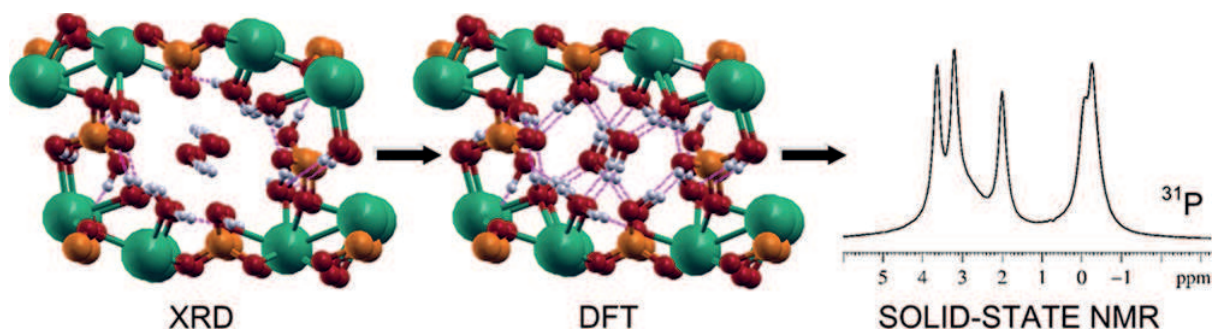




UNIVERSITY OF
CAMBRIDGE

Department of Chemistry

Part II Chemistry:
A Guide to the Course



Academic Year 2017/2018

Contents

| | | |
|-----------|--|-----------|
| 1 | Introduction | 2 |
| 2 | Introductory talk and welcome party | 2 |
| 3 | Careers for chemists | 2 |
| 4 | Outline of the course | 2 |
| 5 | Lecture Course Synopses | 3 |
| 6 | Continuously assessed work | 19 |
| 6.1 | Requirements | 19 |
| 6.2 | Special arrangements for those taking course A6 | 20 |
| 6.3 | Arrangements for laboratory work | 20 |
| 6.4 | Techniques in modern synthetic chemistry | 20 |
| 6.5 | Joint Physical & Theoretical chemistry course | 21 |
| 6.6 | Chemical Informatics (Michaelmas Term) | 21 |
| 6.7 | Language option (Michaelmas and Lent Terms) | 22 |
| 6.8 | Programming option | 22 |
| 6.9 | Mathematical methods (Lent Term) | 23 |
| 6.10 | Assessment of practical work | 23 |
| 7 | Plagiarism | 23 |
| 8 | Examinations | 24 |
| 8.1 | Format of the papers | 25 |
| 8.2 | Timetable | 26 |
| 8.3 | Past papers | 26 |
| 8.4 | Pass marks | 26 |
| 8.5 | Disclosure of examination marks | 26 |
| 9 | Carrying forward marks | 26 |
| 10 | Admission to Part III Chemistry for the academic year 2018/19 | 27 |
| 11 | Part II Physical Sciences: Half Subject Chemistry | 27 |
| 12 | Chemistry teaching website | 28 |
| 13 | Chemistry Consultative Committee | 28 |
| 14 | Library, photocopying and computing | 28 |
| 15 | Further details of the Department | 29 |
| 16 | Titles of lecture courses | 31 |
| | Timetable | 31 |

1 --- 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 offer 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 27 concerning the requirements for admission to Part III.

2 --- Introductory talk and welcome party

On Wednesday 4th October at 12:00 in the Bristol–Myers Squibb Lecture Theatre there will be an introductory talk about the course; it is vital that you attend.

There will be a ‘Welcome Party’ in the foyer above the entrance to the Bristol–Myers Squibb Lecture Theatre for all new Part II students on Friday 6th 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.

3 --- Careers for chemists

On 17th October at 17:00 in the Wolfson Lecture Theatre, Madelaine Chapman, from the Careers Service, will give a short talk on 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. Madelaine’s talk is highly recommended for all the class.

4 --- 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. Melinda Duer’s website and depicts some recent work from her group where by combining X-ray crystallography, first-principles density functional theory calculations, and solid-state NMR, it has been possible to refine the crystal structure of octacalcium phosphate, a key mineral in the structure of bone. For more details about research in the Duer group please refer to www.ch.cam.ac.uk/group/duer/

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 three 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.

5 Lecture Course Synopses

A courses

A1: Inorganic I – structure and bonding

This course focuses on 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.

Dr Sally Boss: 5 lectures

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 shapes of molecules. The synthesis and reactivity of electron deficient compounds will be described and the physical methods used to probe the structures of these species will be briefly 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.

Prof. Melinda Duer (4 lectures) and Dr Daniel Beauregard (3 lectures)

The second half of this course examines the heavier transition metals and f-block elements, focusing on the availability (or otherwise) of valence d and f orbitals in bonding. 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 view point, reinforced with bonding and thermodynamics arguments. Whilst the lanthanide and actinides comprise almost a quarter of the periodic table, they receive comparatively little attention despite their intrinsically interesting properties and widespread applications. A comparison of the chemistry of the lanthanide and actinides reveals strongly differing behaviour which is attributed to the extent of f orbital availability. The effect on bonding and structures is discussed: predominantly ionic bonding in lanthanides and significant covalency in actinide complexes. A good knowledge of IB coordination chemistry is desirable.

Topics Metal–metal multiple bonding in the d block. Metal–ligand multiple bonding in d block chemistry. Ionic vs covalent bonding in the f block. f-Block atomic orbitals, ionic bonding, and covalent bonding.

Recommended books

- N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, Butterworth-Heinemann Ltd, 2nd Edn. [QD466.G74]
F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, Wiley 5th Edition, 1988. [QD151.C68]
J. E. Huheey, *Inorganic Chemistry*, Longman, 4th Edn. [QD157.H84]
N. C. Norman, *Periodicity in the s- and p-block Elements*, Oxford Primer, 2nd Edn. [QD466.N67]
N. Kaltsoyannis and P. Scott *The f elements*, OUP, 1999. [QD172.R2.K35]
S. A. Cotton and F. A. Hart, *The Heavy Transition Metals*, Macmillan, 1975. [QD172.T6.C68]
S. F. A. Kettle, *Physical Inorganic Chemistry*, Spectrum Books, 1996. [QD475.K48]
Inorganic Chemistry, Housecroft and Sharpe, 4th edn., 2012. [QD151.H68] Reference only.
Inorganic Chemistry, Shriver and Atkins, 4th edn. 2006. [QD151.S57] Reference only.
Periodicity and the s- and p-block Elements - (OUP), N. Norman, 1997. [QD466.N6] Reference only.

A2: The Foundations of organic synthesis

Dr Bill Nolan

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.

