



Department of Chemistry
Undergraduate Course Handbook
Academic Year 2019-20

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

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How to use this Handbook

This Handbook applies to students starting the course in Michaelmas Term 2019. The information in this Handbook may be different for students starting in other years. First Year students should read the whole Handbook. Those in subsequent years need only look at the relevant year sections. Suggestions for future editions are always welcome – please contact the Faculty Office (undergraduate.studies@chem.ox.ac.uk).

Further information about the course is available on the [Undergraduate Course](#)¹ section of the Department of Chemistry website and from the Faculty Office in the Inorganic Chemistry Laboratory.

The information in this handbook is accurate as at September 2019. Changes may be necessary in certain circumstances and all relevant web pages will be updated to reflect these changes.

Examinations

The Examination dates given in this handbook are based on information available in September 2019. They are only a rough guide and the definitive dates are those published by the Examiners. For up to date information regarding the Examinations students should check the [Latest Examination Information](#)².

The Examination Regulations are available on the University web pages. There are separate regulations for the [Preliminary Examination](#)³ (Prelims) and for the [Honour School of Chemistry](#)⁴ (Part IA, Part IB, Part II).

To find the Examination Regulations for students starting in previous years, return to the [search](#)⁵ and choose the examination and year.

If there is a conflict between information in this Handbook and the Examination Regulations then students should follow the Examination Regulations. Students should contact the Faculty Office (undergraduate.studies@chem.ox.ac.uk) with any concerns.

Lectures

This Handbook contains a Syllabus and Lecture List for each year. Students should note that lecture timetables are subject to change. Full and up to date information on lecture timetables is available on the [Timetables](#)⁶ section of the Department website. From this page, it is possible to choose to view a weekly or termly timetable for each year group, using the left hand menu.

Other Information

In the Introduction of this Handbook there is information about safety, libraries, IT, communication, welfare and disability support and the Chemists' Joint Consultative Committee (CJCC). Towards the back of the Handbook is a list of academic staff and their contact details, links to University policies, wellbeing & welfare resources and a list of important dates. Academic Staff will be happy to answer any questions that students might have, but for particular information about college teaching students should contact their Tutors. Administrative queries should be directed to the Faculty Office (undergraduate.studies@chem.ox.ac.uk).

¹ <http://teaching.chem.ox.ac.uk/>

² <http://teaching.chem.ox.ac.uk/latest-examination-information.aspx>

³ <http://www.admin.ox.ac.uk/examregs/2019-20/pexaminchem/studentview/>

⁴ <http://www.admin.ox.ac.uk/examregs/2019-20/hschoofchem/studentview/>

⁵ <http://www.admin.ox.ac.uk/examregs/>

⁶ <http://teaching.chem.ox.ac.uk/timetables.aspx>

Message from the 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 Oxford 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. The Department ranks consistently amongst the very best for teaching in the UK, and its research standing places it in the top 10 of Chemistry departments worldwide. 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 and 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. There is also 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. In 2018 we opened the new Chemistry Teaching Laboratory, and the new, integrated Practical Course that is taught here is now in its second year.

Over the next few years you will come to understand just how broad Chemistry is as a subject, and how central as 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. 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 where many of you will have an opportunity to work on 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 reached the 100th anniversary of the completion of the first Part II year at Oxford. I hope you will have the opportunity to celebrate the successful submission of your Part II thesis at the end of the course.

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.



Professor Mark Brouard

Head of the Department of Chemistry
University of Oxford

Introduction

The Oxford Chemistry School has recently been admitting around 180 undergraduates p.a. There are approximately 80 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. The [Safety](#)⁷ section of the Practical Course web pages details the main safety requirements in the Teaching Labs. In addition, lab manuals contain more detail on each experiment and the procedure for risk assessment.

Libraries

As an undergraduate student you will find most of your needs met by well-resourced College libraries. If your library is without a book that you need you should tell your College Tutor or your College Librarian, or inform the librarians in the Radcliffe Science Library (RSL). The RSL 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. From the [RSL website](#),⁸ you can access details of both print and electronic [chemistry resources](#)⁹ available.

Information Technology

You will have Chemistry-focused IT skills training, including programming, as part of the undergraduate practical course. There is also the opportunity to use the central IT Services training courses for more general IT training requirements. Colleges have computing facilities for their undergraduates and there is a University-wide network and wireless network, which enables you to access the Internet, department sites, the practical course, and a wide variety of chemistry journals without charge.

All undergraduates receive an e-mail account with the address firstname.surname@college.ox.ac.uk. The University [IT Services](#)¹⁰ department offers a wide range of IT support to the whole University and there is lots of useful information on their website. The Chemistry Department follows the University's [Data Protection Policy](#)¹¹.

Communication Channels

Academic Staff have pigeon-holes in the Chemistry Department buildings where they have offices, and also in their Colleges. Staff may also be contacted by telephone or e-mail. Most prefer e-mail, which is usually the most efficient option. A list of e-mail addresses and College affiliations is given in the [Academic Staff List](#).

Most administrative information about the course will be sent to you by e-mail, including important information from the Department such as last minute lecture changes, examination information and other deadlines. It is very important, therefore, that you check your e-mail regularly and ensure that your mailbox is kept clear and does not become full. If you are using an e-mail account other than your university account (@college.ox.ac.uk) you should set the forwarding facility appropriately.

Support for Students

Colleges provide pastoral support through subject tutors, Deans and other welfare officers. The university Counselling Service offers confidential help and advice to students, and can be accessed either through college welfare officers or independently.

The Disability Advisory Service 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 Chemistry is Professor Nick Green, who is responsible for strategic oversight of provision for disabled students. The disability co-ordinator is Laura

⁷ <http://course.chem.ox.ac.uk/safety.aspx>

⁸ <https://www.bodleian.ox.ac.uk/science>

⁹ <https://libguides.bodleian.ox.ac.uk/chemistry>

¹⁰ <https://www.it.ox.ac.uk/>

¹¹ <https://compliance.admin.ox.ac.uk/data-protection-policy>

Fenwick, who organises the implementation of this provision.

Further health & welfare resources can be found towards the back of this handbook.

Chemists' Joint Consultative Committee

The [Chemists' Joint Consultative Committee \(CJCC\)](#)¹² is a forum for the exchange of views concerning the undergraduate course. The matters covered by this committee include (i) teaching arrangements, lectures and seminars, organisation and coverage; (ii) the practical course composition, organisation, safety and requirements; (iii) the syllabus and structure of examinations; (iv) library facilities; (v) the general welfare of students, in so far as it affects the Department.

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. The CJCC has fourteen undergraduate members, three postgraduate representatives and six senior members. The chair is the Deputy Director of Studies Dr. Martin Galpin. There is a separate committee for graduate students.

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

There is also student representation on the Chemistry Teaching Committee, which is the committee that oversees the teaching in the department. The student representatives are generally Part II students as they have an overview of the whole course.

Aims and Objectives

The Chemistry Course – Aims and Objectives

- To engender the qualities that 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.

¹² <http://teaching.chem.ox.ac.uk/chemists-joint-consultative-committee-cjcc.aspx>

Teaching

Research and Teaching

The Department of Chemistry has an international reputation for research and this University believes that this high level of research activity provides many benefits to the teaching of the course. 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 are recognised internationally as leaders in their own field of [specialism](#)¹³.

The impact of research on teaching in this department takes 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 Part II); special topics provided as options in the third year; the use of research equipment in the practical course; 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. In other words, you will become a part of the scientific community.

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 they are not compulsory. No attendance checks are made, but only foolish idlers cut lectures. Printed notes, problem sheets and other handouts support lectures and where appropriate they are available on the [Course Material](#)¹⁴ section of the department website. Students need to learn how to take good lecture notes and supplement these with their own private study using textbooks and other sources recommended by the Lecturers and their Tutors. Lecture feedback questionnaires are provided and their completion is encouraged because your feedback helps us to improve what we offer.

Practical work is assessed and practicals have to be written up in detail for marking. The marks for second and third year practicals count towards the final degree class. Both you and your tutors can follow your progress through the practical course on a database that you will be given access to at the beginning of term. During the first three years of the course practical work is compulsory. More information can be found on the [Practical Course](#)¹⁵ section of the department website.

Tutorial teaching (typically in groups of 2 or 3) is based in your college. Your tutor will provide guidance on 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 (known as "Collections") are used to monitor your progress during the intervals between University Examinations. Every term your tutors will write a report on your progress for your College, which you may view via an online system called [OxCORT](#)¹⁶. You will 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 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

¹³ <http://www.chem.ox.ac.uk/research.aspx>

¹⁴ <http://course.chem.ox.ac.uk/home.aspx>

¹⁵ <http://course.chem.ox.ac.uk/practicals.aspx>

¹⁶ <http://www.oxcort.ox.ac.uk/>

you with problems. They will also (as far as possible) tailor your tutorials to your needs. Lecturers also supply problem sets to their courses on the web and these will sometimes 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 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.

