Department of Chemistry

Undergraduate Course Handbook

Academic year 2016 - 2017

http://www.chem.ox.ac.uk
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This Handbook applies to students starting the course in Michaelmas Term 2016. The information in this handbook may be different for students starting in other years. Suggestions for future editions are always welcome please contact nina.jupp@chem.ox.ac.uk.

The Examination Regulations relating to this course are available at http://www.admin.ox.ac.uk/examregs/2016-17/pexamchem/studentview/ and http://www.admin.ox.ac.uk/examregs/2016-17/hschoofchem/studentview/. If there is a conflict between information in this handbook and the Examination Regulations then you should follow the Examination Regulations. If you have any concerns please contact Nina Jupp, <nina.jupp@chem.ox.ac.uk>.

The information in this handbook is accurate as September 2016, however it may be necessary for changes to be made in certain circumstances, as explained at http://admissions.chem.ox.ac.uk/course.aspx (www.ox.ac.uk/coursechanges)/PG (www.graduate.ox.ac.uk/coursechanges) webpage. [If such changes are made the department will publish a new version of this handbook together with a list of the changes and students will be informed.]
Message from Head of Department

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 180-190 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, 450 postgraduates and 500 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 walks 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 discipline, 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. The Part II experience – a full year of research – remains unique amongst UK Chemistry courses. In 2017 we reach the 100th anniversary of the completion of the first Part II year at Oxford and I hope you will have the opportunity to celebrate this anniversary with us.

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.

Mark Brouard, Head of Department

How to use this Handbook

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).

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.

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://teaching.chem.ox.ac.uk/ 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 September 2016. 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.ox.ac.uk/students/academic/exams/entry the only official timetable.
Introduction

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

Safety

Chemistry is a practical subject, and an important part of the course is to train you to conduct experiments safely and to assess and minimise any risks before starting an experiment. Your safety is our top priority, but a large part of this is dependent on you. An important resume of the main safety concerns in the lab can be found on the web at http://course.chem.ox.ac.uk/safety.aspx. In addition the lab manuals have more detail on each experiment and the procedure for risk assessment.

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 (RSL). The 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. 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

Undergraduates will have Chemistry focused IT skills training workshops as part of the undergraduate practical course and opportunity to use the central IT services training courses for more general IT training requirements. 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.it.ox.ac.uk/rules/. The URL for the University Computing Service is http://www.it.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/council/sec/dp/index.shtml for details).

Channels of Communication

Academic Staff have pigeon-holes in the buildings where they have offices and in their Colleges. Staff may also be contacted by telephone or by e-mail. Most of them prefer email, 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), 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 email. It is therefore necessary for mailboxes to be kept clear at all times.

Support for Students

Colleges provide pastoral support through subject tutors and other welfare officers. The university counselling service offers confidential help and advice to students, who can access it through their college welfare officers.

The Disability Advisory Service

https://www.ox.ac.uk/students/welfare/disability should be contacted for advice on sensory or mobility impairments, health conditions, specific learning difficulties, autistic spectrum conditions or mental health difficulties. The disability lead in the Department is nicholas.green@chem.ox.ac.uk who is responsible for strategic oversight or provision for disabled students, and the disability co-ordinator is nina.jupp@chem.ox.ac.uk, who coordinates and organises the implementation of this provision.

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, i) the teaching arrangements, lectures, and seminars; organisation and coverage; ii) the practical courses: composition, organisation, and formal requirements, safety; iii) the syllabus and structure of Examinations; iv) library facilities; v) 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 http://teaching.chem.ox.ac.uk/

The CJCC comprises fourteen undergraduate members, three postgraduate representatives and
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 Master of Chemistry degree is fully accredited at the Masters level by the Royal Society of Chemistry. The University Awards Framework (UAF) award the course FHEQ Level 7, minimum credit value of 180. The full course specification can be found from web address: http://teaching.chem.ox.ac.uk/

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 flow from 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; 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. 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 course 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 lectures and where appropriate they are online: 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. During the first three years practical work is compulsory. Practical work is assessed 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. There is a practical course database on which both you and your tutors can follow your progress and where you can book laboratory slots. You can find this at http://teaching.chem.ox.ac.uk/. Details of arrangements for the practical courses is online: http://course.chem.ox.ac.uk/practicals.aspx

Tutorial teaching (typically 2 or 3 in a group) is based in your College. Your tutor will provide 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. Each term your tutors will write a report on your progress, which will be available to your College and to you via an online system called OxCORT, and you also have the opportunity to give feedback on your tutorials.

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 design an appropriate experiment to solve a problem.
  - 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.

A wide range of information and training materials is available to help you develop your academic skills – including time management, research and library skills, referencing, revision skills and academic writing – through the Oxford Students website http://www.ox.ac.uk/students/academic/guidance/skills

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.

Guidance on paid work

www.ox.ac.uk/students/life/experience

Examinations

There are Examinations in the first three years: Prelims, Part IA and Part IB 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://teaching.chem.ox.ac.uk/. Part II is examined by thesis and viva.

Instructions for entering University Examinations and examination timetables can be found via http://www.ox.ac.uk/students/academic/exams/en try

Information on (a) the standards of conduct expected in examinations and (b) what to do if you would like examiners to be aware of any factors that may have affected your performance before or during an examination (such as illness, accident or bereavement) are available on the Oxford Students website www.ox.ac.uk/students/academic/exams/guidance

The current examiners responsible for examinations in years 1 - 4, can be found from http://intranetchem.ox.ac.uk/committee-membe rmembers.aspx

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 is 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 the first two years of the course; the results are carried forward to be taken into account together with Parts IB and II to determine your final degree 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 options 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.

**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 M.Chem Degree. Part II is weighted 25% in the final classification.

The oral Examinations will be usually held in 10th and 11th 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 

http://www.admin.ox.ac.uk/examregs/ and the Examination Conventions below. 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 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.

Written Examinations are marked anonymously, candidates are identified by number only; at Part II any Examiner who knows a candidate personally will neither 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://teaching.chem.ox.ac.uk/

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 that 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 Procedure

If your concern or complaint relates to teaching or other provision made by the faculty/department, then you should raise it with the Associate Head (teaching) (Dr. N.J.B. Green) or his deputy (TBA). The officer concerned will attempt to resolve your concern/complaint informally. General areas of concern about provision affecting students as a whole should be raised through Chemists' Joint Consultative Committee (CJCC).

If you are dissatisfied with the outcome, you may take your concern further by making a formal complaint to the Proctors under the University Student Complaints Procedure (https://www.ox.ac.uk/students/academic/complaints).

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/index.shtml

If your concern or complaint relates to teaching or other provision made by your college, you should raise it either with your tutor or with one of the college officers / Senior Tutor. Your college will also be able to explain how to take your complaint further if you are dissatisfied with the outcome of its consideration. Further information on the complaints procedure is on the web at http://teaching.chem.ox.ac.uk/.

Academic appeals

An academic appeal is an appeal against the decision of an academic body (e.g. boards of examiners, transfer and confirmation decisions etc.), on grounds such as procedural error or evidence of bias. There is no right of appeal against academic judgement.

If you have any concerns about your assessment process or outcome it is advisable to discuss these first informally with your subject or college tutor, Senior Tutor, course director, director of studies, supervisor or college or departmental administrator as appropriate. They will be able to explain the assessment process that was undertaken and may be able to address your concerns. Queries must not be raised directly with the examiners.

If you still have concerns you can make a formal appeal to the Proctors who will consider appeals under the University Academic Appeals Procedure (https://www.ox.ac.uk/students/academic/complaints).

Examination Conventions in Chemistry

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 (available online at http://www.admin.ox.ac.uk/examregs/information/contents/) and the Undergraduate Course Handbook (http://teaching.chem.ox.ac.uk/Data/Sites/58/media/courseinfo/undergradhandbook2016.pdf). 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). Such enquiries are welcome, as clarification helps everybody. It is not appropriate to address Chairmen of Examiners on such matters.

