Imperial College
London

Department of Chemistry

First Year Syllabus

2004 - 2005

Contents

Page

Foundation Course

Inorganic I

Organic I

Physical I

Department of Chemistry – Imperial College

INTRODUCTION TO FIRST YEAR CHEMISTRY

Aims

The first year of the degree in Chemistry aims to provide the students with an introduction to the fundamental concepts required to rationalise and predict molecular structure and chemical reactivity. To achieve this goal the students study the behaviour of a wide range of chemicals (both organic and inorganic) and rationalise their behaviour using a theoretical framework (quantum mechanics, thermodynamics and kinetics). Furthermore, we aim to provide the students with a basic understanding of the most important spectroscopic techniques for characterisation. These aims can only be achieved by a combined theoretical and practical approach, this being one of the most important strengths of our degree. By the end of the year it is expected that the students will have a good understanding of the factors affecting chemical reactions, the rationalisation of such factors and the ability to explain them within a theoretical framework based on basic quantum mechanics, thermodynamics and kinetics.

Summary of Content

The first year consists of 153 hours of chemistry lectures (plus approximately 50, maximum 60, hours of ancillary courses), 230 hours of practical work (one laboratory course each term) including a maths laboratory (24 hours) and three tutorials a week (in small groups of 4 to 6 students). Moreover the students attend workshops (arrow pushing and symmetry). The first year is evaluated by exams (the Foundation Course in January and three examinations – inorganic, physical and organic – in June) and coursework (which consists of tutorial sheets, laboratory reports, etc). An examination for the ancillary courses is also given.

During the first term the students take 60 hours of lectures, 60 hours of practical work (basic laboratory techniques) and two workshops (maths and arrow-pushing), which all together conform the Foundation Course. This course aims to provide a bridge in knowledge between school chemistry and the start of university chemistry, and to bring students of different backgrounds to the same point. We also aim to indicate the threads which link the three main areas of chemistry (inorganic, organic and physical). More specifically, the Foundation Course aims to provide the students with an appreciation of the quantum mechanical basis of the Periodic Table and in turn with the ability to explain trends in the chemical behaviour of the different elements. The course moves on to provide the students an insight into chemical bonding in simple molecules and also into spectroscopy. Parallel to these three components of the course, an introduction to thermodynamics and kinetics is also provided allowing the students to rationalise and predict chemical reactivity. Synthetic chemistry is taught jointly by organic and inorganic lecturers, using a reaction type/mechanistic approach, to emphasise the links between the two branches. To tackle these courses appropriately, maths is also taught in the Foundation Course.

The second and third term of the first year helps to consolidate the fundamental concepts taught in the foundation course. The inorganic courses concentrate in developing the concepts of periodicity and inorganic reactivity discussing specific examples for the main group elements. In parallel to this, a course on characterisation of inorganic compounds is provided (covering IR, NMR and UV/Vis). While main group chemistry is covered in the periodicity course, an introduction to transition metal chemistry is provided in the coordination chemistry course.

The three organic chemistry courses given during the second and third terms aim to give an introduction to the principal functional groups, their properties and reactivity. More specifically a course on aliphatic and aromatic hydrocarbons is provided where the properties of alkanes, alkenes, alkynes and aromatic compounds is presented. A second course covers the chemistry of haloalkanes, alcohols and amines while the third one deals with the carbonyl and carboxyl groups.

Ancillary courses

The students are given the option to choose one of several ancillary courses (approximately 50, maximum 60, lectures). Besides a wide range of languages (which are mandatory for those students doing a year in Europe) courses in physics, mathematics, chemical engineering (F1H8 an F1HV only) and medicinal biology are offered. The physics ancillary (given by staff from the Physics Department) covers the following topics: vibrations and waves; electricity and magnetism; and nuclear physics. In the mathematics course (given by staff from Maths Department), linear analysis, differential equations and applications of advanced calculus are given. This provides a good mathematical background to those students with interests in the fundamental physical basis of chemistry. The medicinal biology ancillary covers various courses: basic anatomy and physiology; macromolecules structure and biosynthesis; cellular organisation; enzymes and metabolic pathways; and chemicals and man. These provide the students with an important background to understand the molecular basis of the bio-medical sciences.

Foundation Course

Aims

- To provide a bridge in knowledge between school chemistry and the start of university chemistry and to bring students of different backgrounds to the same point.
- To emphasise the threads that link the three main areas of chemistry (inorganic, organic and physical).

(Topics in italics are covered to some extent in the EDEXCEL A-level course)

Foundation Lectures

Atomic and Molecular Structure:

Bohr atom, hydrogen spectrum, particle-wave duality, *orbitals*, wave function, quantisation, *quantum numbers, spin*, hydrogenic atoms, radial and angular functions: radial distribution function, *angular shapes of s,p,d*,f orbitals, Pauli exclusion principle, *Aufbau principle*, screening penetration and *effective nuclear charge*, Hund's rule, *trends in atomic size, ionisation energies, electron affinity, electronegativity, polarizability and polarizing powers.*

NL (8 lectures + 2 problem classes)

This part of the course deals with molecules and builds directly on the earlier part given by Dr Long that deals with atoms.
Lewis Theory, hypervalence, the shapes of molecules and the *VSEPR model*, valence bond theory applied to homodinuclear, heterodinuclear and polyatomic molecules, hybridisation, Linear Combination of Atomic Orbitals and molecular orbital theory for diatomic and small polyatomic molecules. **PDL** (8 lectures + 2 problem classes)

Chemical Equilibria:

Introduction to Thermodynamics: work, temperature, systems, 1st Law, heat, state and path functions. Implications of 1st Law: *enthalpy, calorimetry, Hess's Law*. Entropy: direction of spontaneous change, disorder, 2nd Law, statistical view of entropy. Development of idea of free energy from entropy, application to physical equilibria. *Chemical equilibria*, molar free energy, chemical potential, *dependence upon concentration* , activity, $\ln K_{eq} = -\Delta G/RT$, *temperature dependence*. Colligative properties, Raoult's Law, thermodynamics of freezing-point depression, liquid-liquid extraction . *Acids and Bases, pH, buffer action, pK*.