More Tools of the Trade: Synthesis of More Complex Systems. Control of Mixed Functionality.
Use of Latent Functionality

Concepts and Methods for Ring Synthesis: Heterocyclic. Carbocyclic

Recommended books

Warren, S., *Organic Synthesis – The Disconnection Approach*, Wiley 1982. [QD262.W37]

Clayden J., Greeves N., Warren S. and Wothers P. *Organic Chemistry*, OUP, 2001. [QD251.074]

Clayden J., Greeves N. and Warren S. *Organic Chemistry*, 2nd Edn, OUP, 2012. (either edition is fine)
[QD251.074]

A3: High-resolution molecular spectroscopy

Dr James Keeler

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 Franck–Condon principle. Vibrational and rotational fine structure.

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

Recommended books

J M Hollas, *Modern Spectroscopy*, 4th edit (Wiley, 2004). [QC451.H65]

C N Banwell and E M McCash, *Fundamentals of Molecular Spectroscopy*, 4th edit, (McGraw–Hill, 1994).[QD96.M65.B36]

the following texts are for reference.

D A McQuarrie and J D Simon, *Physical Chemistry, a Molecular Approach*, (University Science Books, 1997). [QD453.M37]

J M Hollas, *High Resolution Spectroscopy*, 2nd edit, (Wiley, 1998) [QC454.H618.H65]

P F Bernath, *Spectra of Atoms and Molecules*, (Oxford,1995). [QC454.A8.B47]

P W Atkins and R S Friedman, *Molecular Quantum Mechanics*, 3rd. edit, (Oxford, 1997). [QD462.A85]

A4: Theoretical techniques

Dr Alex Thom

A central goal of theoretical chemistry is the prediction and rationalization of molecular properties and reactivity. Much qualitative insight can be obtained from molecular orbital theory, which you have already encountered in the Part IB Symmetry and Bonding lectures. In this course we expand on this topic introducing some theoretical techniques and ideas, such as perturbation theory, applied to MO calculations, which enable one to extract chemical insight. For more quantitative understanding electronelectron repulsion must be taken into account and we therefore also continue the more rigorous treatment of the Part IB Quantum Mechanics course with a brief introduction of self consistent field (SCF) theory and techniques used in practical calculations of chemical systems as well as empirical techniques for larger systems.

Topics Recap of Hückel theory: symmetry; linear and ring systems; population and bond-order analysis; alternant hydrocarbons; perturbation theory and heteroconjugated systems.
Many-electron wavefunctions: Slater determinants; Hartree-Fock theory of two electron-systems; electron correlation and molecular dissociation; density functional theory.
Empirical descriptions: intermolecular forces; molecular vibrations.
Chemical Reactivity: state and orbital correlation diagrams; the Woodward–Hoffman rules.

Recommended books

Atkins, P.W. and Friedman, R.S., *Molecular Quantum Mechanics*, 3rd edit., OUP, 1997 (other editions are fine) [QD462.A85]
Cotton, F.A., *Chemical Applications of Group Theory*, Wiley, 1990. [QD461.C68]
Leach, A. R., *Molecular Modelling: Principles and Applications*, Prentice Hall, 2001 (Longmans edition of 1996 is acceptable). [QD480.C43]
Stone, A. J., *The Theory of Intermolecular Forces*, OUP. [QD461.S76]

A6: Concepts in physical chemistry

Dr Volker Deringer 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

P W Atkins, *Concepts in Physical Chemistry*, any edition, Oxford University Press. [Not held in the Chemistry library]

A Vincent, *Molecular Symmetry and Group Theory*, 2nd edition, Wiley 2001. [QD461.V56]

B courses

B1: Inorganic II – Transition metal reactivity and organometallic catalysis¹

Dr Nick Bampos: 6 lectures

Inorganic coordination chemistry can be broadly typified by the following types of reactions: substitution chemistry, redox chemistry and photochemistry. We initially focus on the two extrema 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 we consider factors affecting the rate of electron transfer in both inner sphere and outer sphere mechanisms. The last lecture will focus on uni- and biomolecular photochemistry of coordination compounds.

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.

Inner-sphere electron-transfer: rate determining steps.

Uni- and biomolecular photochemistry, photo-induced redox chemistry.

Dr Paul Wood: 6 lectures

In this part of the course we examine the mechanisms of substitution, electron–transfer and photochemical reactions in coordination compounds. In the second half of the course we extend our arguments to 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. The course will also consider several stoichiometric metal-assisted organic transformations and again examine the particular traits of the metal that allow such reactions to occur.

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.

H₂ & HX reactions. Hydrogenation; hydrosilylation; hydrocyanation.

¹This course may be given as two separate six-lecture courses

Alkene reactions. Isomerization; polymerization with heterogeneous and metallocene catalysts; chain-end and ligand control in stereospecific propene polymerizations; late transition metal catalysts; alkene dimerization and trimerization; ethene oligomerization; SHOP process; alkene oxidation.

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

Selective Catalysis. $\alpha\beta$ -unsaturated aldehyde hydrogenation; epoxidation/aziridination with SALEN- & Sharpless-type catalysts.

Modern Hybrid Systems. Examples of single-site heterogeneous catalysts with enhanced turnover rates, product selectivities and recovery.

Recommended books

D. F. Schriver, P. W. Atkins and C. H. Langford, *Inorganic Chemistry*, 2nd Edn., OUP, 1995 [QD151.S57]

I. S. Butler and J. F. Harrod, *Inorganic Chemistry: Principles and Applications*, Benjamin Cummings, 1989. [not held in the Chemistry library]

S. F. A. Kettle, *Inorganic Chemistry: A Coordination Chemistry Approach*, Spektrum, 1996. [QD475.K48]

K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*, Holt & Saunders., 1977. [not held in the Chemistry library]

M. L. Tobe and J. Burgess, *Inorganic Reaction Mechanisms*, Longman, 1999. [QD502.5.T63]

C. Elschenbroich and A. Salzer, *Organometallics*, 2nd Edn, VCH, 1992. [QD411.E47]

R. H. Crabtree. *The Organometallic Chemistry of the Transition Metals*, 3rd Edn, Wiley, New York, 2001. [QD411.8.T73.C73]

G. W. Parshall, *Homogeneous Catalysis*, 2nd Edn, Wiley, New York, 1992. [QD505.P37]

F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, Wiley, New York, 1988. [QD151.C68]

G. O. Spessand, and G. L. Miessler, *Organometallic Chemistry*, Prentice Hall, New Jersey, 1996 [QD411.S64]

B2: Structure and reactivity

Dr Bill Nolan (6 lectures) and Prof. Ian Paterson (6 lectures)

In the first half of this lecture series (Dr Nolan), 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*.

The focus will shift during the second part (Prof. Paterson) to build on last year's work on NMR spectroscopy and on the relationship between molecular geometry and reactivity. It will introduce powerful new methods for structure determination that have revolutionised NMR spectroscopy. These will be applied to problems of conformation and configuration, both in simple ring systems and bicyclic structures.

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.

7–12 NMR Spectroscopy. Pulsed NMR. Chemical exchange. Shift reagents. Nuclear Overhauser effect. Two-dimensional spectra.

