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This Handbook for the Academic Year 2013-14 has been produced in the Chemistry Faculty Office. Suggestions for future editions are always welcome: [nina.jupp@chem.ox.ac.uk](mailto:nina.jupp@chem.ox.ac.uk)

## Message from the Head of Department

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I would like to offer a warm welcome to all new students starting the Chemistry course here in Oxford. You are joining a group of 170-180 chemists in the first year from all over the UK, Europe and the World. Although many of your initial contacts at Oxford will be with students and tutors from your own college, I am sure that you will also get to know many of the chemists from other colleges as you meet them in lectures and in the teaching labs here in the Department. In fact the Chemistry Department is one of the largest, if not THE largest, chemistry departments in the world with around 750 undergraduates, 400 postgraduates and 300 or so academic, research, support and administrative staff. This Department is consistently ranked amongst the very best for teaching in the UK and its research standing places it in the top 10 of chemistry departments worldwide. But Oxford Chemistry is also a vibrant and friendly community and I am sure that as time goes on you will start to feel a sense of belonging here!

We hope that you will find Chemistry an exciting, challenging, satisfying and enjoyable subject to study at University. Our aims are not simply to provide you with a vast knowledge of chemistry but also to help you develop your intellectual and creative skills, (such as logical and lateral thinking, problem solving), and your practical skills. We aim to encourage and stimulate you to become the next generation of leading researchers and teachers in chemistry. At the same time there is a need for scientifically educated leaders in all ways of life, and whatever your ultimate career choice we are confident that an Oxford Chemistry degree will provide a valuable foundation.

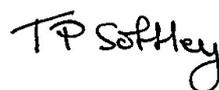
Over the next few years you will come to understand just how broad Chemistry is as a subject, and how central a science. The Chemistry curriculum ranges

from the boundaries with applied mathematics to molecular biology and has important applications in most of the major global challenge areas such as Health, Energy, Environment and Climate, Security and Communications. But you will also experience the rigour and depth of Chemistry as an academic subject, which enables it to lie at the core of many scientific endeavours.

Oxford has world-class Chemistry research facilities, provided by our Chemistry Research Laboratory, and many of you will have an opportunity to work there in a research project or in your Part II year.

My final word is simply to remind you of the fantastic opportunity you have here – but like many things in life, you will only get out what you put in, and it is up to you whether you make the most of that opportunity.

Although we will teach you in lectures, lab classes and tutorials, an Oxford Chemistry education is also about you developing your ability to learn for yourself, to research new materials and engage your mind in the intellectual rigour and excitement of this subject. I wish you all an enjoyable and successful time at Oxford.



Tim Softley, Head of Department

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## How to use this Handbook

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First Year students should read the whole Handbook. Those in subsequent years need only look at the relevant year sections.

Appendices give the lecture contents relevant for the various Examinations. Also given are some important e-mail addresses for contacting members of the Academic Staff, a short reading list for the First Years and information about the Chemist's Joint Consultative Committee (CJCC).

Lecture timetables are subject to change. Full and up to date information on lecture timetables may be found on the Department's lecture timetable web page: <http://www.chem.ox.ac.uk/teaching/timetables.html> or in diary form from the main Chemistry web page: <http://www.chem.ox.ac.uk/> by selecting Course Information from the Undergraduate menu and then clicking on Lecture timetable.

The Examination dates given in this handbook are based on information available in August - September 2013. They are only a rough guide, and the definitive dates are those published by the Examiners. For up to date information regarding the Examinations check on the web page: <http://www.chem.ox.ac.uk/teaching/examindex.html>.

Members of the Academic Staff will be happy to answer any questions you might have, but for particular information about College teaching, students should contact their Tutors.

Further information about the course can be obtained from the Department of Chemistry Website <http://www.chem.ox.ac.uk/> and from the Faculty Office in the Inorganic Chemistry Laboratory.

# Introduction

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The Oxford Chemistry School has recently been admitting around 180 - 200 undergraduates per year. There are approximately 65 full-time Professors and Lecturers with a large support staff.

## Libraries

Undergraduates will find most of their needs met by well-resourced College libraries. If your library is without a book you need, you should tell your Tutor or your College Librarian or inform the librarians in the Radcliffe Science Library. The Radcliffe Science Library (RSL) in Parks Road has a comprehensive collection of chemistry books and journals, which you may borrow provided you have your university card with you. The RSL is both a reference and a lending library and incorporates all the books that were formerly in the Hooke Lending Library. It is an invaluable resource for students. Access to the RSL is from Parks Road.

The RSL has a web page detailing both print and electronic chemistry resources available, <http://www.bodleian.ox.ac.uk/science/subjects/chemistry>.

## Information Technology

There are several networked computers in the IT Centre in the Physical and Theoretical Chemistry Laboratory. All undergraduates can use this open access computing facility, and will be timetabled to undertake practicals in small groups using these computers. The Colleges also have computing facilities for their undergraduates and there is a University-wide network and wireless network, which enables students to access departmental sites, the practical course and the Internet, without charge.

Undergraduates will also receive an e-mail account on the University computing system. All new users will be asked to sign an undertaking to abide by the University rules on the use of computers, <http://www.ict.ox.ac.uk/oxford/rules/>. The URL for the University Computing Service is <http://www.oucs.ox.ac.uk/>

The Chemistry Department follows the general guidelines laid down by the University in regard to the provisions of the Data Protection Act 1998 (<http://www.admin.ox.ac.uk/councilsec/dp/index.shtml> for details).

## Channels of Communication

Academic Staff have pigeon-holes in the buildings where they have offices and in their Colleges. There is a messenger service between Colleges and Departments. Staff may also be contacted by telephone or by e-mail. Most of

them prefer e-mail, which is usually the most efficient way. A list of e-mail addresses and college affiliations is given in **Appendix F**.

Much administrative information about the course and the Examinations is sent to students by e-mail. It is very important therefore that students using e-mail accounts other than their college account ([joe.bloggs@college.ox.ac.uk](mailto:joe.bloggs@college.ox.ac.uk)), set the forwarding facility appropriately and check their e-mail regularly. The majority of information that is sent from the Faculty, for example, regarding last minute lecture changes, examination information and deadlines that need to be met, is sent to individual students using e-mail. It is therefore necessary for mailboxes to be kept clear at all times.

## The Chemist's Joint Consultative Committee (CJCC)

The CJCC is a forum for the exchange of views concerning the undergraduate and postgraduate courses. The matters covered by this Committee include:

- the teaching arrangements, lectures, and seminars; organisation and coverage;
- the practical courses: composition, organisation, and formal requirements; safety;
- the syllabus and structure of Examinations;
- library facilities;
- the general welfare of students, in so far as it affects the Department (welfare matters are primarily a College concern).

Meetings are held twice a term (except in Trinity Term, when there is only one meeting). Colleges are paired, and each pair of Colleges provides a representative for one year. For further details see the web pages at:

<http://www.chem.ox.ac.uk/teaching/oxfordonly/CJCCfolder/CJCCindex.html>.

The CJCC comprises fourteen undergraduate members, three postgraduate representatives and six senior members. It is chaired by the Director of Studies. There is a separate committee for graduates.

The Maths, Physical and Life Sciences Division (MPLS) on has a similar forum with a broader agenda, on which the chemistry department has student representation.

There is also student representation on the Chemistry Academic Board, which is the committee that oversees the teaching in the department.

# Aims and Objectives, Teaching and Examinations

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## The Chemistry Course - Aims and Objectives

- to engender such qualities as will be needed by our students for them to become the next generation of outstanding research chemists and teachers of chemistry
- to stimulate in our students a deep interest in chemistry as a rich academic discipline in its own right, and an appreciation of how modern chemistry underpins a vast range of science, technology and medicine
- to provide intellectual development, skills development and academic challenge for the best and brightest of students in this country, so as to equip them for a wide range of careers and roles in society

The M.Chem. degree is fully accredited by the Royal Society of Chemistry. A new course structure has operated for all years starting since 2009. The full course specification can be found from web address:

<http://www.chem.ox.ac.uk/teaching/>

## Research and teaching

The department of Chemistry has an international reputation for research and this University believes that there are many benefits to the teaching of its courses that are a consequence of this high level of research activity. The tutors and lecturers with whom you will interact during this course are not only employed to teach you, but are also (in nearly all cases) actively engaged in the direction of, or participation in, one or more of the wide range of research projects that contribute to the department's research reputation. Many of the academic staff in this department are recognised internationally as leaders in their own field of specialisation.

The impact of research on teaching in this department may take many forms: tutors and lecturers including their own data or ideas from research in their teaching; the regular updating of reading lists and curricula to reflect research developments; the development of research skills and research-based approaches to study through your participation in research projects (particularly in the Part II); special topics provided as options in the third year; the use of research equipment in practical classes; access to research seminars in the latter years of your course; the many opportunities to meet with research students and members of the faculty, particularly at the research project stage; experience of preparing research reports including papers for external publication in some cases. In general you will be encouraged to

develop the ability to interpret and critically appraise new data and the research literature, and to build the sense that scientific knowledge is contestable and that its interpretation may be continually revisited.

## Departmental and College Teaching

The teaching of the courses is carried out through lectures, practical work in the laboratories, tutorials in the colleges (to which academic staff are also attached), and classes.

The lecture courses are comprehensive and challenging. Lecturers are allowed flexibility in their approach, which frequently leads to the inclusion of material reflecting developments in the field, not contained in standard textbooks. Lectures are generally regarded as essential, but technically they are not compulsory. No attendance checks are made, but only foolish idlers cut lectures. Printed notes, problem sheets and other handouts frequently support them and where appropriate they may be available on the web at <http://course.chem.ox.ac.uk/home.aspx>. Students need to learn how to take good lecture notes, and supplement them with their own private study, using textbooks and other sources recommended by the Lecturers and their Tutors. Feedback questionnaires are provided and their completion is encouraged because it helps us improve what we offer.

Practical work is recorded and practicals have to be written up in detail and marked. The marks for second and third year practicals count towards the final degree class. Termly progress reports on laboratory work are sent to College Tutors. During the first three years practical work is compulsory. Details of arrangements for the practical courses may be found at web address <http://course.chem.ox.ac.uk/practicals.aspx>.

The College-based tutorial teaching (2-4 in a group) provides guidance as to what to study, and in what order, coupled with week-by-week work assignments. These assignments are generally problems, with the occasional essay. College Examinations ('Collections') monitor students' progress during the intervals between University Examinations, and students are given termly reports on their progress.

## The Relationship between Tutorial Teaching and the Lecture Course

There is no formal link between the lecture courses and the tutorial teaching you will get

from your College Tutors, but most of the College Tutors are also University Lecturers and so know what is needed and will match what they teach to the lecture courses, backing up areas of difficulty and helping you with problems. They will also as far as possible tailor your tutorial work to your needs. Lecturers supply problem sets to their courses on the Web at <http://course.chem.ox.ac.uk/home.aspx> and these may be used as the basis of tutorial work.

### Teaching norms

In each of the first three academic years students can expect a minimum of 190 lectures provided by the department, and a norm of 48 hours of college tutorials and classes. The department will also provide at least 400 timetabled hours of practicals over the first three years.

### Skills development

*Students taking the Oxford Chemistry course are expected to gain the following skills via lectures, classes and tutorials:*

- The ability to collate, assimilate and rationalise a wide range of chemical facts, concepts and principles.
- An awareness and understanding of issues where chemistry impinges on other disciplines.
- The ability to reason logically and creatively.
- The ability to communicate effectively, both in writing and orally.
- Problem solving in a variety of contexts, both familiar and unfamiliar, including the demonstration of both self-direction and originality.
- Numeracy and mathematical skills including the appropriate use of units and the assessment and propagation of errors.
- Numerical, computational and IT information retrieval capabilities.

*and the following skills, primarily via the undergraduate practicals, including compulsory IT practicals, and the Part II research year:*

- The ability to conduct an experimental investigation precisely and safely.
- The ability to interpret complex experimental information and infer appropriate conclusions.
- The ability to apply IT methods for data retrieval and archiving and to use a wide variety of standard Chemistry orientated software packages such as those for structure drawing, spectral simulation etc.

- The ability to read and interpret the primary literature.
- Ability to work in a team and interact positively with other people, including those in other disciplines.
- The ability to exercise initiative and personal responsibility.
- Time management, project organisation and decision making abilities
- An ability to communicate effectively via both written and verbal reports and presentations.

### Vacations

At Oxford the teaching terms are short. It is therefore essential that you set aside a significant amount of time each vacation for academic work. The course assumes that you will do this. Your Tutors may also set you some specific vacation work.

### Examinations

There are Examinations in all four years: Prelims, Part IA, Part IB and Part II respectively. The Part IA and Part IB system was introduced in 2004/5 and a revised system was introduced in 2010/11. Past papers and examiners' reports can be viewed from the link <http://www.chem.ox.ac.uk/teaching/>.

### Prelims

This Examination comprises four papers covering the traditional areas of Inorganic, Organic and Physical chemistry, together with Mathematics for Chemistry. The first three of these are very broadly based, and include topics from Biological Chemistry and Physics, which are presented in a chemical context. Students sit the Preliminary Examination in all four subjects in June of the first year. The level of the Examinations is set so that with reasonable commitment the vast majority of students are capable of passing. Distinctions are awarded for excellent performance in the Examination. Failed papers can be re-taken in the following September, with the permission of the student's College, but all must be passed at no more than two sittings. It is necessary to have passed all the examinations in Prelims, including fulfilling practical and IT requirements, before proceeding to the second year course.

The material in the first year course comprises fundamental core material. It is necessary to assimilate it all thoroughly, not just to pass Prelims but also because later parts of the course depend and build on it. Prelims material is generally assumed knowledge in later Examinations.

### **Part IA**

This Examination, taken at the end of the second year, comprises three general papers\* covering aspects of the subject covered in year two of the course; the results are carried forward to be taken into account together with Parts IB and II to determine your final classification. Part IA must normally be sat before Part IB, and not in the same year. Part IA is weighted 15% in the final classification.

### **Part IB**

Part IB consists of six general papers\* covering all the core material in the course and one 3 hour option paper with a wide choice of options. At the end of this Examination candidates are divided into those judged worthy of Honours (who can proceed to Part II, but who may leave, if they wish, with an unclassified BA Honours Degree), those passing (who cannot proceed but who get a BA Pass Degree) and those failing. Part IB is weighted 50% in the final classification at the end of Part II.

\*The duration of these papers is being revised. Students will be informed as soon as possible.

### **Part II**

This is a research year, culminating in presentation of a thesis and a *viva* (oral examination), followed by classification and award of the MChem Degree. Part II is weighted 25% in the final classification.

The oral Examination will be usually held in 10<sup>th</sup> and 11<sup>th</sup> week of Trinity Term. The main purpose of the *viva* is to assure the Examiners that you have carried out and understood the work described in the thesis, but you may be asked more general questions relating to your project. The *viva* may also provide an opportunity for you to clarify points in your thesis that were unclear to the Examiners.

The above notes summarise the main points, but are neither authoritative nor complete; the detailed and authoritative regulations are contained in the Examination Regulations of the University and the Examination Conventions. In cases of difficulty consult the Senior Tutor of your College. The Proctors are the ultimate authority for interpreting the Regulations at the detailed level.

Appropriate allowances and arrangements may be made by Examiners at the request of the Proctors for medical or other special circumstances affecting Examination performance. Senior Tutors will advise and assist; but candidates are

not allowed to communicate directly with the Examiners themselves.