In addition, students are expected to gain the following skills, primarily via the undergraduate practicals and the Part II research year:

- The ability to conduct an experimental investigation safely and to report its results precisely.
- The ability to design an appropriate experiment to solve a problem.
- The ability to interpret complex and incomplete experimental information and to infer appropriate conclusions.
- The ability to apply IT methods for data retrieval and archiving, and to use a wide variety of Chemistry orientated software for

chemical structure and energetics and for spectra simulation etc.

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

A wide range of information and training material is available to help you develop your academic skills – including time management, research and library skills and academic writing – through the [Study Guidance](#)¹⁷ university web pages.

The Oxford teaching terms are short (8 weeks). It is therefore essential that you set aside a significant amount of time in each vacation for academic work. The course assumes that you will do this. Your tutors may also set specific vacation work.

Colleges will not normally permit you to take paid work during term time. For guidance on paid work, see the [Skills and Work Experience](#)¹⁸ web page.

Complaints Procedures

If you have a concern or complaint about teaching or other provision made by the department then you should raise it with the Chair of the Teaching Committee, Professor Nick Green. We will normally attempt to resolve your concern/complaint informally. If you are dissatisfied with the outcome then you may take your concern further by making a formal complaint to the University Proctors. The [Complaints and Academic Appeals](#)¹⁹ web page details the procedures adopted by the Proctors for the consideration of complaints and appeals. All students may lodge complaints on almost anything (except the weather) with the Proctors. Complaints of a general nature may be discussed at the CJCC.

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, such as the 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.

¹⁷ <https://www.ox.ac.uk/students/academic/guidance?wssl=1>

¹⁸ <https://www.ox.ac.uk/students/life/experience?wssl=1>

¹⁹ <https://www.ox.ac.uk/students/academic/complaints?wssl=1>

Examinations

There are Examinations in all four years: Prelims, Part IA, Part IB and Part II respectively. The Part IA and Part IB system was introduced in 2004-05 and revised in 2010-11. Useful information about Examinations can be found at the following links:

- [Past papers](#)²⁰
- [Examiners' reports](#)²¹
- [Instructions for entering](#)²² University Examinations and examination timetables
- [Exam Guidance](#)²³ on (a) the standards of conduct expected in examinations and (b) what to do if you would like examiners to be aware of any mitigating circumstances that may have affected your performance before or during an examination (such as illness, accident or bereavement).
- The current [Examiners](#)²⁴ responsible for examinations in years 1-4 (scroll to the bottom of this web page) and the nominating committee.

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 Trinity Term of the first year. The level of the Examination is set so that with reasonable commitment the vast majority of students are capable of passing. Distinctions are awarded for excellent performance. Failed papers can be re-taken in September, with the permission of the student's college, but all papers must be passed at no more than two sittings. It is necessary to have passed all examination 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 Inorganic, Organic and Physical Chemistry covered in the first two years of the course. The results are carried forward to be taken into account together with Part IB and Part II to determine the 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

This Examination consists of six general papers covering all of 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. Students who are not awarded Honours may have a second attempt at Part IB, one year later.

Part II

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

The oral examinations are usually held in 10th and 11th week of Trinity Term. The main purpose of the 'viva' is to assure the Examiners that the candidate has carried out and understood the work described in the thesis, but a candidate may also be asked more general questions relating to the scientific context of the project. The viva may also provide an opportunity for a candidate to clarify points in the thesis that were unclear to the Examiners.

²⁰ <http://teaching.chem.ox.ac.uk/past-exam-papers.aspx>

²¹ <http://teaching.chem.ox.ac.uk/examiners-reports.aspx>

²²

<https://www.ox.ac.uk/students/academic/exams/entry?wssl=1>

²³

<https://www.ox.ac.uk/students/academic/exams/guidance?wssl=1>

²⁴ <https://intranet.chem.ox.ac.uk/committee-members.aspx>

Summary

The notes above summarise the main points, but are neither authoritative nor complete. The detailed and authoritative regulations are contained in the [Examination Regulations](#)²⁵ and the Examination Conventions (see below). In cases of difficulty students should consult the Senior Tutor of their college. The Proctors are the ultimate authority for interpreting the Regulations at the most 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**. 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. More details may be found in the Examination Conventions below. Any changes made after the publishing of this document

may be found on the [Examination Conventions](#)²⁶ web page.

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 Teaching Committee (CTC), but the Proctors are the ultimate authority on everything except academic judgement.

Most Colleges set informal examinations of their own known as “Collections”. These are usually held at the start of terms. They are for mutual monitoring of progress and do not form part of the official University assessment at any stage.

Complaints Procedures

Any complaint regarding any examination should be made to the Junior Proctor, through the College Senior Tutor. Students should on no account approach examiners directly on any matter.

²⁵ <http://www.admin.ox.ac.uk/examregs/>

²⁶ <http://teaching.chem.ox.ac.uk/examination-conventions.aspx>

Examination Conventions in Chemistry 2019 - 2020

Introduction

These conventions have been approved by the Chemistry Teaching Committee (CTC) and the MPLS Division. They should be read together with the current Examination Regulations ([available online](#)²⁷) and the [Undergraduate Course Handbook](#)²⁸. CTC 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 Chair of CTC, through the [Faculty Office](#)²⁹ in the first instance. Such enquiries are welcome, as clarification helps everybody. It is not appropriate to address Chairs of Examiners on such matters.

Details of the membership of the examination boards are available [here](#)³⁰. 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 Regulations¹, 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 12 days of skills labs, all of which are compulsory, and 18 days of general labs in which there is some choice.

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

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

The resit attempt shall normally be taken at the next opportunity, but may be deferred once, i.e. it must be taken at one of the next two opportunities.

Failure to attend an examination without good reason, approved by the Proctors, will result in a technical failure of that examination and a mark of 0 will be recorded.

Failure to complete the practical requirement and/or the IT requirement to the satisfaction of the Examiners, in the absence of appropriate documentary evidence, will normally constitute failure of the Preliminary Examination. The practical course cannot normally be retaken. Exceptionally a candidate who has failed this component may be permitted jointly by the Examiners and the candidate's college to retake the entire academic year.

A compensated pass in Mathematics is not permitted for resit examinations.

²⁷ <http://www.admin.ox.ac.uk/examregs/information/contents/>
²⁸ <http://teaching.chem.ox.ac.uk/Data/Sites/58/media/courseinfo/undergradhandbook2019.pdf>

²⁹ undergraduate.studies@chem.ox.ac.uk

³⁰ <https://intranet.chem.ox.ac.uk/committee-members.aspx>

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, except in the event of a technical fail (see below). Practical work will not be taken into account for Part IA.

Failure to attend a Part IA examination without good reason will normally result in a mark of 0 and a technical fail of the whole of Part IA. In this event the candidate must retake the whole of Part IA. This will normally at the first possible opportunity, which will be one year later, but may be deferred once, i.e. it must be taken at one of the next two opportunities.

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. Failure to attend a Part IB examination without good reason will normally result in a mark of 0 and a technical fail of the written component of Part IB.

The views of the External Examiners will be considered carefully before any candidate is denied Honours. The honours threshold is expected to be about 40%. Students below this borderline may be called for a viva voce examination with an examination board normally consisting of the 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 not to be worthy of honours have the opportunity to enter again for Part IB of the examination on one, but no more than one, subsequent occasion subject to the limitations laid out in the Examination Regulations. This resit attempt shall normally be taken at the next opportunity, but may be deferred once, i.e. it must be taken at one of the next two opportunities.

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 Regulation](#)³¹, 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 number, 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 marks reported will be University Standardised Marks (USM), reported as percentages. 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%.

³¹ <http://www.admin.ox.ac.uk/examregs/2019-20/hschoofchem/studentview/>

Practical Course

Except in special circumstances, no candidate may pass Part IB without having completed satisfactorily the second and third year practical courses including 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 24 days (144 credit hours). The experiments will be divided into skills labs and general labs, in a similar way to the first year. From 2019/20 the normal third year stint will be 18 days (108 credit hours). 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 they satisfy the examiners in the Part IB examination. Below this limit a candidate will automatically fail Part I.

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 languages a mark of 70% or more.

These bonus marks will be credited for each Supplementary Subject passed at the appropriate level, up to a maximum of three, 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 Regulation](#)³².

