

Yusuf Hamied Department of Chemistry

Part II Chemistry: A Guide to the Course



Academic Year 2024/2025



The Department of Chemistry endeavours to develop an inclusive, supportive and intellectually stimulating environment for our undergraduate community.

Athena SWAN is an ongoing program to address the underrepresentation of women in the sciences. The Silver Award recognises the progress that the Department has made in recent years, and the actions that benefit not only our female students, but all our undergraduate chemists.

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Introduction

This booklet describes the third-year (Part II) course which is offered by the Department. This course builds on the ideas which you have studied in the first and second year, and offers you the opportunity to both broaden and deepen your knowledge of chemistry. As the year progresses there is the opportunity to narrow your focus somewhat, for example towards chemical biology or chemical physics; however, you can equally well choose to pursue a broad range of topics across all areas of chemistry.

Practical work is given a prominent place, and you will continue to develop your skills in this area by tackling more sophisticated and open-ended experiments. The practical skills which you will acquire this year will be very useful to you if you decide to stay on next year and undertake a research project. In addition to conventional practicals, there will be the opportunity to do other kinds of continuously assessed work such as learning a language.

If you are intending to stay on for Part III, you should be aware that the class you are awarded in Part III will take into account the marks you received for Part II, i.e. marks will be carried forward from Part II to Part III. Further details are given on page 26. Please also refer to the details given on page 26 concerning the requirements for admission to Part III.

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Introductory talk

There will be an introductory talk for Part II Chemistry on Wednesday 9th October at 12:00 in the Pfizer Lecture Theatre.

The Head of Department requires all new Part II students, without exception, to attend the introductory talk

There will be a 'Welcome Party' in the Cybercafé (located on the top floor of the Centre for Molecular Informatics building) for all new Part II and Part III students on Friday 11th October from 17:00. We do hope that you will be able to come along and mark the beginning of the year in a suitable way.

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Careers for chemists

On 22nd October at 17:00 in the Pfizer Lecture Theatre, Dr Raj Sidhu, from the Careers Service, will give a talk about Careers for Chemists. Even if you are thinking of returning for Part III, this is a good opportunity to find out about your career options. Dr Sidhu's talk is highly recommended for all the class.

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Outline of the course

The course consists of a set of lectures alongside a package of continuously assessed work (principally practical work). The requirements for continuously assessed work are given on page 19. The lectures are organised into three groups: A, B, and C.

The image on the cover is taken from Prof. Chris Hunter's website and depicts some recent work from his group concerning the development of new methods for studying solvation and cooperativity. For more details about research in the Hunter group please refer to <u>www-hunter.ch.cam.ac.uk</u>

A courses

The A courses are compulsory and cover a range of core topics. If you have taken Chemistry A *and* Chemistry B in Part IB you must take courses A1–A4. If you have only taken Chemistry B in Part IB you have two options: either you can take courses A1–A4 *or* you can take courses A1, A2, and A6 *Concepts in physical chemistry*. This latter course is specifically designed for those who have not taken Chemistry A at Part IB.

No special arrangements are made for those who have taken *only* Chemistry A in Part IB. However, with some focused reading over the preceding vacation and some additional supervisions, you should find it possible to complete courses A1 and A2 in a satisfactory way. You should consult the Director of Teaching and your Director of Studies if you fall into this category.

B and C courses

The B and C courses cover a wide range of topics from which you have a free choice, subject to the constraints of the examination. Most B and C courses consist of 12 lectures, but some are shorter and consist of 6 lectures. The B courses span the last two weeks of the Michaelmas Term and the first three of the Lent Term. The C courses span weeks 5–8 of the Lent Term and the first two weeks of the Easter Term.

You need to think carefully about your choice of B and C courses so that you develop a coherent programme of study, lay down a good foundation for Part III (if that is your intention), and prepare appropriately for the examinations. The details of the examinations are given on page 24 and you need to understand the implications of the examination structure so that you can choose your courses. In short, you will need – at the absolute minimum – to be prepared to answer questions relating to 24 hours of B course lectures, and 24 hours of C course lectures.

Reading Lists Online (RLO)

The link below gives access to the online reading lists for all the Chemistry courses. They have been compiled to follow the structure of the Course Guides. Each one includes a record of the borrowable items held in the Cambridge University Libraries' collections (including the Chemistry Library) and those accessible as eBook titles.

www-library.ch.cam.ac.uk/reading-lists-online-rlo

Lecture Course Synopses

A courses

A1: Inorganic I – Inorganic reactivity, the heavier transition metals and the f-block elements

This course follows on from the IB Chemistry B course on the structure, bonding and reactivity of transition metal complexes which was predominantly focused on the first-row transition metals.

The lectures will explore the similarities and differences between the first row and the heavier transition metals and f-block elements. The availability (or otherwise) of valence d and f orbitals in bonding and reactivity of complexes which contain these elements will be discussed in detail.

Dr Robert Less (4 lectures)

A huge body of experimental data supports the more extensive participation of the d orbitals in the bonding of the second and third row transition metals. The more expanded nature of the 4d and 5d orbitals of the second and third row transition metals leads to significantly stronger covalency in bonding which leads to greater prevalence for metal–metal as well as metal–ligand multiple bonding for the heavier elements. These aspects will be investigated from a primarily structural viewpoint, reinforced with bonding and thermodynamics arguments.

Topics Metal–metal multiple bonding in the d block. Metal–ligand multiple bonding in d block chemistry.

Dr Robert Less (3 lectures)

The f-block elements comprise almost a quarter of the periodic table and we will examine their interesting properties and widespread applications. A comparison of the chemistry of the lanthanoids and actinoids reveals contrasting behaviour which is attributed to the differing extent of f-orbital availability. The effect on bonding and structures is discussed: predominantly ionic bonding in lanthanoids and significant covalency in actinoid compounds. A good knowledge of IB coordination chemistry is desirable.

Topics f-block atomic orbitals, and bonding: metallic, ionic and covalent models.

Prof. Andrew Wheatley (5 lectures)

The substitution and redox chemistry of transition metal coordination complexes will be covered in these lectures. Initially the focus will be on the two extremes of substitution chemistry (associative and dissociative reaction mechanisms) although experimental evidence often suggests the role of the outer coordination sphere is significant leading to so-called interchange processes. The roles of the inner and outer coordination spheres are also important in electron-transfer processes, and these lectures will consider the factors affecting the rate of electron transfer in both inner sphere and outer sphere mechanisms.

Topics Dissociative reaction mechanisms in octahedral complexes; crystal field stabilization energy: inert and labile complexes; the influence of auxiliary ligands on transition state geometry and the geometric outcome of the reaction.

Associative reaction mechanisms in square-planar complexes; the trans-influence and trans-effect.

Outer-sphere electron-transfer between substitutionally inert complexes; Marcus-Hush theory.

Links to other courses –IB Structure, Bonding and Reactivity of Transition Metal Complexes, Part II Organometallic Catalysis, The Chemistry of Future Energy, NMR.

Recommended books- see Reading Lists Online (RLO)

A2: The Foundations of organic synthesis

Dr Bill Nolan (12 lectures)

This course will apply the basic organic chemistry courses, *Key Organic Reactions* and *Shape and Reactivity* taught in IB Chemistry B to organic synthesis. You will see how a molecule can be logically dissected into simple building blocks by working backwards (retrosynthetic analysis) and how, using these tools, you will be able to devise synthetic strategies towards new molecules.

Topics Retrosynthetic Analysis and the Language of Synthesis: Target Molecules. Disconnections. Synthetic equivalents. Criteria for Good Synthetic Planning

C–X Disconnections: Synthesis of halides, ethers, sulphides and amines (considered as one-group –X disconnections). Two-group disconnections illustrated by the synthesis of 1,1-, 2,2- and 1,3-difunctionalised compounds.

C–C Disconnections and Synthesis using the Carbonyl Group: Carbonyl group as an a¹ (acceptor) reagent. Alkene synthesis and the Wittig reaction.

Carbonyl group as a d² (donor) reagent. Enolate alkylations. The aldol condensation. Synthetic control in carbonyl condensations.

 α , β -unsaturated carbonyl compounds as a³ (acceptor) reagents. Synthesis of 1,5-dicarbonyl compounds. Construction of 1,4-difunctionalised compounds.

Construction of 1,4-difunctionalised compounds using synthons of 'unnatural' polarity.

Protecting groups to control mixed functionality

Use of Latent Functionality (Baeyer Villiger oxidation, Alkene chemistry, Use of 1,3-Dithianes, the Birch Reduction and the Pinacol coupling and rearrangement).

The Diels-Alder reaction (perhaps the most important reaction in Organic chemistry).

Recommended books – see RLO

A3: High-resolution molecular spectroscopy

Prof. James Keeler (12 lectures)

This course will be concerned with the high-resolution spectra of small molecules, mostly in the gas phase. We will look at rotational, vibrational and electronic spectroscopy (including the Raman effect), and the kinds of detailed structural information that can be obtained from each kind of spectrum. The course draws extensively on material previously covered in Part IB Chemistry A, showing how the concepts introduced there can be used and extended to more complex cases.