JD (7 lectures + problem class)

Acids-Base strengths, acidity and basicity of solvents, acid-base reactions, gas phase, solvents and solvolysis, proton affinities, oxoacids, polybasic acids, statistical effect, electrostatic effect, *buffers*. **TW** (2 lectures + problem class)

Electrochemistry and Redox Reactions: Half-reactions, oxidation/reduction potential, electrochemical cell, reversibility, reference electrodes, Nernst Equation, chemical potential from Nernst equation **JD** (3 lectures + problem class)

Electrolysis, reductions, oxidations, electrochemical windows, commercial production of aluminium.

TW (2 lectures + problem class)

Chemical Kinetics:

Basic definitions, differential equation view of rate*, rate constant, rate law, reaction order*, 1st and 2nd order kinetics, maths of determination of kinetics from rate laws, *half-life*. Empirical determination of reaction order and reaction kinetics*: initial rates, kinetic analysis, experimental methods*. Reversible 1st order equilibria: $K = k_1/k_{-1}$, relation to ΔG.

AT (10 lectures + problem class)

Inorganic and Organic Reactivity and Characterisation:

Simple organic mechanistic definitions for *additions, eliminations and substitutions*. Reaction types in inorganic and organic chemistry: *additions, eliminations, substitutions, insertion/extrusions, metatheses.*

TW/ES (4 lectures + 2x3-hour arrow-pushing workshops **ES/JS**)

Mathematics:

Differentiation: limits and continuity, gradient and derivative. Techniques of differentiation: first principles, rules, implicit. Applications: stationary and inflection points (link to free energy and system stability).
Integration: definite and indefinite integration, fundamental theorem of calculus, standard integrals (link to thermodynamics such as work expansion of a gas, quantum mechanics).
First order differential equations: separable and linear equations (links to chemical kinetics).
Statistics: basic error analysis, regression analysis (links to experimental, quantum mechanics, Arrhenius equation).

NQ and **FB** (6 lectures + 9x1.5-hour computer-aided Mathslab sessions)

Aromatic Chemistry:

Aromaticity: resonance theory. Aromaticity: Huckel's rules and MO theory. *Electrophilic substitution: arenium ion mechanism*, reactivity and orientation, ipso-substitution, reversible sulphonation (kinetic vs thermodynamic control). Nucleophilic substitution: SNAr mechanism, benzyne mechanism. Sandmeyer and related radical reactions of diazonium salts.

EHS (5 lectures + problem class)

Building upon:
A-level material.

Looking forward to:
Remaining first year organic, inorganic and physical chemistry.

Learning Outcomes:

Students should:

1. Have an appreciation of the quantum mechanical basis of the Periodic Table
2. Account for the horizontal and vertical trends for some atomic properties such as atomic size, ionisation potential, electron affinity and electronegativity
3. Know how to describe chemical bonding in small molecules of the main group elements
4. Be familiar with the three different models describing those chemical bonds
5. Rationalise the major reactivity of organic and inorganic compounds in mechanistic types
6. Analyse experimental data on chemical equilibria to obtain underlying thermodynamic and kinetic parameters
7. Apply thermodynamic principles of equilibria to practical examples of chemical equilibria, including acid/base and redox systems
8. Predict the chemical reactivity of molecules from thermodynamic data
9. Understand the quantum mechanical background for the absorption of electromagnetic radiation and associated spectroscopies (IR, NMR)
10. Be aware of the major fragmentations patterns in mass spectrometry
11. Understand the MO explanation of aromaticity
12. Predict the site of electrophilic substitution in multi-substituted benzenes
13. Be familiar with conditions favouring reactions other than electrophilic substitution in benzenes
14. Understand the mathematics associated with the chemical lectures

Foundation Laboratory

Timetable

Laboratory to be open 2-5pm on Mondays, Tuesdays, Fridays and 3-6 pm Thursdays alternate weeks starting from Week 2 for a total of five weeks.

Programme

Week 2: Recrystallisation
Week 4: Thin Layer Chromatography
Week 6: Steam Distillation and Iodination of Vanillin (relates to **JD** colligative properties lecture and **EHS** aromatic chemistry lectures)
Week 8: pH Experiment (relates to **JD** and **TW** acid base lectures)
Week 10: New inorganic experiment (tba)

Foundation Course Tutorials

Three tutorials per week, one each in organic, inorganic and physical chemistry.

Lectures in Detail

Atomic Structure

Long, Nick

8 hours + 2 problem classes

Aims

This course aims to give an introduction to the relation of the electronic configuration of atoms with their behavior.

Structure

The course will start with an introduction covering the wide range of reactivity and properties in the chemical world. The origins of the classification of the elements will be discussed (periodic table introduced). After some historical remarks during the first lecture, the course will concentrate on answering the following question: How do modern chemists explain the periodic table? The second and third lectures will deal with the fundamentals of quantum mechanics: quantization of matter; wave-like properties of matter and its mathematical representation (wave-function and its meaning). What is an atomic orbital? Relation of the wave-function with the properties of the system.

Lectures 3 and 4 will discuss the structure of hydrogenic atoms, more specifically: energy levels; quantum numbers; shells, subshells and orbitals; electron spin. Lectures 5 and 6 introduce the idea of radial and angular components of the wave-function; radial nodes, angular nodes and nodal planes; the angular shapes of atomic orbitals (s, p, d and f orbitals); polyelectronic atoms; shielding and penetration. effective nuclear charge (Slater rules); Pauli exclusion principle and the building-up principle.

In lectures 7 and 8 the students will make use of the above concepts to understand the modern periodic table; distribution of elements into blocks; periodicity and trends in atomic parameters; atomic and ionic radii; trends in electron affinity and ionisation energies; lanthanide and transition metal contractions; exceptions in the trends; electronegativity and polarisation power.

Objectives

- By the end of the course the students should have a basic understanding of quantum mechanics (a conceptual picture not a mathematical one).
- The students will be able to write the electronic configuration of all the elements (including those that are exceptions to the Aufbau principle) and understand the reasoning behind this.
- The students will have an appreciation of the quantum mechanical basis of the periodic table.
- The students will be able to account for the horizontal and vertical trends of some atomic properties such as atomic size, ionisation potential, electron affinity and electronegativity.

Looking forward to

The material from this course will specifically lead onto Dr. Lickiss's course on 'Molecular Structure' but the underlying principles are relevant to many of the lectures throughout the degree course.

Molecular Structure

Lickiss, Paul

8 hours + 2 problem classes

Aims

- To extend the first part of the course given by Dr Long in which the electronic structure of atoms and the Periodic Table were introduced.
- To describe simple molecular structures using different models and theories.
- To describe bonding using different theoretical models.