Part II is examined by Thesis and by viva voce examination. The Chair 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, or by an Examiner and an Assessor, 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](#)³³.

The two principal readers of the thesis will also conduct the viva, which will be marked out of 20. Thesis marks may only be altered following the viva with the agreement of 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, although the supervisor's report will be taken into account by the examiners.

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 reported to the Part IB examiners will be allowed: candidates who have not completed the practical requirement will not have been adjudged worthy of honours and will not be permitted to start the Part II year.

The two thesis marks and the viva mark will be added to give the Part II mark. The Part II mark will be aggregated with the total Part I mark with a weighting 25:75.

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, 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.

³² <http://www.admin.ox.ac.uk/examregs/2019-20/hschoofchem/studentview/>

³³ <http://teaching.chem.ox.ac.uk/assessment-guidelines.aspx>

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

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.

Mitigating Circumstances

Applications for consideration of [mitigating circumstances](#)³⁴ should be submitted by your College Officer (normally the Senior Tutor) to the University Examinations and Assessments team, together with the relevant supporting material.

Applications will be considered and graded according to severity by a subgroup of the examination board. The full examination board will decide what action to take at the marks meeting, or make a recommendation for future examination boards. Most commonly, action will be deferred until the candidate's full results are available after Part II. However, mitigating circumstances will also be considered for candidates at the Pass/Fail or Pass/Honours borderline after Part IB. Examination boards may take account of circumstances covering a single paper by finalising the mark on the basis of

work completed, or ultimately by disregarding the paper in deciding a classification.

Marking Conventions

All written papers are marked according to the outline marking scheme printed on the examination paper. The mark scheme is a guide, and examiners have the discretion to vary it. Papers will either be double-marked or the marks checked against the marking scheme by a second examiner. University Standard Marks (USM) will be used for each paper, in which class boundaries are drawn at or close to 70%, 60%, 50% and 40%, i.e. marks 70% and above are first class, marks between 60% and 70% are 2.1, etc. Marks may be rescaled to ensure that they conform to the University Standardised Mark (USM) scale (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 part of a question that has 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 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 question 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

³⁴

<https://www.ox.ac.uk/students/academic/exams/guidance?wssl=1>

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, including a safety assessment, in-lab practical skills, the sign-off and the write-up. Practical marks may be scaled to ensure uniformity of standard between experiments and markers. The final assessment will be performed by a Departmental Lecturer in Practical Chemistry or approved by the Director of Teaching Labs or the Deputy. Marks for practicals submitted for marking beyond the 2-week deadline without good reason will be capped at 40%. Practical submitted for marking more than 4 weeks after the start without good reason will be awarded zero marks. Practical 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).

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](#)³⁵ can be found on the website.

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:

$$y = x \exp(\alpha(100 - x)^2)$$

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:

Each Part IA paper	5%
Each Part IB General paper	7%
Part IB Option paper	8%
Part I Practical course	10%
Part II	25%

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

³⁵ <http://course.chem.ox.ac.uk/practicals.aspx>

The following Qualitative Descriptors of Classes have been adopted:

Class	General	Mark range	Problems	Part II and essays
Class 1	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.	90% - 100%	Complete understanding, formulation correct, all steps and assumptions explained properly. Technically without fault.	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.
		80% - 90%	Excellent understanding, formulation correct, clear explanations, very few errors.	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.
		70% - 80%	Very good understanding, formulation correct, principal steps clear, any errors are minor.	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.
Class 2.1	Good or very good problem-solving skills, and good or very good knowledge of much of the material over a wide range of topics.	60% - 70%	Sound to good understanding, principal steps explained. Some errors.	Evidence of some intellectual input. Competent and coherent writing. Good presentation, literature knowledge and analysis of data.
Class 2.2	Basic problem-solving skills and adequate knowledge of most of the material.	50% - 60%	Adequate understanding, not all steps explained and maybe some gaps in logic. Some errors leading to incorrect or incomplete answers.	Routine treatment of data, literature coverage may have gaps, writing competent, but little sign of critical thinking or intellectual input.
Class 3	Reasonable understanding of at least part of the basic material and some problem-solving skills. Although there may be a few good answers, the majority of answers will contain errors in calculations and/or	40% - 50%	Incomplete understanding and formulation. Steps not explained, assumptions not stated. Errors lead to impossible answers. Lack of critical thought.	Shallow, narrow approach. Poor understanding and little sign of thought in selection of material or structure of report. Conclusions may be lacking or flawed.

	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, and it is therefore hard to apply these descriptors to problems.

Calculators for Written Examinations in Chemistry

A candidate may bring a pocket calculator into any Examination, except the **Preliminary Examination 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 mathematic functions such as $\sin(x)$, $\log(x)$, $\exp(x)$ and $(x)^y$ and it may contain constants such as π

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

The intention of these rules is to prevent the possibility of a candidate obtaining an advantage by having a powerful calculating aid (or of a candidate 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 a 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.

First Year 2019 - 2020

The Course

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

- Atomic structure and the periodic table
- The ionic model, pre-transition metal chemistry and solid state structures
- Reactions in solutions
- Introductory transition metal chemistry
- Chemical bonding and molecular orbital theory
- Non-metal chemistry
- Introduction to organic chemistry
- Reactivity in organic chemistry
- Substitution and elimination at saturated carbons
- Introduction to organic synthesis
- Carbonyl group chemistry
- Chemistry of C-C π bonds
- Introduction to biological chemistry
- Physical basis of Chemistry
- Quantum theory of atoms and molecules
- Chemical thermodynamics
- Reaction kinetics
- Equilibrium electrochemistry
- States of matter

For more detail, see the [Syllabus](#).

The [Lecture Timetable](#)³⁶ is published on the department website.

Practicals

[Practical Chemistry](#)³⁷ is taught in the new Chemistry Teaching Laboratory, which opened in 2018. You will be timetabled an introductory week plus 30 days in the laboratory (180 hours). The practical course teaches essential experimental skills, from the synthesis and characterisation of compounds to the operation of spectrometers and instruments for analytical measurements. It makes tangible much that is covered in lectures and tutorials, whilst giving you different and complementary skills. There are also IT practicals, and parts of practicals, which cover programming, the use of chemistry specific software and other relevant skills.

For the Practical Course you will be assigned a group, based on your College, and this group will determine your timetable. Attendance is compulsory. Strict deadlines for submission of laboratory reports must be adhered to. Problems resulting in delay of submissions should be reported to the Senior Laboratory Staff at the earliest opportunity. The following people are responsible for the first year Practical Course:

- Dr. Malcolm Stewart
- Dr. Craig Campbell

They will also welcome your comments and suggestions on the practical course.

All practical work must be completed and signed off by 5pm 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 or skill, and you will not be permitted to proceed to the second year unless the first year practical course has been successfully completed. You should speak to the Senior Laboratory Staff about any problems that you may have in the Practical Course, either with the written work or in the laboratory.

The Practical Course uses a database called [myPracticals](#)³⁸ to log your progression through the course. Both you and your Tutor will have access to this in order to track your progress.

Tutorials and Classes

Chemistry tutorials are organised within the colleges. Classes will also be offered in other subjects, particularly mathematics.

Examinations

See page 10 – Prelims.

Books

Do not rush out immediately and buy new books. There are frequently second-hand books advertised on departmental notice boards for a fraction of the cost. Many of the books you will need and want are also available in college libraries with enough copies

³⁶ <http://www.chem.ox.ac.uk/timetableweek.asp>

³⁷ <http://course.chem.ox.ac.uk/practicals.aspx>

³⁸ <https://mypracticals.chem.ox.ac.uk/>

for you to take them out on a long-term loan. If you do buy, you are advised to buy only the latest editions of texts, since old editions may be out of date. A Reading List of the books recommended by the lecturers for the first year course can be found later in this Handbook. Your tutors will also advise you as to which books you should obtain.

Societies

The [Chemistry and Biochemistry Society \(OUCB\)](http://oucb.uk/)³⁹ holds regular social functions, special interest lectures and other activities. It is open to all chemistry undergraduates. You will receive

information directly from the officers of the Society. The [Scientific Society \(OUSS\)](https://ouscisoc.org/)⁴⁰ also arrange talks by distinguished visiting speakers on a wide variety of topics.

Refreshments

There are vending machines in the foyers of the CTL, ICL and PTCL.

If in doubt about anything, you can always ask your College Tutor. They will be able to direct you to someone else if they cannot answer your query themselves.