Topics Electromagnetic radiation and its interaction with molecules. Transition moments and Einstein coefficients. Linewidths. Lasers.

Instrumentation. Dispersive spectrometers: diffraction gratings, sources and detectors. Fourier transform instruments: advantages. Spectroscopy with lasers.

Rotational spectroscopy. Classification of molecules and the resulting spectra. Intensities. Centrifugal distortion. Electric field effects (Stark effect).

Vibrational spectroscopy. Classification of normal modes and vibrational wavefunctions according to symmetry. Selection rules. Overtones and combination lines. Rotational fine structure: parallel and perpendicular bands.

Raman spectroscopy. Origin of the Raman effect. Practicalities. Rotational and vibrational Raman spectroscopy of linear molecules and symmetric tops. Rule of mutual exclusion. Molecular identification using IR and Raman spectra.

Electronic spectroscopy. Diatomic molecules. Electronic structure and term symbols. Selection rules and the Franc–Condon principle. Vibrational and rotational fine structure.

Electronic spectroscopy of larger molecules: Jablonski diagram. Fluorescence and phosphorescence. Applications.

Recommended books – see RLO

A4: Theoretical techniques

Prof. Angelos Michaelides (6 lectures) and Dr Alex Thom (6 lectures)

It is an incredibly exciting time for theoretical chemistry, which is now a central and "core" part of modern chemistry. Theory and simulation now enables accurate predictions on a wealth of complex chemical systems to be made, providing insights for experiments and in many cases driving experimental innovation. This course will provide an introduction to theoretical chemistry by providing an overview of the core concepts and current simulation methods in theoretical chemistry. This will include techniques such as classical force fields, and self-consistent field (SCF) theories: density functional theory and Hartree-Fock theory. While these methods are expressed in terms of molecular orbitals, their behaviour is underpinned by the many-electron wavefunction, and this course will introduce a framework to qualitatively predict the progress chemical reactions using these wavefunctions.

TopicsBorn Oppenheimer Approximation, Potential Energy Surfaces; Classical Force Fields;
Density Functional Theory (DFT):- underlying theorems, exchange-correlation functionals,
DFT in practice, basis sets, effective core potentials / pseudopotentials, benchmark
Using Molecular Orbitals: population and bond-order analysis; Model one-electron
Hamiltonians; alternant hydrocarbons; perturbation theory and heteroconjugated systems.
Many-electron wavefunctions: Slater determinants; Hartree--Fock theory of two
electron-systems; electron correlation and molecular dissociation; Empirical descriptions:
Chemical Reactivity: state and orbital correlation diagrams; the Woodward-Hoffman rules.
Examples applications in computational chemistry.

Recommended books – see RLO

A6: Concepts in physical chemistry

Dr Andrea Chlebikova and Dr Chris Truscott

This course is aimed at giving you a more detailed understanding of chemical bonding than was possible in the Part IA course. This will require us to introduce some quantum mechanics, which we will do by taking an approach which is always firmly rooted in your chemical understanding and avoids excessive formality or mathematical detail. We will develop the key principles of quantum mechanics using simple model systems, which involve relatively easy mathematics, and then go on to see how these ideas can be applied in atoms and molecules.

The course concludes by showing how molecular symmetry, in the form of *group theory*, can be used to great effect in drawing up MO diagrams of simple molecules.

Topics Revision of some basic mathematics. Functions and curve sketching (polynomials and trigonometric functions). The exponential function and logarithms. Differentiation: the chain rule; differentiation of a product. Integration. Introduction to complex numbers and the complex exponential.

Introducing quantum mechanics. What is quantum mechanics and why is it useful? Wavefunctions, operators and energy levels. Exemplifying these ideas for two simple systems.

Atomic orbitals. Review of AOs, their shapes and energies. Multi-electron atoms: the energies of singlets and triplets. Term symbols.

Molecular orbitals. The two orbital problem. Homo- and hetero-nuclear diatomics. Extended arrangements of orbitals (π systems) in rings and chains. Computational aspects.

Symmetry. The description of symmetry. Symmetry elements operations. Point groups. Character tables. Representations and reduction of representations. Constructing molecular orbital diagrams using symmetry as an aid. Transition metal complexes.

Recommended books – see RLO

B courses

B0: Inorganic II – Electron deficient compounds

Prof. Sally Boss (6 lectures)

This course brings together the bonding models that are currently used to rationalise main group and transition metal inorganic complexes and how these bonding models can help us to understand their structures. You will learn how the bonding models are different in their approach to the ones covered by Dr Less in A1 and further your understanding of cluster complexes of the main group and transition metal elements.

The first part of the course introduces the types of bonding models displayed by polyhedral architectures (electron-deficient, electron-precise and electron-rich bonding models). The interesting class of electron deficient compounds is discussed in depth and used to rationalise the structures of cluster molecules of the p and d block. The isolobal, isoelectronic and isostructural principles will be introduced and used to predict and rationalise the (sometimes elaborate!) shapes of molecules. The synthesis and reactivity of electron deficient compounds will be described and categorised and the physical methods used to probe the structures of these species will be discussed.

Topics Electron-deficient, -precise, and -rich cluster complexes. Electron-counting. Cluster shapes. Wade's Rules. Main Group clusters. Transition Metal clusters. Synthesis and reactivity of electron deficient compounds. Characterisation methods used in cluster chemistry.

Links to other courses –Chemistry B, IB Structure, bonding and reactivity of transition metal complexes, Structure, bonding and the p-block elements. Part II, A1 - Inorganic I - Heavier transition metals and the lanthanoids and actinoids.

Recommended books – see Reading Lists Online (RLO)

B1: Inorganic III – Organometallic catalysis

Dr Paul Wood (6 lectures)

In this part of the course we examine metal-promoted organic transformations which play a fundamental role in catalytic processes such as alkene polymerization and enantioselective

synthesis. Well-defined transition metal systems are particularly effective homogeneous catalysts due to the ability of the metal to adopt different geometries, coordination numbers, and oxidation states. By considering a variety of catalytic processes, we shall examine the exact role of the metal in such cycles and discuss how it is possible to 'tune' the metal centre by varying both the steric and electronic properties of its ancillary ligands in order to favour a specific reaction outcome.

Links to other courses – A good knowledge of both the IB courses *Coordination Chemistry* and *Organometallic Chemistry* is assumed.

CO Reactions. Alkene carbonylation, hydroformylation; alcohol carbonylation; the Monsanto and BP Cativa processes.

Hydrogenation Alkenes, chiral induction and other C=X bonds.

Alkene reactions. Polymerization with heterogeneous and metallocene catalysts; chain-end and ligand control in stereospecific propene polymerizations; late transition metal catalysts; ethene oligomerization; SHOP process.

Metathesis reactions. Alkene and alkyne metathesis; Ring-Opening Metathesis Polymerisation (ROMP), Ring-Closing Metathesis (RCM) *etc.*

Recommended books – see RLO

B2: Organic spectroscopy

Prof. Ian Fleming (6 lectures)

In this lecture series, Prof. Fleming, will build on last year's work on NMR spectroscopy as a tool for the determination of structure and stereochemistry. He will introduce powerful new methods of 1D and 2D NMR spectroscopy, which have expanded its reach. He will show how they can be combined to determine the structure and stereochemistry of molecules more complex than those amenable to the older techniques of organic spectroscopy.

1–6 NMR Spectroscopy. FT-NMR. Chemical shift. Magnitude of coupling constants. Deviations from 1st-order spectra. Exchange. Enantiomeric and diastereomeric ratios. DEPT. 1-D nuclear Overhauser effect.

Two-dimensional spectroscopy, COSY, HSQC, HMBC and NOESY, applied to structure determination. Deconvoluting overlapping multiplets. TOCSY.

Recommended books – see RLO

B3: Chemical biology I – Biological catalysis

Prof. Finian Leeper (6 lectures) and Prof. David Spring (6 lectures)

Enzymes are the main catalysts in the cell. They catalyse an amazing array of reactions, with high chemo-, regio- and stereoselectivity and at rate enhancements of up to 10¹⁵! Consequently, about half of the drugs currently being developed in the pharmaceutical industry are targeted at enzymes. It is therefore very important for us to understand how enzymes achieve catalysis, and how to use this information to design specific inhibitors.

In IB some of the basic concepts behind enzymatic catalysis were introduced. Now we will build on that foundation and explain the diversity of chemical reactions that enzymes catalyse. The examples are chosen to illustrate how enzymes are studied and to introduce concepts that you will need for subsequent biological courses in Part III.

Prof Finian Leeper

Topics Enzyme basics – a reprise (kinetics, free energy profiles, inhibition, isotope effects); Elimination reactions (enolase, dehydroquinase, dehydroquinate synthase, ammonia lyases); Phosphoryl transfer (phosphatases, kinases, ribonuclease, tyrosyl t-RNA synthetase); Aldol and Claisen condensations (thioesters, citrate synthase, Schiff base, aldolase); One carbon transfer reactions (THF, SAM, chiral methyl groups, thymidylate synthase); Carboxylation and decarboxylation (acetoacetate decarboxylase, biotin, rubisco, vitamin K).