Structure

Lecture 1: Introductory remarks emphasising continuation from atomic ideas and periodicity from Dr Long's course. Classification of chemical bond types and their strengths. Lewis theory and the construction of a molecular structure using this model. The octet rule. Resonance

Lecture 2: The idea of hypervalence. The use of the VSEPR model in the construction of molecular structures. Limitations of the VSEPR model.

Lecture 3: The valence bond model. The H_2 molecule. Homodinuclear molecules, N_2, F_2.

Lecture 4: Heterodinuclear molecules, HF.

Lecture 5: Polyatomic molecules, BeH_2, BH_3, CH_4, NH_3, H_2O.

Lecture 6: Molecular orbital theory, the LCAO method. The H_2 molecule.

Lecture 7: Homodinuclear molecules of the second period elements, Li_2, N_2, O_2, N_2, F_2.

Lecture 8: MO theory for Heterodinuclear molecules e.g. HF and small polyatomic molecules.

Objectives

- Knowledge of how to describe chemical bonding in small main group molecules.
- Prediction of molecular structure of small molecules of the main group elements.
- Application of the three different models described and an appreciation of their different strengths and weaknesses.

Looking forward to

The material from this course will be the basis for lectures on Periodicity and Inorganic Reactivity at the end of the 1st year and main Group Chemistry in the 2nd year.

Foundation Mathematics

Quirke, Nicholas and Bresme, Fernando

6 lectures + 8 x 1.5 hour Mathslab sessions

Aims

To introduce students with the basic mathematical tools needed in the chemistry courses, in particular: kinetics and thermodynamics and experimental laboratories.

Structure

Differentiation: limits and continuity, gradient and derivative. Techniques of differentiation: first principles, rules, implicit. Applications: stationary and inflection points (link to free energy and system stability).

Integration: definite and indefinite integration, fundamental theorem of calculus, standard integrals (link to thermodynamics such as work expansion of a gas, quantum mechanics).

First order differential equations: separable and linear equations (links to chemical kinetics).

Statistics: basic error analysis, regression analysis (links to experimental, quantum mechanics, Arrhenius equation).

Objectives

By the end of the course the students should be able to:

- carry out calculations involving differentiation and integration of functions of one and two variables.
- solve first and second order differential equations relevant to kinetics and thermodynamics.
- analyse and interpret experimental data, evaluate their statistical significance and be able to fit them to theoretical functions.

Chemical Kinetics

Taylor, Alan

10 hours + 2 problem classes

Aims

- Introduce subject of chemical kinetics from an empirical viewpoint
- Provide conceptual framework for understanding molecular reaction dynamics
- Link with and compliment the Foundation, Thermodynamics and Mathematica courses.

Structure

- Empirical Reaction Kinetics
- Rates of Reaction, Rate Laws, Order of Reaction, Integrated Rate Laws, 1st and 2nd order kinetics. Arrhenius Behaviour
- Complex Reactions: Unravelling the Rate Law
- Elementary Reactions, Consecutive Reactions, Lindemann-Hinshelwood Mechanism, Reversible Reactions, Enzyme Kinetics, Chain Reactions, Explosions.
- Experimental Methods
- Monitoring Techniques, Initiation Techniques, Single Molecule Spectroscopy.
- Molecular Reaction Dynamics
- Collision Theory, Diffusion Control, Transition State Theory.

Objectives

By end of course, students should be able to:

- Conduct quantitative analyses of kinetic data
- Relate such analyses to underlying mechanisms of chemical reactions
- Explain on a molecular level the origin of observed kinetics for simple chemical reactions.

Chemical Equilibria

Durrant, James and Welton, Tom

13 lectures + 3 problem classes

Aims

- Introduce the subject of chemical equilibrium from the viewpoint of thermodynamics
- Provide a conceptual framework for relating thermodynamic and electrochemical approaches to equilibria.
- Demonstrate that this conceptual approach can be used in practice to quantify chemical reactivity.

Structure

Lecture 1*:* Introduction to chemical equilibria. Introduction to Thermodynamics: work, temperature, systems, 1st Law, heat, state and path functions (JD)
Lecture 2*:* Implications of first law: thermochemistry, Hess's Law, enthalpy, experimental thermochemistry: calorimetry, example: respiration (JD)
Lecture 3*:* Entropy. Concept of direction of spontaneous change, disorder, 2nd Law, statistical view of entropy, system and surroundings, example: hydrogen combustion.
(JD)
Lecture 4*:* Free Energy. Development of idea of free energy from concept of entropy. Example: respiration. Application to physical equilibria: the free energy of freezing / melting. (JD)
Lecture 5*:* Chemical equilibria. Equilibrium Constants. Molar free energy, chemical potential, dependence upon concentration, activity. (JD)
Lecture 6*:* Temperature dependence of chemical equilibria, $\ln K = -\Delta G / RT$, example of temperature dependent equilibrium. (JD)
Lecture 7*:* Acids and bases. pH, buffer action, pK. (JD)
Lectures 8 & 9: Thermodynamics of acid and base function, why one acid /base is stronger than another (TW)
Lecture 10*:* Electrochemistry. Half reactions, oxidation / reduction potentials, electrochemical cell, reversibility, reference electrodes, example: Zn/Zn^{2+} & Cu/Cu^{2+}. (JD)
Lecture 11*:* Nernst equation. Development from concept of chemical potential to Nernst equation. example: Cu / Cu^{2+} (JD)
Lecture 12*:* Thermodynamics of the Hydrogen Economy: hydrogen production, water electrolysis, fuel cells.
Lectures 13 & 14*:* Electrolysis, reductions, oxidations, overpotential, electrochemical windows, commercial production of aluminium. (TW)

Objectives

- Analyse experimental data on chemical equilibria to obtain underlying thermodynamic and kinetic parameters
- Apply thermodynamic principles of equilibria to practical examples of chemical equilibria, including acid / base and redox systems.
- Predict the chemical reactivity of molecules from thermodynamic data.

Chemical Reactivity

Smith, Ed and Welton, Tom

4 lectures

Aims

This course aims to provide a framework within which the huge number of possible chemical reactions can be rationalized and understood. Chemical reactivity is interpreted in terms of the reaction type (addition, substitution etc.) and particularly the electronic behaviour of the reacting species, *i.e.*, Lewis acid-base, redox and radical reactions.