Conformational Analysis. Conformation of six-membered rings, including ketones, alkenes and heterocycles. Larger and smaller rings. Fused ring systems including steroids. Cis- and trans-ring-fusion. Axial and planar chirality.

Structure determination. How to determine absolute configuration and enantiomeric excess. Combined use of spectroscopic techniques to determine structure and conformation.

Recommended books

- Kirby, A. J., *Stereoelectronic Effects*, OUP 1996. [QD481.K57]
Moody, C. J. and Whitham, G. H., *Reactive Intermediates*, OUP, 1992. [QD476.M66]
Eliel, E. L., Wilen S.H. and Mander, L.N., *Stereochemistry of Organic Compounds*, Wiley, 2nd Edn. 1994. [QD481.E45]
Fleming, I., *Pericyclic Reactions*, OUP, 1999. [QD281.R5.F54]
Fleming, I., *Frontier Orbitals and Organic Chemical Reactions*, Wiley, 1996. [QD461.F54]
Fleming, I., *Molecular Orbitals and Organic Chemical Reactions*, Wiley, 2009. [QD461.F54]
Clayden, J., Greeves, N., Warren, S. and Wothers, P., *Organic Chemistry*, OUP, 2001. [QD251.074]
Williams, D. H. and Fleming, I. *Spectroscopic methods in Organic Chemistry*, McGraw-Hill, 5th Edn 1995. [QD272.S6.W55]
Sanders, J, K, M. and Hunter, B. K., *Modern NMR Spectroscopy*, OUP, 2nd Edn., 1993 [QD96.N8.S26]

B3: Chemical biology I – Biological catalysis

Dr 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 10^{15} ! 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.

Dr Finian Leeper

Topics Enzyme basics - a reprise (kinetics, free energy profiles, inhibition); carbon-carbon bond forming reactions; the biological Claisen condensation (thioesters, citrate synthase, fatty acid biosynthesis); the biological aldol reaction (Schiff base, aldolase, acetoacetate decarboxylase); elimination reactions (dehydroquinase, enolase, dehydroquinone synthase, PAL); One carbon transfer reactions (THF, KPHMT, SAM, chiral methyl groups, thymidylate synthase); phosphoryl transfer (tyrosyl t-RNA synthetase, ribonuclease, phosphatases, kinases); metal ion activation of substrates.

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

- T D H Bugg, *An Introduction to Enzyme and Coenzyme Chemistry* Blackwell Science 2004. [QP601.B84]

The following texts are for reference

R B Silverman, *Organic Chemistry of Enzyme-Catalysed Reactions* Academic Press 2002.

[QP601.S55]

R B Silverman, *The Organic Chemistry of Drug Design and Drug Action* Academic Press 1992.

[RS403.S58]

A Fersht, *Structure and Mechanism in Protein Science*, Freeman 1999 [QD431.25.F47]

B4: Chemistry in the atmosphere

*Dr Paul Griffiths (5 lectures), Dr Alex Archibald (5 lectures)
and Dr Anja Schmidt (2 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 NO_x, HOX, ClO_x.

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 be discussed. Sources, formation processes and chemical composition of tropospheric aerosol particles.

Measurements of atmospheric composition and their applications. Remote sensing. Raman 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

Chemistry of atmospheres, Wayne, R P, OUP [QC879.6.W39]

Further reading/reference:

Atmospheric change – an earth system perspective, Graedel, T and Crutzen, P Freeman and Co, NY [QC981.8.G73]

The physics of atmospheres, Houghton, J T, OUP [QC880.H68]

Chemistry of the upper and lower atmospheres, Finlayson-Pitts and Pitts, Academic Press [QC879.6.F56]

Aeronomy of the middle atmosphere, Solomon and Brasseur, Reidel [QC881.2.M53.B73]

Reaction kinetics, Pilling and Seakins, OUP [QD502.P55]

B5: Biomaterials

Dr Silvia Vignolini (6 lectures) and Prof. Melinda Duer (6 lectures)

The first six lectures will cover the chemistry of biopolymers in the natural world, starting from the properties of polysaccharides to the most recent application of such materials in research and industry.

Leading on from this, the second half of the course considers how biological materials, such as bone, hair, skin etc. present an opportunity to learn from Nature how to build functional materials

that have different functions on different lengthscales. For instance, on a macroscopic lengthscale, bone provides structural support whilst on a nanoscopic lengthscale, it provides a home for cells and on an even smaller lengthscale, the molecules that make up the tissue are key in providing a communication system between 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. We will study these materials to gain perspective on how they perform their various material roles. Dealing with complex materials like these however means that we have to investigate different ways of examining their structure from the more conventional diffraction techniques. Thus this part of the course will begin with an overview of solid-state NMR and how it can be applied to determine molecular structures, then lead on to a detailed examination of keratin tissues (hair, nails etc.), and collagenous tissues (bone, tendon, skin, muscle, etc), to focus throughout being on understanding how the underlying molecular structures and dynamics lead to the required material properties.

- 1–2 Polysaccharides, their properties and production in nature, chemical and structural properties of cellulose, chitin, lignin and other natural polymers
- 3–4 Mechanical properties of cellulose and chitin and their role in living systems
- 5–6 Nano-cellulose and applications and their use in bio-materials
- 7–8 Solid-state NMR spectroscopy; applications to studying molecular structure and dynamics.
- 9–10 Keratin ('dead') tissues; basic protein structures, primary and secondary structures. Composite structure of keratin tissues. The importance of fibril structures for mechanical strength; the role of the α -helix protein structure in mechanical properties
- 11–12 Collagen tissues; their composite structure, and self-assembly of collagen fibrils; the role of proteoglycans in organizing collagen fibrils. Mineralization of collagen matrices.

Recommended books

Basic Solid State Chemistry, A R West, John Wiley and Sons Ltd. (2nd Edition) [QD478.W47]
Molecular Crystals, J D Wright, Cambridge University Press. (1st or 2nd Edition). [QD291.W75]
Reactions and Characterisation of Solids, S E Dann, RSC, Tutorial Chemistry Texts. [QD478.D36]
Structural Biomaterials, Julian Vincent, Princeton University Press, 1990. [QP801.B69.V56]
Biomaterialization, S. Mann, Oxford Chemistry Masters, OUP, 2001. [QH512.M36]
Organic Molecular Solids: Properties and Applications, Edited by W Jones, CRC Press.[TA418.9.C7.074]
An Introduction to Solid-State NMR, M.J. Duer, Blackwell Science Ltd, 2004. [QD96.N8.D84]
Core Concepts in Supramolecular Chemistry and Nanochemistry, J. W. Steed, D. R. Turner & K.J. Wallace. Wiley, 2007. [QD878.S74]

B6: Statistical mechanics

Dr Aleks Reinhardt (6 lectures) and Prof. Daan Frenkel (6 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 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

K. A. Dill and S. Bromberg, *Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience*, Garland Science, 2010. [QC311.5.D55]

D. A. McQuarrie, *Statistical Mechanics*, University Science Books, 2000. [QC174.8.M37]

For reference:

D. Chandler, *Introduction to Modern Statistical Mechanics*, Oxford University Press, 1987. [QC174.8.C43]

N. R. Davidson, *Statistical Mechanics*, Dover, 2003. [QC174.8.D38]

K. Huang, *Statistical Mechanics*, Wiley, 1987. [QC174.8.H83]

L. D. Landau and E. M. Lifshitz, *Statistical Physics: Part 1*, Butterworth–Heinemann, 1980. [QC174.8.L36]

J. P. Sethna, *Statistical Mechanics: Entropy, Order Parameters, and Complexity*, Oxford University Press, 2006.

ON ORDER but available online at

pages.physics.cornell.edu/~sethna/StatMech/EntropyOrderParametersComplexity.pdf

B7: Further quantum mechanics

Dr Aleks Reinhardt (6 lectures)

In this course, we will continue to explore some 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 discuss time dependence in quantum mechanics more generally, and 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, and we will in particular touch upon how lasers work, what dispersion and induction forces really are, how selection rules arise in spectroscopy, and how ultrafast femtochemistry can be used to investigate reaction mechanisms at the level of individual molecules.

Topics Non-degenerate perturbation theory. The Hellmann–Feynman theorem. Polarisability of the hydrogen atom. Rayleigh–Schrödinger perturbation theory. Linear operators and Dirac notation. Creation and annihilation operators. Anharmonic vibrations. The helium atom: shielding and penetration. Variation perturbation theory. Degenerate and nearly degenerate

perturbation theory. The linear Stark effect. Fermi resonance for CO₂ and the CO₂-N₂ laser. Time dependence in quantum mechanics. Non-stationary states and wave packets. The Ehrenfest theorem, symmetries and conservation laws. Variation of constants and time-dependent perturbation theory. Transition probabilities. Fermi's golden rule. Dynamic polarisabilities. The closure approximation. Dispersion and induction forces. The London formula.

Recommended books

P. W. Atkins and R. S. Friedman, *Molecular Quantum Mechanics*, Oxford University Press, 2010. [QD462.A85]

for reference:

C. Cohen-Tannoudji, B. Diu and F. Laloë, *Quantum Mechanics*, Wiley, 1977. [QC174.12.C64]

N. J. B. Green, *Quantum Mechanics 2: The Toolkit*, Oxford Chemistry Primer 65, Oxford University Press, 1998. [QC174.12.G74]

C. S. Johnson Jr and L. G. Pedersen, *Problems and Solutions in Quantum Chemistry and Physics*, Dover, 1986. [QD462.J64]

A. J. Stone, *The Theory of Intermolecular Forces*, Oxford University Press, 2013. [QD461.S76]

C courses

C1: Electrochemistry

Prof. Erwin Reisner: 6 lectures

The lectures will give an introduction to electrochemistry and its use to study inorganic redox processes in solution and the solid state.

Topics Overview of electrode processes. Potentials and thermodynamics of cells. Kinetics of electrode reactions. Techniques: Cyclic voltammetry, Film voltammetry, Chrono-amperometry, spectroelectrochemistry. Applications: Electrode reactions with coupled homogeneous chemical reactions, Protein film voltammetry.

Recommended books

Electrochemical Methods, Fundamentals and Applications, 2nd Edition A. J. Bard and L. R. Faulkner, Wiley, 2001. [QD553.B37]

Understanding Voltammetry, 2nd Edition. R. G. Compton, C. E. Banks, ICP, 2011. [QD116.V64.C66]

Inorganic Electrochemistry, Theory, Practice and Application, 2nd Edition P. Zanello, F. Fabrizi de Biani, C. Nervi, RSC Publ., 2012. [QD553.Z36]

Electrode Dynamics. A. C. Fisher, Oxford Chemistry Primers, 1996. [QD571.F57]

C2: Electron paramagnetic resonance (EPR) and magnetism

Prof. Clare Grey: 6 lectures

These lectures examine a technique that is used to characterize the electronic structure of a paramagnetic complex, namely EPR spectroscopy. Magnetic responses of (isolated) paramagnetic molecules are briefly reviewed.

Topics Paramagnetism and diamagnetism: Spin (*S*), orbital (*L*) and total angular momentum (*J*) contributions to magnetism.
Magnetism of the free ion: Term symbols and magnetism of the lanthanides.
Quenching of orbital angular momentum; Term symbols for common Oh and Td complexes; the Van Vleck formula and spin-only magnetic moment for d-block metals.
Basics of EPR spectroscopy focusing on $S = \frac{1}{2}$ systems: electron-Zeeman, nuclear-Zeeman interactions and electron- nuclear interactions.

The g-value and hyperfine coupling.
Sources of g anisotropy.
Information that can be extracted from EPR spectra: localized and delocalized magnetic orbitals; spin-polarisation.

Recommended books

Magnetochemistry, A. F. Orchard, Oxford Chemistry Primers, 2003. [QD596.073]
Introduction to Magnetic Resonance, A. Carrington and A. D. McLachlan, Harper International Edition, 1967. [QD471.C37]
Chemical and Biochemical Aspects of Electron Spin Resonance Spectroscopy, M. Symons, Van Nostrand Reinhold Co. Ltd, 1978. [QD96.E4.S96]
General Inorganic text books such as: *Inorganic Chemistry*, Shriver and Atkins [QD151.S57], *Inorganic Chemistry: Principles of Structure and Reactivity*, Huheey, Keiter and Keiter [QD151.H84] and *Chemical Applications of Group Theory*, Cotton. [QD461.C68]

C3: NMR

Dr Daniel Beauregard (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 ^{13}C 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

NMR Spectroscopy in Inorganic Chemistry J.A. Iggó, Oxford University Press, 2000. [QD96.N8.I34]

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

Dr Priyanka Joshi (6 lectures) and Prof. Sophie Jackson (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 and computational 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

- A. R. Fersht, *Structure and Mechanism in Protein Science*, Freeman. [QD431.25.F47]
T. Creighton, *Proteins: Structures and Molecular Properties*, Freeman. [QP551.C74]
S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books. [QP531.L57]
T. D. H. Bugg, *An introduction to Enzyme and Coenzyme Chemistry*, Blackwell Science. [QP601.B84]

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.

Recommended books

- Clayden, J., Greeves, N., Warren, S. and Wothers, P., *Organic Chemistry*, OUP 1st Edn, 2000 or 2nd Edn, 2012. [QD251.074]

C6: Diffraction methods in chemistry

Dr Andrew Bond

This course provides the background knowledge for the main use of diffraction methods in chemistry, namely the solution of structures by single-crystal x-ray diffraction. It is not intended to be a course in formal crystallography, and no prior knowledge is assumed, but instead it illustrates the basic principles of diffraction, the fundamental relationship between diffracted x-ray amplitudes and the crystal structure, and the problems arising from the measurement of x-ray intensities rather than amplitudes, together with the manner in which these may be circumvented.