Prof. David Spring

Topics Enzymes and Coenzymes. Vitamins; Reduction and Oxidation, NAD(P)H and Flavins; Thiamine Pyrophosphate (TPP)-Dependent Enzymes; Enzymatic Transformations of Amino Acids, PLP; Glucose Metabolism, Enzymes Work Together.

Recommended books - see RLO

B4: Chemistry in the atmosphere

Prof. Alex Archibald (12 lectures)

This course will introduce key ideas about the chemistry of the atmosphere. It will discuss the chemical processes which control the abundances of ozone, and other trace constituents in the troposphere, and the rather different chemistry of the stratospheric ozone layer. We will use examples to reinforce ideas about reaction rates, gas and solution phase kinetics and spectroscopy.

Topics The physical and chemical structure of the atmosphere: composition and temperature as a function of pressure. Sources, sinks and variability. The concept of lifetimes and steady state. The role of ozone in the atmosphere.

Chemistry of the stratospheric ozone layer. The Chapman reactions. Catalytic cycles for ozone destruction and the idea of 'families', including NOx, HOX, CIOx.

Chemistry of the troposphere. Local air quality. Oxidizing and reducing smogs, photochemical oxidants. The role of nitrogen oxides and volatile organics. The global troposphere. Production and destruction of ozone. The role of OH. Sulphur compounds and acid rain

Reactions of atmospheric interest. Some important gas phase atmospheric reactions will be considered in detail. Heterogeneous reactions of important gas phase compounds on atmospherically relevant aerosol particles surfaces will discussed. Sources, formation processes and chemical composition of tropospheric aerosol particles.

Measurements of atmospheric composition and their applications. Remote sensing. Rovibrational spectroscopy. Ultraviolet spectroscopy. Laser studies of the atmosphere. Chemical methods: chemiluminescence, laser induced fluorescence. Electrochemical methods. Chromatographic techniques. Online and offline aerosol sampling and characterization techniques.

Recommended books - see RLO

B5: Structure and reactivity

Prof. Bill Nolan (6 lectures)

During this lecture course molecular orbital theory will be applied, without mathematics, to explain the preferred structures and conformations of organic molecules, and then extended to explain the reactivity and stereochemistry of a wide range of organic reactions. New reactions having interesting features will be added, greatly extending the range from those already

presented in Part IB (Chemistry B) and building upon some of the ideas presented in the Part II course *The Foundations of Organic Synthesis*.

1–6 The fundamental ideas of molecular orbital theory are used as the basis for understanding reactivity. Through space and through-bond (HOMO/LUMO) interactions, hard/soft nucleophiles and electrophiles are explored in detail, as applied to ambident systems and nucleophilic substitution reactions.

Stereoelectronic effects on fundamental organic reactions are thoroughly examined, as applied to the following: cyclisation (Baldwin's rules and the Thorpe–Ingold effect), elimination, fragmentation, rearrangement (migration). Electronic strain and the topic of carbene chemistry are also introduced.

An introduction to pericyclic reactions is given: cycloadditions and electrocyclic reactions are examined in detail in the context of the Woodward–Hoffman Rules

Recommended books – see RLO

B6: Biomaterials

Prof. Melinda Duer (6 lectures)

The mechanical properties of biological materials, such as bone, tendon, skin etc are defined by their so-called extracellular matrix, a complex material organized around and between the cells of the tissue, whose composition and structure is highly specific to each tissue. The extracellular matrix presents an opportunity to learn from Nature how to build functional materials that have different functions on different lengthscales. On a macroscopic lengthscale, the extracellular matrix of bone, for instance, provides structural support for our bodies whilst on a nanoscopic lengthscale, the protein and glycan molecules that make up the bone extracellular matrix "tell" bone cells to function like bone cells.

Currently, man-made materials generally are designed to perform on one lengthscale only, so studying biological materials gives us insight into designing a new generation of materials – and an essential understanding of what can go wrong with our tissues and how to fix them. We will study the components of typical extracellular matrices to gain perspective on how they perform their various mechanical roles. Dealing with complex materials like these however means that we must find different ways of examining their structure from the more conventional diffraction techniques. Thus, the course will begin with an overview of solid-state NMR and how it can be applied to determine molecular structures and dynamics in biological tissues. We will then examine the basics of protein structure which will lead on to a detailed examination of the extracellular matrix in collagenous tissues (tendon, skin, muscle, etc) and finally, a brief discussion of a calcified tissue (bone). The focus throughout is on acquiring the experimental data we need to understand how the molecular structures and dynamics of the extracellular matrixlead to the required material properties.

No previous experience of biochemistry or biology is required for this course.

- Lectures 1–2 Solid-state NMR spectroscopy: comparison to solution-state NMR; how to record solid-state NMR spectra and the nuclear spin interactions relevant in the solid state; 2D solid-state NMR spectra; applications to studying molecular structure and dynamics.
- Lectures 3–5 Basics of protein structure. Collagen as the primary structural protein of the extracellular matrix; collagen fibril formation through self-assembly; collagen fibril structure; mechanical properties of collagen molecules and fibrils and relationship to structure and dynamics.
 - Lecture 6 Calcified tissues bone; calcification of collagen fibrils; bone mineral composition, structure and organization; experimental methods for probing bone mineral.

B7: Statistical mechanics

Dr Aleks Reinhardt (12 lectures)

In the Part IB course 'Molecular Energy Levels and Thermodynamics', we saw how the thermodynamic properties of a macroscopic sample of matter can be expressed in terms of the energy levels of individual molecules. However, while we have dealt with the internal degrees of freedom, such as rotations and vibrations of molecules, we have not so far considered any interactions *between* molecules. In this course, we investigate how such interactions can be treated. Except in a very limited set of circumstances, approximations must be introduced to allow explicit calculations. One of the generic approximations we will study is mean-field theory, which provides a reasonable description of many systems and phenomena, such as phase transitions, magnetism and electrical double layers around membranes. This course will provide an introduction to ensemble theory, classical statistical mechanics, phase equilibria, mean-field methods and the basic theory of transport phenomena. All concepts will be illustrated by applications to physical chemistry and condensed matter science.

This course is a very useful preparation for a number of the theoretical courses offered in Part III.

Topics *Introduction:* The ergodic hypothesis. Boltzmann entropy. Boltzmann distribution. Microcanonical, canonical, grand canonical and isothermal isobaric ensembles. Fluctuations. Quantum and classical statistical mechanics. Thermodynamic equivalence of ensembles. Pressure of interacting particles.

Applications of elementary concepts: Ideal gas in various ensembles. Lattice paramagnet. Langmuir adsorption. Entropy of mixing. Maxwell–Boltzmann distribution.

Equilibrium: Stability criteria. Maxwell constructions. Widom insertion. Second virial coefficients. Landau theory of phase transitions.

Thermodynamic perturbation theory: Artificial thermodynamic integration. Gibbs–Bogoliubov inequality. Mean-field theory. Van der Waals equation of state. Ising model. Regular solutions. Flory–Huggins model.

Transport: Brownian motion. Fick's laws. Diffusion coefficient from microscopic quantities. Auto-correlation functions. Green–Kubo relations. Langevin equation. Stokes–Einstein and Einstein relations.

Polymers: Freely-jointed chain model. Entropic springs.

Recommended books – see RLO

B8: Symmetry

Prof. Ali Alavi (6 lectures)

The methods by which symmetry can be used to simplify calculations have been introduced in earlier courses. Here we shall examine some of the theory that underlies these methods, and extend it to further applications.

Topics Introduction and basic ideas. Representations. What is a representation? Equivalent representations. Characters and classes. The Great Orthogonality Theorem. The symmetric representation. Symmetry and physical properties of molecules. The projection formula. Spherical harmonics and the full rotation group. Direct product representations. Calculation of integrals. The symmetrized and antisymmetrized square. The Jahn Teller theorem. Choosing the symmetry group. What symmetries can be ignored? Approximate symmetries. Selection rules. Rotational spectroscopy. Vibration–rotation spectroscopy. Electronic spectroscopy.

B9: Polymers: synthesis, characterisation and application

Prof. Oren Scherman (3 lectures) and Prof. Hugo Bronstein (3 lectures)

Plastics have an impact on every aspect of our daily lives. The chemistry and uses of polymers and other large molecules have undergone a revolution in the last twenty years. New synthetic techniques can deliver unparalleled control in the size, shape and properties of macromolecules. Novel applications are being developed every day including displays, drug delivery, sensors, and electronics.

The course will introduce the fundamental aspects of polymers, how they are synthesised and characterised and will illustrate their usefulness by considering a range of applications.

This course assumes knowledge of the organic chemistry covered in Part II, specifically A2.