Structure

- Mechanistic descriptions of organic processes additions/eliminations, substitutions, radical reactions.
- Inorganic addition/elimination reactions, Lewis acid-base adduct formation, typical Lewis acids and bases, comparison with organic additions and eliminations. Insertions and extrusions.
- Substitution reactions, displacement of weak Lewis acids or bases by stronger Lewis acids or bases. Bond breaking/making, dissociative, interchange and associative processes, comparison with S_N1 and S_N2 reactions, hydrolysis of $SiCl_4$. Metathesis reactions.
- Redox reactions, electron transfer, balancing redox equations. Rearrangement reactions of transition metal complexes. Combinations of reaction types, oxidative additions/reductive eliminations, transition metal catalysed reactions.

Objectives

By the end of the course the students should be able to:

- Recognise and categorise a reaction.
- Predict the reactions that a particular reagent may take part in.
- Recognise which spectroscopic tool(s) should allow the best characterisation of the product.

Aromatic Chemistry

Smith, Ed

5 Lectures + problem class

Aims

The course aims to provide an understanding of the basic theory and reactions of aromatic compounds

Structure

Lecture 1: Aromaticity in terms of resonance theory and Huckel MO theory. Anti- aromaticity.
Lecture 2: Electrophilic substitution: the arenium ion mechanism, definition of reactivity and orientation.
Lecture 3: Factors influencing *ortho/para/meta* direction, *ortho/para* ratio.
Lecture 4: Orientation in multiply substituted benzenes, reversible sulphonation in naphthalene, thermodynamic versus kinetic control. Nucleophilic substitution: SNAr mechanism, Meisenheimer complexes.
Lecture 5: Benzyne mechanism, *cine*-direction. Sandmeyer and related radical reactions of diazonium salts, mechanisms, role of copper.

Objectives

By the end of the course students should be able to:

- Predict which cyclic conjugated polyenes will be aromatic or anti-aromatic.
- Understand the mechanism of aromatic electrophilic attack
- Predict the regiochemistry of attack by electrophiles on substituted benzenes
- Define the circumstances of substitution and reaction conditions which will result in reactions of aromatics other than electrophilic substitution

Inorganic I

1st Year Synthesis Lab course

Shaffer, Milo and Steinke, Joachim

54 hours

Aims

The aim of this course is to give the student experience in techniques that are commonly used for the synthesis of inorganic and organic compounds. In this course we aim to expose the student to a wide range of techniques such that he/she is equipped to tackle a variety of synthetic procedures including multi-step synthetic routes.

Course Objectives

- To acquire a fundamental knowledge of the way in which organic and inorganic compounds are handled, prepared and purified.
- To have some practical experience of the analytical techniques used for the characterisation and structural assignment of the compounds that you have prepared.
- To learn how to put together a concise and informative report including the results, procedures, analysis and conclusions.

Experiments

Students will perform five experiments during the laboratory course (each one designed to be carried out during 3 to 4 sessions of 3 hours each). The experiments to be carried out are:

- Synthesis of tetraiodotin(IV) and a triphenylphosphine adduct
- Phosphine complexes of nickel(II)
- Silicon Oxygen Compounds
- Ring-opening reaction of an epoxide
- Synthesis of p-vinyl benzoic acid methyl ester (Wittig reaction and esterification)

By carrying out these five experiments, the students will learn the following laboratory procedures:

- Addition of a solid to a stirred liquid phase
- Liquid/liquid phase extraction
- Drying of organic phase
- Gravity filtration of drying agent
- Recrystallisation
- Reflux
- Distillation
- Removal of solvent in a rotary evaporator
- Suction filtration
- Stirring of a solution
- Dropwise addition of a liquid to a stirred reaction with internal temperature control
- Heating of a solution with temperature control
- Column Chromatography
- How to warm (or heat) up a solution in various vessels (round-bottom flask, Erlenmeyer flask, and beaker)

Characterisation of Inorganic Compounds

Williams, Charlotte

10 hours

Aims

The course will cover the fundamental principles and techniques used to characterise inorganic compounds. There will be an introduction to the symmetry of molecules and a problem based learning exercise on the assigning of point groups. Spectroscopic techniques, including IR, NMR and UV-Vis and mass spectrometry will be examined both theoretically and in the context of practical inorganic chemistry.

Structure

- Symmetry: Symmetry elements, operations and point groups of compounds. (2 Lectures)
- Spectroscopy: The theory, wavelengths and relative energies. UV/vis spectroscopy: Beer Lambert Law, extinction coefficients and selection rules with examples of coloured transition metal complexes (2 Lectures)
- IR spectroscopy: The theory, stretching and bending modes, the selection rules and how to use them to predict the number of IR active bands. Characteristic frequencies for inorganic compounds such as boron hydrides, phosphines, phosphates and transition metal compounds will be covered (2 Lectures)
- NMR spectroscopy: Basic concepts including chemical shift, integrals and coupling will be introduced and illustrated with examples of the use of multinuclear NMR to characterise phosphines, fluorine containing compounds and transition metal compounds (2 Lectures)
- Mass spectrometry: Some basic ionisation techniques and isotope patterns will be introduced and their application for the characterisation of inorganic compounds discussed (2 Lectures)

Objectives

By the end of the course students will be able to:

- Apply the principles of symmetry to assign the point group to simple inorganic compounds using the Flow Diagram
- Explain the theoretical principles and selection rules for UV-Vis, IR and NMR spectroscopy and mass spectrometry
- Analyse spectra of inorganic compounds
- Propose structures for unknown compounds based on their spectra

Looking forward to

The material from this course will be the basis for lectures on NMR methods in inorganic chemistry (2nd year) and Symmetry and Spectroscopy (3rd year).

Coordination Chemistry

Hii, Mimi

9 hours

Aims

This course is a general introduction to the language and principles of coordination chemistry. The Crystal Field approximation is examined along with its use to interpret spectroscopic and magnetic properties. There is discussion about the formation of complexes, nomenclature and role of ligands and isomerism in coordination compounds, dealing specifically with those of transition metals.