³⁹ <http://oucb.uk/>

⁴⁰ <https://ouscisoc.org/>

Second Year 2019 - 2020

The Course

In the second year, some of the lectures develop further the topics introduced in the first year. There are also many courses on essentially new topics.

- Diffraction
- Bonding in molecules
- Transition metal chemistry
- Coordination chemistry
- Chemistry of lanthanides and actinides
- Organometallic chemistry
- Electronic properties of solids
- Periodic trends in main-group chemistry
- NMR in inorganic chemistry
- Organic synthesis
- Aromatic and heterocyclic chemistry
- Organic spectroscopy
- Conformational analysis and ring chemistry
- Physical organic chemistry
- Heteroatoms in organic synthesis
- Rearrangements and reactive intermediates
- Organic chemistry of biomolecules
- Quantum mechanics: principles and applications
- Liquids and solutions
- Statistical mechanics
- Atomic and molecular chemistry
- Valence
- Rate processes
- Symmetry
- Introduction to NMR
- Maths for chemists

For more detail, see the [Syllabus](#).

Practicals

[Practical Chemistry](#)⁴¹ is taught in the Chemistry Teaching Laboratory. You will be timetabled an introductory talk at the beginning of the year, which is a compulsory part of the course, plus 24 days in the laboratory (144 hours).

For the Practical Course you will be assigned a group, based on your College, and this group will

determine your timetable. Attendance is compulsory. Strict deadlines for submission of laboratory reports must be adhered to. Problems resulting in delay of submissions should be reported to the Senior Laboratory Staff at the earliest opportunity. The following people are responsible for the second year Practical Course:

- Dr. Andrew Worrall
- Dr. Sam Cahill
- Dr. Simon Hibble

They will also welcome your comments and suggestions on the practical course.

The Practical Course uses a database called [myPracticals](#)⁴² to log your progression through the course. Both you and your Tutor will have access to this in order to track your progress.

Supplementary Subjects

A number of [Supplementary Subjects](#)⁴³ are available each year, on an optional basis. On offer for 2019-20 are:

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

Each Supplementary Subject Examination (held at the end of Hilary Term, except Modern Languages at the end of Trinity Term) comprises one paper, which results in fail / pass / distinction. A pass gives exemption from 36 hours of the 3rd year practical course. A mark over 60% in science based subjects or 70% in languages gives extra credit towards the final degree total. 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 or above may not retake the same Supplementary Subject Examination.

⁴¹ <http://course.chem.ox.ac.uk/practicals.aspx>

⁴² <https://mypracticals.chem.ox.ac.uk/>

⁴³ <http://course.chem.ox.ac.uk/supplementary-sub.aspx>

Third Year 2019 - 2020

The Course

In the third year core course, the topics 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 reaction
- Transition metal catalysis in organic synthesis
- Radical reactions in organic chemistry
- Curly arrows of biology
- Strategies in synthesis
- Magnetic resonance
- Photophysics and photochemistry
- Soft condensed matter
- Physical principles of solids
- Statistical mechanics

For more detail, see the [Syllabus](#).

Additionally, 15 option courses are available as listed in the [Scheme of Third Year Lectures](#) and described in detail in the Syllabus. These option courses will each comprise 8 lectures in Hilary Term and 1 problem class in Trinity Term. The single, compulsory examination paper will contain one question on material taken from each of the option courses. Candidates will be required to answer 3 questions.

Practicals

Before sitting Part IB, except in special circumstances, each candidate must have completed the full practical requirement of 252 hours (or 216 if a Supplementary Subject has been taken and passed). In the third year there is a free choice of experiments. All practical work must be

completed and marked off by 5pm on the Friday of 4th week of Trinity Term.

Part II Allocation

During the third year students apply to and are assigned their supervisor for the fourth year research project (see below). Current research now spans a huge range of topics, many of which are interrelated. You are encouraged to look at the [Research Themes](#)⁴⁴ web pages and select the area you wish to work in by following the links to the web pages for individual members of academic staff. Each page will contain a summary of their current research interests and some have links to their own further research information. There will also be Open Days, usually held in Michaelmas Term. Each Section offers an Open Day where you are invited to visit the labs, meet the supervisors (and their students) 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 also possibilities for Part II students to carry out a portion of the research project at a University abroad, or outside of Chemistry.

The [Apply > Part II Year](#)⁴⁵ web pages explain how the Part II allocation process works and contain more information about projects outside of Chemistry / abroad.

Supplementary Subjects

[Supplementary Subjects](#)⁴⁶ are open to third year students. A mark over 60% in science based subjects or 70% in languages gives extra credit towards the final degree total. Supplementary Subjects may be taken in any of years 2, 3 or 4, with a maximum of three in total. Candidates who get a pass or above may not retake the same Supplementary Subject Examination.

⁴⁴ <http://www.chem.ox.ac.uk/research.aspx>

⁴⁵ <http://teaching.chem.ox.ac.uk/apply--part-ii.aspx>

⁴⁶ <http://course.chem.ox.ac.uk/supplementary-sub.aspx>

Fourth Year 2019 - 2020

Research Project

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 are available in both pure and applied Chemistry and 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 25% in the final determination of the class of MChem honours degree.

[Guidance for the Part II Year](http://teaching.chem.ox.ac.uk/guidance-for-the-part-ii-year.aspx)⁴⁷ is available on the web. Detailed instructions to candidates about the preparation and assessment of the thesis will be posted on the web by the Chair of Examiners and sent to you by email.

There is a [Data Analysis lecture course](http://course.chem.ox.ac.uk/data-analysis-course.aspx)⁴⁸ designed for Part II students. There are also induction lectures organised on a Sectional basis and there are Departmental [Colloquia](http://colloquia.chem.ox.ac.uk/)⁴⁹ which Part II students are encouraged (indeed expected) to attend.

Supplementary Subjects

[Supplementary Subjects](http://course.chem.ox.ac.uk/supplementary-sub.aspx)⁵⁰ are open to Part II students. A mark over 60% in science based subjects or 70% in languages gives extra credit towards the final degree total. Supplementary Subjects may be taken in any of years 2, 3 or 4, with a maximum of three in total. Candidates who get a pass or above may not retake the same Supplementary Subject Examination.

⁴⁷ <http://teaching.chem.ox.ac.uk/guidance-for-the-part-ii-year.aspx>

⁴⁸ <http://course.chem.ox.ac.uk/data-analysis-course.aspx>

⁴⁹ <http://colloquia.chem.ox.ac.uk/>

⁵⁰ <http://course.chem.ox.ac.uk/supplementary-sub.aspx>

Prizes

A number of substantial Prizes and Bursaries are available. In 2019 the following were awarded:

- Prizes for outstanding performance in Prelims
- ABinBev Prizes for outstanding performance in Part IA
- OUP Prize for outstanding improvement between Prelims and Part IA
- Gibbs Prizes for outstanding performance in Part IB
- Thesis Prizes in Inorganic Chemistry, Physical & Theoretical Chemistry, and Organic Chemistry & Chemical Biology
- GSK Part II Prizes in Organic Chemistry for student continuing to DPhil studies in Chemistry at Oxford
- Brian Bannister Prize in Organic Chemistry
- Turbutt, Shimadzu and GSK Prizes in Practical Chemistry

In addition to these, Colleges also award prizes for academic excellence.

Recommended Core Textbooks

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

- *Physical Chemistry*, Atkins, de Paula, Keeler; OUP [11th edn. 2017]
- *Inorganic Chemistry*, Weller, Overton, Rourke, Armstrong, Atkins; OUP [6th edn. 2014]
- *Chemistry of the Elements*, Greenwood & Earnshaw; Butterworth-Heinemann [2nd edn. 1997]
- *Foundations of Organic Chemistry*, Hornby & Peach; Oxford Chemistry Primer OUP [1997, illustrated edition 2000]
- *Organic Chemistry*, Clayden, Greeves, Warren; OUP [2nd edn. 2012]
- *Organic Chemistry*, Maitland Jones, Fleming; Norton [5th edn. 2014]
- *A Guide to Mechanism in Organic Chemistry*, Sykes; Pearson [6th edn. 1986]
- *Foundation Mathematics for the Physical Sciences*, K.F. Riley and M.P. Hobson, Cambridge University Press [2011]

Scheme of Lectures, Classes, Tutorials and Practicals

Lectures and Classes

The Department / Faculty provide the following lectures and classes. Maths and Physics classes are 90 minutes in length. Quantum Supplementary Subject classes are 60 minutes in length.