Topics What is a polymer ?: polymer classifications & structure

Synthesis of polymers - general synthetic strategies

Characterisation techniques

Polymer properties in solution & bulk

Functional polymers & applications

Recommended books – see RLO

B10: Electronic structure

Dr Alex Thom (6 lectures)

The aim of this course is to provide an introduction to Electronic Structure theory and, in particular, to go beyond the non-interacting, one-electron picture which has been implicitly assumed in the molecular orbital theory used in nearly all earlier courses. The inclusion of electron–electron repulsion is crucial for the quantitative prediction of molecular properties. Self-consistent field theory provides a way to include e–e repulsion, albeit at an approximate level maintaining a one-electron picture. Wavefunction-based methods building on on Hartree–Fock are then explored as the traditional starting point to more systematic theories of electron correlation.

Topics Basis functions, hydrogenic (Slater) orbitals, atomic orbitals, Gaussian functions, and contracted functions; the antisymmetrizer, Slater determinants, and matrix elements of Slater determinants; the secular equations from which orbitals are determined; self-consistent field theory; beyond Hartree–Fock electron correlation: configuration interaction, Møller-Plesset perturbation theory, coupled cluster theory; size-consistency; multiconfigurational methods.

C1: Electrochemistry

Dr Jenny Zhang (6 lectures)

The lectures will give an introduction to electrochemistry, the physical phenomena underlying this analytical technique, and its use in the study of molecular redox chemistry and electron transfer events between molecules and a solid state electrode. Applications of this technique range from industrial processes, medicinal chemistry research and energy conversion processes.

TopicsWhat is an electrochemical cell
Dynamic electrochemistry
Voltammetry
Coupling electron transfer to chemical reactions
Beyond homogeneous reactions

Recommended books – see Reading Lists Online (RLO)

C2: The chemistry of future energy

Dr Jonathan Slaughter (6 lectures)

This course concerns the fundamentals of the chemistry of green-energy generation and storage. It will cover three main topics.

Topics Nuclear and Solar Power Generation: materials and their function in solar cells, how a nuclear power station works, mitigation of waste problems.

Hydrogen generation, storage and transport: The focus will be on generation using electrolysis and artificial photosynthesis, the problems associated with low gravimetric energy capacity, and the use of energetic molecules and metal organic frameworks (MOFs) in hydrogen storage.

Electrochemical Storage: lithium ion and other batteries for device and grid electricity storage. Understanding the detailed chemistry of the cathode and anode, and the importance of interface chemistry. Quantifying and investigating battery performance using various techniques.

The aims of the course are to provide an introduction to the future energy field, to highlight the important role that chemistry has, and to pinpoint the key barriers to future developments from a chemical standpoint. Although the course crosses a number of disciplines (chemistry, physics and materials) no previous knowledge will be assumed.

Recommended books – see RLO

C3: NMR

Prof. Alex Forse (6 lectures)

Multinuclear NMR spectroscopy will be investigated, particularly for the characterisation of main group compounds and diamagnetic transition metal complexes. It is likely that a combination of supervisions and classes will be offered for this course.

Topics NMR using nuclei other than ¹H and ¹³C for inorganic structure determination.

Pulse sequences. Structural information from relaxation rate constants. Chemical shifts: diamagnetic and paramagnetic shielding. Scalar coupling magnitudes for structure determination. Solid-state and two-dimensional NMR spectroscopy techniques for inorganic chemistry.

Recommended books – see RLO

C4: Chemical biology II – Proteins: structure, stability, folding and misfolding

Prof. Sophie Jackson (6 lectures) and Dr Pietro Sormanni (6 lectures)

This course will start with a detailed review of protein structure - covering all aspects from primary through to quaternary structure. Large macromolecular assemblies will be described in addition to 'alternative' structures such as amyloid fibres. The thermodynamic basis for the stability of the native structure of proteins will be illustrated and methods for studying the stability of proteins described. From this, the factors that contribute to protein stability and how they can be used to rationally increase protein stability will be presented.

Case studies will be used to illustrate strategies to optimise the stability of proteins, particularly therapeutic proteins, as well as the consequences of protein structure instability.

In the second part of the course, the mechanisms by which unstructured polypeptide chains spontaneously fold into their unique three-dimensional structures will be described alongside experimental approaches for studying this complex reaction. In particular, the use of protein engineering techniques and ϕ -value analysis to determine the structure in partially structured intermediates and transition states will be presented.

In addition, the factors influencing the aggregation of proteins into amorphous and highly structured (amyloid) species will be described along with the kinetics of this important process.

Recommended books – see RLO

C5: Control in organic chemistry

Prof. Jonathan Goodman (6 lectures) and Prof. David Spring (6 lectures)

What controls organic reactions? Is it the reagent, the functional group, the catalyst? Questions like this will be explored in the course leading to an analysis of the different types of control - chemo- regio- and stereo- (not enantio-). Reactions you have met earlier this year will be examined in a new light. Building on these more familiar examples, the mechanisms of new reactions will be introduced.

This course will involve a fundamental analysis of organic chemistry and have a strong mechanistic content. This analysis is vital for a mature understanding of the whole of Part II organic chemistry.

C6: Diffraction methods in chemistry

Dr Andrew Bond (12 lectures)

This course provides the background knowledge for one of the most powerful characterisation techniques in chemistry, namely the determination of structures by single-crystal X-ray diffraction. It illustrates the basic principles of diffraction, the fundamental relationship between a crystal structure and its X-ray diffraction pattern, and the problems that arise from the measurement of X-ray intensities rather than X-ray amplitudes. No prior knowledge is assumed and the mathematical content should be accessible to any student.

The main methods of structure determination are described, ranging from relatively simple methods that can be used for structures containing heavy atoms to more general methods that are commonly used for medium-sized molecules in organic and inorganic chemistry. More advanced methods used in the determination of protein structures are also considered. The aim is to provide the underlying principles behind the techniques, with selected worked examples.

The course also includes a description of powder X-ray diffraction, highlighting its complementarity to the single-crystal technique.

Recommended books – see RLO

C7: Further quantum mechanics

Dr John Morgan (12 lectures)

In this course, we will continue to explore theory and application of quantum mechanics relevant to chemistry. One of the main tools that we will use is perturbation theory. Although few systems can be solved exactly, we can study the effects of a small change to the Hamiltonian of a system, and using perturbation theory we can predict, for example, how a molecule responds to an applied electric field or to the presence of a neighbouring molecule. In addition to studying both stationary and time-dependent perturbation theory, we will look at some of the tools you are familiar with, such as operator algebra, in more detail than you have done so far. Many of the theoretical techniques introduced will be illustrated with examples from physical chemistry, such as investigation of what dispersion and induction forces really are, and how selection rules arise in spectroscopy.

Topics Non-degenerate perturbation theory. Polarisability of the hydrogen atom.

Rayleigh–Schrödinger perturbation theory. Linear operators and Dirac notation. Creation and annihilation operators. Anharmonic vibrations. Variation perturbation theory. Degenerate and nearly degenerate perturbation theory. The linear Stark effect. Normal modes. The Fermi resonance in CO₂. Time-dependent perturbation theory. Fermi's golden rule. and transition probabilities. Dynamic polarisabilities. Dispersion and induction forces.

Recommended books – see RLO

C8: Computer simulation methods

Prof. Rosana Collepardo (6 lectures)

In the last few decades computer simulations have emerged as a new scientific methodology – sandwiched between mathematical theories and experiment – with applications across the sciences and engineering. Because the parameters can be carefully controlled, these "theoretical experiments" provide powerful ways to develop fundamental understanding of the

connection between microscopic models of the interactions between atoms and molecules and observable properties of many-particle systems.

This course is an introduction to the two basic simulation techniques, namely molecular dynamics, in which the equations of motion are solved step by step, and Monte Carlo, in which configuration space is explored by a series of "smart" random steps. We will emphasise the basic techniques and their statistical mechanical origins instead of attempting to cover the vast array of special tools now available. Knowledge of computer language or programming skills are not required. Instead, concepts will be detailed in "pseudocode", describing the steps involved in setting up a simulation for simple model systems.

Topics Molecular Dynamics basics: Verlet algorithm, time and ensemble averages, temperature scaling, force calculation under periodic boundary conditions. thermostats and barostats.

Force fields: atomistic, coarse-grained, and multiscale models

Error estimation and convergence: Block averaging, finite size effects, systematic errors. **Monte Carlo Basics:** Importance sampling, Metropolis algorithm, Markov chains, Detailed balance

Advanced Monte Carlo methods: Biased Monte Carlo Simulations and Hybrid Monte Carlo

Advanced simulation methods: Enhanced sampling methods, Simulations of Phase Equilibria, Simulations of Non-Equilibrium Processes.

Recommended books – see RLO

C9: Chemical biology III – Nucleic acids

Dr Julian Willis (6 lectures) and Prof. Sir Shankar Balasubramanian (6 lectures)

Nucleic acids are fundamental to life and to the study and exploitation of the life sciences. Understanding the chemistry of nucleic acids is as important now as it has ever been given the recent groundbreaking discoveries that relate to DNA, RNA and genome function. These lectures will provide detailed insights into the chemistry of nucleic acids and how this relates to their structure and function in living systems.

Specific themes will include: DNA/RNA structure; the chemical synthesis of DNA and RNA; the recognition of nucleic acids by organic (drug) molecules and by natural proteins; chemical modification of DNA; the chemical biology of enzymes that mediate DNA- or RNA-related reactions (e.g. synthesis, cleavage, ligation and repair); the chemistry of DNA sequencing; and nucleic acid-based molecular medicine.