Details of the membership of the examination boards can be found at the following web address: https://intranet.chem.ox.ac.uk/committee-members.aspx. The Part IA, Part IB and Part II boards each consist of 9 internal and 3 external examiners in addition to the chair. The Prelims board consists of 8 examiners, one of whom is also chair. Candidates must not contact examiners or the chair on examination matters directly under any circumstances.

Prelims

See especially the relevant part of the Examination Regulations: (http://www.admin.ox.ac.uk/examregs/2016-17/examinchem/studentview/), but general regulations found elsewhere also apply.

Each paper is set as a two and a half hour exam, except for the Organic Chemistry paper, which will be a three hour exam.

Each paper will be marked out of 100, according to the outline marking scheme printed on the question paper. Marks may be rescaled if necessary. 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 (45%) 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 (70%) 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.

A candidate who has failed in one or two subjects may offer those subjects at a subsequent examination, and will be deemed to have passed all Parts of Prelims if they pass these resit examinations.

A candidate who has failed in three or four subjects may retake Prelims at a subsequent examination, but must offer all four subjects and will not be deemed to have passed Prelims unless they pass all four resit examinations.

The maximum number of attempts permitted at Prelims is two.

**Progression and classification**

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, together with the second and third year practical course and Part II, are conceived as parts of one examination, the Second Public Examination.

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.

After Part IB a decision is made to identify those who are worthy of Honours. This decision is based on an aggregate of Part IA and Part IB exam marks and marks for the practical course with a relative weighting of 15:50:10 respectively. The award of Honours is also conditional on completion of the minimum practical requirement.

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 Chair of Examiners and the External Examiners.

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.

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.

**Parts IA and IB**

See Examination Regulations, [http://www.admin.ox.ac.uk/examregs/2016-17/hsooofchem/studentview/](http://www.admin.ox.ac.uk/examregs/2016-17/hsooofchem/studentview/), but general regulations found elsewhere also apply.

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, with 10 minutes reading time, 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. The length and difficulty of the questions will be the same as when the exams were two and a half hours, but candidates will be given three hours to attempt them, giving time for reading, reflection and reviewing answers. Candidates are discouraged from wasting the extra time by attempting additional questions. The Options Paper is three hours, plus 10 minutes reading time, 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. The mark scheme is a guide, and examiners have the discretion to vary it if necessary. Marks may be rescaled 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, and contribute 15% to the final degree classification. The six General Papers in Part IB have equal weight, and contribute 42% towards the final degree. The Options paper contributes 8%.

**Practical course**

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 (a reduced third year course may be offered if a Supplementary Subject has been passed, as outlined below).

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
Supplementary subjects

A pass or distinction in a Supplementary Subject may be offered as an alternative to 6 days (36 credit hours) 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. Good marks in Supplementary Subjects will be recognised by the allocation of extra credit for the final assessment after Part II. For science based subjects this applies to marks of 60% or more, and for modern languages a mark of 70% or more.

These bonus marks will be credited for each Supplementary Subject passed at the appropriate level, 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:

(http://www.admin.ox.ac.uk/examregs/2016-17.hschoochem/studentview/)

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. Examiners may refuse to examine a thesis if it fails to conform to these instructions.

Theses will be read by two Examiners, each of whom will assign a 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


The two principal readers of the thesis will also act as examiners in 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 Chair. Other than in exceptional circumstances, the viva cannot result in a decrease in the thesis marks.

The pass mark for Part II shall be an overall score of 40% (88/220).

Supervisors will be asked to report on the work of all candidates and on any special difficulties or advantages the candidates may have had. No part of the Part II mark is given by the supervisor or allocated to the supervisor's report.

Supplementary Subjects may be taken during the Part II year, and mark bonuses will be allocated for good performance, as outlined previously. However, no retrospective compensation for shortfalls in practical work or IT work reported to the Part II 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 good performance in Supplementary Subjects will be added after aggregation.

Part II theses must be submitted to the Examination schools before the deadline of noon on the Friday of 7th week. Applications for late submission, for example because of illness, must be made to the Proctors. All unauthorised submissions after the deadline will be reported to the Proctors for investigation of the reasons for late submission, 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.

<table>
<thead>
<tr>
<th>Lateness</th>
<th>Penalty marks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Up to 5 pm on the Friday of 7th week</td>
<td>2.2 (1%)</td>
</tr>
<tr>
<td>Up to 5 pm on the Monday of 8th week</td>
<td>11 (5%)</td>
</tr>
<tr>
<td>Up to 5 pm on the Tuesday of 8th week</td>
<td>22 (10%)</td>
</tr>
<tr>
<td>Up to 5 pm on the Wednesday of 8th week</td>
<td>44 (20%)</td>
</tr>
<tr>
<td>Up to noon of the Friday of 8th week</td>
<td>66 (30%)</td>
</tr>
<tr>
<td>More than a week late</td>
<td>Fail</td>
</tr>
</tbody>
</table>

For example, a thesis given an overall Part II mark of 141/220 (64%) by the examiners on the basis of the thesis and the viva, but submitted on the Monday of 8th week will be penalised 11 marks (5%) and awarded a final mark of 130/220 (59%). Any penalty assessed will be capped so that it does not take the Part II mark below the pass mark, 40%, 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.

Medical certificates

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. Medical certificates will also be considered for 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 or by disregarding that mark in deciding a classification.

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 (USMs) 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. Marks may be rescaled (see below). If scaling is used, details will be provided in the Chair'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 question 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 4 marks will be taken and the lowest mark discarded. Students are strongly advised not to attempt more questions than required: time spent doing an extra question that will not count towards the total is time wasted. Any spare time is much better spent in checking and correcting answers.

Errors may be carried forward at the discretion of the examiner, depending on the nature and severity of the error. Similarly, partial credit may be given at the discretion of the examiner for incorrect but reasonable answers, particularly if they demonstrate that the candidate is thinking through the problem in a rational way. These are both matters of academic judgement.

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

Practical marks will be awarded according to a detailed scheme that assesses the pre-lab, practical skills, results and the write-up. The relative weights of these components vary from experiment to experiment. 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. Marks for practicals submitted for marking beyond the 2-week deadline without good reason will be capped at 40%. Practicals submitted for marking more than 4 weeks after the start without good reason will be awarded zero marks. Practicals must be submitted for marking, and judged satisfactory, in order to be counted towards the Part I requirement (252 or 216 credit hours, according to whether a Supplementary Subject has been passed).

Unless there is very good reason, any student who fails to attend a timetabled or booked lab session and who has not contacted a lab manager in advance to make alternative arrangements will receive a marks penalty of 50% for that session, even if the practical is completed at a later date.

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. 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/practics.aspx

Scaling of examination marks

It is university policy to award University Standard Marks (USMs) for examinations, so that a first class performance corresponds to a mark of 70% or more, an upper second class mark is between 60% and 70%, a lower second class mark between 50% and 60% and a third class mark between 40% and 50%. Examination marks may be scaled for any or all of the following reasons:

(a) a paper was easier or more difficult than in previous years;

(b) an option was more or less difficult than other options taken by students in a particular year;

(c) a paper has generated a spread of marks which is not a fair reflection of student performance on the University's standard scale for the expression of agreed final marks.

Scaling is not automatic. The decision about whether to scale, the extent of the scaling and the method of scaling will be made by the examination board according to their academic judgement.