First Year	Term	Lectures	Classes
<i>Inorganic Chemistry</i>			
Atomic Structure and Periodic Trends	M	6	
Ionic Model and Structures of Solids	M	9	
Molecular Shapes, Symmetry and Molecular Orbital Theory	H	6	
Acids, Bases and Solution Equilibria	H	4	
Transition Metal Chemistry	H	5	
Non-metal Chemistry	T	6	
Revision Topics	T	4	
<i>Organic Chemistry</i>			
Introduction to Organic Chemistry	M	7	
Introduction to Organic Spectroscopy	M	2	
Orbitals and Mechanisms	M	7	
Substitution and Elimination at Saturated Carbons	H	8	
Chemistry of C-C π Bonds	H	8	
Core Carbonyl Chemistry	H	8	
Introduction to Biological Chemistry	T	12	
Revision Course	T	4	
<i>Physical Chemistry</i>			
Foundations of Physical Chemistry: Chemical Thermodynamics	M	13	
The Physical Basis of Chemistry: Classical Mechanics	M	4	1
The Physical Basis of Chemistry: Property of Gases	M	4	1
The Physical Basis of Chemistry: The Role of Charge I	M	4	1
The Physical Basis of Chemistry: The Role of Charge II	H	4	1
Quantum Theory of Atoms and Molecules	H	10	
Reaction Kinetics	H	6	
Electrochemistry	H	4	
States of Matter	T	4	
<i>Mathematics for Chemistry</i>			
The Calculus of One and Two Variables	M	20	6 + 1 in H
Introduction to Vectors	M	2	1
Vectors and Determinants	H	6	3
Complex Numbers, Multiple Integrals and Ordinary Differential Equations	H	10	4 + 1 in T
Matrix Algebra	T	8	4
Revision	T		1

Second Year	Term	Lectures	Classes
<i>Inorganic Chemistry</i>			
Diffraction	M	4	
Bonding in Molecules	M	8	
Transition Metal Chemistry	M	6	
Coordination Chemistry	H	4	
Chemistry of the Lanthanides and Actinides	H	4	
Organometallic Chemistry	H	8	
Electronic Properties of Solids	H	8	
Periodic Trend in Main Group Chemistry	T	5	
NMR in Inorganic Chemistry	T	4	
Course Overview (and Transition Metals)	T	8	
Revision Topics	T	2	
<i>Organic Chemistry</i>			
Organic Synthesis I	M	4	
Aromatic and Heterocyclic Chemistry	M	4	
Organic Spectroscopy I	M	6	
Conformational Analysis and Ring Chemistry	M	10	
Physical Organic Chemistry	H	8	
Heteroatoms in Organic Synthesis	H	8	
Rearrangements and Reactive Intermediates	H	8	
Organic Synthesis II	T	8	
Organic Chemistry of Biomolecules	T	8	
Problem Solving	T	2	
<i>Physical Chemistry</i>			
Quantum Mechanics: Principles and Applications	M	12	
Liquids and Solutions	M	8	
Statistical Mechanics	H	12	
Atomic and Molecular Spectroscopy	H	10	
Valence	H	8	
Rate Processes	T	8	
Revision Lectures	T	3	
<i>General Chemistry</i>			
Symmetry I	M	5	
Introduction to NMR	M	4	
Maths for Chemists	M	5	2
Symmetry II	M	4	
<i>Supplementary Subjects</i>			
Aromatic and Heterocyclic Pharmaceutical Chemistry	M	16	
Aromatic and Heterocyclic Pharmaceutical Chemistry	H	14	
Quantum Chemistry	M	16	
Quantum Chemistry: Operators and Commutators	M		4
Quantum Chemistry: Group Theory	M		3 + 1 in H
Quantum Chemistry	H	14	
Quantum Chemistry: Perturbation Theory	H		4
Quantum Chemistry: Electronic Structure Theory	H		3
Chemical Crystallography	M	12	
Chemical Crystallography	H	9	
History and Philosophy of Science: The Origins of Modern Science	M	8	
History and Philosophy of Science: Science in Philosophy	H	8	
Chemical Pharmacology	M	3	
Chemical Pharmacology	H	12	
Modern Languages (Language Options TBC at time of printing)	H+T		32

Third Year	Term	Lectures	Classes
<i>Inorganic Chemistry</i>			
Inorganic Reaction Mechanisms	M	4	
Modern Main Group Chemistry	M	5	
Solid State Chemistry	M	5	
Spectroscopy and Magnetism in Inorganic Chemistry	M	5	
Organometallic Chemistry	M	5	
Bioinorganic Chemistry	M	4 + 1 in T	
Revision of Topics in Inorganic Chemistry	T	3	
Review of Periodic Table	T	3	
<i>Organic Chemistry</i>			
Advanced Organic Spectroscopy	M	6	
Organic Synthesis III	M	8	
Curly Arrows of Biology (Primary Metabolism)	M	4	
Transition Metal Catalysis	M	4	
Pericyclic Reactions	M	6	
Radical Reactions	M	4	
Revision Lectures	T	4	
<i>Physical Chemistry</i>			
Physical Principles of Solids	M	8	
Soft Condensed Matter	M	8	
Photophysics and Photochemistry	M	8	
Magnetic Resonance	M	8	
Revision Lectures	T	4	
<i>Option Courses</i>			
Molecular Spectroscopy	H	8 + 1 in T	
Structural Methods	H	8 + 1 in T	
Organometallic Catalysts: From Fundamentals to Application	H	8 + 1 in T	
Solid State Compounds in Technology	H	8 + 1 in T	
Supramolecular, Nano and Medicinal inorganic Chemistry	H	8 + 1 in T	
Natural Product Chemistry	H	8 + 1 in T	
Advanced Synthesis and Total Synthesis	H	8 + 1 in T	
Contemporary Methods in Catalysis for Organic Synthesis	H	8 + 1 in T	
Advanced Chemical Biology	H	8 + 1 in T	
Functional Organic Polymers and Materials Chemistry	H	8 + 1 in T	
Molecular Reaction Dynamics	H	8 + 1 in T	
Theoretical Chemistry	H	8 + 1 in T	
An Introduction to the Liquid State	H	8 + 1 in T	
Magnetic Resonance	H	8 + 1 in T	
Molecular Surface Science	H	8 + 1 in T	

Fourth Year	Term	Lectures	Classes
Data Analysis	M	8	

Third Year Option Courses

The Third Year option courses assume knowledge of the core material from the first three years of the course and build on this. They are designed to develop advanced concepts and methods in chemistry and to cover areas of contemporary interest. They will be updated annually to reflect developments.

Tutorials

Tutorials are the college teaching system. A Tutor (usually a Fellow of the college) teaches undergraduates in very small groups (usually 2 or 3 students). Undergraduates attend, on average, one or two tutorials every week of approximately 90 minutes in length. Students must undertake a considerable number of hours of preparatory work for each tutorial, including background reading, essay-writing and problem-solving. Colleges may, at their discretion and as appropriate, provide teaching quantities or formats other than those indicated here.

Practicals

The Department coordinates practical teaching. The table below outlines the Practical Course requirements in each year group.

	Skills Labs	General Labs	Total
<i>First Year</i>	12 days (72 hours)	18 days (108 hours)	30 days (180 hours)
<i>Second Year</i>	18 days (108 hours)	6 days (36 hours)	24 days (144 hours)
<i>Third Year</i>	Students have free choice of experiments in the third year. The requirement is 18 days (108 hours), or 12 days (72 hours) if a Supplementary Subject has been taken and the exam passed.		

For First Year students there will be an introduction session to assess practical skills on the second day of each group's timetabled practical days in the 1st week of Michaelmas Term.

Students should raise any issues with teaching or supervision as soon as possible so that they can be addressed promptly.

Syllabus for Prelims 2019 - 20

Chemistry 1: Inorganic

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

Atomic Structure and Periodic Trends

The Bohr model, wave properties of electrons, the Born Interpretation: probability densities. The Schrödinger equation and the H atom. The quantum numbers n , l , m_l , their values and interpretation (hence 2s, 3d, 4f, etc.) Shapes and energies of orbitals. Radial wavefunction and the radial distribution function. Polyelectronic atoms: Orbital approximation, spherical average of electron repulsion. Helium and the Pauli Exclusion Principle: electron spin, antisymmetry. Screening and penetration, effective nuclear charge. Structure of the Periodic Table: s-, p-, d-, f-blocks. Trends in ionisation energies, electron affinities, ionic radii, 3d and 4f contractions.