Candidates who have a year out for any reason (permission and arrangements for this are a matter for Colleges) are not disadvantaged in any way.

In the written Examinations, candidates are identified by number only; at Part II any Examiner who knows a candidate personally will not examine their thesis nor conduct their viva.

For the conventions regarding marking and the weighting of the various parts see *Examination Conventions in Chemistry* below, any changes made after the printing of this book may be found on the web version <http://www.chem.ox.ac.uk/teaching/>.

Each Board of Examiners is nominated by a small committee within the department, and approved by the MPLS Division. The Board of Examiners is formally appointed by the University.

Once appointed, the Examiners operate as a body sharing responsibility with considerable discretion within guidelines set by the Regulations and the Chemistry Academic Board (CAB), but the Proctors are the ultimate authority on everything except academic judgement.

The current set of examiners and the members of the nominating committee may be found at <https://intranet.chem.ox.ac.uk/committee-members.aspx>

See **Appendix B** for information about the types of calculators which may be used in written Examinations.

For syllabuses see the relevant Appendices.

Most Colleges set informal examinations of their own called 'Collections', usually at the start of each term. They are for mutual monitoring of progress and do not form part of the official University assessment at any stage.

### **Complaints Procedures**

Undergraduates who have a complaint concerning their own academic activities should raise it with their College Tutor(s), the Senior Tutor of their College, or their Head of House. In cases of difficulty the Director of Studies ([nicholas.green@chem.ox.ac.uk](mailto:nicholas.green@chem.ox.ac.uk)) or the Chairman of Chemistry ([tim.softley@chem.ox.ac.uk](mailto:tim.softley@chem.ox.ac.uk)) will advise. Complaints of general nature may be discussed at the CJCC. All students may lodge complaints on almost anything except the

weather with the Proctors and Assessor. Any complaint regarding any Examination should be made to the Junior Proctor, through the Senior Tutor of the candidate's College. For further information on the complaints procedure it is on the web from <http://www.chem.ox.ac.uk/teaching/>. On the role of the Proctors and Assessor, see their *Essential Information for Students*, on the web at <http://www.admin.ox.ac.uk/proctors/info/pam/ind>

ex.shtml. Students should on no account approach the examiners directly on any matter.

### Disclaimer

The Department aims to run the course as indicated in this Handbook, but reserves the right to alter the timetable, lecture titles and their content. Up to date details will be available on-line.

## Examination Conventions in Chemistry

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### Introduction

These conventions have been approved by the Chemistry Academic Board (CAB) and the MPLS Division. They should be read together with the current *Examination Regulations* and the Undergraduate Course Handbook. CAB reviews the conventions, regulations and handbook annually, and the Examination Conventions may be subject to minor adjustment during any academic year. The Examiners have discretion to deviate slightly from what is laid down, where appropriate and according to circumstances.

If any student or academic staff member finds any part of the Regulations, Conventions or Handbook obscure, enquiries should be addressed to the Chairman of CAB, through the Faculty office in the first instance ([nina.jupp@chem.ox.ac.uk](mailto:nina.jupp@chem.ox.ac.uk)). Such enquiries are welcome, as clarification helps everybody. It is not appropriate to address the Chairmen of Examiners on such matters.

### Prelims

See especially the relevant part of the *Examination Regulations*: (p92 in the 2013 edition), but general regulations found elsewhere also apply.

Each paper will be marked out of 100, according to the outline marking scheme printed on the question paper. Marks will be rescaled if necessary to eliminate imbalance between papers. All Prelim papers have equal weightings.

The pass mark on each paper will be 40. A fail mark in Mathematics of 38 or higher will be allowed as a compensated pass, provided that the candidate passes all three Chemistry papers and has an aggregate mark on all four papers of 180 or more. The aggregate will be the sum of all four agreed marks. No compensation will be allowed on any of the three Chemistry papers.

Distinctions are usually awarded to candidates with an aggregate score of about 280 or higher, approximately the top 30% of candidates.

Except in special circumstances no candidate may pass Prelims without having completed satisfactorily the practical requirement. The first year practical requirement consists of 11 days in each of the three teaching labs and a compulsory IT exercise, including an introductory day in each lab.

No student may enter for Part IA unless they have already passed all parts of Prelims. Prelims marks do not count towards the classification of the degree.

### Parts IA and IB

See *Examination Regulations*, (p168-171 in the 2013 edition), but general regulations found elsewhere also apply.

Parts IA and IB, together with the second and third year practical course and Part II, are conceived as parts of one examination, the Second Public Examination. After Parts IA, IB and the Practical course a decision is made to identify those who are worthy of Honours. The final degree classification for those worthy of honours depends on performance in Parts IA, IB, the practical course and Part II together, weighted 15:50:10:25 respectively.

Part IA consists of three General Papers, and is taken at the end of year two. Each General Paper is set as a two and a half hour exam and students will be expected to attempt six out of eight questions.

Part IB consists of six General Papers and one Options Paper, and is taken at the end of year three. General Papers are three hour exams and students will be expected to attempt four out of six questions. General papers will be set as two and a half hour exams but candidates will be

given three hours to attempt them, giving time for reading, reflection and reviewing answers. Candidates will be expected to answer four questions out of six. The Options Paper is three hours, and students will be expected to attempt three questions from a wide choice.

All papers will be marked according to the outline marking scheme shown on the question paper. Marks will be rescaled if necessary to ensure that they conform to the University Standardised Mark (USM) scale. The mark will be reported as a percentage. The three General Papers in Part IA have equal weight. The six General Papers in Part IB have equal weight, and will contribute 40% towards the final degree. The Options paper will contribute 10%.

There will be no pass/fail mark in Part IA; all candidates who complete this Part of the examination will have their marks carried forward to Part IB, and candidates will not be permitted to take Part IA again. Practical work will not be taken into account for Part IA.

Except in special circumstances, no candidate may pass Part IB without having completed satisfactorily the second and third year practical courses, and the IT practicals (as outlined below, a reduced third year course may be offered if a Supplementary Subject has been passed).

The second year practical course consists of a stint of 10 days (60 credit hours) in each of the three laboratories. The normal third year practical stint is 12 days (72 credit hours), with a free choice of experiments across the three laboratories, plus the third year IT practical. A candidate who has not completed the core requirement outlined above may still qualify for a Pass Degree if they have satisfactorily completed at least 20 days of the second and third year laboratory course in addition to the first year requirement and provided that he/she satisfies the examiners in the Part IB examination. Below this limit a candidate will automatically fail Part IB.

The views of the External Examiners will be considered carefully before any candidate is denied Honours. The honours threshold is expected to be about 40%. Students below this borderline may be called for a *viva voce* examination with an examination board normally consisting of the Chairman of Examiners and the External examiners.

Medical and other certificates will be considered by the Examination board for the set of

examinations they apply to and in each subsequent year up to Part II. Most commonly, action will be taken when the candidate's full results are available after Part II. Exceptions are candidates at the Pass/Fail or Pass/Honours borderline after Part IB. Examination boards may take account of medical and other certificates covering a single paper by an appropriate adjustment of the mark.

Candidates who are judged not to be worthy of honours may not enter for Part II. The examiners may recommend that they be awarded a B.A. Pass Degree or that they fail outright. In recent years the number of outright failures in Part I has been 0 or 1 and the number of Pass degrees awarded has been 0-2 (total candidate numbers were of the order 150-190). Candidates who are judged worthy of honours but who do not wish to continue to Part II may graduate with an unclassified B.A. Honours degree.

A pass or distinction in a Supplementary Subject may be offered as an alternative to half of the third year practical requirement. While the majority of candidates who choose to take a Supplementary Subject will take a single course during their second year, a Supplementary Subject may be taken in years 2, 3, or 4, with the proviso that a maximum of three Supplementary Subjects may be passed. Distinctions in Supplementary Subjects will be recognised by a marks bonus after Part II of 10 (i.e.1%). Marks above 60% not awarded a distinction will attract a bonus of 5 marks (0.5%). These bonus marks will be credited for each Supplementary Subject passed, but only one Supplementary Subject pass may be offered in lieu of practical work. Candidates who achieve a pass may not retake the same Supplementary Subject in a subsequent year.

## **Part II**

See *Examination Regulations*: (p171-2 in the 2013 edition)

Part II is examined by Thesis and by *viva voce* examination. The Chairman of the Part II Examiners will circulate instructions on the preparation of theses and information about other pertinent matters in Hilary Term. Candidates may be penalised for failure to conform.

Theses will be read by two Examiners, each of whom will mark out of 100. Because of the wide range of subject matter in Part II projects it is not appropriate to prescribe a single marking

scheme, but a set of guidelines for examiners is available on the departmental web page at <http://www.chem.ox.ac.uk/teaching/partII.html>.

The two principal readers of the thesis will lead the discussion during the viva, which will be marked out of 20. Thesis marks may only be altered following the viva with the agreement of a third examiner and the Chairman. Other than in exceptional circumstances, the viva cannot result in a decrease in the thesis marks.

Supervisors will be asked to report on the work of all candidates and on any special difficulties or advantages the candidates may have had, although the Supervisor's report makes no numerical contribution to the final mark.

Additional Supplementary Subjects may be taken during the Part II year, and mark bonuses will be allocated as outlined previously. However, no retrospective compensation for shortfalls in practical work or IT work reported to the Part IB examiners will be allowed: candidates who have not completed the practical requirement will not have been adjudged worthy of honours and will not be permitted to start the Part II year.

The two thesis marks and the viva mark will be added to give the Part II mark. The Part II mark will be aggregated with the total (scaled) Part I mark with a weighting 25:75, and expressed as a mark out of 1000. Bonuses for Distinctions in Supplementary Subjects will be added after aggregation.

Part II theses submitted after the deadline (noon on the Friday of 7<sup>th</sup> week) will be reported to the Proctors for investigation, and in addition to any sanction the Proctors may impose, an academic penalty will be applied to the Part II mark at the discretion of the examiners, according to the following scheme.

Lateness	Penalty
Up to 5 pm on the Friday of 7 <sup>th</sup> week	1%
Up to 5 pm on the Monday of 8 <sup>th</sup> week	5%
Up to 5 pm on the Tuesday of 8 <sup>th</sup> week	10%
Up to 5 pm on the Wednesday of 8 <sup>th</sup> week	20%
Up to noon of the Friday of 8 <sup>th</sup> week	30%
More than a week late	Fail

For example, a thesis given an overall Part II mark of 64% by the examiners on the basis of the thesis and the viva, but submitted on the Monday of 8<sup>th</sup> week will be penalised 5% and awarded a final mark of 59%. Any penalty assessed will be capped so that it does not take the Part II mark below the pass mark, with the exception of theses more than a week late. Candidates failing Part II remain entitled to the unclassified BA honours degree they qualified for at Part IB.

In deciding final classifications, account will be taken of any medical or other proper certificates received in Part IA, IB or Part II.

### Marking conventions

All written papers are marked according to an outline marking scheme printed on the examination paper. Examiners have discretion to vary this scheme as necessary. Papers will either be double-marked or the marks checked against the marking scheme by a second examiner. University Standard Marks (USM) will be used for each paper, in which class boundaries are drawn at or close to 70%, 60%, 50% and 40%, i.e. marks 70% and above are first class, marks between 60% and 70% are 2.1, etc. If in the academic judgement of the examiners the raw marks do not conform to this standard when compared against the class descriptors (below), the marks will be rescaled. If scaling is used, details will be provided in the Chairman's report. Any scaling of individual papers at Part IA, Part IB or Part II will be applied in the year the examination is taken.

A mark of zero shall be awarded for any part or parts of questions that have not been answered by a candidate, but which should have been answered.

All parts of questions answered will be marked unless clearly crossed out by the candidate. The best set of marks consistent with the examination rubric will be taken, e.g. if the number of questions specified by the rubric is 4 and a candidate answers 5, then the best 5 marks will be taken and the worst question discarded.

Discrepancies between the marks awarded by different examiners will be resolved as follows. Marks should be averaged if they differ by less than 10% of the maximum available, with a third marker arbitrating if they differ by more than this and the markers cannot agree.

Practical marks will be awarded according to a detailed scheme that assesses the pre-lab, practical skills and the write-up. Practical marks may be scaled to ensure uniformity of standard between experiments and markers. The final sign-off will be performed by a senior demonstrator or approved by a lab manager. Practicals submitted for marking beyond the 2-week deadline will be penalised. The aggregate practical mark will be reported as a percentage, and will be a weighted average of the marks for all the practicals that contribute to the appropriate requirement (252 or 216 credit hours, according to whether a Supplementary Subject has been passed). The relative weight of each practical in this average will be advertised in the laboratory manual. Detailed rules for the practical course can be found on the website at <http://course.chem.ox.ac.uk/practicals.aspx>.

### Classification

The class borderlines will be drawn at or close to 70%, 60%, 50% and 40%. The examination board will have the discretion to decide the exact borderlines, but they will not normally be higher than these norms, nor more than 1% lower. Each paper will contribute the following proportions to the maximum aggregate mark:

Each Part IA paper	5%
Each Part IB General paper	6.67%
Part IB Option paper	10%
Part I Practical course	10%
Part II	25%

It is expected that the percentages of the classes awarded will be in the ranges of recent years, i.e. I, 33-42%; Ii, 42-50 %; Iii, 10-15%; III, 0-5%. These ranges are not mandatory: occasionally a candidate's thesis and viva are deemed inadequate for any class of M.Chem. degree. Such candidates remain entitled to the unclassified B.A. Honours degree gained after Part IB.

### The following Qualitative Descriptors of Classes have been adopted:-

*Class I* The candidate shows excellent problem-solving skills and excellent knowledge of the material over a wide range of topics, and is able to use that knowledge in unfamiliar contexts.

*Class Iii* The candidate shows good or very good problem-solving skills, and good or very good knowledge of much of the material over a wide range of topics.

*Class Iiii* The candidate shows basic problem-solving skills and adequate knowledge of most of the material.

*Class III* The candidate shows reasonable understanding of at least part of the basic material and some problem-solving skills. Although there may be a few good answers, the majority of answers will contain errors in calculations and/or show incomplete understanding of the topics.

*Pass* The candidate shows some limited grasp of basic material over a restricted range of topics, but with large gaps in understanding. There need not be any good quality answers, but there will be indications of some competence.

*Fail* The candidate shows inadequate grasp of the basic material. The work is likely to show major misunderstanding and confusion, and/or inaccurate calculations; the answers to most of the questions attempted are likely to be fragmentary only.

The interpretation of these Descriptors is at the discretion of the Examiners.

## First Year 2013 - 2014

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**Lectures and Practicals.** At the beginning of term you will be given a list of lectures by your College Tutors. The lecture timetable and information regarding practicals can be accessed from the Chemistry web page: <http://www.chem.ox.ac.uk/teaching/>.

Experimental Chemistry is taught in rotation at each of the three main departments. You will be timetabled a single introductory day plus ten days in each of the three laboratories. The practical course teaches essential experimental skills, from the synthesis and characterisation of compounds to the operation of spectrometers and other instruments for physicochemical measurements. It also makes tangible much that is covered in lectures and tutorials. There is also an IT course concerning computer applications and chemistry software packages in the IT centre of the Physical and Theoretical Chemistry Laboratory (approx. 8 hours).