All the main methods of structure determination will be dealt with, ranging from the relatively simple approach used in structures containing heavy atoms, through the so-called 'Direct Methods' used for medium sized molecules in Organic and Inorganic Chemistry, to the advanced isomorphous replacement methods used in the determination of protein structures. In all these cases the aim is to provide, via selected worked examples, the underlying principles behind the techniques.

The course concludes with an introduction to methods of crystal structure refinement, an assessment of what constitutes a 'correct' structure, and an outline of some of the additional information which may be gained from the use of neutron diffraction.

Recommended books

- Dunitz, J.D., *X-ray Analysis and the Structure of Inorganic Solids*, Cornell Univ. Press. [QD945.D86]
Guinier, A., *X-ray Diffraction*, W.H. Freeman and Co. [QD945.G85]
Cowley, J.M., *Diffraction Physics*, North Holland Publishers. [QC415.C69]
Giacovazzo, C., *Fundamentals of Crystallography*, O.U.P. [QD905.2.F86]
Woolfson, M.M., *X-ray Crystallography*, C.U.P. [QD945.W66]
Stout, G.H. and Jensen, L.H., *X-ray Structure Determination – A Practical Guide*, John Wiley & Sons. [QD495.S76]

C7: Investigating organic mechanisms

Dr Peter Wothers

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.

Recommended books

Organic and Bio-organic Mechanisms, M. Page and A. Williams, Longman, 1997. [QD502.P34]
Structure and Reactivity in Organic Chemistry, Howard Maskill, Oxford Chemistry Primer 81, 1999. [QD476.M37]
Modern Physical Organic Chemistry, E. V. Anslyn and D. A. Dougherty, University Science Books, 2004. [QD476.A57]

C8: Electronic structure

Prof. Michael Sprik

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. Two varieties of SCF theory exist: wavefunction-based methods based on Hartree–Fock and density-functional methods. The former provides the traditional starting point to more systematic theories of electron correlation, and is the bedrock of quantum chemistry. The latter have proven a highly popular and efficient alternative to Hartree–Fock, but unlike Hartree–Fock, still account for electron correlation in an approximate way. Both topics will be covered.

Topics Basis functions, hydrogenic (Slater) orbitals, atomic orbitals, Gaussian functions, and contracted functions; the secular equations from which orbitals are determined; self-consistent field theory, and its numerical implementation; beyond Hartree–Fock, electron correlation; the energy functional, the importance of electron density, Hohenberg–Kohn theorems; The Kohn–Sham equations and orbitals; comparison with Hartree–Fock theory; the exchange correlation functional; electronic structure calculations as research tool.

Recommended books

A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry*, 2000, Dover publications. [QD462.S93]
W. Koch and M. C. Holthausen, *A Chemist's Guide to Density Functional Theory*, 2001, Wiley-VCH. [QD472.6.D45.K63]

C9: Chemical biology III – Nucleic acids

Dr Gonçalo Bernardes (4 lectures), Prof. Jason Chin (4 lectures) and Prof. Sir Shankar Balasubramanian (4 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 Nucleic acids analogues as therapeutics; 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 transactions (e.g. synthesis, cleavage and repair); the chemistry of DNA sequencing; and nucleic acids-based molecular medicine.

- 1 (GB) Introduction to nucleic acids
- 2 (GB) Chemical synthesis of nucleic acids
- 3 (GB) Chemical analogues of DNA/RNA therapeutics
- 4 (GB) Recognition of DNA by synthetic organic molecules
- 5 (JC) RNA secondary structure and protein recognition
- 6 (JC) Chemical and enzymatic cleavage of nucleic acids
- 7 (JC) RNA enzymes
- 8 (JC) Ribosomes and translation
- 9 (SB) Chemical reactions on DNA, DNA damage and repair
- 10 (SB) Enzymatic synthesis of DNA – Polymerases
- 11 (SB) DNA replication and medicinal chemistry
- 12 (SB) Chemistry of DNA sequencing

Recommended books

Eds G. M. Blackburn, M. J. Gait, D. Loakes and D. M. Williams, *Nucleic Acids in Chemistry and Biology*, 3rd edition, RSC Publishing Cambridge, 2006. [QD433.N83]

R. B. Silverman, *The Organic Chemistry of Drug Design and Drug Action*, 2nd edition, Elsevier Academic Press 2004. [RS403.S58]

C10: Surfaces and interfaces

Dr Israel Temprano (4 lectures), Dr Stephen Jenkins (4 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

G. Attard and C. Barnes, *Surfaces*, Oxford Chemistry Primer No 59, Oxford Science Publications, 1998. [QD506.A88]

E. M. McCash, *Surface Chemistry*, Oxford University Press, 2001. [QD506.M33]

K. W. Kolasinski, *Surface Science*, Wiley, 2002. [QD506.K65]

P. W. Atkins, *Physical Chemistry*, Oxford University Press, 7th Ed, 2001. [QD453.A85]

J. B. Hudson, *Surface Science: An Introduction*, Wiley, 1998 (reference). [QC173.4.S94.H83]

A. W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces*, Wiley, 1997 (reference). [QD506.A33]

C11: 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.

Recommended books

A. Vincent, *Molecular Symmetry and Group Theory*, Wiley. [QD461.V56]

A. Cotton, *Chemical Applications of Group Theory*, Wiley (The first edition is not recommended as it contains many errors.) [QD461.C68]

P. W. Atkins, *Molecular Quantum Mechanics*, OUP. [QD462.A85]

J. W. Leech and D. J. Newman, *How to use Groups*, Methuen. [QC174.5.L44]

J. P. Elliott and P. G. Dawber, *Symmetry in Physics*, vol. 1, Macmillan. [not held in the Chemistry library]

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

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 two exercises associated with the *Chemical Informatics* course.
- Five additional credits.

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

- Extended experiments offered at the end of each of the core practical courses; you will be able to gain **up to five** 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 |
|---|-----------------|
| <i>Techniques in Modern Synthetic Chemistry</i> (core practical course) | 30 |
| <i>Physical & Theoretical Chemistry</i> (core practical course) | 30 |
| Informatics | 7.5 |
| Each additional credit | 6.5 |

Students may complete more additional credits than the minimum, in which case the five 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

The class will be divided into two equal groups.

Group 1 will follow the core course *Techniques in Modern Synthetic Chemistry* in the Michaelmas term, and the *Physical & Theoretical Chemistry* core course in the Lent Term.

Group 2 will follow the *Physical & Theoretical Chemistry* core course in the Michaelmas term, and the *Techniques in Modern Synthetic Chemistry* core course in the Lent Term.

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.

Due to restriction on the number of computers and apparatus available, the *Physical & Theoretical Chemistry* core course is timetabled rigidly. You must work on the days allocated to you when you register at the start of Term. As in Part IB, your practical write-ups will be assessed in the class by one of the Senior Demonstrators.