Ionic Model, Pre-Transition Metal and Solid State Chemistry

General atomic and chemical properties of elements of Groups 1, 2, within the framework of the Periodic Table. Elements, halides, hydrides, oxides. Born-Haber cycles, Born-Landé and Kapustinskii equation. Hess's Law cycles. Trends in the stability of binary compounds. Structures of ionic solids based on closed packing and filling of interstitial holes. Close packing, unit cells, space efficiency. Fractional coordinates, plan views and projections. Location, number and size of octahedral and tetrahedral interstitial holes. Common AB and 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, metals in liquid ammonia, unusual oxidation states, organometallic chemistry (e.g. methyl lithium).

Shapes, Symmetry and Molecular Orbital Theory

Lewis structures, VSEPR rules. Symmetry of molecules, symmetry elements, point group determination. Molecular orbital theory: H₂⁺, H₂, homonuclear diatomics, s/p mixing, bond strength and bond order, paramagnetism. Heteronuclear diatomics, HF and CO. 3-centre/2-electron, 4-centre/2-electron bonds: H₃⁺, H₃⁻, HF₂⁻, B₂H₆.

Acids, Bases and Solution Equilibria

Definitions (Brønsted, Lewis), pK_a, trends in acid strength, Pauling's rules for oxy-acids. Buffers. Redox potentials, Nernst equation, pH dependence, Latimer diagrams, Frost diagrams - construction and interpretation. Calculation of equilibrium constants from redox potentials.

Non-Metal Chemistry

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

Transition Metal Chemistry

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

Chemistry 2: Organic

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

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

these data and concepts to chemical problem solving.

Introduction to Organic Chemistry

Lewis bonding, bond polarisation. Lewis acids. Structures and isomers. Stereochemistry. Enantiomers: chirality, stereogenicity. Molecular orbital theory hybridisation. Functional groups: carbonyls, imines, oximes, nitriles. Lewis acids and bases. Curly arrows and mechanism. Resonance.

Introduction to Organic Spectroscopy

Introduction to spectroscopy. Nuclear spin and resonance. The chemical shift. Factors that influence carbon chemical shifts. Spin-spin coupling. Multiplet patterns for carbon-hydrogen couplings. Correlating carbon chemical shifts with organic structures.

Orbitals and Mechanisms

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

A unified approach to mechanism. Neutralisation and ionisation, S_N1 . 1,2-Addition to $C=O$ and β -elimination ($E1cB$, $E2$). S_N2 . Electrophilic addition with H^+ & regiochemistry. $E1$. Electrophiles and stereospecificity including simple reactions of arenes and alkenes.

Substitution and Elimination at Saturated Carbons

Substitution and Elimination at Saturated Carbons. Substitution reactions and mechanisms. Synthetically useful variants of eliminations.

Core Carbonyl Chemistry

Nucleophilic addition to $C=O$, reversible and irreversible. Nucleophilic substitution of $C=O$, (acetals; imines, oximes and hydrazones; enamines, Wittig and Horner-Emmons reactions, Wolff-Kishner reaction). Nucleophilic substitution at $C=O$, (acid chlorides; anhydrides; esters; amides). Simple IR stretch of $C=O$ groups. Chemistry of carboxylic acids. Keto-enol tautomerism: α -racemisation in acid or base. pK_a of simple FGs including malonates. Reactions of enolates. Alkylation, Claisen condensation, halogenation of ketones. The haloform, Reformatsky and Darzens reactions.

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

Chemistry of $C-C \pi$ -Bonds

Alkene and alkyne chemistry: influence of orbitals on reactivity. Overview of types of reaction. Alkene reactivity: electrophilic addition, pericyclic addition, free radical addition, catalytic hydrogenation. Allylic bromination. Alkyne reactivity: electrophilic addition, hydration to ketones, alkylation of terminal alkynes, reduction. Conjugation/delocalisation in non-aromatic systems: conjugated alkenes and alkynes, allenes. Modifications to reactivity, conjugate addition reactions. Structure and Reactivity of Aromatic compounds. Electrophilic aromatic substitution. Mechanism. Reactions: halogenation, nitration, sulfonation, Friedel-Crafts alkylation/acylation, formation of azo dyes (coupling with diazonium salts). Directing effects. Nucleophilic aromatic substitution.

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. Mechanism of transcription (DNA to RNA) and translation (RNA to protein) in cells. Consequences of DNA mutations. Modified DNA and RNA bases in nature. PCR and nucleic acid sequencing methods.

Revision and Problem Solving

The course will cover recent Prelims questions.

Chemistry 3: Physical

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

States of Matter and Equilibrium Thermodynamics

Le Chatelier's principle. Equations of state. Systems and surroundings. Work and heat. First law. Internal energy. State functions. Expansion work. Reversible and irreversible changes. Heat capacity and enthalpy. Thermochemistry. Standard states. Standard enthalpy changes (transition, reaction, formation). Kirchhoff law. Second law. Direction of change. Entropy. Condition of equilibrium. Entropy changes of phase transition. Temperature and pressure dependence of entropy. Third law. Statistical interpretation. Free energy. A and G . Available work. Temperature and pressure dependence of Gibbs energy. Phase equilibria. Clapeyron and Clausius-Clapeyron equations. One-component phase diagrams. Chemical equilibrium. Thermodynamics of mixtures. Chemical potential. Entropy and enthalpy of mixing. Extent of reaction. Reaction quotient. Condition for equilibrium, equilibrium constant and its temperature dependence; relation to standard Gibbs function.

Electrochemistry

The metal/solution interface. Electrochemical potential. Equilibrium Nernstian electrochemistry. Activity and activity coefficients and their determination. Nernst equation. Cells and half cells. Reference electrodes. Reversibility and irreversibility of cells. Relation of standard potentials to thermodynamic quantities. Conductivity of ionic solutions - liquid junction potentials. Measurement of standard electrode potentials.

States of Matter

Microscopic view of structure and motion in the three states; radial distribution function. Density, mechanical properties, diffusion and viscosity, degrees of freedom, equipartition and heat capacity. Intermediate states of matter: liquid crystals, gels, glasses. Intermolecular forces and pair potentials. Gas imperfection, van der Waals equation, virial expansion. Relationship between potential energy curve and the virial coefficients/internal energy. Single component phase diagrams (e.g., H_2O , CO_2 , 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

Quantum theory. Failures of classical physics. Quantization of electromagnetic radiation. Wave-particle duality. The de Broglie relation. The Schrödinger equation. Solution for particle in a one-dimensional square well and results for an n -dimensional square well; particle on a ring and the rigid rotor; simple harmonic oscillator; hydrogen atom. Born interpretation. Correspondence principle. Zero point energy. Quantum Tunnelling. Eigenvalue equations. Position, momentum and Hamiltonian operators. Expectation values, uncertainty principle. Atomic spectra: one-electron atoms and alkali metals. Orbitals, energy levels and quantum numbers. Radial and angular distributions. Term and level symbols. Spin-orbit coupling. Penetration and shielding. Selection rules and spectra. Structure of many-electron atoms and the Aufbau principle.

The Physical Basis of Chemistry: Classical Mechanics and Properties of Gases

Newton's Laws of motion: forces, momentum and acceleration. Work, and kinetic and potential energy. Rotations: angular momentum and moments of inertia. Vibrations: simple harmonic motion. Properties of gases: the perfect gas

equation. Kinetic theory of gases, origin of pressure, Maxwell-Boltzmann distribution. Molecular motions and equipartition. Collisions between molecules, mean free path, collision frequency, effusion, diffusion.

Reaction Kinetics

Rates of reactions. Order and molecularity. Rate laws and their determination. Experimental measurement of reaction rates. Sequential and reversible reactions, pre-equilibrium, the steady state approximation: applications to unimolecular reactions (Lindemann) and enzyme catalysis. Temperature dependence of reaction rates: Arrhenius Equation, activation energies, elementary collision theory.

Mathematics for Chemistry

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

Linear equations and determinants. Vector algebra and calculus, and applications to mechanics. Plane

polar, spherical polar and cylindrical polar coordinates. Inverse functions. Hyperbolic functions. Limits and their determination. Elementary calculus of one and of two variables. Taylor series and L'Hopital's rule. Integration, integration by parts. Transformation of coordinates. Theory of errors. Multiple Integrals in two and three dimensions. Complex Numbers. Argand diagram, Euler equation, de Moivre's theorem. Solutions of the equation $z^m = a + ib$

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

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

Syllabus for Part IA 2019 - 20

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

Atomic properties. Relative energies of s and d orbitals. Electronic configurations. Ionisation energies. Z_{eff} . The relative stability of oxidation states. The stability of the half-filled shell. Sublimation energies of the elements. Heats of formation of cations. Trends in stability of binary compounds. Rationalisation of electrode potentials. Ligand field splittings: high and low spin complexes, spin-pairing energies; LFSE effects in lattice energies, heats of formation, hydration energies, etc.; site preference energies in spinels, dependence on ligand type, oxidation state, and transition metal series.