The need to cope with large numbers of students means that you will go through the First Year laboratories on a rota system and you will be designated to a Group through your College. Attendance is compulsory, therefore please check the practical information web page: <http://course.chem.ox.ac.uk/practicals.aspx>

Strict deadlines for submission of laboratory reports must be adhered to. Problems resulting in delay of submissions should be reported to the practical organiser at the earliest opportunity. Each practical is designed to teach you an important technique, and you will not be permitted to proceed to the second year unless the first year practical course has been successfully completed.

Ask for the Demonstrators' advice over any problems that you may have in the laboratories. They will be helpful. The following people are responsible for the first year practical courses:

Organic Practicals: Dr. Malcolm Stewart  
Inorganic Practicals: Dr. Phil Wiseman  
Physical Practicals: Dr. Fabrice Birembaut  
IT practical: Dr. Karl Harrison

They will welcome your comments and suggestions on the practical course. All practical work must be completed and marked off by 5 pm on the Friday of 6<sup>th</sup> week of Trinity Term. This is a University examination deadline and may only be relaxed by permission of the Proctors.

**Tutorials and Classes.** Most chemistry tutorials are organised through your colleges, and classes will also be offered in other subjects, particularly mathematics. Your College Tutors will arrange these.

**Computing.** The Chemistry IT centre is located in the Physical and Theoretical Chemistry Laboratory (PTCL) and is available for Undergraduates to access chemistry software. Additionally there is an area of the web site called 'my Degree' which produces online timetable information and practical booking, marking and completion information. The Department World Wide Web site <http://www.chem.ox.ac.uk> provides a gateway to a vast array of useful information. If you are interested in doing more computing, numerous courses are organised at the Computing Services, 13 Banbury Road.

**e-mail.** Please make sure you keep your e-mail boxes in good working order and delete old/unwanted messages as important information will be circulated to you via e-mail from the Faculty Office. You should check your e-mail daily.

**Books.** Do not rush out immediately and buy new books as there are frequently second-hand books advertised on departmental notice boards for a fraction of the cost. However, you are strongly advised to buy only the latest edition of texts, since old editions are often out-of-date; Lecturers usually use and give references to only the most recent edition. A list of the books recommended by the Lecturers for the first-year course is given in **Appendix A**. Your Tutor will advise you as to what books you should obtain.

**Societies.** The Chemistry Society holds regular social functions, special interest lectures and other activities and is open to all chemistry undergraduates. You will receive information directly from the officers of the Society. The Scientific Society also arranges talks by distinguished visiting speakers on a wide variety of topics.

**Refreshments.** Coffee and chocolate machines are available in the laboratories.

As ever, if in doubt, ask your College Tutor.

## The Course

Chemistry lectures in the first year will provide introductory coverage of the following topics:

- physical basis of chemistry
- quantum theory of atoms and molecules
- chemical thermodynamics
- reaction kinetics
- equilibrium electrochemistry
- states of matter
- atomic structure and the periodic table
- the ionic model, pre-transition metal chemistry and solid state structures
- reactions in solution
- introductory transition metal chemistry

- chemical bonding and molecular orbital theory
- non-metal chemistry
- introduction to organic chemistry
- reactivity in organic chemistry
- substitution and elimination at saturated carbons
- introduction to organic synthesis
- carbonyl group chemistry
- chemistry of C–C  $\pi$ -bonds
- introduction to biological chemistry

For more detail, see **Appendix D**.

### Examinations (Prelims)

See page 7.

## Schedule for First Year Lectures

For more details see the Chemistry Department's Lecture web page (<http://www.chem.ox.ac.uk/teaching/timetables.html>).

M = Michaelmas Term, H = Hilary Term, T = Trinity Term

Subject	Hours per Term		
	M	H	T
<i>Inorganic Chemistry</i>			
The Periodic Table	1		
Atomic Structure and Periodic Trends	5		
Ionic Model and Structures of Solids	10		
Molecular Shapes, Symmetry and Molecular Orbital Theory		6	
Acids, Bases and Solution Equilibria		4	
Non-metal Chemistry		6	
Transition Metal Chemistry			8
<i>Organic Chemistry</i>			
Introduction to Organic Chemistry	8		
Orbitals and Mechanisms I	8		
Substitution and Elimination at Saturated Carbons		8	
Chemistry of C–C $\pi$ Bonds		8	
Core Carbonyl Chemistry		8	
Introduction to Biological Chemistry			12
Revision Course and introduction to Organic Synthesis			4
<i>Physical Chemistry</i>			
Foundations of Physical Chemistry: Chemical Thermodynamics	13		
The Physical Basis of Chemistry: Properties of gases and classical mechanics	8		
The Physical Basis of Chemistry: The Role of Charge	4	4	
Quantum Theory of Atoms and Molecules		10	
Reaction Kinetics		6	
Electrochemistry		4	
States of Matter			4
<i>Mathematics for Chemistry</i>			
The Calculus of one and two Variables	20		
Introduction to Vectors	2		
Vector Algebra and Determinants		6	
Complex Numbers, Multiple Integrals and Ordinary Differential Equations		10	
Matrix Algebra			8

## Second Year 2013 - 2014

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### The Course

Some of the lectures develop further the topics introduced in the first year. There are additionally many courses on essentially new topics.

- principles of quantum mechanics
- symmetry and its implications
- bonding in molecules
- solid state chemistry
- diffraction methods
- atomic and molecular spectroscopy
- statistical mechanics
- liquids and solutions
- rate processes
- valence
- transition metal chemistry
- coordination chemistry
- non-metal chemistry
- organometallic chemistry
- high energy intermediates
- chemistry of the lanthanides and actinides
- liquids and solutions
- reactive intermediates in organic chemistry
- aromatic and heterocyclic chemistry
- heteroatom chemistry
- biological chemistry
- organic synthesis
- physical organic chemistry
- conformational analysis and ring chemistry
- maths for chemists
- introduction to NMR

### Practicals

There will be an introductory talk at the beginning of each part of the course. Attendance is compulsory, therefore please check the practical information web page: <http://course.chem.ox.ac.uk/practicals.aspx>. You will go through the laboratories on a rota system and you will be designated to a Group through your College.

Strict deadlines for submission of laboratory reports must be adhered to. Problems resulting in delay of submissions should be reported to the practical organiser at the earliest opportunity.

Ask for the demonstrators' advice over any problems that you have in the laboratories.

The following people are responsible for the second year practical courses:

Organic Practicals: Dr. Malcolm Stewart  
Inorganic Practicals: Dr. Phil Wiseman  
Physical Practicals: Dr. Fabrice Birembaut  
IT practical: Dr. Karl Harrison

### Supplementary Subjects

A number of Supplementary Subjects is available each year, on an optional basis; the titles will be advertised in the final term of the previous year. For up to date information see the Supplementary Subject page:

<http://course.chem.ox.ac.uk/supplementary-sub.aspx>

On offer for 2013-14 are:

- Quantum Chemistry
- Aromatic, Heterocyclic and Pharmaceutical Chemistry
- Chemical Crystallography
- Chemical Pharmacology
- Modern Languages
- History and Philosophy of Science

Each Supplementary Subject Examination (all at the end of Hilary Term except for languages which is sat in Trinity Term) comprises one paper; which results in fail/pass/distinction. A Pass gives exemption from one year's practical requirement in one laboratory (see page 8); a Distinction gives extra credit for the final assessment in Part II.

Although it is usual for Supplementary Subjects to be taken in the Second Year, they may be taken in any of years 2, 3 or 4, with a maximum of three in total. Candidates who get a Pass may not retake the same Supplementary Subject Examination.

For more detail, see **Appendix E1**.

### Examination (Part IA)

See page 7

## Schedule for Second Year Lectures

For more details see the Chemistry Department's Lecture web page (<http://www.chem.ox.ac.uk/teaching/timetables.html>).

M = Michaelmas Term, H = Hilary Term, T = Trinity Term

Subject	Hours per Term		
	M	H	T
<i>Inorganic Chemistry</i>			
Transition Metal Chemistry	6		
Co-ordination Chemistry	4		
Bonding in Molecules	8		
Chemistry of the Lanthanides and Actinides		4	
Organometallic Chemistry		8	
Structures and Electronic properties of solids		12	
Non-Metal Chemistry			4
NMR in Inorganic Chemistry			4
Course overview			8
<i>Organic Chemistry</i>			
Aromatic and Heterocyclic Chemistry	4		
Organic Spectroscopy I	8		
Conformational Analysis and Ring Chemistry	10		
Physical Organic Chemistry		8	
Rearrangements and Reactive Intermediates		8	
Heteroatoms in Organic Synthesis		8	
Problem solving for Synthesis		2	
Organic Synthesis II			8
DNA, Proteins and Enzyme Catalysis			8
Problem Solving			2
<i>Physical Chemistry</i>			
Quantum Mechanics: Principles and Applications	12		
Liquids and Solutions	8		
Statistical Mechanics		12	
Atomic and Molecular Spectroscopy		10	
Valence		8	
Rate Processes			8
Revision Lectures			4
<i>General Chemistry</i>			
Symmetry I	5		
Symmetry II	4		
Maths for Chemists	7		
Introduction to NMR	4		
<i>Supplementary Subjects</i>			
Aromatic, Heterocyclic and Pharmaceutical Chemistry	16	14	
Quantum Chemistry	16	14	
Chemical Crystallography	13	6	
History and Philosophy of Science	8	8	
Chemical Pharmacology	4	14	
Modern Language			32

## Third Year 2013 - 2014

### The Course

In the third year core course, the topics to be covered are

- post transition metal chemistry
- inorganic reaction mechanisms
- solid state chemistry
- spectroscopy and magnetism
- organometallic reaction mechanisms and catalysis
- organic spectroscopy
- pericyclic reactions
- transition metal catalysts in organic synthesis
- strategies in synthesis
- magnetic resonance
- photophysics & photochemistry
- surfaces & soft matter
- statistical mechanics

*Additionally 16 option courses are available as listed in the "Schedule for 3<sup>rd</sup> year Lectures" below and described in detail in the appendix. These option courses will each comprise 8 lectures in Hilary Term and 1 problem class in Trinity Term. The single, compulsory examination*

*paper will contain one question on the material taken from each of the 16 option courses. Candidates will be required to answer a total of 3 questions in 3 hours.*

### Practical Work

Before sitting Part IB, except in special circumstances, each candidate must have completed their practical requirement, which is a core second year requirement of 60 credit hours in each laboratory plus a third year requirement of 72 credit hours plus the IT practicals; except that those candidates who take and pass a Supplementary Subject will have a reduced third year requirement of 36 credit hours plus the IT practicals. The third year requirement is a free choice of third year experiments offered by the three teaching labs. All practical work must be completed and marked off by 5 pm, Friday, 4<sup>th</sup> week of Trinity Term.

For more detail, see **Appendix E2**.

### Examination (Part IB)

See page 7.

### Schedule for Third Year Lectures

For more details see the Chemistry Department's Lecture web page

(<http://www.chem.ox.ac.uk/teaching/timetables.html>)

M = Michaelmas Term, H = Hilary Term, T = Trinity Term

Subject	Hours per term		
	M	H	T
<i>Inorganic Chemistry</i>			
Inorganic Reaction Mechanisms	4		
Post-Transition Metal Chemistry	4		
Organometallic Chemistry	5		
Solid State Chemistry	5		
Spectroscopy and Magnetism in Inorganic Chemistry	4		
Bioinorganic Chemistry	4		
Revision of Topics in Inorganic Chemistry			5
Review of Periodic Table			3
<i>Organic Chemistry</i>			
Organic Spectroscopy II	8		
Organic Synthesis III	8		
Organic Catalysis	8		
Orbitals and Mechanisms III	8		
Revision – Molecular structure and reactivity			4
<i>Physical Chemistry</i>			
Applications of Statistical Mechanics	8		
Surface and Soft Matter Chemistry	14		
Photophysics and Photochemistry	8		
Magnetic Resonance	8		
Revision			4

Subject	Hours per term		
	M	H	T
<i>Option Courses</i>			
Molecular Spectroscopy		8	1
Structural Methods		8	1
Organometallic Chemistry: Structures, Bonding and Catalysis		8	1
Solid State Compounds in Technology		8	1
Supramolecular and Medicinal Inorganic Chemistry		8	1
Natural Product Chemistry		8	1
Advanced Synthesis and Total Synthesis		8	1
Contemporary Methods in Catalysis for Organic Synthesis		8	1
Advanced Chemical Biology		8	1
Functional Organic Polymers and Materials Chemistry		8	1
Fundamentals of Atmospheric and Astrochemistry		8	1
Molecular Reaction Dynamics		8	1
Biophysical Chemistry		8	1
Theoretical Chemistry		8	1
An Introduction to the Liquid State		8	1
Magnetic Resonance		8	1

## Fourth Year 2013 - 2014

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The fourth year is spent exclusively on research, providing you with the opportunity to immerse yourself in a significant project. A wide choice of research projects is available in both pure and applied Chemistry and also in related sciences. You will be supervised by a senior member of the academic staff and have full access to the research facilities of your host laboratory. The year's work results in a thesis, the assessment of which is weighted one quarter in the final determination of the class of M.Chem honours degree.

Current research now spans a huge range of topics, many of which are interrelated. The students are encouraged to look at the web pages on <http://www.chem.ox.ac.uk/researchguide/> and to select the area they wish to work in by following the links to the individual members of academic staff world wide web pages. Each page will contain a recent summary of their current research interests and some have links to their own further research information. This will be followed up by Open Days usually held in Michaelmas Term. Each Laboratory offers an Open Day where you are invited to visit the labs, meet the supervisors and discuss potential Part II projects. You may wish to return later for further discussion, but Open Days provide the ideal opportunity to learn about the research conducted in Oxford.

There are possibilities for Part II students to carry out a portion of the research project at a University abroad.

Supplementary Subject courses (see <http://course.chem.ox.ac.uk/supplementary-sub.aspx> and Examinations are open to Part II students.

For further information regarding the allocation process look at the web pages accessed from: <http://www.chem.ox.ac.uk/teaching/PartII/part2tl.html>.

Guidance for approaching the Part II may be found on the departmental web page from <http://www.chem.ox.ac.uk/teaching/partII.html>.

Detailed instructions to Part II candidates about the preparation and assessment of the thesis will be posted on the Departmental website by the chairman of examiners, and notified to you by e-mail.

There is a Data Analysis lecture course designed for Part II students. There are also induction lectures organised on a Sectional basis and there are Departmental Colloquia which Part II students are encouraged (indeed expected) to attend. These can be found on the following web page:

<http://www.chem.ox.ac.uk/faculty/colloquia.html>

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## Prizes

A number of substantial Prizes and Bursaries are available. In 2013 the following were awarded:

- (1) Bruker (UK) Ltd. for excellence in Prelims: total of £300
- (2) Eisai Limited for excellence in Part IA: total of £1,000
- (3) OUP Book Prize £100 X 2 for the most improved candidate/s between Prelims and Part IA
- (4) Gibbs Prize in Chemistry for excellence in Part IB: first prize, proxime accessit and three book prizes totalling £1,000
- (5) In addition there were Thesis Prizes for excellence in Part II, and in practical work, and there are College Prizes as well.

## APPENDIX A

### Recommended Core Textbooks

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The following will be useful from the outset; more detailed recommendations will be made by Lecturers and Tutors.

*Physical Chemistry*, Atkins, de Paula, OUP [9<sup>th</sup> edn., 2009].

*Inorganic Chemistry*, Atkins, Overton, Rourke, Weller, Armstrong, Oxford University Press [5<sup>th</sup> ed. 2009].