Structure

(i) ***Introduction and Scope:*** The language of coordination chemistry. Basic definitions of ligands, complexes, modes of coordination. Nomenclature: rules for naming complexes. Denticity: mono-, bi-, tri-, poly- and ambi-dentate ligands. The chelate, macrocyclic and cryptate effects. Stability constants

(ii) ***Types of Complexes Encountered:*** Charge: neutral, cationic, anionic. Nuclearity: mononuclear, polynuclear, clusters, oligomeric. Common geometries, coordination numbers and oxidation states. Isomerism: geometrical (examples for square planar and octahedral), linkage, coordination, ionisation, optical.

(iii) ***Introduction to Bonding in Coordination Complexes:*** Hard and soft acids and bases theory. Calculation of oxidation state and *d*-occupancy for a complex *i.e.* matching ligands to oxidation states (π-donors vs. π-acids). Crystal field theory for homoleptic complexes. *d*-orbital splittings for O_h, T_d and D_{4h} electric fields. Implications: magnetism, stabilities. Jahn-Teller distortion O_h ---> D_{4h}. Inadequacies: introduction to MO approach (π-bonding).

(iv) ***Colour in Coordination Complexes:*** Overcoming selection rules: (i) Laporte (vibronic transitions, reduction in symmetry); (ii) $\Delta S = 0$ (d^5 case); charge-transfer transitions.

Objectives

By the end of the course , students should be able to (i) calculate the metal oxidation state, coordination number and *d*-occupancy, (ii) suggest the most likely geometry based on CF arguments, (iii) predict the number of unpaired electrons and magnetic moment, (iv) address any questions of isomerism and correctly name these (*cis*, *trans*, *mer*, *fac*, *D*, *A*, etc.), (v) if octahedral, indicate whether Jahn-Teller distortions are to be expected, (vi) suggest whether a complex should be labile or inert towards ligand substitution, (vii) identify the origin of any colours and compare these to related complexes and have begun to develop a familiarity with first-row *d*-block metals and the more common ligands.

Looking forward to

The material from this course will be the basis for lectures on Transition Metal Chemistry (2nd year) and Organometallic Chemistry (2nd year).

Periodicity and Inorganic Reactivity

Davies, Rob

8 hours

Aims

This course presents an overview of the properties, bonding and structures of the s- and p- block elements and their compounds, with particular emphasis being placed upon the trends down the Groups and across the Periods.

Structure

- General principles: types and strengths of bonds, review of hybridisation and VSEPR theory and oxidation states
- Group 1, the alkali metals: elements, compounds, macrocycles
- Group 2, the alkaline earth metals: elements, compounds, covalent character of Be compounds
- Group 13, the boron group: elements, compounds, inert pair effect, boron trihalides (including discussion of Lewis acids and bases), diborane, other group 13 trihalides
- Group 14, the carbon group: elements and allotropes, compounds and oxidation states, catenating ability, halides of group 14 including Lewis acidity of SiF_4 due to vacant d-orbitals
- Group 15, the pnictogens: elements, structure of white phosphorus, strength of N-N triple bond and unusual weakness of N-N single bond, +3 vs +5 oxidation state for the halides, Lewis basicity of R_3M species and effect of changing R and M, hydrides of group 15, oxides of group 15
- Group 16, the chalcogens: elements, colour and paramagnetism of oxygen (MO diagram), oxidation states, hydrides and bond angles in H_2O vs H_2S and H_2Se, halides – structures and reactivities, oxides
- Group 17, the halogens: elements, colours of elements, compounds – covalent vs ionic bonding in compounds, hydrides, interhalogens, oxides and oxo-acids
- Group 18, the noble gases: elements, compounds, halides, oxides
- Diagonal relationships: Li / Mg, Be / Al and B / Si

Objectives

By the end of the course students should understand and be able to discuss:

- Types of bonding in main-group compounds, bond strengths and the orbitals involved: ionic, covalent, metallic, electron deficient, single bonds, multiple bonds and hybridization.
- Physical trends in and structures of the elemental forms down each Group
- Trends in reactivity (including valence and oxidation states) down each Group
- Structure and reactivity of electron deficient molecules such as the boron trihalides, $BeCl_2$ and Al_2Cl_6
- The inert pair effect
- Lewis acidity and basicity in main group compounds
- The use of VSEPR to predict the shape and hybridization of molecules, and the exceptions H_2S and XeF_6
- The origin of the colour of the halogens and oxygen using MO theory
- Hydrogen bonding

Looking forward to

The material from this course will be the basis for lectures on Main Group Chemistry (2nd year) and Advanced Main Group Chemistry (3rd year).

Organic I

Synthesis Lab

Shaffer, Milo and Steinke, Joachim

54 hours

Aims

The aim of this course is to give the student experience in techniques that are commonly used for the synthesis of inorganic and organic compounds. In this course we aim to expose the student to a wide range of techniques such that he/she is equipped to tackle a variety of synthetic procedures including multi-step synthetic routes.

Course Objectives

- To acquire a fundamental knowledge of the way in which organic and inorganic compounds are handled, prepared and purified.
- To have some practical experience of the analytical techniques used for the characterisation and structural assignment of the compounds that you have prepared.
- To learn how to put together a concise and informative report including the results, procedures, analysis and conclusions.

Experiments

Students will perform five experiments during the laboratory course (each one designed to be carried out during 3 to 4 sessions of 3 hours each). The experiments to be carried out are:

- Synthesis of tetraiodotin(IV) and a triphenylphosphine adduct
- Phosphine complexes of nickel(II)
- Silicon Oxygen Compounds
- Ring-opening reaction of an epoxide
- Synthesis of p-vinyl benzoic acid methyl ester (Wittig reaction and esterification)

By carrying out these five experiments, the students will learn the following laboratory procedures:

- Addition of a solid to a stirred liquid phase
- Liquid/liquid phase extraction
- Drying of organic phase
- Gravity filtration of drying agent
- Recrystallisation
- Reflux
- Distillation
- Removal of solvent in a rotary evaporator
- Suction filtration
- Stirring of a solution
- Dropwise addition of a liquid to a stirred reaction with internal temperature control
- Heating of a solution with temperature control
- Column Chromatography
- How to warm (or heat) up a solution in various vessels (round-bottom flask, Erlenmeyer flask, and beaker)

Stereochemistry

Spivey, Alan

3 hours

Aims

To provide an introduction to the shapes of organic molecules and the basic principles and nomenclature of stereogenic elements in organic molecules.