The choice of scaling method will depend on an analysis of the examination scripts, the marks distribution, marks obtained on the other papers taken by the candidates in question, the historical record and the class descriptors. For example, if an examination has been harder than expected, and this has persisted across the whole school, as judged by a cumulative sum analysis, then a straightforward linear scaling may be selected. However, if the best candidates have been less affected by the problem, but the majority of candidates have found the examination too hard, then regular scaling may be employed. This is a single parameter scaling, based on the theory of regular solutions:

\[ y = x \exp \left( \alpha (100 - x) \right)^2 \]
**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:

<table>
<thead>
<tr>
<th>Part</th>
<th>Contribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Part IA paper</td>
<td>5%</td>
</tr>
<tr>
<td>Each Part IB paper</td>
<td>7%</td>
</tr>
<tr>
<td>Part IB Option paper</td>
<td>8%</td>
</tr>
<tr>
<td>Part I Practical course</td>
<td>10%</td>
</tr>
<tr>
<td>Part II</td>
<td>25%</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Class</th>
<th>General</th>
<th>Mark range</th>
<th>Problems</th>
<th>Part II and essays</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class 1</td>
<td>Excellent problem-solving skills and excellent knowledge of the material over a wide range of topics, and ability to use that knowledge in unfamiliar contexts.</td>
<td>90% - 100%</td>
<td>Complete understanding, formulation correct, all steps and assumptions explained properly. Technically without fault.</td>
<td>High degree of commitment to the project. Clear evidence of initiative and independence. Excellent organisation, logical development, thorough critical analysis of literature and data, excellent presentation.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80% - 90%</td>
<td>Excellent understanding, formulation correct, clear explanations, very few errors.</td>
<td>Strong intellectual input into design and implementation of project. Excellent, original, well written and structured. Critical analysis of data and command of the literature. High quality presentation.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>70% - 80%</td>
<td>Very good understanding, formulation correct, principal steps clear, any errors are minor.</td>
<td>Clear evidence of intellectual input and engagement with project. Good understanding of the topic and the literature. Critical analysis of data. Well written and clearly structured.</td>
</tr>
<tr>
<td>Class 2.1</td>
<td>Good or very good problem-solving skills, and good or very good knowledge of much of the material over a wide range of topics.</td>
<td>60% - 70%</td>
<td>Sound to good understanding, principal steps explained. Some errors.</td>
<td>Evidence of some intellectual input. Competent and coherent writing. Good presentation, literature knowledge and analysis of data.</td>
</tr>
<tr>
<td>Class 2.2</td>
<td>Basic problem-solving skills and adequate knowledge of most of the material.</td>
<td>50% - 60%</td>
<td>Adequate understanding, not all steps explained and maybe some gaps in logic. Some errors leading to incorrect or incomplete answers.</td>
<td>Routine treatment of data, literature coverage may have gaps, writing competent, but little sign of critical thinking or intellectual input.</td>
</tr>
<tr>
<td>Class 3</td>
<td>Reasonable understanding of at least part of the basic</td>
<td>40% - 50%</td>
<td>Incomplete understanding and formulation. Steps not explained, assumptions not</td>
<td>Shallow, narrow approach. Poor understanding and little sign of thought in selection of material</td>
</tr>
</tbody>
</table>
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 | 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. | 30% - 40% | Limited understanding, large gaps. Some sign of thought, but little actually correct. | Little evidence of understanding or attempt to approach the topic. |
| Fail | 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. | < 30% | Inadequate understanding, fragmentary answers. | No engagement with the project. No sign of effort or thought |

The interpretation of these Descriptors is at the discretion of the Examiners. For problem questions answers may be very patchy, excellent in some places and erroneous or missing in others, it is therefore hard to apply these descriptors to problems, although it should still be a helpful check list.
Lectures and Practicals  The lecture timetable and information regarding practicals can be accessed from the Chemistry web page:  
http://teaching.chem.ox.ac.uk/.

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 makes tangible much that is covered in lectures and tutorials. There is also an IT course concerning computer applications and chemistry software packages (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 responsible practical coordinator at the earliest opportunity. The following people are responsible for the first year practical courses:

Organic: Dr. Malcolm Stewart
Inorganic: Dr. Vlad Kuznetsov
Physical: Dr. Zsuzsa Mayer
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 6th week of Trinity Term. This is a University examination deadline and may only be relaxed by permission of the Proctors. 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.

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 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 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 IT Services, 13 Banbury Road, and in week 8 of TT you will be given a short course in programming using Python.

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 each of the foyers of 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
- introduction to organic spectroscopy
- substitution and elimination at saturated carbons
- introduction to organic synthesis
- carbonyl group chemistry
- chemistry of C–C π-bonds
- introduction to biological chemistry

For more detail, see Appendix D.

Examinations (Prelims) See page 6.

Schedule for First Year Lectures

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

http://teaching.chem.ox.ac.uk/timetables.aspx  M = Michaelmas Term, H = Hilary Term, T = Trinity Term

<table>
<thead>
<tr>
<th>Subject</th>
<th>Hours per Term</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Inorganic Chemistry</strong></td>
<td></td>
</tr>
<tr>
<td>Atomic Structure and Periodic Trends</td>
<td>6</td>
</tr>
<tr>
<td>Ionic Model and Structures of Solids</td>
<td>10</td>
</tr>
<tr>
<td>Molecular Shapes, Symmetry and Molecular Orbital Theory</td>
<td>6</td>
</tr>
<tr>
<td>Acids, Bases and Solution Equilibria</td>
<td>4</td>
</tr>
<tr>
<td>Non-metal Chemistry</td>
<td>6</td>
</tr>
<tr>
<td>Transition Metal Chemistry</td>
<td>4</td>
</tr>
<tr>
<td>Revision topics</td>
<td>4</td>
</tr>
<tr>
<td><strong>Organic Chemistry</strong></td>
<td></td>
</tr>
<tr>
<td>Introduction to Organic Chemistry</td>
<td>7</td>
</tr>
<tr>
<td>Introduction to Organic Spectroscopy</td>
<td>2</td>
</tr>
<tr>
<td>Orbitals and Mechanisms</td>
<td>7</td>
</tr>
<tr>
<td>Substitution and Elimination of Saturated Carbons</td>
<td>8</td>
</tr>
<tr>
<td>Chemistry of C–C π Bonds</td>
<td>8</td>
</tr>
<tr>
<td>Core Carbonyl Chemistry</td>
<td>8</td>
</tr>
<tr>
<td>Introduction to Biological Chemistry</td>
<td>12</td>
</tr>
<tr>
<td>Revision Course</td>
<td>4</td>
</tr>
<tr>
<td><strong>Physical Chemistry</strong></td>
<td></td>
</tr>
<tr>
<td>Foundations of Physical Chemistry: Chemical Thermodynamics</td>
<td>13</td>
</tr>
<tr>
<td>The Physical Basis of Chemistry: Classical mechanics</td>
<td>4</td>
</tr>
<tr>
<td>The Physical Basis of Chemistry: Property of gases</td>
<td>4</td>
</tr>
<tr>
<td>The Physical Basis of Chemistry: The role of charge I</td>
<td>4</td>
</tr>
<tr>
<td>The Physical Basis of Chemistry: The role of charge II</td>
<td>4</td>
</tr>
<tr>
<td>Quantum Theory of Atoms and Molecules</td>
<td>10</td>
</tr>
<tr>
<td>Reaction Kinetics</td>
<td>6</td>
</tr>
<tr>
<td>Electrochemistry</td>
<td>4</td>
</tr>
<tr>
<td>States of Matter</td>
<td>4</td>
</tr>
<tr>
<td><strong>Mathematics for Chemistry</strong></td>
<td></td>
</tr>
<tr>
<td>The Calculus of One and Two Variables</td>
<td>20</td>
</tr>
<tr>
<td>Introduction to Vectors</td>
<td>2</td>
</tr>
<tr>
<td>Vector Algebra and Determinants</td>
<td>6</td>
</tr>
<tr>
<td>Complex Numbers, Multiple Integrals and Ordinary Differential Equations</td>
<td>10</td>
</tr>
<tr>
<td>Matrix Algebra</td>
<td>8</td>
</tr>
</tbody>
</table>
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
- 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
- organic spectroscopy

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](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. Vlad Kuznetsov
- Physical Practicals: Dr. Zsuzsa Mayer
- 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](http://course.chem.ox.ac.uk/supplementary-sub.aspx)

On offer for 2016-17 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 mark over 60% in the science based supplementary subjects, gives extra credit for the final assessment in Part II. For modern languages a mark over 70% gives extra credits.