*Chemistry of the Elements*, Greenwood & Earnshaw, Butterworth-Heinemann [2<sup>nd</sup> edn.], 1997 [1<sup>st</sup> edn. 1985]

*Foundations of Organic Chemistry*, Hornby & Peach, Oxford Chemistry Primer, OUP, 1993: Illustrated edition 2000

*Organic Chemistry*, Clayden, Greeves, Warren, OUP, [2<sup>nd</sup> ed. 2012].

*Organic Chemistry*, Maitland Jones, Norton [5<sup>th</sup> edn. 2013]

*A Guide to Mechanism in Organic Chemistry*, Sykes, Pearson [6<sup>th</sup> edn.] 1986

*Foundation Mathematics for the Physical Sciences*, K. F. Riley and M. P. Hobson, Cambridge University Press, 2011

## APPENDIX B

### Calculators for Written Examinations in Chemistry

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A candidate may bring a pocket calculator into any Examination, **except the Prelims Mathematics for Chemistry paper**, provided the calculator meets the conditions set out as follows:

- The calculator must not require connection to any external power supply
- It must not be capable of communicating with any other device
- It must not make a noise that could irritate or distract other candidates
- It must not be capable of displaying functions graphically
- It must not be capable of storing and displaying text, other than the names of standard functions such as 'sin' or 'cosh'
- It must not be able to store programs or user-defined formulae
- It must not be able to perform symbolic algebra, symbolic integration or differentiation
- Within the above, the calculator may be capable of evaluating elementary mathematical functions such as  $\sin(x)$ ,  $\log(x)$ ,

$\exp(x)$ ,  $x^y$  and it may contain constants such as  $\pi$ .

#### Notes

These guidelines follow the regulations but, supersede on detail, the 'Use of calculators in Examinations' in the University Examination Regulations.

The intention of the rules is to prevent the possibility of a candidate obtaining an advantage by having a powerful calculating aid (or of reading stored information as a substitute for knowing it). It is appreciated that candidates may already own calculators that are excluded by these rules. In such case the candidate is responsible for obtaining a more basic calculator that is within the rules, and for becoming familiar with it in advance of the Examination.

## Important Dates

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### ***DATES OF FULL TERM 2013-14***

MICHAELMAS TERM  
Sunday 13 October - Saturday 7 December

HILARY TERM  
Sunday 19 January - Saturday 15 March

TRINITY TERM  
Sunday 27 April - Saturday 21 June

### ***DATES OF EXTENDED TERM for Part II Candidates in Chemistry 2013-14***

MICHAELMAS TERM  
Thursday 26 September - Sunday 22 December

HILARY TERM  
Monday 6 January - Thursday 17 April

TRINITY TERM  
Monday 28 April - Saturday 12 July

### ***DATES OF FULL TERM 2014-15***

MICHAELMAS TERM  
Sunday 12 October - Saturday 6 December

HILARY TERM  
Sunday 19 January - Saturday 15 March

TRINITY TERM  
Sunday 27 April - Saturday 21 June

### ***DATES OF EXTENDED TERM for Part II Candidates in Chemistry 2014-15***

MICHAELMAS TERM  
Thursday 25 September – Tuesday 23 December

HILARY TERM  
Tuesday 6 January - Wednesday 1 April

TRINITY TERM  
Monday 13 April - Saturday 11 July

### ***Important dates for the Diary***

Examination entries must be made through your College, who will advise you of the appropriate deadlines: detailed dates are not available at the time of printing, but may be found on the university web page <http://www.admin.ox.ac.uk/schools/oxonly/entries/index.shtml> and more examination information can be found on <http://www.ox.ac.uk/students/exams/timetables>. Students need to enter for optional examinations, i.e. Supplementary subjects and Prelims resits. All other entries will take place automatically. Special arrangements will be made for Chemistry Part II because of the need to register the Thesis title.

Supplementary Subject Examinations (except Modern Languages)	Begins 8 <sup>th</sup> week Hilary Term To be taken in 8 <sup>th</sup> week Trinity Term
Prelims	Begins 7 <sup>th</sup> week Trinity Term
Part IA Examination	Begins 8 <sup>th</sup> week Trinity Term
Part IB Examination	Begins 6 <sup>th</sup> week Trinity Term
Part II Thesis deadline	7 <sup>th</sup> week (Friday, 12 noon) Trinity Term
Part II Vivas	Begin 10 <sup>th</sup> week Trinity Term

### **These dates are provisional and subject to change**

Students may be required to be in attendance by Colleges (Part I students) or Sections and Supervisors (Part II students) outside the Full Term and Extended Term dates given.

## Syllabus for Prelims 2013-14

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### SUBJECT 1, Chemistry 1: Inorganic

*Aims: The aim of the first year inorganic chemistry course is to lay foundations in the areas of atomic structure, bonding and the structures of molecules and solids, and chemical reactivity. These areas and their importance will be illustrated by a wide-ranging descriptive chemistry of the elements.*

#### Atomic Structure and Periodic Trends

The Bohr model, wave properties of electrons, the Born Interpretation: probability densities.

The Schrödinger equation and the H atom. The quantum numbers  $n$ ,  $l$ ,  $m_l$ , their values and interpretation (hence  $2s$ ,  $3d$ ,  $4f$ , etc.) Shapes and energies of orbitals. Radial wavefunction and the radial distribution function.

Polyelectronic atoms: Orbital approximation, spherical average of electron repulsion. Helium and the Pauli Exclusion Principle: electron spin, antisymmetry. Screening and penetration, effective nuclear charge.

Structure of the Periodic Table:  $s$ -,  $p$ -,  $d$ -,  $f$ -blocks. Trends in ionisation energies, electron affinities, ionic radii,  $3d$  and  $4f$  contractions.

#### Ionic Model, Pre-Transition Metal and Solid State Chemistry

General atomic and chemical properties of elements of Groups 1,2, within the framework of the Periodic Table. Elements, halides, hydrides, oxides.

Born-Haber cycles, Born-Landé and Kapustinskii equation. Hess's Law cycles. Trends in the stability of binary compounds. Structures of ionic solids based on closed packing and filling of interstitial holes. Close packing, unit cells, space efficiency. Fractional coordinates, plan views and projections. Location, number and size of octahedral and tetrahedral interstitial holes. Common AB and AB<sub>2</sub> structures. Factors affecting structure: relative sizes, charges, ionicity, van der Waals, the NiAs class of compounds.

Chemistry in aqueous solution, trends in solubility of compounds, complex formation, nature of ligands and driving force. Chemistry in non-aqueous solution, metals in liquid ammonia, unusual oxidation states, organometallic chemistry (e.g. methyl lithium).

#### Shapes, Symmetry and Molecular Orbital Theory

Lewis structures, VSEPR rules. Symmetry of molecules, symmetry elements, point group determination.

Molecular orbital theory: H<sub>2</sub><sup>+</sup>, H<sub>2</sub>, homonuclear diatomics,  $s/p$  mixing, bond strength and bond order, paramagnetism. Heteronuclear diatomics, HF and CO. 3-centre/2-electron, 4-centre/2-electron bonds: H<sub>3</sub><sup>+</sup>, H<sub>3</sub><sup>-</sup>, HF<sub>2</sub><sup>-</sup>, B<sub>2</sub>H<sub>6</sub>.

#### Acids, Bases and Solution Equilibria

Definitions (Brønsted, Lewis),  $pK_a$ , trends in acid strength, Pauling's rules for oxy-acids. Buffers.

Redox potentials, Nernst equation, pH dependence, Latimer diagrams, Frost diagrams - construction and interpretation. Calculation of equilibrium constants from redox potentials.

#### Non-Metal Chemistry

General atomic and chemical properties of elements of Groups 13,14,15,16,17 within the framework of the Periodic Table. Elements, halides, hydrides, oxides, oxoacids. Structure, bonding, trends in stability, acid/base properties and reactivity patterns.

#### Transition Metal Chemistry

Transition elements and the Periodic Table. Survey of atomic properties, oxidation states, energetics and coordination environments. Key ideas of coordination chemistry. Introduction to ligand fields.

### SUBJECT 2, Chemistry 2: Organic

*A knowledge of the dynamic and evolving science of Organic Chemistry is central to the discovery, understanding and development of many important breakthroughs in biology, medicine, and materials science. This course will provide an introduction of the concepts and fundamental reactions of Organic Chemistry, show how these discoveries are supported experimentally, and how this knowledge can be used in a problem-solving and predictive capacity.*

*Aims: The course is designed to introduce and develop the fundamental concepts of organic chemistry; to show some of the key experimental evidence which supports these concepts; to apply these data and concepts to chemical problem solving.*

#### Introduction to Organic Chemistry

Lewis bonding, bond polarisation. Lewis acids. Structures and isomers. Stereochemistry. Enantiomers: chirality, stereogenicity. Molecular orbital theory hybridisation.

Functional groups: carbonyls, imines, oximes, nitriles. Lewis acids and bases. Curly arrows and mechanism. Resonance.

#### Orbitals and Mechanisms I

Acids and bases: resonance and inductive effects. Thermodynamics and kinetics. Hammond postulate. FMO interactions. Conjugation; vinylogy. Reactions: curly arrow rules, formal charges, mechanism and structure as a consequence of FMO interactions. Solvent effects, reactive intermediates: C<sup>-</sup>, C<sup>•</sup>, C<sup>+</sup>.

A unified approach to mechanism. Neutralisation and ionisation, S<sub>N</sub>1. 1,2-Addition to C=O and β-elimination (E1cB, E2). S<sub>N</sub>2. Electrophilic addition with H<sup>+</sup> & regiochemistry. E1. Electrophiles and stereospecificity. Attack by carbenes, dienes = pericyclic. Attack by radicals, orientation. Redox concepts.

#### Substitution and Elimination at Saturated Carbons

Kinetics and mechanism of S<sub>N</sub>1 and S<sub>N</sub>2 reactions. MO theory of substitution reactions. Stereoelectronics.

Nucleophilicity and basicity. Activation of leaving groups. Carbocations. Substrates, leaving group, nucleophile and solvent. Intermolecular substitutions giving alkyl halides, ethers, esters, amines, azides, thiols and sulfides, phosphonium salts. Substitution with nitriles/isonitriles. Intramolecular substitutions giving cyclic products.

Kinetics and mechanism of E1 and E2 reactions, mechanism of E1cb reactions. MO theory of elimination. Stereoelectronics. Competition between substitution and elimination. Elimination for alkene and alkyne synthesis. E1cb in carbonyl chemistry.

### Core Carbonyl Chemistry

Nucleophilic addition to C=O, reversible and irreversible. Nucleophilic substitution of C=O, (acetals; imines, oximes and hydrazones; enamines, Wittig and Horner-Emmons reactions, Wolff-Kishner reaction). Nucleophilic substitution at C=O, (acid chlorides; anhydrides; esters; amides). Simple IR stretch of C=O groups. Chemistry of carboxylic acids: factors that affect pKa.

Keto-enol tautomerism:  $\alpha$ -racemisation in acid or base. pKa of simple FGs including malonates. Reactions of enolates. Alkylation, Claisen condensation, halogenation of ketones. The haloform, Reformatsky and Darzens reactions.

Condensation reactions with carbonyl groups. The aldol reaction. Conjugate additions.

### Chemistry of C–C $\pi$ -Bonds

Alkene and alkyne chemistry: influence of orbitals on reactivity. Overview of types of reaction. Alkene reactivity: electrophilic addition, pericyclic addition, free radical addition, catalytic hydrogenation. Allylic bromination.

Alkyne reactivity: electrophilic addition, hydration to ketones, alkylation of terminal alkynes, reduction.

Conjugation/delocalisation in non-aromatic systems: conjugated alkenes and alkynes, allenes. Modifications to reactivity, conjugate addition reactions.

Structure and Reactivity of Aromatic compounds. Electrophilic aromatic substitution. Mechanism. Reactions: halogenation, nitration, sulfonation, Friedel-Crafts alkylation/acylation, formation of azo dyes (coupling with diazonium salts). Directing effects. Nucleophilic aromatic substitution. Radical reactions at the benzylic position.

### Introduction to Biological Chemistry.

The chemical blueprint of a cell. Towards a chemical understanding of biology.

Amino Acids and Peptides. Peptides and Proteins: analysis of primary sequence. Protein Structure. Protein function and enzymes. Enzyme Kinetics. Enzyme Inhibition.

## SUBJECT 3, Chemistry 3: Physical

*Aims: The first-year physical chemistry course lays foundations in the key areas of quantum mechanics, physics, thermodynamics and reaction kinetics, upon which the whole of modern physical chemistry is based.*

### States of matter and equilibrium

#### Thermodynamics

Le Chatelier's principle. Equations of state. Systems and surroundings. Work and heat.

First law. Internal energy. State functions. Expansion work. Reversible and irreversible changes. Heat capacity and enthalpy.

Thermochemistry. Standard states. Standard enthalpy changes (transition, reaction, formation). Kirchhoff law.

Second law. Direction of change. Entropy. Condition of equilibrium. Entropy changes of phase transition. Temperature and pressure dependence of entropy. Third law. Statistical interpretation.

Free energy,  $A$  and  $G$ . Available work. Temperature and pressure dependence of Gibbs energy.

Phase equilibria. Clapeyron and Clausius-Clapeyron equations. One-component phase diagrams.

Chemical equilibrium. Thermodynamics of mixtures. Chemical potential. Entropy and enthalpy of mixing. Extent of reaction. Reaction quotient. Condition for equilibrium, equilibrium constant and its temperature dependence; relation to standard Gibbs function.

### Electrochemistry

The metal/solution interface. Electrochemical potential.

Equilibrium Nernstian electrochemistry. Activity and activity coefficients and their determination. Nernst equation. Cells and half cells. Reference electrodes. Reversibility and irreversibility of cells. Relation of standard potentials to thermodynamic quantities.

Conductivity of ionic solutions - liquid junction potentials. Measurement of standard electrode potentials.

### States of Matter

Microscopic view of structure and motion in the three states; radial distribution function. Density, mechanical properties, diffusion and viscosity, degrees of freedom, equipartition and heat capacity.

Intermediate states of matter: liquid crystals, gels, glasses.

Intermolecular forces and pair potentials. Gas imperfection, van der Waals equation, virial expansion. Relationship between potential energy curve and the virial coefficients/internal energy.

Single component phase diagrams (e.g., H<sub>2</sub>O, CO<sub>2</sub>, He); phase coexistence and stability, triple point, critical point, multiple solid phases.

The interface between phases; qualitative discussion and definition of surface tension. Kinetics of crystallization.

### Quantum Mechanics and Spectroscopy

#### The physical basis of Chemistry: Electromagnetism

Coulomb's Law, electric fields, electric potentials. Electric dipoles (inc. molecules) and dielectric materials

Magnetic dipoles and magnetic materials.

The Biot-Savart Law.

E.M. induction: the Faraday-Lenz Law, Lorentz forces.

Waves, the E.M. spectrum and the Doppler effect.

Superposition and diffraction.

Reflection and Refraction (Snell's Law).

## Quantum theory of atoms and molecules

Quantum theory. Failures of classical physics. Quantization of electromagnetic radiation. Wave-particle duality. The de Broglie relation.

The Schrödinger equation. Solution for particle in a *one*-dimensional square well and results for an *n*-dimensional square well; particle on a ring and the rigid rotor; simple harmonic oscillator (outline); hydrogen atom (brief outline). Born interpretation. Correspondence principle. Zero point energy.