- 1 (JW) The chemical nature of DNA and RNA
- 2 (JW) Restriction endonucleases
- 3 (JW) DNA modifying enzymes
- 4 (JW) The genetic code and DNA amplification
- 5 (JW) DNA cloning
- 6 (JW) DNA assembly techniques
- 7 (SB) Chemical synthesis of DNA and RNA
- 8 (SB) Recognition of DNA by synthetic molecules
- 9 (SB) Chemical reactions on DNA and origins of chemotherapy
- 10 (SB) Enzymatic synthesis of DNA Polymerases
- 11 (SB) DNA replication and medicinal chemistry

Recommended books – see RLO

C10: Surfaces and interfaces

Prof. Stephen Jenkins (8 lectures) and Dr David Madden (4 lectures)

The behaviour of atoms and molecules at surfaces has a central role in many areas of great academic and industrial importance from everyday problems (such as corrosion, lubrication and detergency) to high added value technologies (such as oil recovery, heterogeneous catalysis and novel sensors). Many biological systems also have behaviour that is ultimately dominated by interactions at, or across, interfaces. Therefore it is clearly essential that we understand surfaces and interfaces if we are to optimise and control these important processes.

The objective of this course is to present a coherent, fundamental description of the structure and properties of interfaces, both 'wet' (solid–liquid and liquid-vapour interfaces) and 'dry' (solid–vapour interfaces). We will consider the behaviour over a range of lengthscales, from the atomistic mechanisms involved in surface mediated reactions to the macroscopic, thermodynamic description of adsorption. The focus will be on identifying and drawing together key conceptual ideas (including some gained from IB courses such as *Electrons in Solids* and *Molecular Energy Levels and Thermodynamics*), rather than mathematical aspects, to understand and predict interfacial behaviour. The course also provides the basics for several part III courses including *Electronic Structure of Solid Surfaces* and *Nano Science and Colloid Science*.

Topics Clean Surfaces Macroscopic description (Surface energies of solids and liquids); Microscopic description of single crystal surfaces (Miller indices).

Adsorption: Physisorption vs Chemisorption; Thermodynamic description of adsorption (adsorption isotherms and isosteres); Quantum chemical description of adsorption; Self-assembled Monolayers.

Surface Reactions, Heterogeneous Catalysis: Reaction Mechanisms and their relationship to rate equations; Activity, Selectivity.

Experimental Techniques: including Wilhelmy plate and capillary rise (surface tension); ultraviolet and X-ray photoelectron spectroscopy and Auger electron spectroscopy (chemical composition of surfaces); neutron reflectivity, grazing incidence X-ray diffraction and low-energy electron diffraction (surface crystallography); reflection-absorption infrared spectroscopy and sum-frequency generation (vibrational spectroscopies); atomic force microscopy and scanning tunnelling microscopy (scanning-probe techniques).

Recommended books – see RLO

C11: Investigating organic mechanisms

Prof. Peter Wothers (12 lectures)

How do we know how a reaction proceeds? How much faith should we put in the mechanisms we so readily draw? In this course we will investigate the different methods available to the chemist in order to understand exactly how species react in solution. We will look at the ways of determining and manipulating the reaction pathways from starting materials, through transition states and intermediates to products. The crucial role of the solvent in controlling the outcome of a reaction is also examined.

Topics Kinetics, potential energy surfaces for reactions, interpretation of enthalpy, entropy and volume of activation, interpretation of kinetic isotope effects, acid and base catalysis, linear free energy relationships (Brønsted and Hammett equations). Noncovalent interactions, solvation, water as a solvent and hydrophobic effects and solvent effects on organic reactivity.

Continuously assessed work

You are required to complete a portfolio of continuously assessed work taken from a range of options on offer. Naturally, conventional practical work features heavily as chemistry is above all an experimentally based subject, and to describe yourself as a chemist you need to know how to design and carry out experiments.

Chemists also need to develop a wider range of skills, such as how to find out and sift information, how to write, how to use computers in different contexts and how to communicate your ideas. You will have the opportunity to develop these skills as part of your portfolio of continuously assessed work. It is important to realise that even if you are not intending to carry on as a professional chemist, these skills will nevertheless be very useful to you in your future career.

6.1 Requirements

6

The continuously assessed work you need to complete is made up in the following way (this corresponds to the 'six units of further work' referred to in the University Ordinance which defines the structure of Part II Chemistry):

- The two core practical courses which consist of *Techniques in Modern Synthetic Chemistry* (organic and inorganic) and the joint *Physical & Theoretical Chemistry* course.
- The exercises associated with the Chemical Informatics course.
- Four additional credits.

The four additional credits can be made up by any combination of the following:

- Extended experiments offered during the first two weeks of the Easter term; you will be able to gain **up to four** credits associated with each core course
- The Language Option: four credits
- The Programming Option: one or two credits
- The Mathematical Methods course: three credits

To produce a final mark for the continuously assessed work, each component will be weighted as follows:

Component	% of final mark
Techniques in Modern Synthetic Chemistry (core practical course)	35.5
Physical & Theoretical Chemistry (core practical course)	35.5
Informatics	3.0
Each additional credit	6.5

Students may complete more additional credits than the minimum, in which case the four credits with the highest marks will be used. The one exception to this is that students embarking on the Language Option **cannot** substitute any additional credits for the four associated with this option.

The marks for the continuously assessed component contribute 25% to the overall mark for Part II.

6.2 Special arrangements for those taking course A6

If you are taking the A6 course then you will be required to complete the *Techniques in Modern Synthetic Chemistry* course and the following experiments

- 1. Experiments A, B and D from the joint *Physical & Theoretical Chemistry* core course; you are not expected to do any of the theoretical exercises.
- 2. Exercises 1, 5 and 10 from the Part IB Chemistry A course.
- 3. The Physical experiment *Kinetics of protein folding* (this may only be available in the Lent Term).

6.3 Arrangements for laboratory work

Practical Groups A-D

The Part II class will be split into four groups, **Groups A-D**, and each group attempts the four elements of the Core practical over the course of the Michaelmas and Lent terms. The Core practical consists of the following.

- SYN Synthetic lab (Part II O/I laboratory)
- PHY Physical lab (Part II Physical laboratory)
- THE Theoretical (Room G30)
- CHI Chemical Informatics (online)

IMPORTANT

Please take careful note of which group you are in since it is essential for the safe and smooth running of the practical classes.

The groups will complete their Core practicals according to the following rotation

- Group A SYN/CHI/PHY/THE
- Group B PHY/THE/SYN/CHI
- Group C CHI/SYN/THE/PHY
- Group D THE/PHY/CHI/SYN

Once the core experiments from each set have been completed it will be possible to do further experiments to gain additional credits. The core courses will build on and extend the practical skills you acquired in the second year, and you will also do experiments which illustrate the ideas and concepts presented in last year's and this year's lecture courses.

Extended experiments

In the Easter term all labs will be open to all groups during the period 1 May - 16 May for extended experiments.

6.4 Techniques in modern synthetic chemistry (SYN)

- **Location** East end of the Organic & Inorganic Practical Laboratory which is on the ground floor of the Department on the Union Road side of the building. Please enter the laboratory by the doors which open onto the foyer outside the BMS Lecture Theatre.
- **Time** The laboratory is open weekdays, 11:00 to 18:00; you are free to complete your work during this time.
- **Attendance** For each Group (A D) the course will begin with an Induction Day, in the Part II Laboratory, during which safety issues will be covered, the layout of the laboratory will be explained and some techniques demonstrated. Please follow the timetable for your Group.

You must attend the Induction Day assigned to your group; you will be required to attend in the laboratory from the start of the induction session to the end of the day.

Personnel The technician in change of the class is Dr Atheer Madlool and he is assisted by Maria Cascone. The members of staff responsible are Prof. Sally Boss and Prof Bill Nolan.

6.5 Joint Physical & Theoretical chemistry course

Physical chemistry experiments (PHY)

- **Location** Part IB/II Physical Chemistry Laboratory on the first floor, Lensfield Rd side of the building.
- **Time** The laboratory is open weekdays, 11:00 to 18:00; *on your allotted day* you are free to complete your work during this time.
- **Rough books** As last year, you must record any measurements, as you make them, in a rough book; you need to bring your rough book with you when you have an experiment marked off.
- **Personnel** the technicians in change of the class are Sarah Mitchell and Tom Wilkins. The member of staff responsible is Prof. Peter Wothers.

Theoretical chemistry exercises (THE)

Location Room G30 (UMD), by the lift on the Lensfield Rd side of the building.

- **Time** Weekdays, 14:00 to 17:00; *on your allotted day* you are free to complete your work during this time, but it is recommended that you attend at the start of the session to be briefed about the exercise.
- Personnel The member of staff responsible is Dr John Morgan (jwrm2).

6.6 Chemical Informatics (CHI)

This part of the course consists of two online lectures; you will be required to complete two assessed exercises. Further details will be given out prior to your Group starting the CHI component of the practical.