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://teaching.chem.ox.ac.uk/timetables.aspx).

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

<table>
<thead>
<tr>
<th>Subject</th>
<th>Hours per Term</th>
<th>M</th>
<th>H</th>
<th>T</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Inorganic Chemistry</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Diffraction</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Transition Metal Chemistry</td>
<td>6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bonding in Molecules</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Co-ordination Chemistry</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chemistry of the Lanthanides and Actinides</td>
<td>4</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Organometallic Chemistry</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Electronic properties of solids</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Periodic trends in main-group Chemistry</td>
<td>5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NMR in Inorganic Chemistry</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Course overview</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Revision Topics</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Organic Chemistry</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Aromatic and Heterocyclic Chemistry</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Organic Synthesis I</td>
<td>4</td>
<td></td>
<td></td>
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<tr>
<td>Organic Spectroscopy I</td>
<td>6</td>
<td></td>
<td></td>
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<tr>
<td>Conformational Analysis and Ring Chemistry</td>
<td>10</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Physical Organic Chemistry</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rearrangements and Reactive Intermediates</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heteroatoms in Organic Synthesis</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Organic Synthesis II</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Organic Chemistry of Biomolecules</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Problem Solving</td>
<td>2</td>
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<td>Quantum Mechanics: Principles and Applications</td>
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<td>Liquids and Solutions</td>
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<td>Statistical Mechanics</td>
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<td>Valence</td>
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<td>Rate Processes</td>
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<td>Revision Lectures</td>
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<td>Introduction to NMR</td>
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<td>Aromatic, Heterocyclic and Pharmaceutical Chemistry</td>
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<td>Chemical Crystallography</td>
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<td>History and Philosophy of Science</td>
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<td>Modern Language</td>
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</table>
The Course

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

- post transition metal chemistry
- inorganic reaction mechanisms
- bioinorganic chemistry
- main group chemistry
- solid state chemistry
- spectroscopy and magnetism
- organometallic reaction mechanisms and catalysis
- organic spectroscopy
- pericyclic reactions
- transition metal catalysis in organic synthesis
- radical reactions in organic chemistry
- curly arrows of biology
- strategies in synthesis
- magnetic resonance
- photophysics & photochemistry
- soft condensed matter
- physical principles of solids
- statistical mechanics

Additionally, 15 option courses are available as listed in the “Schedule for 3rd year Lectures” below.

Schedule for Third Year Lectures

For more details see the Chemistry Department’s Lecture web page: (http://teaching.chem.ox.ac.uk/)

<table>
<thead>
<tr>
<th>Subject</th>
<th>Hours per term</th>
<th>M</th>
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<tr>
<td>Inorganic Chemistry</td>
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<td>Inorganic Reaction Mechanisms</td>
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<tr>
<td>Modern main group chemistry</td>
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<tr>
<td>Organometallic Chemistry</td>
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<tr>
<td>Solid State Chemistry</td>
<td>5</td>
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<tr>
<td>Spectroscopy and Magnetism in Inorganic Chemistry</td>
<td>5</td>
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<tr>
<td>Bioinorganic Chemistry</td>
<td>4</td>
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<td>Revision of Topics Inorganic Chemistry</td>
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<td>Review of Periodic Table</td>
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<tr>
<td>Organic Chemistry</td>
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<tr>
<td>Advanced Organic Spectroscopy</td>
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<tr>
<td>Curly Arrows of Biology</td>
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<td>Organic Synthesis III</td>
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<td>Transition Metal Catalysis</td>
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<td>Pericyclic Reactions</td>
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<td>Radical Reactions</td>
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<td>Revision Lectures</td>
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<tr>
<td>Physical Chemistry</td>
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<tr>
<td>Physical Principles of Solids</td>
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<td>Soft Condensed Matter</td>
<td>8</td>
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<tr>
<td>Photophysics and Photochemistry</td>
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</table>

Option Courses

<table>
<thead>
<tr>
<th>Subject</th>
<th>Hours per term</th>
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<tbody>
<tr>
<td>Molecular Spectroscopy</td>
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<tr>
<td>Structural Methods</td>
<td>8</td>
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<tr>
<td>Organometallic Chemistry; Structures, Bonding and Catalysis</td>
<td>8</td>
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<tr>
<td>Solid State Compounds in Technology</td>
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<tr>
<td>Supramolecular Nano and Medicinal Inorganic Chemistry</td>
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<tr>
<td>Natural Product Chemistry</td>
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<td>Advanced Synthesis and Total Synthesis</td>
<td>8</td>
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<tr>
<td>Contemporary Methods in Catalysis for Organic Synthesis</td>
<td>8</td>
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<tr>
<td>Advanced Chemical Biology</td>
<td>8</td>
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<tr>
<td>Functional Organic Polymers and Materials Chemistry</td>
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<tr>
<td>Fundamentals of Atmospheric and Astrochemistry</td>
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<tr>
<td>Molecular Reaction Dynamics</td>
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<td>Theoretical Chemistry</td>
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<td>An Introduction to the Liquid State</td>
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<tr>
<td>Magnetic Resonance</td>
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</table>
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/researchthemes.asp](http://www.chem.ox.ac.uk/researchthemes.asp) 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](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://teaching.chem.ox.ac.uk/](http://teaching.chem.ox.ac.uk/).

Guidance for approaching the Part II may be found on the departmental web page from [http://teaching.chem.ox.ac.uk/](http://teaching.chem.ox.ac.uk/). 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://faculty.chem.ox.ac.uk/](http://faculty.chem.ox.ac.uk/).

A number of substantial Prizes and Bursaries are available. In 2016 the following were awarded:

- **Bruker (UK) Ltd. for excellence in Prelims**: total of £300
- **SAB Miller Plc. for excellence in Part IA**: total of £1,000
- **OUP Book Prize £150** for the most improved candidate/s between Prelims and Part IA
- **Gibbs Prize in Chemistry for excellence in Part IB**: first prize, proxime accessit and three book prizes totalling £1,700

In addition there were Thesis Prizes for excellence in Part II, and in practical work, and there are College Prizes as well.

**History of Alchemy and Chemistry Prize, in Part II, £150**
Appendix A

Recommended Core Textbooks

The following will be useful from the outset, more detailed recommendations will be made by lecturers and tutors.

• Physical Chemistry, Atkins, de Paula; OUP [10th edn., 2014].
• Foundations of Organic Chemistry, Hornby & Peach; Oxford Chemistry Primer, OUP, 1997:
  • Illustrated edition 2000
• Organic Chemistry, Maitland Jones, Fleming; Norton [5th edn. 2014]
• 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

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

### DATES OF FULL TERM 2016-17

<table>
<thead>
<tr>
<th>Term</th>
<th>Dates</th>
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<tbody>
<tr>
<td>MICHAELMAS TERM</td>
<td>Sunday 9 October - Saturday 3 December</td>
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<tr>
<td>HILARY TERM</td>
<td>Sunday 15 January - Saturday 11 March</td>
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<tr>
<td>TRINITY TERM</td>
<td>Sunday 23 April - Saturday 17 June</td>
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### DATES OF FULL TERM 2017-18

<table>
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<th>Term</th>
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<tbody>
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<td>MICHAELMAS TERM</td>
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</tr>
<tr>
<td>HILARY TERM</td>
<td>Sunday 14 January - Saturday 10 March</td>
</tr>
<tr>
<td>TRINITY TERM</td>
<td>Sunday 22 April - Saturday 16 June</td>
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### DATES OF EXTENDED TERM for Part II Candidates in Chemistry 2016-17

<table>
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<tr>
<th>Term</th>
<th>Dates</th>
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<tr>
<td>MICHAELMAS TERM</td>
<td>Thursday 22 September - Tuesday 20 December</td>
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<tr>
<td>HILARY TERM</td>
<td>Tuesday 3 January - Wednesday 12 April</td>
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<tr>
<td>TRINITY TERM</td>
<td>Monday 24 April - Saturday 8 July</td>
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### DATES OF EXTENDED TERM for Part II Candidates in Chemistry 2017-18