Eigenvalue equations. Position, momentum and Hamiltonian operators. Expectation values, uncertainty principle.

Atomic spectra: one-electron atoms and alkali metals. Orbitals, energy levels and quantum numbers. Radial and angular distributions. Term and level symbols. Spin-orbit coupling. Penetration and shielding. Selection rules and spectra; related optical concepts. Determination of ionization energies for one-electron atoms.

Structure of many-electron atoms and Aufbau principle.

## Kinetics

### The physical basis of chemistry: Classical mechanics and properties of gases

Newton's Laws of motion: forces, momentum and acceleration.

Work, and kinetic and potential energy.

Rotations: angular momentum and moments of inertia.

Vibrations: simple harmonic motion.

Properties of gases: the perfect gas equation.

Kinetic theory of gases, origin of pressure, Maxwell-Boltzmann distribution.

Molecular motions and equipartition.

Collisions between molecules, mean free path, collision frequency, effusion, diffusion.

## Reaction kinetics

## APPENDIX E1

# Syllabus for Part IA 2013-14

## INORGANIC CHEMISTRY

*The content of the Part IA Examination in Inorganic Chemistry will be based on the content of the lectures delivered to 2<sup>nd</sup> year students. Candidates will also be expected to be familiar with material covered in the 1<sup>st</sup> year course. In some questions it may be necessary to make use of simple symmetry arguments at the level covered in the Symmetry I and Symmetry II General Chemistry course. Candidates will be expected to be familiar with the content of the 1<sup>st</sup> and 2<sup>nd</sup> year practical courses.*

### Transition Metal Chemistry

Atomic properties. Relative energies of *s* and *d* orbitals. Electronic configurations. Ionisation energies. The stability of the half-filled shell. Sublimation energies of the elements. Heats of formation of cations.

Rates of reactions. Order and molecularity. Rate laws and their determination.

Experimental measurement of reaction rates.

Sequential and reversible reactions, pre-equilibrium, the steady state approximation: applications to unimolecular reactions (Lindemann) and enzyme catalysis.

Temperature dependence of reaction rates: Arrhenius Equation, activation energies, elementary collision theory.

## SUBJECT 4, Mathematics for Chemistry

*Calculators will not be permitted in the Examination but Tables containing standard results from calculus and trigonometry will be provided.*

### Syllabus

Linear equations and determinants. Vector algebra and calculus, and applications to mechanics. Plane polar, spherical polar and cylindrical polar coordinates.

Inverse functions. Hyperbolic functions. Limits and their determination.

Elementary calculus of one and of two variables. Taylor series and L'Hopital's rule. Integration, integration by parts. Transformation of coordinates. Theory of errors. Multiple Integrals in two and three dimensions.

Complex Numbers. Argand diagram, Euler equation, de Moivre's theorem. Solutions of the equation  $z^m = a + ib$ .

First Order Differential Equations, exact, separable, linear, homogeneous.

Second order Linear Differential Equations, linear homogeneous differential equations, equation of harmonic motion, damping terms. Second order linear inhomogeneous differential equations.

Matrix addition and multiplication. Inverse matrices. Orthogonal matrices. Eigenvalues and eigenvectors. Properties of symmetric and of Hermitian matrices.

Trends in stability of binary compounds. Rationalisation of electrode potentials.

Ligand field splittings: high and low spin complexes, spin-pairing energies; LFSE effects in lattice energies, heats of formation, hydration energies, etc.; site preference energies in spinels; dependence on ligand type, oxidation state, and transition metal series. The Jahn-Teller effect and its consequences.

Stability of oxidation states in the 1st transition series. Trends in reduction potentials for  $M^{3+}/M^{2+}(aq)$ . Oxidation state diagrams (Frost and Pourbaix). The effect of pH and of ligands on redox potentials. Factors and ligands stabilising high and low oxidation states.

Stereochemistry and coordination number. Main differences between the 1st and the 2nd and 3rd transition series: stability of oxidation states; trends in

covalence; metal-metal bonding.

Comparative survey of the chemistry of transition metal groups, e.g. titanium, zirconium and hafnium; chromium, molybdenum and tungsten; iron, ruthenium and osmium; nickel, palladium and platinum.

### Lanthanides & Actinides

Lanthanides: Occurrence of the elements; electronic properties: the nature of *f*-electrons; periodicity in the *f*-block. Extraction and separation. Properties of the metals. The predominance of the 3+ oxidation state. Structural chemistry of the lanthanide compounds. Aqueous chemistry, complex formation, nature of ligands, redox chemistry. Examination of binary halides, hydrides, oxides and borides: structures and electronic properties. Organometallic chemistry. Comparisons/contrasts with transition metals.

Actinides: Occurrence and properties of the metals. Periodicity and general chemistry of the actinides including comparisons with lanthanides and transition series: oxidation states; aqueous chemistry; coordination stereochemistry. Focus on uranium chemistry: halides, hydrides, oxides, aqueous chemistry (especially of the uranyl ion), organometallic chemistry.

### Coordination Chemistry

Thermodynamics and kinetics of complex formation: monodentate vs polydentate ligands, including acyclic and macrocyclic examples. Isomerism.

Thermodynamics of complex formation: stability constants. Factors affecting the magnitude of stability constants – Irving Williams series, chelate effect, class a and class b classification, requirements of ligands.

Macrocyclic Ligand Complexes: biological importance, macrocyclic effect. Macrocyclic ligand syntheses – template and non-template syntheses. Template effect: thermodynamic and kinetic contributions.

Occurrence of common geometries: the role of metal electronic configuration and ligand in determining the stereochemistry in  $d^6$ ,  $-d^{10}$  ions.

### Bonding in Molecules

The orbital approximation, the LCAO approach.

The use of symmetry in polyatomic molecules MO treatment of  $AH_2$  (linear and bent),  $AH_3$  (planar and pyramidal),  $AH_4$  ( $T_d$ ).

Walsh diagrams: The shapes of  $AH_2$  molecules, the bonding and shapes of  $H_3^+$  and  $H_3^-$ : 3-centre-2-electron and 3-centre-4-electron bonds.

Photoelectron spectroscopy and "experimental" MO diagrams, spectra of  $AH_n$  molecules.

$AB_2$  molecules from  $CO_2$  to  $XeF_2$ , 12-electron main group octahedral systems:  $SF_6$  as an example. 8-electron main group octahedral systems:  $[C(AuPR_3)_6]^{2+}$  as a relative of  $CH_6^{2+}$ .

Octahedral transition metal systems,  $\sigma$ -bonding, comparison with electrostatic model. MO filling in octahedral complexes:  $p$ -interactions and factors that affect the magnitude of  $D$ .

Molecular orbitals for 4-coordinate geometries:  $ML_4$  ( $T_d$  and  $D_{4h}$ ).

First- and second-order Jahn-Teller distortions.

### Organometallic Chemistry

General principles: valence electron count, formal oxidation state, number of *d*-electrons. The 18- and 16-electron rules: applications and exceptions.

Classification of reactions: addition, dissociation, ligand substitution, migratory insertion, extrusion, oxidative addition, reductive elimination and attack on coordinated ligands.

Synthesis, bonding and selected reactions: Transition metal alkyl, alkylidene (carbene), alkylidyne (carbyne) and carbonyl complexes. Hydride, dinitrogen and dihydrogen complexes. Alkene, alkyne and allyl complexes. Cyclopentadienyl, arene and other  $C_nH_n$  ( $n = 4-8$ ) sandwich and half-sandwich complexes. Synergic bonding and  $\pi$ -complexes: CO as a ligand, alkene complexes, bonding in ferrocene.

Contemporary environments for new organometallic chemistry: anionic N- and O- donor ligands (porphyrins and other macrocycles, amides, imides, alkoxides).

### Structures and Electronic properties of solids

*Diffraction methods* Distinction between lattices and structures. Unit cells and Bravais lattices. Fractional coordinates.

Miller indices ( $hkl$ ) and  $\{hkl\}$ . Calculation of  $d_{hkl}$ . Derivation of Bragg's Law. Indexing powder diffraction patterns.

X-ray powder diffraction: techniques and uses. Consideration of the peak intensity: the structure factor; systematic absences. Use of powder diffraction for following solid-state reactions.

### Bonding in Solids

Models of electronic structure: introduction to energy bands in ionic, covalent and metallic solids. Band gaps and their importance in the properties of solids.

Free Electron and Tight Binding models (treated somewhat mathematically). Simple Tight Binding pictures for elements such as: Li, Be, transition metals, diamond and Si, solid  $I_2$ . Comparison with the molecular picture.

Extension of band model to simple ionic compounds: e.g. NaCl and CaO; transition metal oxides:  $TiO$ ,  $ReO_3$ ,  $TiO_2$  and  $VO_2$ , and sulfides:  $ZrS_2$ ,  $NbS_2$ ,  $MoS_2$ . Trends in the properties of solids and how they relate to the general chemistry of the transition metals in particular.

Brief description of Spectroscopic techniques for studying band structure.

Mott-Hubbard insulators and breakdown of the band model. Chemical trends in the Mott-Hubbard transition – competition between bandwidth and interelectron repulsion.

Low-dimensional metals and the Peierls distortion with examples – electronically-driven structural distortions.

Intrinsic and extrinsic semiconductors; the effect of doping level on the properties.

### Structures of solids

Review of important structure types; relationship between crystal structure and electronic structure – electronic structure-directing effects and comparison with molecular systems.

### **Inorganic NMR**

Brief review of fundamentals of NMR. Chemical shielding: diamagnetic & paramagnetic terms. Multinuclear NMR, shielding ranges (including chemically useful examples). Scalar ( $J$ -) coupling: 1, 2 & 3-bond coupling constants; coupling to  $n$  nuclei (multiplets); sequential stick diagrams; satellites (isotopomers). Structures from NMR: e.g.  $^{19}\text{F}$  NMR of main group fluorides. NMR of quadrupolar nuclei.

### **Non-Metal Chemistry**

Survey of group trends. Electronegativity, size and polarisability: implications for "ionic" compounds formed with metals. Covalent bonds: trends in bond strength; formation of multiple bonds; hypervalence. Bonding models for hypervalent compounds. Catenation and polymerisation. Catenated and multiple bonds with Si, P, and S. Polymeric structures formed by Si-O, P-N and S-N compounds. Boranes: structural classification and Wade's rules; aspects of preparation and reactivity.

Solvent properties: polarity, donor/acceptor properties, and ion transfer. Examples of hydride, oxide and halide solvents. Superacids.

Donor/acceptor properties. Major trends in Lewis acid/base chemistry. HSAB classification. Ligand properties.

High oxidation states. Group trends: the "Alternation effect". Formation of polycations.

Aspects of xenon chemistry.

## **ORGANIC CHEMISTRY**

*The course is designed to develop the concepts of organic chemistry introduced in the first year; to show some of the key experimental evidence which supports these concepts; to apply these data and concepts to chemical problem solving; and to demonstrate that the subject is still evolving and that it has a key role to play in modern technological developments in diverse fields, ranging from chemical synthesis to biological science. Questions on the Part IA Examination will be based upon topics covered by both the first and second year lecture courses and in the practical courses.*

Topics to be covered are:

### **Organic Spectroscopy I**

NMR. Nuclear spin and resonance, chemical shifts, factors that influence  $^1\text{H}$  chemical shifts. Spin-spin coupling, coupling patterns and resonance multiplicities, coupling to chemically equivalent spins, weak and strong coupling. Chemical and magnetic equivalence;  $^1\text{H}$  spin couplings and chemical structure-geminal, vicinal and long-range couplings, chirality and NMR, chiral solvating agents.  $^{13}\text{C}$  NMR spectroscopy, Spectrum editing, NMR instrumentation, Fourier transform NMR, example  $^1\text{H}$  &  $^{13}\text{C}$  spectra.

UV spectroscopy; electronic transitions as a source of bonding information; Beer-Lambert Law; common chromophores and Woodward's rules; interpretation of simple spectra. Donor-acceptor conjugations and effects on HOMO/LUMO.

IR spectroscopy; vibrational transitions as a source of bonding information; characteristic group frequencies; interpretation of spectra

Application of all the above spectroscopic techniques

to the solution of structural problems.

### **Aromatic and Heterocyclic Chemistry**

The nature and origin of aromaticity; the reactions of aromatic compounds; the introduction of functional groups onto aromatic substrates; and the difference in reactivity of heteroaromatic compounds (furan, pyrrole, thiophene; pyridine; indole; quinoline; isoquinoline).

### **Organic Synthesis Problem Solving**

Problem-solving lectures relating to the 1<sup>st</sup> year course 'Introduction to Organic Synthesis'.

### **Conformational Analysis and Ring Chemistry**

Structure, conformation and stereoelectronic effects in acyclic and cyclic systems (with emphasis on 6-membered rings). Stereoselectivity in addition reactions of C=O and C=C in cyclic and acyclic systems. Effect of ring size on reactivity. Ring synthesis: examples of cyclisation reactions; pericyclic ring-forming processes; dependence on ring size and cyclisation conditions.

### **Physical Organic Chemistry**

Structure and reactivity in organic chemical reactions. Kinetics, thermodynamics, transition states, intermediates. Rate equations and kinetics, kinetic isotope effects, solvent effects, linear free energy relationships, elucidating reaction mechanism. Catalysis of organic reactions.

### **Rearrangements and Reactive Intermediates**

Structure, reactivity and rearrangement reactions of carbocations and carbanions. Neutral reactive intermediates including carbenes, nitrenes and radicals, structure, synthesis, and reactivity. Rearrangements, including to electron deficient oxygen and nitrogen. General reactions of radicals.

### **Heteroatoms in Organic Synthesis**

The chemistry of organic compounds containing boron, silicon, phosphorus and sulfur including their use in the construction of complex organic molecules and mechanistic and stereochemical aspects. Brief extension to other elements e.g. Se

### **Organic Synthesis II**

Regioselectivity, chemoselectivity, and stereoselectivity. Oxidation, reduction, selective alkene oxidation and reduction. Site blocking and protecting groups and their utility; selective carbohydrate manipulations as exemplars. Principles of retrosynthetic analysis and worked examples.

### **DNA and Proteins**

Chemistry, structure and role of nucleic acids / nucleotides. ATP, coenzyme A, RNA and DNA structures. Synthesis and analysis of oligonucleotides. Chemistry of genetics. Chemistry of protein biosynthesis. Nucleic acid pharmacology

## **PHYSICAL CHEMISTRY**

*The Examination will consist of questions relating to the lecture courses given in the second year, together with all the first year material:*

### **Quantum Theory**

Operators: basic notions and properties; linear

operators, eigenvalue equations; degeneracy; expansion in a complete set.

Postulates of QM and deductions there from; expectation values and the meaning of measurement in QM; the time-dependent Schrödinger equation; stationary states and the time-independent Schrödinger equation.

Commutators: definition, evaluation, properties. Physical significance of commutators; complementary observables, simultaneous dispersion-free measurement and the uncertainty principle (weak and strong). Bra-ket notation; definition and properties of Hermitian operators.

One-body problems: the free particle (wave-particle duality; commutation and measurement; peculiarities). The particle in a  $d$ -dimensional box (quantization *via* boundary conditions; zero-point energy; the correspondence principle; degeneracy). Rotational motion: angular momentum; angular momentum operators, commutation relations and their significance; particle on a ring; particle on a sphere and eigenfunctions of  $L^2$ ; the rigid rotor. The H-atom. The simple harmonic oscillator: wavefunctions, energy levels and properties. The variational principle.