Extended experiments

Extended Physical and Theoretical experiments will be available throughout both the Michaelmas and Lent Terms. Students in either Group may attempt these once they have completed the *Physical & Theoretical Chemistry* core course.

Extended experiments associated with the *Techniques in Modern Synthetic Chemistry* course can *only* be undertaken in the Michaelmas Term for students in Group 1 and in the Lent term for students in Group 2.

6.4 Techniques in modern synthetic chemistry

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 There will be 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. For Group 1 the Induction Day will commence at 11:15 on Thursday 5th October. For Group 2 the Induction Day will commence at 14:00 on Thursday 18th January.

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 charge of the class is Mykola Karabyn and he is assisted by Maria Cascone. The members of staff responsible are Dr Sally Boss, Dr Deborah Longbottom and Dr Bill Nolan.

6.5 Joint Physical & Theoretical chemistry course

Physical chemistry experiments

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 technician in charge of the class is Chris Brackstone. The member of staff responsible is Dr Peter Wothers.

Theoretical chemistry exercises

Location Room G30 (MCS), 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 Andreas Bender (ab454@cam.ac.uk).

6.6 Chemical Informatics (Michaelmas Term)

This part of the course consists of four lectures; you will be required to complete two assessed exercises. Further details will be given out in the first lecture.

Lectures 1 & 2: 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, SciFinder, Reaxys (Beilstein), CSD, ChemSpider, National Chemistry Database Service etc.). The problems and challenges of finding and analysing chemical information will be discussed.

Lectures 3 & 4: Computer representation of molecules and molecular data analysis

Prof. Robert Glen

How can large collections of molecules be described and analysed? Is it possible to design a new molecule with specific physical or biological properties? Some methods of representing molecules in computers will be described, showing how different approaches are best for different contexts. Molecular data can be generated and analysed from these molecular representations. Methods of property generation and analysis will be described.

6.7 Language option (Michaelmas and Lent Terms)

There are around twenty places on offer to study Chinese, French, German, Japanese or Spanish in the Department of Engineering's excellent Language Unit:

www.eng.cam.ac.uk/teaching/language

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 lecturers (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 3rd October (in the Unilever 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 4th 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 morning.

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 will be done will be announced in the introductory lecture. Classes will commence in Week 2, starting Thursday 12th 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 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.

If you are thinking of taking the programming option it will make sense to be in Group 1 so that the skills you learn can be used to complete some of the optional Theoretical exercises offered in the Lent Term.

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 (mv245@cam.ac.uk) and Dr Robert Jack (rlj22@cam.ac.uk) will lead the course: please address any questions you have to them. 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) 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 you must hand in a folder containing all 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.cam.ac.uk/plagiarism. 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

The format of all the Papers have been changed for 2017/18. The details given here are subject to final confirmation.

Paper 1 Duration 2 hours 40 minutes. There will be two sections and candidates must answer all the questions in each section. Section A will contain four 30 minute questions: two relating to A1, two relating to A2. Section B will contain 4 5 minute questions relating to A1, and 4 5 minute questions relating to A2. Candidates should allocate 2 hours to Section A, and 40 minutes to Section B.

Paper 2A Duration 2 hours 40 minutes. There will be two sections and candidates must answer all the questions in each section. Section A will contain four 30 minute questions: two relating to A3, two relating to A4. Section B will contain 4 5 minute questions relating to A3, and 4 5 minute questions relating to A4. Candidates should allocate 2 hours to Section A, and 40 minutes to Section B.

Paper 2B Duration 2 hours 40 minutes. There will be two sections and candidates must answer all the questions in each section. Section A will contain four 30 minute questions relating to A6. Section B will contain 8 5 minute questions relating to A6. Candidates should allocate 2 hours to Section A, and 40 minutes to Section B.

Paper 3 Duration 3 hours. This paper will contain questions relating to the B courses. There will be two 45 minute questions from each 12 lecture B course and one 45 minute question from each 6 lecture B course; candidates should answer four questions, without restriction.

Paper 4 Duration 3 hours. This paper will contain questions relating to the C courses. There will be two 45 minute questions from each 12 lecture C course and one 45 minute question from each 6 lecture C course; candidates should answer four questions, without restriction.

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 be scheduled as follows: Paper 1 Monday 4th June, Papers 2A & 2B Tuesday 5th June, Paper 3 Thursday 7th June, and Paper 4 Friday 8th June, all at 09:00 apart from Papers 2A & 2B which are likely to be at 13:30. You will be given an extra 10 minutes of reading time for all of these papers.

We also expect that oral examinations, if required, will be held in the late morning of Tuesday 19th June, and that the results will be available in CamSIS on the afternoon of Wednesday 20th June. You must be in Cambridge and available for an oral examination on the day announced.

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* (www.vle.cam.ac.uk), 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 James Keeler.

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. However, the final allocation of a class will not simply be done by a mechanical process. Rather, the Examiners will consider each candidate's mark profile and will give particularly careful consideration to candidates who fall on class boundaries or for whom there is a large discrepancy between their Part II and Part III marks.

10

Admission to Part III Chemistry for the academic year 2018/19

The minimum standard required for entry to Part III in 2018/19 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 University Applications Committee 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 two 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: www.vle.cam.ac.uk. If you find that you do not have access to the Chemistry part of Moodle, please email the Teaching Office on teaching@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 and the composition of the committee can be found on the teaching website

www.ch.cam.ac.uk/teaching/student-consultative-committee

14

Library, photocopying and computing

www-library.ch.cam.ac.uk

The Departmental Library, which is located in the Centre for Molecular Informatics (linked to the main building), is available for you to use when the department is open. You will need your University Card to gain access to the library. Evening and weekend library access is available to Part II Chemistry students. Please ask your Director of Studies to apply in advance on your behalf, specifically confirming your status as a Part II Chemistry student, in an email to cmi-admin@ch.cam.ac.uk. Eligibility for access to the Library and details of borrowing rights can be found on this website: www-library.ch.cam.ac.uk/access-library. Extended library access is available to Part II Chemistry students: the details of how this can be applied for are given in Section 15 below. It is forbidden to bring food into the Library. The only drink permitted in the Library is water in a container with a non-spill cap.

The *Blue Book* collection of core texts is shelved in Unit 17, on the right hand side as you enter the library. Most of this collection is for short loan (three days) or for reference only. The rest of the book collection is shelved on the wall to the left and on the shelves behind the periodical display. All Chemistry books are listed on iDiscover, www.idiscover.lib.cam.ac.uk, the online catalogue for the libraries of the University. There is a dedicated computer in the library for searching the catalogue.

Short undergraduate induction sessions are held in October and you are welcome to attend. These sessions will be advertised by email. Part II students may borrow from the library and should call in to the library office to set up a borrowing account on the automated system.