The Jahn-Teller effect and its consequences. Stability of oxidation states in the 1st transition series. Trends in reduction potentials for $M^{3+}/M^{2+}(\text{aq})$. Oxidation state (Frost) diagrams. The effect of pH and of ligands on redox potentials. Factors and ligands stabilising high and low oxidation states (e.g. pi acceptor ligands versus pi donor ligands). Role of entropy. Triad trends: stability of oxidation states; trends in covalence; metal-metal bonding. High coordination numbers. Pi bonding effects with ligands. Comparative survey of the chemistry of transition metal groups, e.g. titanium, zirconium and hafnium; chromium, molybdenum and tungsten, nickel, palladium and platinum. Introduction to transition metals in biology.

Lanthanides & Actinides

Lanthanides: Occurrence of the elements; electronic properties: the nature of f-electrons; periodicity in the f-block. Extraction and separation.

Properties of the metals. The predominance of the 3+ oxidation state. Structural chemistry of the lanthanide compounds. Aqueous chemistry, complex formation, nature of ligands, redox chemistry. Examination of binary halides, hydrides, oxides and borides: structures and electronic properties. Organometallic chemistry. Comparisons/contrasts with transition metals.

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

Coordination Chemistry

Thermodynamics and kinetics of complex formation: monodentate vs polydentate ligands, including acyclic and macrocyclic examples. Isomerism. thermodynamics of complex formation: stability constants. Factors affecting the magnitude of stability constants – Irving Williams series, chelate effect, class a and class b classification, requirements of ligands. Macrocyclic Ligand Complexes: biological importance, macrocyclic effect. Macrocyclic ligand syntheses – template and non-template syntheses. Template effect: thermodynamic and kinetic contributions. Occurrence of common geometries: the role of metal electronic configuration and ligand in determining the stereochemistry in d^6 , – d^{10} ions.

Bonding in Molecules

The orbital approximation, the LCAO approach. The use of symmetry in polyatomic molecules MO treatment of AH_2 (linear and bent), AH_3 (planar and pyramidal), AH_4 (T_d). Walsh diagrams: The shapes of AH_2 molecules, the bonding and shapes of H_3^+ and H_3^- : 3-centre-2-electron and 3-centre-4-electron bonds.

Photoelectron spectroscopy and "experimental" MO diagrams, spectra of AH_n molecules. AB_2 molecules from CO_2 to XeF_2 , 12-electron main group octahedral systems: SF_6 as an example. 8-

electron main group octahedral systems: $[C(AuPR_3)_6]^{2+}$ as a relative of CH_6^{2+} .

Octahedral transition metal systems, σ -bonding, comparison with electrostatic model. MO filling in octahedral complexes: at-interactions and factors that affect the magnitude of Δ . Molecular orbitals for 4-coordinate geometries: ML_4 (T_d and D_{4h}).

First- and second-order Jahn-Teller distortions.

Organometallic Chemistry

General principles: valence electron count, formal oxidation state, number of d-electrons. The 18- and 16-electron rules: applications and exceptions. Classification of reactions: addition, dissociation, ligand substitution, migratory insertion, extrusion, oxidative addition, reductive elimination and attack on coordinated ligands. Synthesis, bonding and selected reactions: Transition metal alkyl, alkylidene (carbene), alkylidyne (carbyne) and carbonyl complexes. Hydride, dinitrogen and dihydrogen complexes. Alkene, alkyne and allyl complexes. Cyclopentadienyl, arene and other C_nH_n ($n = 4 - 8$) sandwich and half-sandwich complexes. Synergic bonding and 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 (hkl) and {hkl}. Calculation of dhkl. 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: TiO, 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. Brief description of Spectroscopic techniques for studying band structure.

Mott-Hubbard insulators and breakdown of the band model. Chemical trends in the Mott-Hubbard transition – competition between bandwidth and interelectron repulsion. Low-dimensional metals and the Peierls distortion with examples – electronically-driven structural distortions. Intrinsic and extrinsic semiconductors; the effect of doping level on the properties.

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

Inorganic NMR

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

Survey of group trends. Electronegativity, size and polarisability: implications for "ionic" compounds formed with metals. Covalent bonds: trends in bond strength; formation of multiple bonds; hypervalence. Bonding models for hypervalent compounds. Catenation and polymerisation. Catenated and multiple bonds with Si, P, and S. Polymeric structures formed by Si-O, P-N and S-N compounds. Boranes: structural classification and Wade's rules; aspects of preparation and reactivity. Donor/acceptor properties. Major trends in Lewis acid/base chemistry. HSAB classification. Ligand properties. High oxidation states. Group trends: the "Alternation effect". Formation of polycations. Aspects of xenon chemistry.

Organic Chemistry

The course is designed to develop the concepts of organic chemistry introduced in the first year; to show some of the key experimental evidence which supports these concepts; to apply these data and

concepts to chemical problem solving; and to demonstrate that the subject is still evolving and that it has a key role to play in modern technological developments in diverse fields, ranging from chemical synthesis to biological science.

Questions on the Part IA Examination will be based upon topics covered by both the first and second year lecture courses and in the practical courses.

Organic Synthesis I

A logical approach to synthesis with a focus on applying concepts from the carbonyl chemistry course. Review of reactions from the 1st year. Retrosynthesis, disconnections, and synthons. 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,n-difunctionalised molecules.

Organic Spectroscopy

IR spectroscopy: Vibrational transitions as a source of bonding information; characteristic group frequencies; interpretation of spectra. NMR Spectroscopy. Proton NMR spectroscopy. Chemical shifts: factors that influence proton chemical shifts. Spin-spin coupling: proton coupling patterns and resonance multiplicities, coupling to chemically equivalent spins, weak and strong coupling, chemical and magnetic equivalence. Proton spin coupling constants and chemical structure: geminal, vicinal and long-range couplings. Chirality and NMR, chiral solvating agents. Carbon NMR spectroscopy: interpreting carbon chemical shifts. Example proton and carbon spectra.

Mass Spectrometry: Introduction to Mass Spectrometry as an analytical technique in chemical and biochemical analysis. Basic principles, instrumentation 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 aliphatic, aromatic and simple heteroatom compounds. Examples. Application of the above spectroscopic techniques to the solution of structural problems.

Aromatic and Heterocyclic Chemistry

What is Aromaticity? Resonance energy; molecular π -orbitals of benzene and cyclobutadiene; Huckel $4n + 2$ rule; aromatic ring currents; examples of non-benzenoid aromatic and anti-aromatic compounds; synthesis and characterisation of cyclobutadiene; homoaromaticity. Pyrrole, thiophene and furan.

Dipole moments; electrophilic aromatic substitution; deprotonation; comparison with pyridine; indole: reactivity with electrophiles; synthesis of pyrrole, thiophene and furan; Fischer indole synthesis. Pyridine and related compounds. Reactivity towards electrophiles; activation via N-oxide formation; pyridones; nucleophilic substitution; reduction of pyridinium salts; reactivity of methyl pyridines; synthesis of pyridine derivatives. Benzene, benzyne and nanographenes. Synthesis of the benzene ring: from acetophenone and from cyclopentadienones. Benzyne: synthesis and reactivity of ortho and para-benzyne.

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 stereoelectronic 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

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

Rearrangements and Reactive Intermediates

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

Heteroatoms in Organic Synthesis

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

Organic Synthesis II

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

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. Solid-phase RNA synthesis: protecting group strategies. Mechanisms of common molecular biology techniques used for the synthesis of entire genomes. Biological applications of oligonucleotides: blotting, qPCR, siRNA, CRISPR-Cas9. Common genomic/transcriptomic analysis: chromatin immunoprecipitation sequencing, RNA sequencing.

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 of inhibitors on enzyme kinetics and use of kinetic data to identify potent inhibitors. Concepts will be illustrated throughout with a range of 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 there from; expectation values and the meaning of measurement in QM; the time-dependent Schrödinger equation; stationary states and the time-independent Schrödinger equation. Commutators: definition, evaluation, properties. Physical significance of commutators; complementary observables, simultaneous dispersion-free measurement and the uncertainty principle (weak and strong). Bra-ket notation; definition and properties of Hermitian operators. One-body problems: the free particle (wave-particle duality; commutation and measurement; peculiarities). The particle in a d-dimensional box (quantization via boundary conditions; zero-point energy; the correspondence principle; degeneracy). Rotational motion: angular momentum; angular momentum operators, commutation relations and their significance; particle on a ring; particle on a sphere and eigenfunctions of L^2 ; the rigid rotor. The H-atom. The simple harmonic oscillator: wavefunctions, energy levels and properties. The variational principle.