Chemical information

Prof. Jonathan Goodman

How do you write a recipe for a reaction? The answer might be in the chemistry department library which contains reports of molecular experiments performed over more than a century, or in an on-line database. The lectures will describe how this huge quantity of information can be searched and analysed, using the main databases available to us (Web of Science, Reaxys (Beilstein), CSD, ChemSpider, National Chemistry Database Service etc.). The problems and challenges of finding and analysing chemical information will be discussed.

6.7 Language option (Michaelmas and Lent Terms)

There are around twenty five places on offer to study Chinese, French, German, Japanese or Spanish in the Centre for Languages and Inter-Communication (CLIC) based in the Department of Engineering:

www.clic.eng.cam.ac.uk

The courses are aimed at enabling you to understand both the written and spoken word; the emphasis is not on technical vocabulary but rather on the day-to-day language that you might need when working overseas. The courses cope with a wide range of starting abilities, from beginners to A-level standard.

The Language Unit is very well set up and has two full-time lectors (one French, one German), a part-time Director and many skilled language teachers who work alongside the permanent staff. Teaching is through the medium of conventional classes and computer-based audio-visual material, much of which has been written specifically for the courses. The Unit is housed in the Baker Building at the Lensfield Rd end of Trumpington St and those who are registered for the course will have unrestricted access to the Unit's facilities.

Finding out about the course and registering interest

At 14:00 on Tuesday 8th October (in the Pfizer lecture theatre) David Tual, the Director of the Language Programme, will give an introductory talk on the courses offered by the Language Unit. If you are thinking of taking one of these, it is vital that you attend this introduction.

If, after hearing the talk, you wish to take up one of the places, you need to fill in an electronic form (a link will be provided) giving some basic details, describing your motivation for the course, and indicating which language you would like to study. The deadline for submitting these forms is 09:00 on Wednesday 9th October. If the course is oversubscribed, names will be selected by drawing lots. The names of those successful in gaining a place will be announced, by EMAIL, on Wednesday afternoon.

Further details and assessment

If you are allocated a place on the Language Course you will need to take a self assessment test (LASSIE). Further details will be available nearer the time.

You will also need to be issued with a swipe-card so that you can access the Language Unit outside normal hours. Details of how this can be done will be announced in the introductory lecture. Classes will commence in Week 2, starting Thursday 17th October, and continue for the rest of the Michaelmas Term and all of the Lent Term – the starting date will be confirmed to you when you register.

The Language option will be challenging and will demand self discipline as each week you need to complete a number of hours of unsupervised work. There may be some difficulties in fitting the Language classes in with your timetable for practical work; we will do our best to be accommodating, but some compromises may have to be made. You are expected to attend the Language classes and complete the homework assigned; if you fail to do this, you will be withdrawn from the course.

There will be a formal assessment of your progress at the end of both the Michaelmas and Lent Terms. You must attend these assessments. Details will be announced nearer the time.

6.8 Programming option

This option provides a structured introduction to scientific computer programming in the language Python. The course is largely self-taught and runs for the whole of Michaelmas and Lent Terms. Dr Alex Thom (ajwt3@cam.ac.uk) will lead the course; please address any questions you have to him. Assessment is by means of programming exercises which are submitted and marked. The course consists of two parts, so it is possible to complete just the introductory part of the course to gain one credit, or the whole course to gain two credits. A weekly drop-in session (times to be announced) will be available to help with the exercises.

6.9 Mathematical methods (Lent Term)

This course covers mathematical methods which are relevant for those interested in advanced courses in theoretical and physical chemistry. Part of the course will involve revisiting topics covered in Part IB NST Mathematics, and part will involve the extension of this material and the study of some new material. If you have not done Part IB NST Mathematics, then this course will still be accessible to you.

The course will consist of eight two-hour sessions, held weekly during the Lent Term (exact times to be announced). Prof. Michele Vedruscolo (<u>mv245@cam.ac.uk</u>) will lead the course: please address any questions you have to him. Assessment will be via weekly take-home problem sets, which you will be asked to complete.

Topics to be covered include: linear algebra; probability theory and inference methods; tensors; series; integral transforms; ordinary and partial differential equations; stochastic processes; and optimization theory.

6.10 Assessment of practical work

Most of your practical work will be assessed in front of you on a week-by-week basis, so you will know your marks as the year progresses. All marks awarded for continuously assessed work are subject to moderation by the relevant member of staff in charge of that part of the course and/or the Examiners. This is done so that comparability between kinds of work can be maintained.

All continuously assessed work must either have been assessed (in the case of conventional practical work) or be submitted for assessment (in the case of other work) by the end of the Term in which it was undertaken. You must not accumulate unmarked practicals throughout the Term and then expect to have them marked in the last few days. There will be penalties imposed on work of any kind which is submitted after the deadline.

At the end of the year the External Examiners may wish to see samples of your continuously assessed work. It is therefore important that you keep your write-ups etc. together and in a safe place.

7 — Plagiarism

Plagiarism is defined as submitting as one's own work that which derives in part or in its entirety from the work of others without due acknowledgement. It is both poor scholarship and a breach of academic integrity. The University views plagiarism as a serious matter and, under Discipline Regulation 6, has the power to take disciplinary action against those found guilty of plagiarising the work of others.

The general university statement on plagiarism, and further general advice on plagiarism and how to avoid it, is given on the University's plagiarism and good academic practice website www.plagiarism.admin.cam.ac.uk/definition. Generally the Department follows the advice and policies set out by the University. This section gives further guidance as to how

these policies apply to study in the Department of Chemistry.

Supervision work and Tripos questions

The majority of questions set as supervision work and in Tripos examinations take the form of problems to be solved. In presenting their solutions to these problems students are not expected to quote the source or authority of the facts, theories and concepts they use to formulate their solutions.

Continuously assessed work (principally practical work)

Here the rules against plagiarism are especially relevant as they prohibit copying and colluding. Basing a write-up on data or answers provided by another student is an example of plagiarism (or, more simply, cheating). The following rules apply to all continuously assessed work

- Unless otherwise instructed, you must work alone. Where you are permitted to work in a group, the names of those you have worked with must be stated on your practical write-up.
- The write-up must be entirely your own work. In particular, you may not use spreadsheets or templates prepared by others.
- It is expressly forbidden to invent, falsify or modify data, spectra or observations, or to use data, spectra or samples obtained from other persons unless authorised to do so by a Senior Demonstrator.
- Where data from other sources is quoted in a write-up, the source must be identified.

The following summarizes succinctly the key point:

The Golden Rule: The examiners must be in no doubt as to which parts of your work are your own original work, and which are the rightful property of someone else.

8

Examinations

The basic rules are

- Candidates must offer four papers in total.
- Candidates must offer Paper 1 and either Paper 2A or Paper 2B, Paper 3 and Paper 4.

Next come the rules about which out of Papers 2A & 2B you can do.

- Candidates who have taken Part IB Chemistry A and Part IB Chemistry B must take Paper 2A.
- Candidates who have taken only Part IB Chemistry B may take *either* Paper 2A *or* Paper 2B.

The point of these is that they allow students who have only done Chemistry B to attempt all the core courses if they wish, or to take the alternative course (A6) especially designed for them.

8.1 Format of the papers

Note that the format of all the Papers changed in 2017/18.

Paper 1 is of duration 3 hours and will consist of two sections. Section A will contain 4 compulsory 5 minute questions relating to course A1 and 4 compulsory 5 minute questions relating to course A2. Section B will contain 2 compulsory 30 minute questions relating to course A1 and 2 compulsory 30 minute questions relating to course A2.

Section A carries 25% of the marks and Section B carries 75% of the marks. Within a section each question has equal weight.

Paper 2A is of duration 3 hours and will consist of two sections. Section A will contain 4 compulsory 5 minute questions relating to course A3 and 4 compulsory 5 minute questions relating to course A4. Section B will contain 2 compulsory 30 minute questions relating to course A3 and 2 compulsory 30 minute questions relating to course A4.

Section A carries 25% of the marks and Section B carries 75% of the marks. Within a section each question has equal weight.

Paper 2B is of duration 3 hours and will consist of two sections. Section A will contain 8 compulsory 5 minute questions relating to course A6. Section B will contain 4 compulsory 30 minute questions relating to course A6.

Section A carries 25% of the marks and Section B carries 75% of the marks. Within a section each question has equal weight.

- Paper 3 is of duration 3 hours and will contain two 45 minute questions relating to each 12 lecture B course and one 45 minute question relating to each 6 lecture B course; candidates should answer four questions, without restriction. Each question is of equal weight.
- Paper 4 is of duration 3 hours and will contain two 45 minute questions relating to each 12 lecture C course and one 45 minute question relating to each 6 lecture C course; candidates should answer four questions, without restriction. Each question is of equal weight.

You will be given an extra 10 minutes of reading time for all of these papers. Each of the four papers sat by a given candidate is of equal weight and together they contribute 75% of the final mark.

In all of the examinations you will be provided with a Data Book which contains a simple Periodic Table, values of physical constants, certain mathematical formulae and definitions and selected character tables. You will be provided with a copy of the Data Book when you register for the course (accessible on line at www.ch.cam.ac.uk/teaching/data-book). You may take (unassembled) molecular models into the examinations.