If you would like to recommend any resources, make suggestions or discuss anything related to the Library, please contact the student representative on the Committee for the Library and Scholarly Communication (web address below) or email the Library directly on library@ch.cam.ac.uk.

www-library.ch.cam.ac.uk/committee-library-and-scholarly-communication

Photocopying, printing, scanning, and computing facilities

The library has 20 PCs and 2 Macs which are hosted on the MCS (Managed Cluster Service) network and 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, as well as photocopying and free scanning. Online payment for printing and photocopying on this machine is made through the *common balance* scheme, there is more information at

www.ucs.cam.ac.uk/desktop-services/ds-print/paying-for-ds-print

There is also a traditional photocopier by the lift on the second floor of the Lensfield Road side of the Department and photocopy cards for this machine can be purchased from the Library Office. Computers and MFDs which are also attached to the MCS network are available in room G30 (by the lift on the Lensfield Rd side of the building), and in the Part IB/II Physical Chemistry Laboratory. When practicals are being run, access to the computers in G30 and the Physical Lab. may be restricted.

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, please contact Susan Begg (smb28@cam.ac.uk) straight away so she can make authorised changes.

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 only give you access to the building from 09:00–20:00 on weekdays, and from 09:00–13:00 on Saturdays. Outside these times you are not permitted to be in the Department unless some specific arrangement has been made. If you remain in the Department after 20:00 you risk becoming trapped by the security doors and/or the turnstiles. Should this happen use one of the emergency red telephones and contact 36330 or Central Security on 101 to let them know where you are.

If you would like access to the Departmental library outside normal working hours you will need to go and see Susan Begg to arrange this (her office is on the ground floor of the Centre for Molecular Informatics building, Room UG05, next to the Unilever Lecture Theatre). She will ask you to sign the following declaration before enabling your card.

I understand that my security access is being increased to allow entry to the Department of Chemistry via the main entrance, to enable me to use the library after 20:00 Monday to Friday and during weekends.

I hereby confirm that I will not contravene the rules laid down in the Department Safety Handbook, and will not undertake any work in any laboratory. I will sign in and out in the book at the front entrance when I am here after 18:00 weekdays or at anytime over the weekend. I am aware that I cannot be in any part of the building after midnight. I accept that the privilege will be withdrawn if I am found to have breached this agreement.

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 15:45; you may also use the room outside these hours. Hot and cold drinks, as well as a selection of snack foods are available. At busy times, please make sure that you are not occupying too much space i.e. by spreading out all your books and papers.

Part II students may also use the small common room located in the centre of the Organic and Inorganic Part II Laboratory at any time that the lab. is open. The room is set out with tables and food may be eaten there. Facilities are provided for making tea and coffee.

Part II Chemistry 2017/2018: Titles of lecture courses

| Code | Hours | Title | Lecturer(s) |
|---|-------|---|---|
| A courses | | | |
| A1 | 12 | <i>Inorganic I</i> : Structure and bonding | Boss (5), Duer (4), Beauregard (3) |
| A2 | 12 | The foundations of organic synthesis | Nolan |
| A3 | 12 | High resolution molecular spectroscopy | Keeler |
| A4 | 12 | Theoretical techniques | Thom |
| A6 | 12 | Concepts in physical chemistry | Deringer, Truscott |
| B courses | | | |
| B1 | 12 | <i>Inorganic II</i> : Transition metal reactivity and organometallic catalysis | Bamos (6), Wood (6) |
| B2 | 12 | Structure and reactivity | Nolan (6), Paterson (6) |
| B3 | 12 | <i>Chemical biology I</i> : Biological catalysis | Leeper (6), Spring (6) |
| B4 | 12 | Chemistry in the atmosphere | Griffiths (5), Archibald (5), Schmidt (2) |
| B5 | 12 | Biomaterials | Vignolini (6), Duer (6) |
| B6 | 12 | Statistical mechanics | Reinhardt (6), Frenkel (6) |
| B7 | 6 | Further quantum mechanics | Reinhardt (6) |
| C courses | | | |
| <i>Inorganic III, characterisation methods:</i> | | | |
| C1 | 6 | Electrochemistry | Reisner (6) |
| C2 | 6 | Electron paramagnetic resonance (EPR) and magnetism | Grey (6) |
| C3 | 6 | NMR | Beauregard (6) |
| C4 | 12 | <i>Chemical biology II</i> : Proteins: structure, stability, and folding | Joshi (6), Jackson (6) |
| C5 | 12 | Control in organic chemistry | Goodman (6), Spring (6) |
| C6 | 12 | Diffraction methods in chemistry | Bond |
| C7 | 12 | Investigating organic mechanisms | Wothers |
| C8 | 12 | Electronic structure | Sprik |
| C9 | 12 | <i>Chemical biology III</i> : Nucleic acids | Bernardes (4), Chin (4), Balasubramanian (4) |
| C10 | 12 | Surfaces and interfaces | Temprano(4), Jenkins (4), Madden (4) |
| C11 | 6 | Symmetry | Alavi (6) |
| Other | | | |
| CI | 6 | Chemical informatics | Goodman (3), Glen (3) |
| MM | 12 | Mathematical Methods | Vendruscolo, Jack |

Part II Chemistry : Michaelmas Term 2017

| Week | Date | Day | 9 | 10 | 11 | 12 | Courses | Other activities / comments |
|------|-------|-----|-------|-------|----|----|-----------------------------|--|
| 0 | 3/10 | Tu | | | | | | Lang. Intro. 14:00 (ULT) Introductory Lect. 12:00 (BMS) |
| | 4/10 | We | | | | | | |
| 1 | 5/10 | Th | A3/A6 | A4/A6 | | | A1 A2 A3 A4 A6* | 11:15 Group 1 induction |
| | 6/10 | Fr | A1 | A2 | | | | |
| | 9/10 | Mo | A1 | | | | | |
| | 10/10 | Tu | A3/A6 | A4/A6 | | | | |
| | 11/10 | We | A1 | A2 | | | | |
| 2 | 12/10 | Th | A3/A6 | A4/A6 | | | | Language courses start |
| | 13/10 | Fr | A1 | A2 | | | | |
| | 16/10 | Mo | A1 | A2 | | | | |
| | 17/10 | Tu | A3/A6 | A4/A6 | | | | |
| | 18/10 | We | A1 | A2 | | | | |
| 3 | 19/10 | Th | A3/A6 | A4/A6 | | | | |
| | 20/10 | Fr | A1 | A2 | | | | |
| | 23/10 | Mo | A3/A6 | A2 | | | | |
| | 24/10 | Tu | A3/A6 | A4/A6 | | | | |
| | 25/10 | We | A1 | A2 | | | | |
| 4 | 26/10 | Th | A3/A6 | A4/A6 | | | | |
| | 27/10 | Fr | A3/A6 | A2 | | | | |
| | 30/10 | Mo | A1 | A4/A6 | | | | |
| | 31/10 | Tu | A3/A6 | A4/A6 | | | | |
| | 1/11 | We | A1 | A2 | A3 | | | |
| 5 | 2/11 | Th | A6 | A4/A6 | | | | |
| | 3/11 | Fr | | A2 | | | | |
| | 6/11 | Mo | A1 | A4/A6 | | | | |
| | 7/11 | Tu | A3/A6 | A4/A6 | | | | |
| | 8/11 | We | A1 | A2 | | | | |
| 6 | 9/11 | Th | B1 | B5 | | | | |
| | 10/11 | Fr | B3 | B2 | B4 | CI | | |
| | 13/11 | Mo | B1 | B2 | B6 | | | |
| | 14/11 | Tu | B3 | B5 | | CI | | |
| | 15/11 | We | B4 | B6 | | | | |
| 7 | 16/11 | Th | B1 | B5 | | CI | | |
| | 17/11 | Fr | B3 | B2 | B4 | | | |
| | 20/11 | Mo | B1 | B2 | B6 | | | |
| | 21/11 | Tu | B3 | B5 | | CI | | |
| | 22/11 | We | B4 | B6 | | | | |
| 8 | 23/11 | Th | B1 | B5 | | CI | | |
| | 24/11 | Fr | B3 | B2 | B4 | | | |
| | 27/11 | Mo | B1 | B2 | B6 | | | |
| | 28/11 | Tu | B3 | B5 | | CI | | |
| | 29/11 | We | B4 | B6 | | | | |