The existence of electron spin. Spin functions for a single electron. Spin functions for two electrons; singlet and triplet states. The Pauli principle, antisymmetric wavefunctions, Slater determinants

Introduction to atomic spectra. He atom: variational calculation of ground state  $1s^2$ ; orbital approximation.  $1s^2 2s^1$  configuration; singlets and triplets. Atomic states:  $LS$  coupling; treatment of spin-orbit coupling. The Zeeman effect in atoms (magnetic fields),  $g$ -factors. The Stark effect (electric fields).

### Liquids and Solutions

Ideal solutions. Basis (entropy of mixing, zero enthalpy of mixing). Raoult's law, ideal solubility, depression of freezing point (the phase diagram of a eutectic mixture will be included), osmotic pressure.

The effects of non-zero interactions. Starting point from Henry's law (link with radial distribution functions). The effect of non-zero enthalpy of mixing on activities. Phase separation conditions.

Electrolyte solutions. Hydration structure of ions (link with radial distribution functions, *e.g.* hydrated Cl ion). Simple treatment of Debye-Hückel (D-H) theory of activity. Application of D-H to solubility, dissociation.

Polymer solutions. Flory-Huggins model. Non-ideality of polymer solutions as manifested in osmotic pressure behaviour. Polymer dimensions in solution (theta and good solvents, radius of gyration).

Surface of liquids and solutions. The Gibbs equation for surface tension. A brief introduction to hydrophobicity, amphiphilicity and surface activity.

### Statistical Mechanics.

Systems of independent particles. Aims of statistical mechanics. Distribution of molecules over molecular quantum states: microstates, configurations and the weight of a configuration. The most probable configuration and derivation of Boltzmann distribution for independent molecules. Definition and significance of molecular partition function,  $q$ . Factorization of  $q$  into translational, rotational etc. components; calculation of  $q_{\text{trans}}$  and  $q_{\text{elec}}$ . Determination of internal

energy,  $E$ , and specific heat,  $C_v$ , from  $q$ ; application to monatomic gas. Limitations of Maxwell-Boltzmann statistics. Mean values of observables; applications to bulk magnetization, paramagnetic susceptibility and derivation of Curie Law.

Interacting particles. Concept of an ensemble. The canonical ensemble and the canonical distribution. The canonical partition function,  $Q$ , its physical significance and determination of internal energy from  $Q$ . Entropy in statistical mechanics, and its relation to  $Q$ . Determination of enthalpy, Helmholtz free energy, Gibbs free energy and chemical potential from  $Q$ .

Independent particles II. Reduction of  $Q$  for special case of independent molecules: the relation of  $Q$  to  $q$  for (i) independent distinguishable and (ii) independent indistinguishable particles. Summary of thermodynamic functions for independent particles expressed in terms of  $q$ ; separability of thermodynamic functions into contributions from different modes.

Calculation of molecular partition function and selected applications.  $q_{\text{trans}}$ ,  $q_{\text{elec}}$  and the statistical thermodynamics of a monatomic gas; molar entropies and the Sackur-Tetrode equation. Rotational contribution to  $q$  for heteronuclear molecules; the high temperature limit and characteristic rotational temperature,  $\theta_{\text{rot}}$ . Rotational contributions to  $S$  and  $C_v$ . The effects of nuclear spin: symmetry numbers and  $q_{\text{rot}}$  for homonuclear diatomics and other symmetrical molecules. Applications to rotational spectroscopy. Vibrational partition functions,  $q_{\text{vib}}$ , for diatomic molecules and polyatomics.

Chemical equilibrium. Statistical mechanical result for the equilibrium constant  $K$  of a general chemical reaction. Calculating the equilibrium constant and selected examples: dissociation reactions, isotope exchange reactions, thermal ionization equilibria.

Transition state theory – the derivations. Concept of the transition state and the reaction coordinate. Transition state theory in terms of separable motion. The quasi equilibrium hypothesis. Derivation of the explicit expression for  $k(T)$  in terms of partition functions.

### Molecular Spectroscopy

Introduction. Energy levels of molecules; Born-Oppenheimer separation; interaction of radiation with matter; absorption; emission; transition moments; selection rules

Rotational Spectroscopy (Microwaves). Rotors and their symmetry; moments of inertia; isotope effects; centrifugal distortion; selection rules; Stark effect

Vibrational Spectroscopy (Infrared) I. Selection rules; anharmonicity; rotation-vibration transitions; normal mode vs. local mode

Vibrational Spectroscopy (Infrared) II. overtone and combination bands; vibrational modes: individual molecules vs. molecules in condensed phases

Raman Spectroscopy. Stokes, Anti-Stokes and Rayleigh scattering; rotational and vibrational transitions; selection rules; mutual exclusion in centrosymmetric molecules; Raman vs. IR

Selected Topics and Examples. Experimental methods; effects of nuclear spin statistics; applications and examples

Atomic Spectroscopy I. Resumé of atomic spectroscopy. Wavefunctions. Atomic orbitals. Hydrogen atom. Hydrogenic atoms. Helium atom. Alkali metals (and pseudo-1-electron) atoms. The orbital approximation. SCF procedure. Penetration and shielding. The quantum defect. Selection rules and spectra. Determination of ionisation energies.

Atomic Spectroscopy II. Many electron atoms. Russell Sanders coupling and  $j-j$  coupling. Term symbols. Hund's rules, selection rules and spectra.

Molecular spectroscopy I. Electronic energy levels. (Born Oppenheimer separation of energies). Potential energy curves/surfaces. Description of diatomic (linear) molecules. Classification of electronic states. Electronic selection rules.

Molecular spectroscopy II. Vibrational structure. Franck-Condon Principle.

Rotational structure in electronic spectroscopy. Band heads. Dissociation energies. Birge-Sponer extrapolation. Predissociation.

### Valence

Born-Oppenheimer Approximation. Bonding in  $H_2^+$  (LCAO approximation). Many-electrons - the Orbital Approximation. Deficiencies of the orbital approximation. binding of  $He_2$ , splitting of degenerate configurations, dissociation of  $H_2$ .

Application of Variation Principle to find LCAOs - the Secular Equations. Simplification due to symmetry and electronegativity differences.

Examination of energy levels of diatomic molecules. Splitting into terms ( $O_2$ ) and levels (NO).

Electronic and Photoelectron Spectra of Molecules. Franck-Condon Effects. Selection Rules.

Examination of vibrational and rotational structure. Band heads. Birge-Sponer extrapolation. Predissociation. Radiationless transitions.

Polyatomics - Hückel simplifications of the secular equations. Use of symmetry. Properties from the wavefunction - bond-order, electron density, dipole moments, spectral properties, organic reactivity.

### Rate Processes

Simple collision theory. Collision frequency and collision cross section. Reaction cross section and steric factor. Potential energy surfaces. Classical motion over PES's. Link between reaction cross sections and rate constants.

Transition state theory. Comparison with simple collision theory. Calculation of rate constants. Estimation of pre-exponential factors. Temperature dependence of rate constants. Kinetic isotope effects. Quantum mechanical tunnelling. Non-Arrhenius behaviour. Thermodynamic formulation of TST.

Liquid-phase kinetics. Comparison of liquid-phase and gas-phase reactions. Encounter pairs, cage effect, and geminate recombination. Wavelength and viscosity dependence of photodissociation, radical scavenging, kinetics of  $I_2$  photodissociation, cluster reactions, spin effects.

Diffusion controlled reactions. Smoluchowski theory. Stokes-Einstein relation. Effects of solvent viscosity and temperature, reactions between ions, spin effects.

Activation controlled reactions. Gibbs energy of reaction, effect of electrostatic interactions, influence of solvent permittivity, entropy and volume of activation, electrostriction, influence of pressure and ionic strength.

Electron transfer reactions. Marcus theory. Gibbs energy and reorganization energy. Marcus inverted region. Homogeneous and heterogeneous electron transfers.

Interfacial kinetics. Electric potential and its effect on interfacial reaction rates. Butler-Volmer equation. Transfer coefficients. Overpotential. Tafel relations. Voltammetry.

## GENERAL CHEMISTRY

### Symmetry I - Molecular symmetry, group theory, and chemical bonding

Symmetry operations and symmetry elements. Symmetry classification of molecules - point groups. Symmetry and physical properties: Polarity, Chirality. Combining symmetry operations: 'group multiplication'

Mathematical definition of a group. Review of Matrices. Definitions, matrix algebra, inverse matrices and determinants. Transformation matrices. Matrix representations of groups. Properties of matrix representations. Similarity transforms. Characters of representations.

Reduction of representations. Irreducible representations and symmetry species. Character tables. Orthogonality relationships in group theory. Using the LOT to determine the irreps spanned by a basis. Symmetry adapted linear combinations.

Bonding in diatomics. Bonding in polyatomics - constructing molecular orbitals from SALCs. The variation principle. Solving the secular equations. Matrix formulation of a set of linear equations. Solving for the orbital energies and expansion coefficients. Summary of the steps involved in constructing molecular orbitals. Hückel molecular orbital theory

### Symmetry II

Character tables and their meaning:  $C_{2v}$ ,  $C_{3v}$  and  $T_d$  revisited.

The reduction formula and its application to SALCs in  $CH_4$ . Projection operators and the SALCS of  $NH_3$ . p orbitals in  $C_6H_6$ .

Another look at the origins of degeneracy in molecular systems. Ligand field splitting of d levels. Tables of descent in symmetry. Jahn-Teller theorem. 2nd order Jahn Teller effect.

Direct products - symmetry of many electron states. Selection rules in electronic spectroscopy: octahedral versus tetrahedral systems. IR and Raman selection rules. Overtones and combination bands. Vibronic transitions.

Vibrational spectroscopy: stretching vibrations of  $CF_4$ ,  $SF_4$  and  $XeF_4$ . The mutual exclusion rule. Complete 3N basis sets and the vibrations of  $NH_3$ . The vibrations of  $C_{60}$ .

### Maths for Chemists

Solution of separable Partial Differential Equations. The complete set. Orthogonality of sine and cosine. Fourier series. The delta function. Fourier transforms.

## Introduction to NMR

Introduction to magnetic resonance, including the background physics of magnetic resonance, the origin of shielding, the physical origin of the splitting of

NMR transitions due to  $J$ -coupling, a short introduction to spin relaxation processes, and an overview of experimental methods

## APPENDIX E2

# Syllabus for Part IB 2013-14

## INORGANIC CHEMISTRY

### General Papers

The examination papers in Part IB will include all the topics considered in the core courses in Inorganic Chemistry delivered in the 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> years of the course. Candidates should also be familiar with the material covered in the practical course. The style of questions will be similar to questions used recently in Part IB examination papers. For each paper, candidates will be required to answer 4 questions taken from a choice of 6.

### Core Lecture Courses

#### Inorganic Spectroscopy and Magnetism

##### Electronic spectra of metal complexes

The different types of electronic transition. Characteristics of absorption bands: transition energy and intensity (and the implications for colour) and band widths.

Selection rules: allowed and forbidden transitions. Charge-transfer spectra: (a) ligand-to-metal CT transitions; focus on tetrahalide complexes, tetroxo-anions and hexahalide complexes; the redox connection; (b) metal-to-ligand CT transitions; focus on octahedral  $ML_6$ .

Ligand field ( $d-d$ ) spectra: trends in the orbital splitting parameter, including the spectrochemical series; R-S terms in the ligand field; Orgel diagrams for the simpler cases. The Racah parameter  $B$  and the nephelauxetic effect.

Tanabe-Sugano diagrams (in outline).

##### Magnetic properties of metal complexes

Definition of magnetic quantities.

Brief survey of the different forms of bulk magnetism, focusing on paramagnetism.

Curie paramagnetism: the Curie law and the effective magnetic moment; the spin-only formula. The saturation moment; Curie-Weiss law.

Lanthanide compounds: the Hund-Landé formula and its scope.

Compounds of the transition elements: (a) quenching of the orbital magnetic moment; scope of the spin-only formula; (b) residual orbital angular momentum and deviations from the spin-only expectation.

#### Bioinorganic Chemistry

Introduction to bioinorganic chemistry: Cellular compartmentalisation. The roles of the Group 1 and Group 2 ions  $Na^+$ ,  $K^+$ ,  $Mg^{2+}$ ,  $Ca^{2+}$ . Electrolytes, ion channels, signalling. Properties of complexes between metals and proteins – how one influences the chemistry of other.

Haem proteins and enzymes. Cytochrome  $c$  and electron transfer. The biological chemistry of oxygen: haemoglobin, peroxidases, catalases, and monooxygenases. Oxygen binding. Reactive oxygen species and oxidative damage.

Cobalt and radical chemistry. The cobalamin co-factor. Cobalt oxidation states and their stabilization and chemistry. Mutases and methyl transferases.

The bioinorganic chemistry of proteins and enzymes containing M–S and M–O clusters. Iron-sulphur clusters in electron transfer, nitrogen fixation, and hydrogenases. Manganese-oxo chemistry and the oxygen-evolving centre.

#### Solids state chemistry

Overview of the material covered in the 2<sup>nd</sup> year: the basic electronic properties of stoichiometric solids and the effect of introducing defects.

##### Defects and ion transport

Defects in solids: thermodynamic and structural aspects. Non-stoichiometry and electronic consequences. Applications to metal oxides and other inorganic solids.

Outline of experimental techniques used to study defects – diffraction, EXAFS, solid state NMR, electron microscopy (without detail on the techniques: focus is on information they provide)

Ionic mobility in the solid state: factors affecting ionic conductivity in various types of solid. Applications in technology.

##### Structures, Reactivity and Synthesis

Chemical aspects of solid state chemistry: general synthetic methods. Low temperature reactivity of solids illustrated by intercalation chemistry (e.g. graphite, layered oxides and sulfides,  $C_{60}$ ). Application of redox processes in solid state systems, for example in Li-ion secondary batteries).

#### Post-Transition Metals

Position of the elements in the Periodic table, relation to transition elements, and distinctive properties of the atoms and their compounds. Ionisation energies and radii; oxidation states and relative stabilities; failings of the ionic model; structural features; complex formation and HSAB; relativistic effects; inert pair and alternation effects; geometric issues; organometallic chemistry and properties of representative compounds; colours and band gaps in the group oxidation state; metal-metal bonding; mixed valence compounds; low oxidation states and clusters.

#### Inorganic Reaction Mechanisms

Ligand substitution reactions in square planar metal complexes (including the *trans* effect) and in

octahedral metal complexes:  $D$ ,  $A$ ,  $I_a$ ,  $I_d$  mechanisms, anation and solvolysis reactions.

Electron transfer reactions: inner sphere and outer sphere electron transfer. Introduction to Marcus theory: interplay between donor-acceptor overlap, thermodynamic driving force and reorganisation energy. Two-electron transfer and non-complementary reactions.

### Organometallic Reaction Mechanisms and Catalysis

Oxidative addition and reductive elimination. Mechanistic evidence including: dihydrogen compounds, agostic bonding. Brief mention of C-H bond activation.

$\alpha$ - and  $\beta$ -hydrogen transfer; migratory insertion reactions.

Introduction to homogeneous catalysis and a consideration of various important and representative systems. Including the isomerisation and hydrogenation of olefins; hydroformylation; Monsanto acetic acid process; Wacker process. Brief introduction to olefin polymerization by metallocene or similar systems.