Material from the Part IB course will not be examined explicitly in the Part II examinations. However, you should be aware that a sound understanding and firm grasp of the IB material is essential for success in the Part II papers.

In addition to the written papers, all candidates must submit the specified amount of continuously assessed course work as described above.

Example exam entries

- 1. If you have taken Chemistry A and B at Part IB you should be entered for Papers 1, 2A, 3 & 4.
- 2. If you have only taken Chemistry A but have nevertheless decided to tackle the four core courses A1–A4 you should be entered for the papers as in 1.

- 3. If you have only taken Chemistry B and followed the course A6, then you should be entered for Papers 1, 2B, 3, & 4.
- 4. All candidates must be entered for the 'six units of further work' this is the continuously assessed part of the course.

8.2 Timetable

Although the Examination timetable will not be announced formally until early in the Easter Term, our understanding is that the papers will all be sat in the week commencing Monday 9th June. We expect that the results will be available in CamSIS on the afternoon of Friday 27th June. Please note that these dates are all provisional and subject to confirmation.

8.3 Past papers

Past papers are available from the relevant section of *Moodle* (<u>www.vle.cam.ac.uk</u>), and suggested answers to questions more than five years old are also available.

8.4 Pass marks

The marks obtained on the written papers are combined with marks obtained from the continuously assessed work; the intention is that 75% of the final mark is for the theory and 25% for the continuously assessed work. The Examiners may, however, at their discretion alter the weight given to different papers or different parts of the continuously assessed work. The Examiners may also scale the raw marks obtained in any component of the examination e.g. the continuously assessed part.

Please note that to be awarded a pass in the whole examination candidates will need to achieve: (1) a pass mark (40%) in the combined total of the theory papers, **and** (2) a pass mark (40%) in the total from the continuously assessed work.

The Senior Examiner for Part II Chemistry is Dr Paul Wood.

8.5 Disclosure of examination marks

The marks which are disclosed (via *CamSIS*) are those for each of the papers, a total mark for the continuously assessed component of the course, and the final overall total and class. Please note that the marks from the continuously assessed component may be scaled by the Examiners. In addition you will be notified separately of your question-by-question marks.

9

Carrying forward marks

Exam regulations allow the Part III examiners to take into account a candidate's performance in Part II from the previous year. In effect, this means that marks will be 'carried forward' from Part II to Part III.

The practice is that the Part III examiners will draw up the class list by combining the Part II and Part III marks, with a weighting of 15% for the Part II marks.

10 Admission to Part III Chemistry for the academic year 2025/26

The minimum standard required for entry to Part III in 2025/26 will be a II.1 in Part II Chemistry.

Students who have not achieved the required standard may appeal to the Faculty Board of Physics and Chemistry to be admitted to Part III. In assessing such appeals the Faculty Board will be looking for evidence that the student has performed consistently at the II.1 level in the past, and has performed at this level for a significant part of the Part II written examination. Strong support of the student's Tutor or Director of Studies will be expected.

Please note that where a student has failed to meet the II.1 level as a result of illness or other incapacity, the appeal is made to the Examinations, Access and Mitigation Committee (EAMC) and not to the Faculty Board.

The appeals procedure is set out at

www.ch.cam.ac.uk/teaching/admission-part-ii-and-part-iii.

11 — Part II Physical Sciences: Half Subject Chemistry

This paper is offered in NST Part II Physical Sciences, the full details of which can be found at

www.cam.ac.uk/about/natscitripos/students/thirdps.html

Students taking this option also need to complete a 5000 word dissertation on an approved topic (the word limit does not include: acknowledgements, contents lists, figure captions, references), as well as a further subject from Part IB NST. The marks for Part II Physical Sciences are divided as follows: Half Subject 60%, Part IB Subject 25%, Dissertation 15%.

You should consult your Director of Studies early in the Michaelmas Term to discuss the selection of the topic. Your topic needs to be agreed with the Director of Teaching by the end of the Michaelmas Term, and your dissertation (three copies, soft bound, along with a PDF version) needs to be handed in by the first day of the Easter Full Term.

The programme of work for Half Subject Chemistry is a sub-set of that set out for Part II. You are required to take two of the core courses A1 - A4, and have a free choice of B and C courses. You will need to consider carefully how many B and C courses to prepare, but the absolute minimum will be 12 hours of lectures from the B courses, and the same from the C courses.

You will sit Paper 1 *or* Paper 2A (as described above), Paper 3 and Paper 4 but with the following modified rubrics: (a) for Papers 3 and 4 you will be given 90 minutes to write the examination and (b) for these papers you will be required to answer two questions.

The requirements for continuously assessed work are:

- EITHER the joint Physical & Theoretical Chemistry core course OR the Techniques in Modern Synthetic Chemistry course.
- The exercises associated with the *Chemical Informatics* course.
- Two additional credits.

The Language option is not normally available to students taking half subject chemistry.

12 Chemistry teaching website

You can find up-to-date information on the course and other related matters from the teaching website: www.ch.cam.ac.uk/teaching.

Handouts and other course materials will be posted on *Moodle*: <u>www.vle.cam.ac.uk</u>. If you find that you do not have access to the Chemistry part of Moodle, please email the Teaching Office on teaching.office@ch.cam.ac.uk.

13 Chemistry Consultative Committee

The Chemistry Consultative Committee consists of representatives of students and academic staff. It meets towards the end of each term and is a forum for the discussion of all aspects of the teaching of Chemistry in the Department. Student representatives are elected during the Michaelmas term; comments and suggestions can be passed on to them so that they can be discussed at the meetings.

The minutes of previous meetings may be found on Moodle and the composition of the committee can be found on the teaching website

www.ch.cam.ac.uk/committees/consultative-committee

14 Department of Chemistry Library

www-library.ch.cam.ac.uk

Library, photocopying, printing, scanning and computing

The Chemistry Library is located in the Centre for Molecular Informatics (CMI) building (first floor, beneath the Cybercafe). You can access it between 08:00 and 21:00 (Monday to Friday only), 08:00 and 16:00 Saturdays only) using your University Card. You can apply for evening and weekend access by contacting the Mifare Admin Team at the department; please visit the 'Access to the library website': www-library.ch.cam.ac.uk/access-library for further information.

Books recommended in the Blue Book are either short loan and can be borrowed for four days, or are for reference only. Main loan books can be borrowed for 28 days and are auto-renewed until you return them or someone else requests them from you; short loan books cannot be renewed. You can borrow up to 10 books (incl. max. two short loan books) at a time. All Chemistry books and ebooks are listed on iDiscover, the online catalogue for the libraries of the University: //idiscover.lib.cam.ac.uk There is a dedicated computer in the Library for searching the catalogue. A self-service machine is available for borrowing and returning books.

The Library has four PCs which are hosted on the UMD (University Managed Desktop) network. Print jobs can be sent from these to a MultiFunctional Device (MFD) situated in the small room next to the Library Office. The MFD offers colour printing, photocopying and free scanning. Online payment for printing and photocopying is made through the Common Balance scheme. You can send print jobs to the MFD from your own desktop, laptop, tablet, or phone; there are instructions for setting this up and information on paying for printing/photocopying at help.uis.cam.ac.uk/service/printing

There are also six docking solutions you can connect your laptop to, consisting of a 27" monitor, VGA and HDMI cables. Wifi and power points are available throughout the Library.

For comprehensive guidance on the library collections (printed and online), services and much more consult the Chemistry Library website at:

www-library.ch.cam.ac.uk

Reading Lists Online (RLO)

The link below gives access to the online reading lists for all the Chemistry courses. They have been compiled to follow the structure of the Course Guides. Each one includes a record of the

borrowable items held in the Cambridge University Libraries' collections (including the Chemistry Library) and those accessible as eBook titles.

www-library.ch.cam.ac.uk/reading-lists-online-rlo

15 Further details of the Department

In order to access areas of the Department other than the lecture theatres you will need your University card so that you can pass the turnstiles and the appropriate internal doors. You should therefore make it a point to *always* bring your card with you when you come to the Department. By the time of the registration process for the practical classes we should have collected sufficient information to have already programmed your University card for the appropriate access. If you find that your access rights are different to others in your year group, or access suddenly stops, please contact Mifare Admin (<u>mifareadmin@ch.cam.ac.uk</u>).

Please note that undergraduates will *not* be given access to research areas. If you need to meet supervisors and so on, you will need to arrange for them to meet you in a general access area. Do make sure you know who they are and how to contact them, so that Security can help you locate them if necessary.

Your card will give you access to the building from 08:00–20:00 on weekdays and 09:00–14:00 on Saturdays. Outside these times you are not permitted to be in the Department unless some specific arrangement has been made (see below) If you remain in the Department after 20:00 you risk becoming trapped by the security doors and/or the turnstiles.

If you would like access to the Departmental library outside normal working hours you will need to contact Mifare Admin (<u>mifareadmin@ch.cam.ac.uk</u>) and they will be able to arrange the usual extension for a Part II student.