Structure

***Lecture 1*:** Hybridisation and shape; Stereogenic centres; other stereogenic elements.
***Lecture 2*:** (R)- and (S)- nomenclature, Cahn-Ingold-Prelog priority rules.
***Lecture 3*:** Enantiomers, diastereomers and epimers: consequences of symmetry for synthesis and spectroscopy

Objectives

By the end of the course, students should:

- Be able to distinguish chiral molecules from achiral ones.
- Be able to assign (R)- and (S)-descriptors to stereogenic centres in chiral molecules.
- Appreciate the difference between enantiomers and diastereomers.

Alkanes, Alkenes and Alkynes

Gibson, Sue

8 hours

Aims

To introduce the chemistry of alkanes, alkenes and alkynes, using the mechanistic framework of radical reactions, electrophilic additions and concerted reactions.

Structure

A) GENERAL

Line notation; guidelines for drawing organic molecules.
Nomenclature; advice on chemical names, names for the hydrocarbon framework, practice in understanding the names of alkanes, alkenes, and alkynes.
Isomerism; constitutional isomers, stereoisomers, E/Z notation for alkenes, practice.
Bonding in alkanes, alkenes and alkynes; methane, ethene, ethyne, acidity of ethyne.
Shape: conformation of straight chains; ethane, butane;
Shape: conformation of cyclohexane; drawing the chair conformation, ring inversion of cyclohexanes.

B) REACTIVITY OF ALKANES

Heterolysis and homolysis.
Alkyl radical stability.
Radical chain reactions.
Chlorination of alkanes; mechanism, product distribution.

C) REACTIVITY OF ALKENES I – ELECTROPHILIC ADDITION (mainly)

Carbocation stability
Addition of HX; HBr, HI, HCl, H_2S, radical addition of HX.
Addition of bromine; mechanism, addition to cyclohexene.
Addition of water; acid catalysed hydration, $Hg(OAc)_2$ / $NaBH_4$, (hydration of alkynes).

D) REACTIVITY OF ALKENES II – CONCERTED ADDITIONS (mainly)

Epoxidation.
Dihydroxylation (OsO_4); syn and anti diols *via* dihydroxylation or epoxidation / ring opening.
Ozonolysis.
The Diels-Alder reaction.
Hydroboration; borane-diborane, sources of BH_3, hydroboration of alkenes, oxidation of organoboranes using alkaline hydrogen peroxide, hydroboration / oxidation of alkynes.

E) THE VERSATILITY OF ETHYNE

Deprotonation of alkynes.
Alkynes to Z-alkenes.
Alkynes to E-alkenes.
Overview.

Objectives

At the end of this course you should be able to:

- Identify and draw correctly alkanes, alkenes and alkynes.
- Use the bonding picture presented for alkanes, alkenes and alkynes to explain their reactivity.
- Undertake a conformational analysis of ethane and butane.
- Draw the chair form of cyclohexane, invert it, and understand why equatorially substituted cyclohexanes are more stable than axially substituted cyclohexanes.
- Draw a mechanism for the halogenation of alkanes.
- Predict the reactions of alkenes with a range of reagents, and draw mechanisms for these reactions.
- Predict the reactions of alkynes with a range of reagents, and draw mechanisms for these reactions.

Haloalkanes, Alcohols and Amines

Braddock, Chris

11 hours

Aims

To introduce the chemistry of haloalkanes, alcohols and amines via consideration of the unifying mechanistic framework of nucleophilic aliphatic substitution and 1,2-elimination.

Structure

1. **General**
    1) Nomenclature and structure; 1°, 2°, 3°, hydrogen bonding
    2) General reactivity considerations; haloalkanes as electrophiles, (deprotonated) alcohols and (neutral) amines as nucleophiles.
2. **Reactivity of Haloalkanes, Alcohols and Amines**
    1) Nucleophilic Aliphatic Substitution: S_N1 & S_N2
        - (i) Mechanisms;
        - (ii) Kinetics and reactivity; *rate laws, 1° vs 2° vs 3°, steric effects, carbocation stability - hyperconjugation, allylic and benzylic substrates.*
        - (iii) Stereochemical consequences; *complete inversion in* S_N2*, racemisation in* S_N1
        - (iv) Solvent effects; S_N1 *in protic solvent,* S_N2 *in dipolar aprotic solvent*
        - (v) Electrophiles; *Comparison of leaving group ability of halides – bond strengths and pKa of HX; converting an alcohol to a halide; activation of alcohols as tosylates, cleavage of aryl methyl ethers.*
        - (vi) Nucleophiles; *Halide based: Finkelstein reaction. Oxygen based: hydroxide, alkoxide, carboxylate - Williamson ether synthesis, ether formation with diazomethane. Nitrogen based: Amines – overalkylation, Gabriel synthesis, azides. Carbon based: nitriles.*
    2) 1,2-Elimination (□-elimination): E1 & E2
        - (i) Mechanisms;
        - (ii) Regioselectivity (Orientation) & Reactivity; *stability of alkenes, Saytzeff orientation, 3° vs 2° vs 1°*
        - (iii) Stereochemistry of E2 elimination; *anti-periplanar stereospecific elimination*
        - (iv) E1 vs E2; *conc strong base favours E2*
        - (v) Elimination vs Substitution; *steric factors*
        - (vi) Elimination of $HOCr(O)_2OH$ from chromate esters: *oxidation of alcohols.*

Objectives

At the end of this course the student should be able to:

- Identify correctly the various functional groups introduced on this course;
- Identify the product of a given nucleophilic aliphatic substitution or elimination product when presented with the substrate and reagent;
- Select reagents to achieve a given nucleophilic aliphatic substitution or 1,2-elimination reaction when presented with the starting material and desired product;
- Predict whether a given nucleophilic aliphatic substitution occurs via an S_N2 or S_N1 mechanism, and the consequences for any stereochemistry at the reacting centre;
- Predict whether a given 1,2-elimination reaction occurs via an E2 or E1 mechanism, and the regioselectivity of the elimination;
- Explain, with arrow-pushing, the mechanistic rationale underpinning the above.

Introduction to Carbonyl and Carboxyl Chemistry

Blackmond, Donna

12 hours

Aims

To provide the students with the fundamentals of carbonyl and carboxyl chemistry. To recognise a wide variety of different carbonyls in different structures, to understand the nature of carbonyl reactivity (e.g. electrophilic, □-position)., to be able to apply simple mechanistic ideas to explain carbonyl reactivity, to familiarise themselves with common carbonyl reactions (e.g. aldol, Claisen) to understand how to characterise the carbonyl group from various spectroscopic methods (e.g. infra-red, NMR and UV-visible spectroscopy).