<table>
<thead>
<tr>
<th>Term</th>
<th>Dates</th>
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</thead>
<tbody>
<tr>
<td>MICHAELMAS TERM</td>
<td>Thursday 21 September - Tuesday 19 December</td>
</tr>
<tr>
<td>HILARY TERM</td>
<td>Tuesday 2 January - Wednesday 28 March</td>
</tr>
<tr>
<td>TRINITY TERM</td>
<td>Monday 9 April - Saturday 7 July</td>
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</table>

### 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.ox.ac.uk/students/exams/timetables/](http://www.ox.ac.uk/students/exams/timetables/) and more examination information can be found on [http://teaching.chem.ox.ac.uk/examinations.aspx](http://teaching.chem.ox.ac.uk/examinations.aspx). 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** begins 8th week Hilary Term (except Modern Languages) to be taken in 8th week Trinity Term
- **Prelims** begins 7th week Trinity Term
- **Part IA Examination** begins 8th week Trinity Term
- **Part IB Examination** begins 6th week Trinity Term
- **Part II Thesis deadline** 7th week (Friday, 12 noon) Trinity Term
- **Part II Vivas** begin 10th 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.
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, their values and interpretation (hence 2s, 3d, 4f, etc.) Shapes and energies of orbitals. Radial wavefunction and the radial distribution function.


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 AB₂ 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, metal ions in 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.


Acids, Bases and Solution Equilibria


Non-Metal Chemistry


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


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


Introduction to Organic Spectroscopy


Orbitals and Mechanisms

Acids and bases: resonance and inductive effects. Thermodynamics and kinetics. Hammond postulate. FM0 interactions. Conjugation; vinylogy. Reactions: curly arrow rules, formal charges, mechanism and structure as a consequence of FM0 interactions. Solvent effects, reactive intermediates: C₂, C₃, C₄.

Substitution and Elimination at Saturated Carbons


Core Carbonyl Chemistry

Keto-enol tautomerism: α-racemisation in acid or base. pKs of simple FGs including malonates. Reactions of enolates. Allylation, 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 σ-Bonds

Alkyne reactivity: electrophilic addition, hydration to ketones, alkylation of terminal alkenes, reduction. Conjugation/localisation in non-aromatic systems: conjugated alkenes and alkenes, allenes. Modifications to reactivity, conjugate addition reactions.


Introduction to Biological Chemistry.
Introduction, context and structure of a cell, highlighting molecules that are important in biology. Amino acid structure, chemistry and synthesis. Peptide structure, conformation and simple synthesis. Primary protein structure and sequencing, secondary, tertiary and quaternary protein structure.

Introduction to the importance of enzymes in catalysing the diverse chemical reactions of life; how enzyme active sites enable catalysis including through the use of cofactors; how enzymes achieve specificity in catalysis; introduction to transition state stabilisation and the thermodynamics of enzyme-catalysed reactions; a simple enzyme mechanism to illustrate how the conformation of amino acid side chains enables efficient catalysis.

The chemical structure and fundamental properties of nucleic acids and their building blocks; the nucleobases that occur in DNA and RNA, their physical properties, the ribose and deoxyribose sugars, nucleosides, nucleotides, and single stranded nucleic acids.

The chemical structure of double stranded DNA, A, B, and Z-DNA structures, how the structure of the double helix was determined. Chargaff’s rules. Watson-Crick A,T and G,C base pairs, the importance of base stacking and hydrogen bonding in stabilising the double helix. Replication, involvement of dNTPs and the importance of enzymatic control to ensure a high level of efficiency and accuracy. Base mispairing and the structures and physical properties of mispaired bases.

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


Electrochemistry
The metal/solution interface. Electrochemical potential.


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., H2O, CO2, He); phase coexistence and stability, triple point, critical point, multiple solid phases.

Quantum Mechanics and Spectroscopy
The physical basis of Chemistry: Electromagnetism
Coulomb's Law, electrostatic forces and fields. Electric energy and potential.
Electric dipole moment.
Electric current, resistance and conductivity.
Magnetic forces – the Lorentz force.
Magnetic fields and the Biot-Savart law.
Magnetic dipoles and magnetic materials.
Waves, the E.M. spectrum.
Superposition and diffraction.
Refraction (Snell’s Law).

Quantum theory of atoms and molecules

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; hydrogen atom. Born interpretation. Correspondence principle. Zero point energy. Quantum Tunnelling.


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


Molecular motions and equipartition.

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

Reaction kinetics
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, enzyme catalysis, and chain reactions.

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.


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


Appendix E1

INORGANIC CHEMISTRY

The content of the Part IA Examination in Inorganic Chemistry will be based on the content of the lectures delivered to 2nd year students. Candidates will also be expected to be familiar with material covered in the 1st 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 1st and 2nd year practical courses.

Transition Metal Chemistry


The effect of pH and of ligands on redox potentials. Factors and ligands stabilising high and low oxidation states (eg $\pi$ acceptor ligands versus $\pi$ donor ligands). Role of entropy. Main differences between the 1st and the 2nd and 3rd transition series. Main differences between the 1st and the 2nd and 3rd transition series: stability of oxidation states; trends in covalence; metal-metal bonding. High coordination numbers. 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.

Introduction to transition metals in biology: iron and copper in electron transfer proteins, a brief survey of haem iron and cobalt enzymes.

Lanthanides & Actinides

Coordination Chemistry

Bonding in Molecules
The orbital approximation, the LCAO approach. The use of symmetry in polyatomic molecules MO treatment of AH2 (linear and bent), AH3 (planar and pyramidal), AH4 (Td).

Walsh diagrams: The shapes of AH2 molecules, the bonding and shapes of H2 and H3+: 3-centre-2-electron and 3-centre-4-electron bonds.

Photoelectron spectroscopy and "experimental" MO diagrams, spectra of AH4 molecules.

AB2 molecules from CO2 to XeF2: 12-electron main group octahedral systems: SF6 as an example. 8-electron main group octahedral systems: [C(AuPR3)3]2+ as a relative of CH2=.

Octahedral transition metal systems, σ-bonding, comparison with electrostatic model. MO filling in octahedral complexes: π-interactions and factors that affect the magnitude of Δσ. Molecular orbitals for 4-coordinate geometries: ML6 (T2g and D5h).

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), alkylidene (carbyne) and carbonyl complexes. Hydride, dinitrogen and dihydrogen complexes. Alkene, alkyne and allyl complexes. Cyclopentadienyl, arene and other C4Hn (n = 4 - 8) sandwich and half-sandwich complexes. Synergic bonding and π-complexes CO as a ligand, alkene complexes, bonding in ferrocene.

Structures and Electronic properties of solids
Diffraction methods Distinction between lattices and structures. Unit cells and Bravais lattices. Fractional coordinates.

Miller indices (hkI) and (hkI). Calculation of dAB 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.

Electronic properties of 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 I2. Comparison with the molecular picture.

Extension of band model to simple ionic compounds: e.g. NaCl and CaO; transition metal oxides: TiO2, ReO3, TiO2 and VO2, and sulfides: ZrS2, NbS2, MoS2. Trends in the properties of solids and how they relate to the general chemistry of the transition metals in particular.


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
Multinuclear NMR. Review of the fundamentals: chemical shielding (diamagnetic & paramagnetic shielding terms) and scalar spin-spin coupling (multiplets, sequential stick diagrams, coupling constant values, satellites). Structures from NMR data (e.g. 19F NMR of main group fluorides). Quadrupolar Nuclei. Introduction to NMR in the solid state. Dynamical processes and NMR: a range of examples including trigonal bipyramidal molecules and organometallic systems.

Non-Metal Chemistry
compounds. Boranes: structural classification and Wade’s rules; aspects of preparation and reactivity.