## ORGANIC CHEMISTRY

*The course is designed to develop the concepts of organic chemistry introduced in the first and second years; to show some of the key experimental evidence which supports these concepts; to apply these data and concepts to chemical problem solving. The core course will provide a comprehensive treatment of more elaborate aspects organic chemistry, with an emphasis on synthesis and biological chemistry.*

### General Papers

*The examination papers will be based upon topics covered by the third year organic chemistry core lecture courses below, and will also include topics covered in the first and second year organic chemistry lecture courses and possibly from the practical laboratory course. For each paper, candidates will be required to answer 4 questions taken from a choice of 6.*

### Organic Spectroscopy II

Applications of NMR and mass spectrometry to problem solving in organic chemistry. Using 1D NMR; decoupling and spectrum editing. Establishing molecular connectivity with 2D NMR. Establishing molecular stereochemistry with the nuclear Overhauser effect. Introduction to mass spectrometry: History, instrumentation, methods and applications. Principles of the detection of ions, characteristics of the mass spectrum; isotopes and ion abundance. Mass Spectra and their interpretation: accurate mass, structural elucidation, tandem mass spectra and fragmentation patterns. Hyphenated techniques: Chromatography and mass spectrometry. Biological mass spectrometry: Protein, peptide and oligonucleotide identification. Proteomics and identification of post-translational modifications (PTMs).

### Organic Synthesis III

The following questions will be addressed: Why do we want to synthesise molecules- what sort of molecules do we need to make? What aspects of selectivity do we

need to exert to accomplish a good synthesis (think about chemo-, regio- and stereoselectivity, control of absolute stereo-chemistry). What is the perfect synthesis? What are the constraints imposed on an academic versus an industrial synthesis? Where does chirality come from?

Other topics covered include: Protecting group chemistry, which is central to almost any synthetic effort (including the major types of PG and tactics for protecting most and least hindered functional groups). Retrosynthesis - learning to think backwards. Importance of making C-C bonds and controlling oxidation state. Umpolung. Examples of retrosynthesis/synthesis in action.

For each case-study molecule, there will be a detailed retrosynthetic analysis and then a full discussion of the completed synthesis. Key points of interest in each synthesis are described.

### Orbitals and Mechanisms III

Hückel molecular orbitals; conservation of orbital symmetry; frontier molecular orbital theory; Woodward-Hoffmann rules. Cycloaddition Reactions. Diels-Alder reaction: endo-preference, Lewis acid catalysis; [2+2] cycloaddition of ketenes, dipolar cycloaddition, cheletropic reactions; photochemical reactions. Electrocyclic Reactions. ring opening of cyclobutenes, ring closure of hexatrienes, cyclopropyl halide solvolysis; charged systems. Sigmatropic Rearrangements. Dewar method compared to FMO approach, [1,n] H-atom shifts, Cope and Claisen variants; ene reactions. Applications of pericyclic reactions in synthesis.

**Catalysis in Organic Synthesis** Introduction to organometallic chemistry of transition metals. Organopalladium chemistry: Suzuki coupling, Heck coupling and related cross couplings. Alkene metathesis. Catalytic oxidation and reduction, including hydrogenation, epoxidation and dihydroxylation. Organocatalysis.

### Revision – Molecular Structure and Reactivity

This course provides revision for essential knowledge of the organic chemistry course taken over the three years of the undergraduate course, considered under two broad headings, molecular structure and molecular reactivity. Each of the reaction types will be illustrated with examples showing their application to synthetic organic chemistry.

## PHYSICAL CHEMISTRY

### General Papers

*Candidates will be required to answer 4 questions out of 6. The style of questions on the two papers will be the same and will be similar to that of the 2012 and 2013 papers and of Part IB papers in the years up to 2011.*

### Magnetic Resonance

A revision of the principles of Nuclear Magnetic Resonance (NMR): magnetic moment, space quantization, the resonance condition, the vector model, populations and bulk magnetization, selection rules, the origin of shielding, diamagnetic and paramagnetic shielding, neighbouring group anisotropy, ring current effects, electronic effects, intermolecular interactions.  $J$ -coupling, multiplet splitting, coupling to spins with  $I$  greater than  $\frac{1}{2}$ ,

discussion of Fermi contact interaction), an introduction to dipolar coupling. Magnetic resonance spectroscopy of two coupled spin- $\frac{1}{2}$  particles: a quantum mechanical treatment. The rotating frame, linear and circularly polarized fields, NMR as a coherence phenomenon; experimental methods: continuous wave and pulsed NMR, Free Induction Decay (FID) and Fourier Transformation for simple FIDs. Spin relaxation: spin-lattice and spin-spin relaxation, the rotational correlation time and the spectral density function, spin relaxation and the vector model, measurement of relaxation times, the inversion recovery experiment, the spin-echo experiment. An introduction to Electron Paramagnetic Resonance (EPR): hyperfine interactions and  $g$ -values in EPR, use of hyperfine coupling to probe molecular orbitals via spin densities, connection to Hückel theory. Double resonance techniques in NMR and EPR: Principles and applications (spin decoupling techniques, NOE, DNP, ENDOR, ELDOR).

### **Surfaces and Soft Matter Chemistry**

#### *Solid surfaces*

Nature and atomic structure of solid surfaces. Chemical adsorption and thermodynamics; Adsorption isotherms; Langmuir model. Kinetics of adsorption processes; competitive adsorption; heterogeneous catalysis; Physical adsorption. Experimental investigation of solid surfaces.

#### *Wet surfaces*

Interaction between surfaces: dispersion forces; Van der Waals attraction; Hamaker constant; double layer repulsion; measurements of forces. Surfactants: Gibbs adsorption equation; thermodynamics of micelle formation; geometric model for micelle shapes; interface curvature, wetting, capillarity.

#### *Soft Matter*

Brownian motion; Langevin equation; Einstein-Smoluchowski equation; velocity auto-correlation function; diffusion; mean square displacement; Timescales. Colloidal phase behaviour; hard sphere crystallization; fluid-fluid phase separation; entropy driven phase transitions; polymers; elastic properties of polymers; depletion interaction; polymer brushes

### **Photophysics and photochemistry**

Electronic transitions of polyatomic molecules. Beer-Lambert law, selection rules and absorption strength, vibronic transitions, radiative lifetime, Franck-Condon Principle.

Fates of excited states: Jablonski diagram, fluorescence and phosphorescence, vibrational relaxation, intersystem crossing and internal conversion, intramolecular vibrational redistribution, dissociation/predissociation.

Lifetimes of excited states: quantum yield, photochemical kinetics, fluorescence / phosphorescence quenching, Stern-Volmer plot.

Spectroscopy and dynamics: wavepackets and the semiclassical method.

Intramolecular energy transfer: application of Fermi's Golden Rule, rates of intersystem crossing (El-Sayed rule), and internal conversion, energy-gap law, isotope effects, conical intersections. Delayed fluorescence.

Intermolecular energy transfer, Electronic energy transfer, long-range (dipolar, FRET) and short-range (exchange) mechanisms, spin correlation rules. Triplet

annihilation. Triplet sensitization and delayed fluorescence. Exciplex formation.

Chemical reactivity of electronically excited molecules; isomerisation, acidity, redox, orbital character etc. The role of intersections in returning to the ground state.

Geminate recombination, escape probability and recombination timescale.

Photoionisation and photoelectron spectroscopy. Ion chemistry, ZEKE.

Photodissociation, and predissociation, ozone destruction.

Ultrafast photochemistry and photophysics. Pulsed lasers. Pump-probe spectroscopy. Generation and fate of nuclear wavepackets. Chemistry in real time.

Applications of photochemical and photophysical phenomena to single molecule imaging. The diffraction limit. Super-resolution fluorescence microscopy. Stimulated emission depletion. Photo activated localization and stochastic optical reconstruction microscopies (PALM, STORM).

### **Applications of Statistical Mechanics**

*A. Solids* Recap of statistical mechanics with some new aspects (heat capacity of simple gasses, ortho-para hydrogen etc, effects of thermal dissociation). Third law entropy and residual entropy - various examples. Heat capacity of solids, Einstein and Debye models - successes and failures. Simple applications (vapour pressure, thermal conductivity). Heat capacity of the electron gas. Configurational entropy in defective solids and adsorbed layers - equilibrium concentration of defects, Langmuir isotherm.

*B. Interacting systems: imperfect gases* Canonical Ensemble (revision) – v/d Waals canonical partition function. Classical Statistical Mechanics (phase space, configuration integral), Equipartition. Virial expansion, in particular second virial coefficient (in terms of interparticle potential) within the canonical ensemble. Application to hard-sphere, square-well and van der Waals gases.

### **Options Paper**

*The option courses are designed to develop advanced concepts and methods in chemistry to cover some areas of contemporary interest, for example in technology and in the environment. The options are dynamic, and will be updated annually to reflect modern developments. The courses are M (Masters level), assume knowledge of the core material in the first three years of the course and build on it. The options examination will be three hours and students will be expected to answer three questions. Each of the 16 options offered will have one 1-hour question on the paper. Each option course comprises 8 lectures in Hilary Term and 1 problem class in Trinity term.*

### **Inorganic Molecular Spectroscopy**

How various spectroscopic techniques are used to characterise inorganic systems. The complementary nature of all the techniques will be illustrated. 1. Electronic spectroscopy – The use of spectroscopic techniques to probe transition metal and lanthanide systems. 2. Vibrational spectroscopy – Underpinned by the course “Symmetry II”, but going further and

demonstrating the value of matrix isolation, the use of polarised light and time resolved studies to probe various systems. 3. Molecular Photoelectron spectroscopy – Valence and core level PES as a probe of molecules. 4. Applications of NMR spectroscopy quantitative dynamics, 2D spectra.

### Structural Methods

The focus is on using various structural methods to probe materials in the solid state. The complementarity of the various techniques will be emphasised and modern instrumentation will be described. 1. Diffraction techniques – X-ray, neutron and electron diffraction techniques for characterising long range order in extended and molecular solids. 2. Local Probes – EXAFS and X-ray absorption techniques for elucidating local structure. Pair distribution function analysis. X-ray photoelectron spectroscopy for probing electronic structure. NMR spectroscopy

### Organometallic Chemistry: Structures, Bonding and Catalysis

An advanced-level options course that will cover structure and bonding in organometallic chemistry from an experimental and theoretical viewpoint, and the application of organometallic compounds in various catalytic processes.

#### *Homogeneous olefin polymerisation*

Homogeneous vs. heterogeneous olefin polymerisation catalysts; examples of homogeneous transition metal catalysts focussing on metallocene-types; co-catalysts: types and mode of operation; polymerisation mechanism: initiation, propagation, termination;  $\alpha$ -olefins and control of tacticity.

#### *Ring opening Polymerisation*

Introduction to synthesis of “green” polymers using ROP focussing on  $\epsilon$ -caprolactone and lactide; examples of types of catalyst (initiator); initiator and propagation by coordination-insertion and activated monomer mechanisms; transesterification processes; living and immortal ROP; control of tacticity.

#### *Structure and Bonding in Organometallic Chemistry*

Electronic structure of transition metal and main-group metallocenes - comparison with benzene analogues. Development and basis of the isolobal analogy and its importance in organometallic chemistry.

#### *E-H sigma complexes: structure and bonding*

Fundamental issues of electronic structure and bonding in sigma complexes featuring H-H, C-H, Si-H and B-H bonds, relevance to oxidative addition chemistry, spectroscopic probes of the nature of the interaction with the metal.

#### *C-H activation: Fundamentals and catalysis*

C-H...M bonds in organometallic chemistry, a brief survey. C-H activation processes and their mechanisms. Use of C-H activation in synthesis. A discussion of representative catalytic processes using C-H activation, concentrating on mechanism.

#### *Catalytic functionalisation of organic molecules by borane reagents.*

Metal catalysed hydroboration and diboration of alkenes and alkynes, direct borylation of C-halogen and C-H bonds in arenes and alkanes.

### Solid State Compounds in Technology

This builds on the core topics of solid state chemistry. The focus is on properties which confer technological value on solid state compounds (e.g. telecommunications, ICT, energy generation and

storage). For example:

1. Materials for Energy applications. Photovoltaics, Battery Materials, Transparent Conductors, Fuel Cell materials, Thermoelectric materials. How do we use our knowledge of Inorganic Chemistry to devise new compounds with particular properties?
2. Superconductivity. Classical and non-BCS superconductors. Factors affecting T<sub>c</sub>. Recent developments; superconductors in action.
3. Magnetism. The collective magnetism in solids. The uses of magnetic materials in technology – magnetoresistance, multiferroic materials.
4. Thin Films. Methods for Growth of Thin Films. Molecular beam epitaxy, chemical vapour deposition, pulsed laser deposition. Application to III-V and II-VI semiconductors. Bandgap engineering. Heterostructures and device applications.
5. Zeolites and porous material in separation and catalysis.

### Supramolecular and Medicinal Inorganic Chemistry

This course focuses on specific examples of uses of coordination compounds. 1. Supramolecular Chemistry: nature of the non-covalent interactions involved, illustrated with biological and synthetic examples of cation, anion and neutral guest recognition. Importance of preorganisation in host design. Extension of Template Effect to self-assembly, in particular metal-directed self-assembly of polymeric architectures dictated by polydentate ligand design and stereochemical preference of metal. Catalysis within polymeric cage frameworks. Anion coordination chemistry: biological importance; exploiting electrostatics, hydrogen bonding and Lewis acidity in anion receptor design illustrated with synthetic examples. Simultaneous cation and anion (ion-pair) binding by heteroditopic host systems for extraction, salt solubilisation and membrane transport applications.

Case studies will be discussed which highlight the principles of transition metal optical and redox selective sensing of cation and anion analytes of biological and environmental importance.

2. Inorganic Medicinal Chemistry: how inorganic compounds and complexes can be used to treat and diagnose disease. For example: *Therapy*: platinum complexes in cancer chemotherapy, lithium carbonate, photodynamic therapy using porphyrin complexes), radiotherapy (choice of radioisotopes. Ligand design), targeted radiotherapy (bifunctional chelating agents, antibody and peptide targeting, antibody directed prodrug therapies). *Diagnosis: Magnetic Resonance Imaging*: principles of contrast imaging, development of paramagnetic contrast agents; factors influencing contrast agent design; targeted and responsive MRI imaging agents. *Radioisotope Tomography* (Positron Emission Tomography and Single Photon Computer Tomography): blood pool and organ targeted imaging agents, application of bifunctional chelating agents to targeted imaging of receptors. *Luminescent imaging* (responsive probes for endogenous metal ions and anions): time-resolved imaging using lanthanide complexes, lanthanide based bioassay in drug discovery and diagnosis. *Multi-modal imaging* (MRI-PET, optical-PET and optical-MRI).

### Natural Product Chemistry

This course builds upon previous courses on primary metabolism and synthesis and covers secondary

metabolism and biosynthesis of polyketides, fatty acids, terpenes, and alkaloids. The total synthesis of members of these classes of natural product using a biomimetic approach will be discussed.

### **Advanced Synthesis and Total Synthesis**

This course builds from the core 3<sup>rd</sup> year lecture course Organic Synthesis III and will draw together many core synthesis topics. The course will illustrate advances in the total synthesis of major classes of natural products, selected pharmaceuticals, and other challenging molecules, with asides to cover important reactions, reagents, reactivity and strategy principles.