Structure

Electronic structure
Reactivity
Intermediates
Common reactions
Characterisation

Objectives

By the end of the course the students should be able to:

- Understand the basic structure and how it relates to carbonyl chemistry
- Using simple mechanistic ideas explain reactivity
- Understand how it is possible to characterise carbonyl using spectroscopic techniques
- Apply these ideas to explain reactions that have been undertaken in the synthetic laboratory

Macromolecule structure and biosynthesis - 1st year ancillary [Medicinal Biology]

Leatherbarrow, Robin

8 hours

Aims

The course introduces students to the structure and function of the main biological macromolecules.

Structure

- Structure of amino acids, peptides and proteins
- Structure of nucleic acids
- Description of the role of DNA as the genetic material; account of methods for DNA sequencing
- The biology of DNA replication
- The biology of DNA Transcription
- The mechanism of protein biosynthesis
- Oligosaccharide structure

Objectives

The students will know the basic biological macromolecule structures and their biochemical role.

Enzymes and Metabolic pathways - 1st year ancillary [Medicinal Biology]

Leatherbarrow, Robin

8 hours

Aims
The course introduces students to the concepts of metabolic pathways within the cell and describes the basic features of enzyme-catalysed reactions.

Structure
- Basic enzyme kinetics
- The glycolysis pathway
- The TCA cycle
- Oxidative Phosphorylation
- Control of metabolism

Objectives
The students will know the fundamental metabolic pathways, their role and significance and the structures of the core metabolic intermediates. They will know how control of these enzyme-catalysed pathways regulates the flux of the pathways and controls the amounts of product that is generated.

Physical I

1st Year Physical Lab course

De Mello, Andrew

60 hours

Objectives

- To teach good laboratory practice and the keeping of laboratory notebooks
- To teach the writing of experimental reports.
- To introduce the assessment of errors and of the accuracy of experiments
- To introduce data handling, analysis and fitting to calculate results.
- To introduce some basic principles of measurement in physical and analytical chemistry.

Experiments

Students will perform five experiments during the laboratory course. These will be selected from 15 possible experiments covering the following key subject areas:

- Electrochemistry
- Analytical Chemistry
- Spectroscopy
- Vacuum Techniques
- Kinetics

Complete List of Experiments

Electrochemistry
Silver Electrodes
Amalgam Cell
Conductance of Solutions

Analytical
Spectrophotometric Determination of Iron
Gas Chromatography
Electrodeposition

Spectroscopy
NO_2/N_2O_4 equilibrium
IR Spectrum of CO
Absorption Spectra of Solutions

Vacuum Techniques
Viscosity of Gases
Vapour Pressure at Low Temperatures

Kinetics
Persulphate Iodide Reaction Kinetics
Peroxide-Iodide Reaction Kinetics
Kinetics of Diacetone Alcohol Decomposition

Building upon

A-level material, Foundation Experimental and Mathematics Laboratories and Lecture Courses. Spring term Spectroscopy course.

Looking forward to

2nd Year Physical Chemistry Laboratory.

Mathslab 1

Bresme, Fernando

16 hours

Aims

To provide the students with analytical and numerical tools to solve chemistry related problems. The course will build upon the Foundation Mathslab, and will continue to use Excel as the primary software programme.

Objectives

- To teach the use of advance symbolic processing mathematics programs.
- To introduce the representation of complex functions of relevance in chemistry (parametric representation, wave functions, …).
- To teach the vector algebra in the context of crystal structure calculations.
- To introduce numerical/analytical techniques to solve ordinary and complex equations of relevance to chemistry problems.

List of Computer Experiments

1) Non Linear and Advanced Linear Least Squares Fitting.
    - Weighted fits, using non linear fitting.
2) Maths Lab on Kinetics:
    - Analytical and Numerical solution of differential equations.
3) Maths Lab on Intermolecular interactions:
    - Work in a conservative field.
    - Introduce concept of conservative fields and path integrals – link to maths lectures.
4) Maths Lab on quantum mechanics:
    - Solution of Schrödinger equation: harmonic oscillator, particle in a box, or anharmonic oscillator. Analytical + numerical
    - Wave functions and probability, energy levels and spectroscopy.

Building upon

A-level material, Foundation Mathematics Laboratories and Lecture Courses. Spring term Theoretical Methods 1 lecture course.

Looking forward to

Spring term physical chemistry lecture courses: Molecular Dynamics, Spectroscopy and Quantum Mechanics. 2nd Year Theoretical Methods Laboratory.

Theoretical Methods 1

Quirke, Nicholas

6 hours

Aims

This course aims to provide the mathematical knowledge and skills required for solving problems in the physical chemistry courses. It is especially linked with the first year courses.

Structure

- Vectors: vectors and scalars; vector components; vector addition; vector dot and cross product; vector differentiation. Examples from Molecular Interactions **1 lecture**

- Partial differentiation, integration and thermodynamic functions **2 lectures**

- Complex numbers **1 lecture**

- Differential equations & kinetics and quantum mechanics. First order, second order linear and homogeneous **2 lectures**

Objectives

By the end of the course the students should be able to:
- Manipulate vectors and complex numbers.
- Manipulate and solve simple differential equations that appear in mechanics, kinetics and quantum mechanics, such as the motion of a diatomic molecule under Newton's law, reaction rates in 1st and 2nd order kinetics, the Schrödinger equation for particle in a box.

Building upon

A-level material, Foundation Experimental and Mathematics Laboratories and Lecture Courses.

Looking forward to

2nd Spring term physical chemistry lecture courses: Molecular Dynamics, Spectroscopy and Quantum Mechanics. Theoretical Methods 1 laboratory.

Molecular Interactions and Dynamics

Templer, Richard

9 hours

Aims

To provide the students with an understanding of the dynamics of linear, vibrational and rotational molecular motion, using concepts of force, energy and momentum. To explore the classical origins of molecular interactions and express these in terms of force, field, potential and potential energy.

Structure

9 lectures with interspersed problem sessions to support lecture and reading material.