*A6 is given in the Todd-Hamied room

All lectures are held in the Pfizer Lecture Theatre unless otherwise stated

Part II Chemistry : Lent Term 2018

| Week | Date | Day | 9 | 10 | 11 | 12 | Courses | Other activities / comments |
|------|------|-----|----|-----|-----|-----|---------|-----------------------------|
| 1 | 18/1 | Th | B1 | B5 | | | | 14:00 Group 2 induction |
| | 19/1 | Fr | B3 | B2 | B4 | | | |
| | 22/1 | Mo | B1 | B2 | B6 | | | |
| | 23/1 | Tu | B3 | B5 | | | | |
| | 24/1 | We | B4 | B6 | | | | |
| 2 | 25/1 | Th | B1 | B5 | | | | |
| | 26/1 | Fr | B3 | B2 | B4 | | | |
| | 29/1 | Mo | B1 | B2 | B6 | | | |
| | 30/1 | Tu | B3 | | | | | |
| | 31/1 | We | B4 | B6 | | | | |
| 3 | 1/2 | Th | B1 | | | | | |
| | 2/2 | Fr | B3 | B2 | B4 | | | |
| | 5/2 | Mo | B1 | B2 | B7 | | | |
| | 6/2 | Tu | B3 | B5 | | | | |
| | 7/2 | We | B4 | B7 | C1 | | | |
| 4 | 8/2 | Th | C1 | C10 | B5 | | | |
| | 9/2 | Fr | C4 | C5 | C10 | | | |
| | 12/2 | Mo | | C5 | B6 | | | |
| | 13/2 | Tu | C4 | C8 | C10 | B5 | | |
| | 14/2 | We | C4 | B6 | C5 | | | |
| 5 | 15/2 | Th | | C6 | C7 | | | |
| | 16/2 | Fr | C4 | C5 | C8 | C10 | | |
| | 19/2 | Mo | C1 | C5 | B7 | C10 | | |
| | 20/2 | Tu | C4 | C6 | C7 | C9 | | |
| | 21/2 | We | C4 | B7 | C5 | C9 | | |
| 6 | 22/2 | Th | C1 | C6 | C7 | C9 | | |
| | 23/2 | Fr | C4 | C5 | C8 | C10 | | |
| | 26/2 | Mo | C1 | C5 | B7 | C10 | | |
| | 27/2 | Tu | C4 | C6 | C7 | C9 | | |
| | 28/2 | We | C1 | B7 | C8 | C10 | | |
| 7 | 1/3 | Th | C4 | C6 | C7 | C9 | | |
| | 2/3 | Fr | C2 | C5 | C8 | C10 | | |
| | 5/3 | Mo | C2 | C4 | C11 | C10 | | |
| | 6/3 | Tu | C2 | C5 | C7 | C9 | | |
| | 7/3 | We | C6 | C11 | C8 | C10 | | |
| 8 | 8/3 | Th | C2 | C6 | C7 | C9 | | |
| | 9/3 | Fr | | C5 | C8 | C10 | | |
| | 12/3 | Mo | C2 | C4 | C11 | | | |
| | 13/3 | Tu | C2 | C5 | C7 | C9 | | |
| | 14/3 | We | C4 | C11 | C6 | C8 | | |

All lectures are held in the Pfizer Lecture Theatre unless otherwise stated

Part II Chemistry : Easter Term 2018

| Week | Date | Day | 9 | 10 | 11 | 12 | Courses | Other activities / comments |
|------|------|-----|----|-----|-----|----|---------|--|
| 1 | 26/4 | Th | | C6 | C7 | | | |
| | 27/4 | Fr | C3 | C8 | C9 | | | |
| | 30/4 | Mo | C3 | C8 | C11 | | | |
| | 1/5 | Tu | | C6 | C7 | | | |
| | 2/5 | We | C3 | C11 | C9 | | | |
| 2 | 3/5 | Th | | C6 | C7 | | | |
| | 4/5 | Fr | C3 | C8 | C9 | | | |
| | 7/5 | Mo | | C8 | | | | |
| | 8/5 | Tu | C3 | C6 | C7 | | | |
| | 9/5 | We | C3 | | C9 | | | |
| 3 | 10/5 | Th | | | | | | ‡Revision lecture (SRB) |
| | 11/5 | Fr | | A1‡ | | | | |
| | 14/5 | Mo | | | | | | |
| | 15/5 | Tu | | | | | | |
| | 16/5 | We | | | | | | |
| 4 | 17/5 | Th | | | | | | |
| | 18/5 | Fr | | | | | | |
| | 21/5 | Mo | | | | | | |
| | 22/5 | Tu | | | | | | |
| | 23/5 | We | | | | | | |
| 5 | 24/5 | Th | | | | | | |
| | 25/5 | Fr | | | | | | |
| | 28/5 | Mo | | | | | | |
| | 29/5 | Tu | | | | | | |
| | 30/5 | We | | | | | | |
| 6 | 31/5 | Th | | | | | | Paper 1* Paper 2A/2B* |
| | 1/6 | Fr | | | | | | |
| | 4/6 | Mo | | | | | | |
| | 5/6 | Tu | | | | | | |
| | 6/6 | We | | | | | | |
| 7 | 7/6 | Th | | | | | | Paper 3* Paper 4* |
| | 8/6 | Fr | | | | | | |
| | 11/6 | Mo | | | | | | |
| | 12/6 | Tu | | | | | | |
| | 13/6 | We | | | | | | |
| 8 | 14/6 | Th | | | | | | Orals (if required)* Class list posted* |
| | 15/6 | Fr | | | | | | |
| | 18/6 | Mo | | | | | | |
| | 19/6 | Tu | | | | | | |
| | 20/6 | We | | | | | | |

*Provisional dates

All lectures are held in the Pfizer Lecture Theatre unless otherwise stated