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


**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 Synthesis I**

A logical approach to synthesis illustrated by arene and carbonyl chemistry. Retrosynthesis, disconnections, and synths. Order of events guided by functional group compatibility and selectivity principles; protecting and blocking groups. Carbon-carbon bond formation and functional group interconversion both separately and in combination. Synthesis of mono- and 1,2-difunctionalised molecules.

**Organic Spectroscopy I**

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

NMR Spectroscopy. Nuclear spin and resonance, chemical shifts, factors that influence ¹H chemical shifts. Spin-spin coupling, ¹H coupling patterns and resonance multiplicities, coupling to chemically equivalent spins, weak and strong coupling. Chemical and magnetic equivalence; ¹H spin couplings and chemical structure-geminal, vicinal and long-range couplings, chirality and NMR, chiral solvating agents. ¹³C NMR spectroscopy, ¹³C chemical shifts.

Mass Spectrometry. An introduction to Mass Spectrometry; basic principles and applications; relationship between molecular weight and chemical composition; processes of ion formation and interpretation of a radical cation mass spectrum. Determining location of charge and predicting fragmentation patterns based on product ion stability. Interpreting fragmentation patterns for saturated and unsaturated aliphatics, aromatics and simple heteroatom compounds. Examples. 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 1st year course ‘Introduction to Organic Synthesis’.

**Conformational Analysis and Ring Chemistry**

This course examines the factors that control conformation and reactivity in organic molecules, covering stereoelectronic, steric, and electronic effects. The conformation of acyclic and cyclic molecules is discussed, and the concept of strain. Using this understanding, we analyze how conformational and stereochemical effects influence the reactivity and selectivity of reactions of cyclic and acyclic organic molecules, focusing particularly on reactions of C=O and C=C functional groups. The course also covers methods for ring synthesis.

**Physical Organic Chemistry**


**Rearrangements and Reactive Intermediates**

Structure, reactivity and rearrangement reactions of carbocations and carbanions. Neutral reactive intermediates including carbones, 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.

**Organic Chemistry of Biomolecules**

Chemical synthesis of nucleic acids: solid-phase phosphoramidite DNA synthesis, synthesis of building blocks, synthesis of modifications that are commonly introduced into synthetic DNA for biological applications. Microarray DNA synthesis for the synthesis of entire genomes. Solid-phase RNA synthesis: protecting group strategies. Large scale oligonucleotide synthesis for diagnostic and therapeutic applications: backbone-modified DNA and DNA analogues. Applications: antisense oligonucleotides, exon skipping oligonucleotides, siRNA.

Enzyme kinetics; Michaelis-Menten model to determine steady state parameters, the use of kinetic parameters to understand enzyme mechanisms, multi-substrate reactions, reaction intermediates, other tools to investigate enzyme mechanisms, e.g. isotopes. Enzyme inhibition; pharmaceutical motivation, classes of enzyme inhibitor and mechanism of action, effects on enzyme kinetics and use of kinetic data to identify potent inhibitors. Concepts will be illustrated throughout with case studies, highlighting the contribution of enzyme structure to function.
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 therefrom; 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; particularities). 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\(^2\)s\(^1\) 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


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 \( Q_{\text{rot}} \). 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. \( Q_{\text{trans}} \), \( Q_{\text{rot}} \) 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, \( \theta \). 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, isotopic 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.

Atomic and Molecular Spectroscopy

General aspects of Spectroscopy: Energy levels of molecules; Born-Oppenheimer separation; the photon; interaction of radiation with matter; absorption; emission; transition moments; Einstein Coefficients, selection rules

Atomic Spectroscopy: Revision of H-atom; wavefunctions; atomic orbitals; selection rules; Grotrian diagrams; Many electron atoms; Alkaline metal (and pseudo-1-electron) atoms; Penetration and shielding: The quantum defect; Selection rules and spectra; Determination of ionisation energies; Russell Saunders coupling; Atomic term symbols; The Helium atom; Singlet and triplet states; configurations, terms and levels; Hund’s rules; electron correlation; Effects of external fields – Zeeman interactions; spin-orbit coupling

Molecular Spectroscopy (General)

Molecular Rotational Spectroscopy; Rotors and their symmetry; revision of rigid rotor; moments of inertia; isotope effects; centrifugal distortion; selection rules; Stark effect; Complications of nuclear spin statistics. Molecular Vibrational Spectroscopy; Revision of harmonic oscillator and selection rules; Anharmonicity; normal vs local modes; symmetry considerations; vibration rotation spectroscopy.

Molecular electronic spectroscopy; Potential energy curves/surfaces; Description of diatomic (linear) molecules; Classification of electronic states;

Electronic selection rules; Franck-Condon Principle; Band heads; Dissociation energies; Birge-Sponer extrapolation; Predissociation.
Valence
Born-Oppenheimer Approximation; nature of the problem and the approximation; limitations in the Born-Oppenheimer approximation.

Solving the electronic problem: bonding in H₂⁺; the LCAO approximation.

Many electron molecules: the orbital approximation and its strengths and weaknesses; Pauli exclusion principle; binding of H₂ and He₂; splitting of degenerate configurations, dissociation of H₂.

Applications of the variation principle: the LCAO approximation and the secular equations; bonding in heteronuclear diatomics.

Bonding in the first row diatomic molecules: general considerations; splitting into terms (O₂) and levels (NO).

Walsh diagrams: bond angles in AH₂ systems.

Hückel theory for polyanatomic molecules: use of symmetry; π-bonding in butadiene bond order, electron densities and organic reactivity.

Applications of Hückel theory: aromaticity; illustrations of use of perturbation theory; correlation diagrams.

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.


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’

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.

Symmetry II
Character tables and their meaning: Cᵥ, Cᵥ, and Tᵥ revisited.

The reduction formula and its application to SALCs in CH₄. Projection operators and the SALCS of NH₃. p orbitals in C₆H₆.

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.


Vibrational spectroscopy: stretching vibrations of CF₆, SF₆ and XeF₆. The mutual exclusion rule. Complete 3N basis sets and the vibrations of NH₃. The vibrations of Co₆.

Maths for Chemists


Fourier series and Fourier transforms. FT infra-red spectroscopy and the Michelson interferometer. The Peltier advantage.

Introduction to NMR
Introduction to magnetic resonance, including the background physics of magnetic resonance, the origin of shielding, multiplet structures, exchange phenomena and an overview of experimental methods.
INORGANIC CHEMISTRY

General Papers
The examination papers in Part 1B will include all the topics considered in the core courses in Inorganic Chemistry delivered in the 1st, 2nd and 3rd 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 1B 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, intensity and bandwidth.
Selection rules: allowed and forbidden transitions. Ligand field (d-d) spectra: trends in the orbital splitting parameter (spectrochemical series); ligand field terms; Orgel diagrams and spectral assignment. The Racah parameter B and the nephelauxetic effect. Tanabe-Sugano diagrams.
Charge-transfer (CT) spectra: (a) ligand-to-metal CT transitions in tetrahalide, tetroxo and hexahalide complexes; the redox connection; (b) metal-to-ligand CT transitions in octahedral ML₆.
Magnetic properties of metal complexes.
Definition of magnetic quantities.
Curie paramagnetism: the Curie law and the effective magnetic moment; the spin-only formula. 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 magnetic moment.

Bioinorganic Chemistry
Introduction to bioinorganic chemistry: Cellular compartmentalisation. The roles of the Group 1 and Group 2 ions Na⁺, K⁺, Mg²⁺, Ca²⁺. Electrolytes, ion channels, signalling. Properties of complexes between metals and proteins – how one influences the chemistry of other.
Cobalt and radical chemistry. The cobalamin co-factor. Cobalt oxidation states and their stabilization and chemistry. Mutases and methyl transferases.

Solids state chemistry
Overview of the material covered in the 2nd year: the basic electronic properties of stoichiometric solids and the effect of introducing defects.
and β-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.