### **Contemporary Methods in Catalysis for Organic Synthesis**

The lecture course will focus on new methods of catalysis, both organometallic and organocatalytic, applied to organic synthesis. Sustainability (Green), industrially relevant chemistry, asymmetric syntheses, mechanistic studies, and applications of key reactions will all be considered.

### **Advanced Chemical Biology**

The course will illustrate how chemical knowledge can be applied to biology with an emphasis on mechanisms and chemical principles. The content of the course may change to reflect current advances. (1) Protein and Peptide Synthesis. Methods, strategy and analysis. Use of protecting groups, coupling reagents and solid phase synthesis. Comparison with non-ribosomal peptide biosynthesis. (2) Protein biosynthesis, proteomics and post-translational modifications (PTMs). Revision of protein bio-synthesis (with an emphasis on translation) and structure. Roles (in brief) and extent of post-translational modifications including proteolysis and protein-splicing. Genetic engineering including recombinant methods, mutants and the polymerase chain reaction. Biological and chemical methods for introducing post translational modifications. Overview of advances in genomics and proteomics highlighting current challenges. (3) Enzymes and biological catalysis I Enzyme families and ways of classifying. Convergent and divergent evolution. Overview of hydrolytic enzymes. Overview of biological catalysts (including ribozymes). Uses and examples involving acyl bond formation and cleavage as a theme (proteasome; proteases; ribosome). Genomic analysis; the problem of identifying substrates/functions and techniques employed. Need for control of enzyme activity. Mechanistic relationships between acyl transfer / hydrolytic enzymes. Enzyme inhibition for medicinal benefit. (4) Enzymes and biological catalysis II. Revision of general principles of enzyme catalysis. Catalytic antibodies. Overview of techniques used to study enzymes in vitro and in vivo - kinetics, crystallography, spectroscopy, synthetic probes. Correlation of structure and chemistry with function. Use of mutants. Kinetics. Enzyme inhibition as illustrated by acyl transfer / hydrolytic enzymes. The penicillin story.

### **Functional Organic Polymers and Materials Chemistry**

#### *Dyes*

Mauveine, chromophores, commercial dyes, synthesis of azo dyes and cyanines, direct dyes, reactive dyes for cellulose, fluorescence, chemiluminescence, photochromics, photoinduced electron-transfer.

#### *Polymers and polymer synthesis*

Polymerisation reactions: condensation vs. addition, step-growth vs. chain-growth, DP, Mn, Mw, polydispersity index, Carothers equation, epoxy-resins, ring opening, stereochemistry, Ziegler Natta, metallocene catalysts, dendrimer synthesis

#### *Living polymerisation*

Anionic, cationic, free radical and ring opening metathesis. Use of living polymerisation to synthesise complex architectures

#### *Liquid Crystals*

Classification: thermotropic/lyotropic, calamitic/isotropic, nematic/smectic/columnar; examples; molecular structural requirements; synthesis; techniques: polarised optical microscopy, differential scanning calorimetry; orientation: by electric fields, by rubbed surfaces, by surfactants; twisted nematic LCD; LC thermometers; LC polymers: main-chain e.g. Kevlar, side-chain

#### *Organic Surface Chemistry*

Comparison of different techniques for preparing and analysing organic surface functions.

#### *Organic Surface Chemistry*

Grafting to and grafting from approaches, polymer brushes, applications of organic surface chemistry.

#### *Organic Semiconductors*

Types of organic metals and semiconductors: charge-transfer salts, conjugated polymers, molecular crystals; polyacetylene and poly-para-phenylene: band structure, solitons and bipolarons, synthesis, precursor routes, substituted derivatives, conformation

#### *Electronic Devices Based on Organic Semiconductors*

Electroluminescence: how an LED works; photovoltaic devices: the basic principles, dye-sensitised cells, polymer blend devices; controlling energy transfer and electron transfer.

### **Fundamentals of Atmospheric and Astrochemistry**

Introduction to the Earth's atmosphere: vertical structure of the atmosphere, pressure, composition, temperature; the hydrostatic equation; blackbody radiation, absorptivity and emissivity, scattering and absorption of solar radiation; radiative balance and the green-house effect; role of boundary layer processes and clouds; photolysis rates.

Half life, residence time and renewal time of chemicals in the atmosphere, the importance of trace species; sources, transformation, transport, and sinks of chemicals in the troposphere; tropospheric chemical cycles; air pollution.

The stratospheric ozone layer, catalytic cycles, perturbations to the ozone layer; polar ozone loss; chemistry of the ionosphere.

Heterogeneous chemistry; aerosol concentration and size distribution, sources of aerosols, transformations, chemical composition, transport, atmospheric effects.

Measurement methods for atmospheric sensing. Ground based methods for minor constituents, absorption, scattering. Remote and satellite sensing.

Introduction to astrochemistry; spectroscopic measurements on extraterrestrial environments; the early universe; synthesis of the elements in stars; cosmic abundance of the elements.

The interstellar medium; molecular gas clouds and chemistry in interstellar space; ionization, gas-phase reaction, and neutralisation processes in interstellar gas clouds.

A simple model for the rate of ion-molecule reactions; dust grain chemistry; chemical modelling of molecular clouds.

## Molecular Reaction Dynamics

Thermally averaged collision properties: state resolved properties. Individual collision events: conservation of energy and angular momentum. Concept of a cross-section, and the relationship with opacity functions and impact parameter.

Elastic and inelastic scattering. Total and differential cross sections: molecular beam scattering experiments. Types of energy transfer and their relationship to intermolecular forces.

Potential energy surfaces. Origin of the PES, and examples. Inelastic and reactive scattering in terms of classical trajectories on surfaces.

Reactive scattering: determining the angular distribution. Crossed molecular beam methods. Reaction mechanisms: stripping mechanism and the harpoon model; rebound reactions; complex formation. Stereochemistry and cones of acceptance.

Reactive scattering: controlling reagents and characterizing products. Selection of reagent states and control molecular orientation. Laser based methods for reagent state selection. Spectroscopic based methods for detecting products. Infrared emission. Laser based methods.

Reactive scattering: interpretation. Potential energy surfaces and attractive and repulsive energy release. Mass effects. Microscopic reversibility: use of reagent energies. Non-adiabatic processes.

Probing the transition state. Half collisions and photodissociation dynamics. Femtochemistry. Photoelectron detachment spectroscopy.

Applications of molecular reaction dynamics. Atomic and molecular lasers. Excimer lasers. Energy transfer and the CO<sub>2</sub> laser. Chemical lasers: CO laser. Chemistry in extreme environments: low and high energy collisions.

## Biophysical Chemistry Option (joint with Inorganic and Organic)

Biophysical chemists seek to understand biological phenomena at the molecular level. They seek to ask questions such as: How do protein machines work? How do proteins pack DNA into viruses? How do viruses invade cells? How do plants harness sunlight to make food? A good historical example of how the application of physical science techniques to biological advances is in the structure of biomolecules: The double-helical model for DNA proposed by Watson and Crick was only possible due to the application of x-ray diffraction to this problem. Many of the skills you have learnt in Physical Chemistry can be applied to tackle similar problems in biology. This course will introduce you to a selection of modern biophysical methods. We will explore the utility of these methods with biological examples.

Single molecule techniques. Introduction. Treatment and analysis of single-molecule data and the connections to ensemble kinetics. Revision of Förster Resonance Energy Transfer & the fundamentals of single-molecule fluorescence imaging. Atomic Force Spectroscopy. Optical Tweezers. Single-channel electrical recording. Applications of single-molecule techniques to biology.

Biological applications of polymer theory. The freely-jointed chain and polymer elasticity. Applications to DNA: genome size and packaging. Beyond the freely-jointed chain: the worm-like chain model.

Biomolecular simulation. Molecular Dynamics and Monte Carlo simulations. Protein folding. Biomolecular mass spectrometry. Mass spectrometry of biomolecules. Mechanisms of ion formation. Methods for ion separation, and activation. Mass measurement of biomolecules, both intact molecules and fragments. Cross-linking. H/D exchange. Oxidative footprinting.

Gas-phase structural biology. Mass spectrometry of protein assemblies. Ion mobility spectrometry. Determination of collision cross section. Relationship to collision cross section with other biophysical parameters. Correlation with other low resolution methods. Electron microscopy

## Theoretical Chemistry

### *Time-Dependent Quantum Mechanics*

Review of time dependence in quantum mechanics; stationary and non-stationary states. Two level system in a rotating field (*e.g.*, ESR/NMR), Rabi oscillations.

Perturbation theory: derivation of 1st order amplitudes, application to two-level systems and a continuous final spectrum (Fermi Golden rule rates). Applications of Fermi Golden rule rates to non-radiative processes in molecules, *e.g.* inter-system crossing and interconversion.

The interaction of light and matter 1: dipole approximation, derivation of the Einstein *A* and *B* coefficients. Derivation of the Einstein *A* and *B* coefficients.

The interaction of light and matter 2: electric susceptibilities, oscillator strengths, and sum rules. Applications to radiative processes in molecules. Molecular electric susceptibilities, oscillator strengths, sum rules.

### *Statistical Mechanics – Mean-field theory*

Recap of statistical mechanics of non-interacting systems; consequences of interactions; role of theory, models and simulation.

Introduction to mean-field theory and concept of molecular field.

Ferromagnetic to paramagnetic transition; Ising model and its mean-field description.

Liquid-gas phase transition; classical partition functions; mean-field derivation of van der Waals equation of state.

### **An Introduction to the Liquid State**

Introduction on waves and interaction between light and matter; point scatterer; Rayleigh Ratio.

Larger particles: Form factor; Rayleigh-Gans-Debye theory; Guinier law; Porod's law. Form factor of a sphere; Radius of gyration; Role of polydispersity; Contrast variation.

More dense suspensions: Structure factor. Solids vs. Liquids; Relation to statistical mechanics (pair distribution function and osmotic compressibility);

Ornstein-Zernike equation; Polymers, micelles, charged spheres, hard spheres.

Dynamic light scattering. Single particle; Van Hove functions, intermediate scattering functions.

Available techniques: light, neutrons, x-rays

### **Magnetic Resonance**

Overview of how modern NMR experiments work. Conceptual and theoretical tools needed to understand something of the inner workings of some of the more important multi-pulse, multi-nuclear, multi-dimensional techniques used to probe the structures and dynamics of molecules.

Brief review of spin interactions in NMR. Zeeman interaction, chemical shift.  $J$ -coupling. Energy levels. Appearance of spectra.

Vector model. Magnetization. Rotating frame. Radiofrequency pulses. Free precession.  $T_1$  and  $T_2$

relaxation. Free induction decay. Spin echoes, echo modulation. Fourier transformation, lineshapes.

Product operators for one spin.

Product operators for two coupled spins. Spin echoes, homonuclear and heteronuclear.

INEPT. Polarization transfer. Multiple quantum coherence. Double quantum filter, INADEQUATE.

Two-dimensional NMR. COSY. NOESY.

Review of quantum mechanics of spin angular momentum. Spin Hamiltonian.

Density matrix. Time-dependent Schrödinger equation. Liouville-von Neumann equation. Pulses and delays.

Two-spin systems.

## APPENDIX F

### Academic Staff

All Staff in the Department can be contacted by e-mail which is generally the best method. Add chem.ox.ac.uk to the e-mail addresses listed below.

<b>Name</b>	<b>Section</b>	<b>Office</b>	<b>College</b>	<b>e-mail</b>
Aarts Prof DGAL	PTC	PTCL	Christ Church	<a href="mailto:dirk.aarts@chem.ox.ac.uk">dirk.aarts@</a>
Adlington Dr RM	OC	CRL	LMH	<a href="mailto:robert.adlington@chem.ox.ac.uk">robert.adlington@</a>
Aldridge Prof S	IC	ICL	Queen's	<a href="mailto:simon.aldridge@chem.ox.ac.uk">simon.aldridge@</a>
Anderson Dr E	OC	CRL	Jesus	<a href="mailto:edward.anderson@chem.ox.ac.uk">edward.anderson@</a>
Anderson Prof HL	OC	CRL	Keble	<a href="mailto:harry.anderson@chem.ox.ac.uk">harry.anderson@</a>
Armstrong Prof FA, FRS	IC	ICL	St. John's	<a href="mailto:fraser.armstrong@chem.ox.ac.uk">fraser.armstrong@</a>
Barford Dr W	PTC	PTCL	Balliol	<a href="mailto:william.barford@chem.ox.ac.uk">william.barford@</a>
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Benesch Dr JLP	PTC	PTCL	University	<a href="mailto:justin.benesch@chem.ox.ac.uk">justin.benesch@</a>
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Brouard Prof M	PTC	PTCL	Jesus	<a href="mailto:mark.brouard@chem.ox.ac.uk">mark.brouard@</a>
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Clarke Dr SJ	IC	ICL	Exeter	<a href="mailto:simon.clarke@chem.ox.ac.uk">simon.clarke@</a>
Clary Prof DC, FRS	PTC	PTC	Magdalen	<a href="mailto:david.clary@chem.ox.ac.uk">david.clary@</a>
Compton Prof RG	PTC	PTCL	St John's	<a href="mailto:richard.compton@chem.ox.ac.uk">richard.compton@</a>
Conway Dr SJ	OC	CRL	St Hugh's	<a href="mailto:stuart.conway@chem.ox.ac.uk">stuart.conway@</a>
Cooper Dr RI	IC	CRL	Pembroke	<a href="mailto:richard.cooper@chem.ox.ac.uk">richard.cooper@</a>
Davies Prof SG	OC	CRL	Magdalen	<a href="mailto:steve.davies@chem.ox.ac.uk">steve.davies@</a>
Davis Prof BG	OC	CRL	Pembroke	<a href="mailto:ben.davis@chem.ox.ac.uk">ben.davis@</a>
Davis Dr JJ	IC	PTCL	Christ Church	<a href="mailto:jason.davis@chem.ox.ac.uk">jason.davis@</a>
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### Commonly used abbreviations:

OC = Organic Chemistry
IC = Inorganic Chemistry
PTC = Physical and Theoretical Chemistry
CB = Chemical Biology
CRL = Chemistry Research Laboratory
ICL = Inorganic Chemistry Laboratory
PTCL = Physical and Theoretical Chemistry Laboratory
DP = Dyson Perrins Building
T.Lab = Teaching Laboratory
MPLS = Mathematical, Physical and Life Sciences Division

## University Policies

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There are formal University Policy documents in the following areas, which are drawn to your attention. To ensure that these are up to date, please consult the relevant University web pages.

Intellectual property: <http://www.admin.ox.ac.uk/researchsupport/ip/>.

Plagiarism: <http://www.ox.ac.uk/students/academic/goodpractice/about/>

Equal opportunities: <http://www.admin.ox.ac.uk/eop/policy/index.shtml>.

Disability: <http://www.admin.ox.ac.uk/eop/disab/>.

Harassment: <http://www.admin.ox.ac.uk/eop/harassmentadvice/>

Health and safety: <http://www.admin.ox.ac.uk/safety/hs-mgement-policy/>

Computer usage: <http://www.ict.ox.ac.uk/oxford/rules/>.

Examination regulations: <http://www.admin.ox.ac.uk/examregs/contents.shtml>.

The Proctors' Memorandum: <http://www.admin.ox.ac.uk/proctors/info/pam/index.shtml>.

Data Protection Act 1998: <http://www.admin.ox.ac.uk/councilsec/dp/>