Contact Hours:	24 hours lectures/tutorials	
Pre-requisites:	None	
Assessment:	One written examination (2 hours, 60%)	plus coursework (40%)

Academic objectives

To be successful in today's economic climate, the chemical industry and chemical laboratories must be dedicated to continuing improvements in the quality of their products and services. This module sets out to define standards and introduce effective methods of quality assurance and control. A number of statistical methods are covered, but no prior knowledge of these techniques will be assumed. The emphasis will be placed on practical procedures of Quality Control.

- Introduction to quality control. Data gathering and presentation. Accuracy and precision. Random and systematic errors. Use of standards
- Statistical methods. Probability distributions: Binomial; Poisson; Normal; Student t. Hypothesis testing. Estimation and confidence limits. Inferences on means, proportion. Errors of type I and II.
- Quality control. Control by acceptance sampling. Process control, sampling by attributes and by variables. Performance of sampling plans. Operating characteristics. Control charts (Shewhart). Cusum.

SCIENTIFIC COMMUNICATION SKILLS

ECTS Credits: 5	Level: 2Semester: 1	Code: CH215-05
Contact Hours:	4 hours lectures, 4 hours individual discussion with supervisor, 8 hours seminars	
Pre-requisites:	None	
Assessment:	Project report (70%) and oral presentation (30%)	

Academic Objectives

The aim of the module is to develop the student's ability to:

- Access chemical and other scientific information from primary literature sources.
- Analyse and disseminate such information.
- Give an oral review presentation of a topic in a professional and lucid manner.
- Produce a concise and informative report on a topic, including a focused bibliography of literature references.

Detailed Syllabus

The module is mainly project based. Whole class tuition will be given in:

- Manual and electronic techniques for information retrieval.
- Analysing, sorting and understanding the significance of information retrieved.
- Preparing a review of scientific material.
- Preparing and presenting an oral presentation.

Titles for the projects will be offered by individual members of staff and will vary from year to year depending on the interests and availability of individual staff members. The member of staff offering the topic will provide some individual guidance to the student. In general, BSc students will be allocated project topics of a more general nature, such as those found in the popular scientific press, whereas MChem students will be allocated more technical based projects to prepare them for their final year research work.

Students will present their oral presentations, in seminar groups, to their peers and members of staff. Written project reports are to be handed in by the end of the semester.