Advanced Organic Spectroscopy

NMR Spectroscopy: Assigning 1H NMR spectra: Spin decoupling and 2D NMR, 1H COSY; Assigning 13C NMR spectra; 13C NMR chemical shifts and their interpretation, carbon spin coupling and spectrum editing (DEPT), 2D NMR- one-bond (HSQC) and multiple-bond (HMBC) 1H-13C correlations. Defining molecular stereochemistry using the nuclear Overhauser effect (NOE).

Mass Spectrometry: Differences between radical cation and pseudomolecular ion formation, stability and chemical determination. Qualitative mass spectrometry analysis: Chemical formulae calculation; nitrogen rule; high resolution analysis of isotopes signatures. Tandem mass spectrometry: Post-source fragmentation processes; molecular and structural identification. Selected applications of mass spectrometry.

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 retro synthesis/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.

Pericyclic Reactions


Transition Metal Catalysis


Curly Arrows of Biology

An Introduction to the Chemistry of Metabolism/ Bioenergy. Primary and secondary metabolism. Glycolysis and the citric acid cycle. Amino acid metabolism and the nitrogen cycle.

Radical Reactions


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 similar to that of the 2012 - 2016 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 spines with I greater than ½, discussion of Fermi contact interaction, an introduction to dipolar coupling. Magnetic resonance spectroscopy of two coupled spin- ½ particles: a quantum mechanical treatment. The rotating frame, line 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.
Soft Condensed Matter

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

Photophysics and photochemistry


Physical Principles of Solids


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.

Advanced Chemical Biology

Functional groups in proteins and nucleic acids. Peptide synthesis: Methods, strategy, factors compromising yields, including loss of stereo-chemistry, and analysis. Use of different types of protecting groups, coupling reagents (including use of protein-splicing and, in outline, enzymes) for solid and solution phase peptide synthesis. Comparison with nucleic acid synthesis, and, in outline, with biological peptide biosynthesis. Roles (in brief) and extent of post-translational modifications including enzyme catalyzed peptide hydrolysis. Preparation and applications of unnatural biopolymers prepared by mutagenesis and chemical methods. Concepts in orthogonal chemistry. Use of reactions that do not occur in nature, e.g. selected cycloaditions.


Advanced Synthesis and Total Synthesis

This course builds from the core 3rd 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 aces 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.

Functional Organic Polymers and Materials Chemistry

Dyes: Chromophores, commercial dyes, synthesis of azo dyes and cyanines, direct dyes, reactive dyes for cellulose, fluorescence, chemiluminescence, photodromics, photoinduced electron-transfer.

Polymers: Polymerisation reactions: condensation vs. addition, step-growth vs. chain-growth, DP, Mn, Mw, polydispersity. Carothers equation, epoxy-resins, ring opening, stereochemistry, Ziegler Natta, metallocene catalysts, living polymerisation (anionic, cationic, ring opening metathesis) architecture, dendrimers.

Living Polymerisation and Conjugated Polymers: Living free-radical polymerisation (nitroxide-mediated polymerization, ATRP and RAFT). Approaches to the synthesis of conjugated polymers, using polycyctylene, polyphenylene vinylene, poly-para-phenylene and polythiophene as examples.

Liquid Crystals: classification: thermotropic/ lyotropic, calamatic/discotic, 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. Keval, side-chain.
**Organic Surface Chemistry:** Why is there a need to modify surfaces? Comparison of different techniques for preparing and analysing organic surface functions: self-assembled monolayers, chemical methods for surface modification, grafting to and grafting from, chemically activated polymers.


**Organic Electronic Materials:** Types of organic metals and semiconductors: charge-transfer salts, conjugated polymers, molecular crystals; band structure, solitons and bipolarons; 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 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, dust-grain chemistry, and neutralisation processes in interstellar gas clouds. A simple model for the rate of ion-molecule reactions; chemical modelling of molecular clouds.

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


**Inorganic Molecular Spectroscopy**

How various spectroscopic techniques are used to characterise inorganic systems. The complementary nature of all the techniques will be illustrated.

Electronic spectroscopy - The use of spectroscopic techniques to probe transition metal and lanthanide systems.

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.

NMR spectroscopy - Examples of applications of a range of NMR methods including double resonance techniques, 2D NMR, cross polarization and magic angle spinning NMR. Use of NMR to study dynamic systems including the extraction of quantitative data, mechanistic information and real time NMR studies.

**An Introduction to the Liquid State**

Classical statistical mechanics: classical partition function, phase space; pairwise additivity, second virial coefficient.

Statistical mechanics of the liquid state: pair distribution function, osmotic compressibility, Ornstein-Zernike equation, structure factor.

Light scattering: Rayleigh scattering (point scatterer), Rayleigh-Gans-Debye theory (larger particles), form factor, Guinier and Porod’s laws, structure factor and link to statistical mechanics of liquids, partial structure factors, contrast variation, computer simulation of liquids.

**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, multidimensional techniques used to probe the structures and dynamics of molecules.


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.


**Molecular Reaction Dynamics**

Introduction: Types of collisions: definitions of impact parameter, cross sections, differential cross sections, state-to-state processes; conservation of energy and momentum.

Potential energy surfaces and trajectories: introduction to potential energy surfaces; types of potential energy surface; quasi-classical trajectory and quantum scattering calculations as a link between experiment and theory; centrifugal barriers.

**Experimental techniques for control of initial states:** spatial/temporal isolation; laser photolysis and pump and probe methods; molecular beam methods, including brief examples of state-selection, deceleration and orientation.

**Experimental techniques for probing product states:** crossed molecular beams with mass spectrometric detection; chemiluminescence and laser induced fluorescence; resonantly enhanced multiphoton ionization and Rydberg tagging; velocity map ion-imaging; the lab to centre-of-mass frame transformation.

**Elastic and Inelastic scattering:** total (integral) and differential cross sections; examples of molecular beam inelastic scattering experiments; types of energy transfer and their relationship to intermolecular forces.

**Reactive scattering:** examples of crossed molecular beam reactive scattering experiments; reaction mechanisms.
including stripping mechanism and the harpoon model, rebound reactions, and complex formation.

**Controlling reagents and characterizing products:** effect of translational energy on the reaction cross-section for reactions with and without a barrier; effect of initial vibrational state on the reaction cross-section and Polanyi’s rules; selective disposal of energy, including microscopic reversibility, and the potential energy surfaces for attractive and repulsive energy release; examples of mass effects and angular momentum conservation effects; statistical reactions.

**Probing the transition state:** examples of control of molecular orientation, stereochemistry and cone of acceptance, angular momentum polarization; applications of femtochemistry; photoelectron detachment spectroscopy.

**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. The course will include: the link between primary and secondary metabolism; enzymes, cofactors and common metabolic pathways; the acetate hypothesis, fatty acid, prostaglandin and polyketide biosynthesis; mevalonic acid formation, terpene, squalene and steroid biosynthesis; amino acid biosynthesis; biosynthesis of alkaloids derived from lysine/ornithine and phenylalanine/tyrosine leading to the biosynthesis of complex polycyclic alkaloids such as morphine.

**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 homogenous transition metal catalysts focussing on metallocene-types; co-catalysts: types and mode of operation; polymerisation mechanism: initiation, propagation, termination; a-olefins and control of tacticity.

**Ring opening Polymerisation**

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

**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**


**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:

**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?

**Superconductivity.** Classical and non-BCS superconductors. Factors affecting Tc. Recent developments; superconductors in action.

**Magnetism.** The collective magnetism in solids. The uses of magnetic materials in technology – magnetoresistance, multiferroic materials.

**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.

**Supramolecular, Nano and Medicinal Inorganic Chemistry**

This course focuses on specific examples of uses of coordination compounds.

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 polymetallic 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.

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).

Supramolecular cation and anion receptors and derived optical and redox sensors. Molecular machine design, examples of molecular switches and surface assembly. Multimodality in molecular imaging, nanoparticle image contrast and drug delivery systems. Supramolecular switches in drug delivery.