- Centre of Mass, The Electrostatic Force, Collision between two ions, forces exerted and outcome.
- The electrostatic dipole, field and potential. Work done moving in a potential. Potential energy and Kinetic energy.
- Morse potential, well depth and curvature, Internal motion, the harmonic oscillator.
- Rotational motion, torque, angular momentum. Rotating dipole in an electrostatic field. Coupling of rotation and vibration.
- Intermolecular forces, dipole dipole , dipole induced dipole, and van der Waals force The Lennard Jones potential.

Objectives:

By the end of the course the student should be able to:

- Calculate, using vectors, the force exerted on an ion in an electrostatic field
- Predict the outcome of a collision between two ions
- Demonstrate a mathematical and pictorial understanding of electrostatic field and potential. Calculate work done moving in a potential
- Demonstrate pictorially and mathematically how interatomic forces are related to the curvature of the Morse potential and be able to calculate binding energies from a given potential form.
- Use the harmonic oscillator as a model and mathematically demonstrate how potential and kinetic energy are related.
- Give an account of amplitude, circular frequency and oscillation period in terms of the mass and force constant of the oscillator
- Relate rotational motion to linear motion, calculate angular momentum, torque and rotational kinetic energy using polar co-ordinates.
- Discuss how rotational and vibrational motion are coupled
- Discuss the origin of weak intermolecular forces and the origin of the Lennard Jones Potential.
- Demonstrate a conceptual understanding of the relative strengths and ranges of intermolecular forces.

Building upon

A-level material, Foundation Experimental and Mathematics Laboratories. Theoretical Methods 1 lectures and laboratory.

Looking forward to

Following spring term lecture courses in Spectroscopy and Quantum Mechanics.

Spectroscopy

de Mello, Andrew

8 hours + 1 problem class

Aims

This course introduces the basic concepts of molecular quantum mechanics and molecular spectroscopy (i.e. how we can use light to view the microscopic world).

Structure

The course will begin by discussing the nature of electromagnetic radiation in terms of both 'wave' and 'particular' models. The concepts of energy quantization and molecular energy levels will be introduced with particular emphasis on how these allow molecular spectra to be interpreted. The course will then focus on two types of spectroscopy routinely used to identify molecular species, namely rotational and vibrational spectroscopies.

In the first students will be introduced to rotational motion in diatomic and polyatomic molecules. Rotational energies will be treated using both the rigid rotor and non-rigid rotor approximations. Molecular rotational spectra will be introduced through consideration of transitions between rotational energy levels and selection rules. Simple techniques will be described to allow for the prediction of spectral features and assignment of spectroscopic bands.

In the second students will be introduced to vibrational motion in diatomic and polyatomic molecules. Vibrational motion will be analyzed using both the harmonic and anharmonic oscillator models. Molecular vibrational spectra will be introduced through consideration of transitions between energy levels and selection rules.

Objectives

- In general the course will teach students to interpret molecular spectra and use this information to determine spectroscopic constants and structural characteristics of molecules. Students should understand the nature of electromagnetic radiation and be able to classify it in terms of wavelength, frequency and energy.
- Students should be able to appreciate the nature of molecular energy quantization and understand the population of energy states in terms of the Boltzmann distribution.
- Students should understand the significance of wavefunctions and Schrödinger’s equation.
- Students will be able to model the rotational behavior of diatomic molecules in terms of the rigid and non-rigid rotor models.
- Students will be able to model the vibrational behavior of diatomic molecules in terms of the harmonic and anharmonic oscillator models.

Building upon

A-level material, Foundation Experimental and Mathematics Laboratories. Theoretical Methods 1 lectures and laboratory. Characterisation of inorganic compounds and Molecular Dynamics Courses.

Looking forward to

Following spring term lecture courses in Quantum Mechanics. 2nd year Photochemistry course.

Measurement and mechanism in physical chemistry

Gould, Ian

8 hours

Aims

- To introduce the spatial and temporal dimensions inherent in chemistry and physical processes
- To illustrate the relationship between structure, function, mechanism, measurement and design
- To integrate the theoretical material of the first year physical course with physical measurement
- To cohesively link quantum mechanics, thermodynamics, molecular dynamics, spectroscopy and kinetics with real chemical systems

Structure

- Experimental techniques used to determine the three dimensional structure of a molecule :-
- IR, UV, CD, NMR and X-Ray
- Illustration of determination of 3D structure of biological molecule, protein or DNA
- Illustration that 3D Structure are not necessarily rigid, i.e. proteins c.f. rigid zeolites
- Demonstration of the complexity of a small molecule such as CO or ozone from the theoretical and experimental perspective

Objectives

To integrate the first year physical course material with “real world” examples and explanation. The students gain perspective in how and why the theoretical background is used in conjunction with experiment to investigate, understand and ultimately engineer at the atomic and molecular level.

Building upon

Spring term physical chemistry lecture courses: Molecular Dynamics, Spectroscopy and Quantum Mechanics.

Looking forward to

2nd and 3rd lecture courses in physical chemistry and biological chemistry.

Quantum Chemistry I

Klug, David

8 hours

Aims

This course introduces Quantum mechanics and its associated formalisms to students.

Summary

- The Schrödinger equation.
- Solving the Schrödinger equation for particle in a box, motion in a circle.
- Expectation values.
- The uncertainty principle.
- The wave nature of the Schrödinger equation.
- Atomic orbitals.
- Tunnelling
- Simple harmonic motion.

Objectives

- The students should understand the mathematical machinery behind expectation values and be able to calculate average energies, positions and momenta in simple cases from a knowledge of the wavefunction.
- The concept of the uncertainty principle should be known and applicable to simple problems. Interpretation of the wavefunction as a probability density and the implications of this should be understood.
- The students should be able to solve the Schrödinger equation for particle in a box and motion in a circle and free particles. They should also be aware of the form of the wavefunctions for simple atoms. The students should be comfortable in manipulating the Schrödinger equation and have an understanding of the mathematical formalities of operators and eigenfunctions.
- The concept of interference should be understood and examples of superposition of wavefunctions known.
- A simple description of tunnelling is required knowledge including the assumptions underlying the description.

Building upon

Foundation Experimental and Mathematics Laboratories. Theoretical Methods 1 lectures and laboratory. Molecular dynamics and spectroscopy lecture courses.

Looking forward to

Summer course on Measurement and Mechanism in Physical Chemistry. 2nd year courses in Statistical Thermodynamics, Photochemistry and Electronic Properties of Solids. 3rd Year Quantum Mechanics 2.