Cybercafé

You are most welcome to use the Departmental tea room (Cybercafé) which is located on the top floor of the Centre for Molecular Informatics Building. Service is available from 09:30 to 15:30. Hot and cold drinks, as well as a selection of snack foods are available.

Please bear in mind there is limited space and it is intended for use by the research workers and staff in the Department (the morning and lunchtime periods are especially busy).

16 _____ Part II Chemistry 2024/2025: Titles of lecture courses

Code	Hours	Title	Lecturer(s)								
		A									
۸.1	10	A courses	Loop (7) Wheatley (5)								
A1 40	12Inorganic reactivity, the heavier transition metals and the f-block elementsLess (7), Whea12The foundations of organic synthesisNolan (12)										
AZ	12	2The foundations of organic synthesisNolan (12)2High resolution molecular spectroscopyKeeler (12)									
A3	12	2 High resolution molecular spectroscopy Keeler (12) 2 Theoretical techniques Theoretical techniques									
A4	12 I heoretical techniques Michaelides (6),										
A6	24	Concepts in physical chemistry	Chiebikova (14), Truscott (10)								
		B courses									
B0	Boss (6)										
B1	6 Inorganic III: Organometallic catalysis Wood (6)										
B2	6	Organic spectroscopy	Fleming (6)								
B3	12	Chemical biology I: Biological catalysis	Leeper (6), Spring (6)								
B4	12	Chemistry in the atmosphere	Archibald (12)								
B5	6	Structure and Reactivity	Nolan (6)								
B6	6	Biomaterials	Duer (6)								
B7	12	Statistical mechanics	Reinhardt (12)								
B8	6	Symmetry	Alavi (6)								
B9	6	Polymers: synthesis, characterisation and application	Scherman (3), Bronstein (3)								
B10	6	Electronic structure	Thom (6)								
		C courses									
		Inorganic IV, characterisation methods:									
C1	6	Electrochemistry	Zhang (6)								
C2	6	The chemistry of future energy	Slaughter (6)								
C3	6	NMR	Forse (6)								
C4	12	Chemical biology II: Proteins: structure, stability, folding and misfolding	Jackson (6),Sormanni (6)								
C5	12	12 Chemical biology II: Proteins: structure, stability, folding and misfolding Jackson (6), 12 Control in organic chemistry Goodman (6)									
C6	12	12Diffraction methods in chemistryBond (12)									
C7	12	12 Further guantum mechanics Morgan (12)									
C8	6	Computer simulation methods	Collepardo (6)								
C9	12	Chemical biology III: Nucleic acids	Willis (6), Balasubramanian (6)								
C10	12	Surfaces and interfaces	Jenkins (8). Madden (4)								
C11	12	Investigating organic mechanisms	Wothers (12)								
		Other									
CHI	2	Chemical informatics	Goodman (2)								
MM	8	Mathematical Methods	Vendruscolo (8)								

9 Week 10 12 Courses Other activities / comments Date Day 11 0 Lang. Intro. 14:00 (Pfizer LT) 8/10 Tu Introductory Lect. 12:00 (PLT) 9/10 We 1 Th Practical: Groups A-D (start) 10/10 A1 A2 A1 A3/A6 A4/A6 A2 11/10Fr 14/10 A3/A6 A4/A6 A3 Mo 15/10Tu A1 A2 A4 16/10 We A3/A6 A4/A6 A6 2 17/10Th A2 Language courses start A1 18/10 A3/A6 A4/A6 Fr 21/10 Mo 22/10Careers talk (Dr Raj Sidhu) 17:00 (PLT) Tu A1 A2 23/10 We A3/A6 A4/A6 3 24/10Th A1 A2 25/10 Fr A3/A6 A4/A6 28/10 Mo A3/A6 A4/A6 29/10 Tu A1 A2 30/10 We 31/10 Th 4 A1 A2 1/11Fr A3/A6 A4/A6 A3/A6 A4/A6 4/11 Mo 5/11 Tu A1 A2 6/11 We 5 7/11 Th A2 Practical: Groups A-D (rotation 1) A1 A3/A6 A4/A6 8/11 Fr 11/11A3/A6 A4/A6 Mo 12/11 Tu A1 A2 13/11 We 6 14/11Th A1 A2 15/11Fr A3/A6 A4/A6 **B**7 18/11 B10 **B**7 Mo A1 A2 19/11 Tu **B**7 20/11We B10 A6 venue: Unilever LT/Todd Hamied 9 Week Date Day 10 11 12 Courses Other activities / comments 7 B0 Boss (6) 21/11Th **B**0 B2 B0 22/11B3 B4 B7 B2 B2 Fleming (6) Fr 25/11 **B**0 B10 **B3** B3 Leeper (4) Mo **B2** B4 26/11 Tu B3 B4 Β7 B4 Archibald (4) We B7 Reinhardt (6) 27/11B0 **B**2 **B**7 B10 Thom (6) 8 28/11Th B0B2 **B**7 B10 29/11 Fr **B**3 B4 B10 2/12Mo **B**0 B2 B10 3/12 Tu B3 B4 **B**7 4/12 We **B**0 **B**2 B10

Part II Chemistry : Michaelmas Term 2024

Week	Date	Day	9	10	11	12	Courses	Other activities / comments
1	23/1 24/1 27/1 28/1 29/1	Th Fr Mo Tu We	B3 B7 B3 B7	B1 B4 B4 B1 B4	B9 B8 B9 B9 B9 B8	B5 B5 B6	B1 B3 B4 B5 B6	Practical: Groups A-D (rotation 2) B1 Wood (6) B3 Leeper (2), Spring (6) B4 Archibald (8) B5 Nolan (6)
2	30/1 31/1 3/2 4/2 5/2	Th Fr Mo Tu We	B3 B7 B7 B3	B1 B4 B4 B1 B4	B9 B8 B9 B9 B9 B8	B5 B6 B5 B6	B7 B8 B9	B6 Duer (6) B7 Reinhardt (6) B8 Alavi (6) B9 Scherman (3), Bronstein (3)
3	6/2 7/2 10/2 11/2 12/2	Th Fr Mo Tu We	B3 B7 B3 B7 B3	B1 B4 B4 B1 B3	B8 B8	B5 B6 B5 B6 B6 B6		
4	13/2 14/2 17/2 18/2 19/2	Th Fr Mo Tu We	C1 C6 C6 C1 C6	C11 C11 C11	C5 C5	C4 C4 C4	C1 C4 C5 C6 C11	C1 Zhang (6) C4 Jackson (6), Sormanni (6) C5 Goodman (6), Spring(6) C6 Bond (12) C7 Morgan (6)
5	20/2 21/2 24/2 25/2 26/2	Th Fr Mo Tu We	C1 C6 C6 C1 C6	C11 C9 C11 C9 C9	C5 C10 C5 C10	C9 C4 C4 C4	C10 C9	Practical: Groups A-D (rotation 3)
6	27/2 28/2 3/3 4/3 5/3	Th Fr Mo Tu We	C1 C6 C6 C1 C6	C11 C9 C11 C9 C9	C5 C10 C5 C5 C10	C7 C4 C4 C7 C4	C7	C8 Collepardo (6) C9 Willis (6), Balasubramanian (6) C10 Jenkins (4), Madden (4) C11 Wothers (12)
7	6/3 7/3 10/3 11/3 12/3	Th Fr Mo Tu We	C7 C6 C6 C7 C6	C11 C9 C11 C9 C9	C10 C5 C5 C10 C5	C4 C4 C4	C8	C8 2 pm Pfizer LT C8 2 pm PLT C8 2 pm PLT
8	13/3 14/3 17/3 18/3 19/3	Th Fr Mo Tu We	C7 C7	C11 C9 C11 C9 C11	C10 C5 C10 C5			C8 2 pm PLT C8 2 pm PLT C8 2 pm PLT

Part II Chemistry : Lent Term 2025

Week	Date	Day	9	10	11	12	Courses	Other activities / comments
1	1/5 2/5 5/5 6/5 7/5	Th Fr Mo Tu We	C3 C3 C3	C7 C7 C7	C10 C2 C2 C10 C2		C2 C3 C7 C10	Extended experiments start C2 Slaughter (6) C3 Forse (6) C7 Morgan (6) C10 Jenkins (4)
2	8/5 9/5 12/5 13/5 14/5	Th Fr Mo Tu We	C3 C3 C3	C7 C7 C7 C7	C10 C2 C2 C10 C2			Part II class photo 12.15
3	15/5 16/5 19/5 20/5 21/5	Th Fr Mo Tu We						Extended experiments end
4	22/5 23/5 26/5 27/5 28/5	Th Fr Mo Tu We						
5	29/5 30/5 2/6 3/6 4/6	Th Fr Mo Tu We						
6	5/6 6/6 9/6 10/6 11/6	Th Fr Mo Tu We						Part II exams start*
7	12/6 13/6 16/6 17/6 18/6	Th Fr Mo Tu We						
8	19/6 20/6 23/6 24/6 25/6	Th Fr Mo Tu We						Class list posted Friday 27 June*

Part II Chemistry : Easter Term 2025

*Provisional dates