Theoretical Chemistry

Time-Dependent Quantum Mechanics

1. 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.

2. 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.


4. Conditions for adiabatic and non-adiabatic transitions, via the Landau-Zener theory, and application to a simplified theory of electron transfer.

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.

APPENDIX E3

Syllabus for Supplementary Subjects 2016-17

CHEMICAL CRYSTALLOGRAPHY

A supplementary course exploring the way in which crystallography is used to determine the atomic scale structure of chemical compounds covering crystal structure, symmetry, diffraction, reciprocal space, experiments, structure solutions, modelling and refinement.

1. Describing structure in real and reciprocal space. Understanding symmetry in diffraction patterns. Relationship between space group symmetry and diffraction patterns.

2. Space group symmetry notation and conventions. Lattices, symmetry operations and space groups.


QUANTUM CHEMISTRY

Time independent quantum mechanics

Operators and Commutators. Postulates of quantum mechanics; Linear operators; Hermitian operators; The unit operator; Commutators; The uncertainty principle; Constants of the motion.

The Harmonic Oscillator. Hamiltonian. Creation and annihilation operators; Eigenvalues and eigenstates; Matrix elements. Angular Momentum. Angular momentum operators; Commutation relations; Raising and lowering operators; Eigenvalues and eigenstates; Coupling of angular momenta.

Matrix Formulation. Matrix representations; Hermitian matrices; Hamiltonian matrices; The variational method; Secular equations; Examples.

Group Theory

Group Theory in the abstract: definition of a group, examples, multiplication tables, abelian groups, conjugacy classes. Symmetry and Quantum Mechanics: ‘true’ symmetries of the molecular Hamiltonian. Molecular point groups, Matrix representations and similarity transformation, Reducible and Irreducible representations.


Perturbation Theory and Time Dependent Quantum Mechanics

Stationary State Perturbation Theory, Non-degenerate and degenerate cases Applications, e.g. helium atom, Stark Effect, Time Dependence in Quantum Mechanics Equations of Motion, Time-independent Hamiltonians, Stationary and Non-stationary States, Time-dependent Hamiltonians

Molecular Electronic Structure

Introduction: Schrödinger equation, Born-Oppenheimer, wavefunctions; The linear combination of atomic orbitals (LCAO) approach to molecular orbitals; Pauli principle, Slater determinants; Formulation of the Hamiltonian for H₂, H₂ Matrix formulation and the secular determinants
for a 1-electron system (H$_2^+$); Formulation of H$_2$* in the LCAO approach; Formulation of Hamiltonian for H$_2$; Coulomb integrals, Triplet state of H$_2$ and the exchange integral, Expansion of the Coulomb and exchange integrals in an atomic basis, Self-consistent fields and Hartree-Fock theory, Hartree-Fock and Roothaan equations, Basis sets, Slater's vs Gaussians, Hierarchy of basis sets, Beyond the HF approximation, Configuration interaction, Density functional theory, Semi-empirical methods, Hückel and Extended Hückel theory.

**AROMATIC AND HETEROCYCLIC CHEMISTRY**

Aromatic and heterocyclic chemistry is a very large and important branch of chemistry with which those students who enter the chemical industry are almost certainly going to intimately involved. Mechanistic rationales for the synthetic basis of aromatic chemistry that is practised today will be presented; more descriptive organic chemistry than would be reasonable in a main lecture course will be given. The relationship of reactions in aromatic chemistry to those of aliphatic chemistry will be emphasised. This is an area that provides a substantial part of the profits of the pharmaceutical industry, the syntheses of some of the past and potential blockbusters will be exemplified. The course will consist of 5 modules each having 5 lectures and 1 problems class.

**Heterocyclic Synthesis I** Objectives of the course. Range of 5 ring heterocycles: synthesis of 1,4-dicarboxyls in many different guises. Cheap natural sources. Fused systems and in particular indole.

**Benzenoid Chemistry** Comparison with heterocyclic reactions. Reactions of benzenoid systems: electrophilic aromatic substitution; early and late transition states; reactivity-selectivity in electrophilic and oxidative attack; electrophilic reactivity; ipso attack; kinetics versus thermodynamics; nucleophilic substitution; SNAr, SRN1, benzene mechanisms; applications in synthesis. Aromatic rearrangements. Arene metallations and cross couplings.

**Heterocyclic Synthesis II** Range of 6 ring heterocycles: 1,5-dicarboxyls by aldol, base-catalysed dehydration and Michael reactions. Synthesis of frameworks with more than one heteroelement towards purines and pyrimidines.


**Introduction to Pharmaceutical Chemistry** - Drug discovery process: sildenafil. Physicochemical properties. Pharmacology: drug targets; potency; enzymes; receptors (cimetidine); transporters (omeprazole). Drug design: drug-protein Interactions; structure-based drug design (crizotinib). Pharmacokinetics: half-life, dose; volume of distribution (amlodipine and azithromycin); clearance. Drug safety: central nervous system; drug-drug interactions (ketoconazole, terfenadine and fexofenadine); anti-HIV (maraviroc).
# Academic Staff

All Staff in the Department can be contacted by e-mail which is generally the best method. Add [chem.ox.ac.uk](http://chem.ox.ac.uk) to the e-mail addresses listed below.

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**Disability Contact:** Ms N. Jupp  nina.jupp@

**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

The University has a wide range of policies and regulations that apply to students. These are easily accessible through the A-Z of University regulations, codes of conduct and policies available on the Oxford Students website www.ox.ac.uk/students/academic/regulations/a-z.

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/guidance/skills/plagiarism

Plagiarism is presenting someone else's work or ideas as your own, with or without their consent, by incorporating it into your work without full acknowledgement. All published and unpublished material, whether in manuscript, printed or electronic form, is covered under this definition. Plagiarism may be intentional or reckless, or unintentional. Under the regulations for examinations, intentional or reckless plagiarism is a disciplinary offence.

- Equal opportunities: http://www.admin.ox.ac.uk/eop/
- Disability: www.ox.ac.uk/students/welfare/disability
- Harassment: http://www.admin.ox.ac.uk/eop/harassmentadvice/
- Health and safety: http://www.admin.ox.ac.uk/safety/hs-management-policy/
- Chemistry Department safety: http://safety.chem.ox.ac.uk/
- Computer usage: http://www.ict.ox.ac.uk/oxford/rules/
- Examination regulations: http://www.admin.ox.ac.uk/examregs/
- The Proctors’ Memorandum: http://www.admin.ox.ac.uk/proctors/info/pam/
- Data Protection Act 1998: http://www.admin.ox.ac.uk/councilsec/dp/
- OUSU Student Advice Service - https://ousu.org/advice/student-advice-service/

Resources

University Careers Service: www.careers.ox.ac.uk
Enterprising Oxford: Enterprising Oxford: http://www.eship.ox.ac.uk/

What are the top skills needed to be an excellent researcher?

Creative problem-solving? Resourcefulness? Confidence and determination? Did you know these are also key attributes of an enterprising or entrepreneurial mind-set?

But what does “enterprising” actually mean? If “Dragon’s Den” or “The Apprentice” is the first thing you think about, then check out Enterprising Oxford, where you will see what being enterprising is and where it can take you.

Enterprising Oxford is an online map and guide to innovation and entrepreneurship in Oxfordshire, developed here at the University of Oxford. Start at the beginning, with Entrepreneurship 101, to discover how being entrepreneurial can help with research or employability, or go straight in to Explore & Build your idea. Read about entrepreneurs at all stages of the journey, mingle with successful start-ups, and find creative ways to fund your ideas and initiatives. Whether you have an idea, a start-up or a well and truly established venture, Enterprising Oxford highlights opportunities to develop further or help support others.
Commonly used abbreviations:

PTCL  = Physical and Theoretical Chemistry Lab.
DP    = Dyson Perrins Building
ICL   = Inorganic Chemistry Laboratory
CRL   = Chemistry Research Laboratory
UM    = University Museum
RSL   = Radcliffe Science Library