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

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

Liquids and Solutions

Ideal solutions: entropy of mixing, zero enthalpy of mixing, Raoult's law, ideal solubility, depression of freezing point, osmotic pressure. Regular solutions: the effects of non-zero interactions, non-zero enthalpy of mixing, Henry's law, vapour pressure, phase separation. Polymer solutions: polymer dimensions in solution (theta and good solvents,

radius of gyration), Flory-Huggins model, entropy and enthalpy of mixing, osmotic pressure.

Electrolyte solutions: activity coefficients of ions in solution, Debye-Hückel (D-H) theory, Debye-length, ionic strength, application of D-H to solubility and dissociation. Surface of liquids and solutions: surface tension, Laplace's law, the Kelvin equation, the Gibbs dividing surface and the Gibbs adsorption equation.

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_{trans} and q_{elec} . Determination of internal energy, E , and specific heat, C_v , from q ; application to monatomic gas.

Limitations of Maxwell-Boltzmann statistics. Mean values of observables; applications to bulk magnetization, paramagnetic susceptibility and derivation of Curie Law. Interacting particles. Concept of an ensemble. The canonical ensemble and the canonical distribution. The canonical partition function, Q , its physical significance and determination of internal energy from Q . Entropy in statistical mechanics, and its relation to Q . Determination of enthalpy, Helmholtz free energy, Gibbs free energy and chemical potential from Q .

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

Calculation of molecular partition function and selected applications. q_{trans} , q_{elec} and the statistical thermodynamics of a monatomic gas; molar entropies and the Sackur-Tetrode equation. Rotational contribution to q for heteronuclear molecules; the high temperature limit and characteristic rotational temperature, Θ_{rot} . Rotational contributions to S and C_v . The effects of

nuclear spin: symmetry numbers and q_{rot} for homonuclear diatomics and other symmetrical molecules. Applications to rotational spectroscopy. Vibrational partition functions, q_{vib} , for diatomic molecules and polyatomics. Chemical equilibrium. Statistical mechanical result for the equilibrium constant K of a general chemical reaction. Calculating the equilibrium constant and selected examples: dissociation reactions, isotope exchange reactions, thermal ionization equilibria.

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

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; Alkali 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. Raman and Rayleigh Scattering; rotational and vibrational transitions; selection rules; mutual exclusion in centrosymmetric molecules; Raman vs. IR.

Valence

Born-Oppenheimer Approximation. Bonding in H_2^+ (LCAO approximation). Many-electrons - the Orbital Approximation. Deficiencies of the orbital approximation. Binding of He_2 , splitting of degenerate configurations, dissociation of H_2 . Application of Variation Principle to find LCAOs - the Secular Equations. Simplification due to symmetry and electronegativity differences. Examination of energy levels of diatomic molecules. Splitting into terms (O_2) and levels (NO). Electronic and Photoelectron Spectra of Molecules. Franck-Condon Effects. Selection Rules. Examination of vibrational and rotational structure. Band heads. Birge-Sponer extrapolation. Predissociation. Radiationless transitions. Polyatomics - Hückel simplifications of the secular equations. Use of symmetry. Properties from the wavefunction - bond-order, electron density, dipole moments, spectral properties, organic reactivity.

Rate Processes

Simple collision theory. Collision frequency and collision cross section. Reaction cross section and steric factor. Potential energy surfaces. Classical motion over PES's. Link between reaction cross sections and rate constants. Transition state theory. Comparison with simple collision theory. Calculation of rate constants. Estimation of pre-exponential factors. Temperature dependence of rate constants. Kinetic isotope effects. Quantum mechanical tunnelling. Non-Arrhenius behaviour. Thermodynamic formulation of TST. Liquid-phase kinetics. Comparison of liquid-phase and gas-phase reactions. Encounter pairs, cage effect, and geminate recombination. Wavelength and viscosity dependence of photodissociation, radical scavenging, kinetics of I_2 photodissociation, cluster reactions, spin effects. Diffusion controlled reactions. Smoluchowski theory. Stokes-Einstein relation. Effects of solvent viscosity and temperature, reactions between ions, spin effects. Activation controlled reactions. Gibbs energy of reaction, effect of electrostatic interactions, influence of solvent permittivity, entropy and volume of activation, electrostriction, influence of pressure and ionic strength. Electron transfer reactions. Marcus theory. Gibbs energy and reorganization energy. Marcus inverted region. Homogeneous and heterogeneous electron transfers. Interfacial kinetics. Electric potential and its effect on interfacial reaction rates. Butler-

Volmer equation. Transfer coefficients. Overpotential. Tafel relations. Voltammetry.

General Chemistry

Material from these courses can be examined in any Part IA paper, but is most applicable to Inorganic and Physical Chemistry.

Symmetry I - Molecular Symmetry, Group Theory, and Chemical Bonding

Symmetry operations and symmetry elements. Symmetry classification of molecules - point groups. Symmetry and physical properties: Polarity, Chirality. Combining symmetry operations: 'group multiplication' Mathematical definition of a group. Review of Matrices. Definitions, matrix algebra, inverse matrices and determinants. Transformation matrices. Matrix representations of groups. Properties of matrix representations. Similarity transforms. Characters of representations. Reduction of representations. Irreducible representations and symmetry species. Character tables. Orthogonality relationships in group theory. Using the LOT to determine the irreps spanned by a basis. Symmetry adapted linear combinations. Bonding in diatomics. Bonding in polyatomics - constructing molecular orbitals from SALCs. The variation principle. Solving the secular equations. Matrix formulation of a set of linear equations. Solving for the orbital energies and expansion coefficients. Summary of the steps involved in constructing molecular orbitals. Hückel molecular orbital theory.

Symmetry II

Character tables and their meaning: C_{2v} , C_{3v} and T_d revisited. The reduction formula and its application to SALCs in CH_4 . Projection operators and the SALCS of NH_3 . p orbitals in C_6H_6 . Another look at the origins of degeneracy in molecular systems. Ligand field splitting of d levels. Tables of descent in symmetry. Jahn-Teller theorem. 2nd order Jahn Teller effect. Direct products - symmetry of many electron states. Selection rules in electronic spectroscopy: octahedral versus tetrahedral systems. IR and Raman selection rules. Overtones and combination bands. Vibronic transitions.

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

Maths for Chemists

Ordinary differential equations: Series solution, Frobenius method. Special functions: Bessel functions, Legendre, Laguerre, Hermite polynomials.

Partial differential equations, separation of variables. The Schrödinger equation; particles in rectangular and circular boxes, the H atom. The diffusion equation. Numerical methods. Finite difference and finite element approaches. Explicit and implicit methods. COMSOL. Fourier series and

Fourier transforms. FT infra-red spectroscopy and the Michelson interferometer. The Fellgett 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.

Syllabus for Part IB 2019 - 20

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 Part1B examination papers. For each paper, candidates will be required to answer 4 questions taken from a choice of 6.

Inorganic Spectroscopy and Magnetism

Electronic spectra of metal complexes. The different types of electronic transition. Characteristics of absorption bands: transition energy, intensity and band width. 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 ML_6 . 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^+ , Mg^{2+} , Ca^{2+} . Electrolytes, ion channels, signalling. Properties of complexes between metals and proteins – how one influences the chemistry of other. Haem proteins and enzymes. Cytochrome c and electron transfer. The biological chemistry of oxygen: haemoglobin, peroxidases, catalases, and monooxygenases.

Oxygen binding. Reactive oxygen species and oxidative damage.

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

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

Solid State Chemistry

Overview of the material covered in the 2nd year: the basic electronic properties of stoichiometric solids and the effect of introducing defects. Defects and ion transport Defects in solids: thermodynamic and structural aspects. Non-stoichiometry and electronic consequences. Applications to metal oxides and other inorganic solids. Outline of experimental techniques used to study defects – diffraction, EXAFS, solid state NMR, electron microscopy (without detail on the techniques: focus is on information they provide). Ionic mobility in the solid state: factors affecting ionic conductivity in various types of solid. Applications in technology. Structures, Reactivity and Synthesis Chemical aspects of solid state chemistry: general synthetic methods. Low temperature reactivity of solids illustrated by intercalation chemistry (e.g. graphite, layered oxides and sulfides, C_{60}). Application of redox processes in solid state systems, for example in Li-ion secondary batteries).

Modern Main Group Chemistry

"Traditional" conceptions of chemical behaviour in main group and transition metal systems. Modern interpretations of electronic structure and bonding in main group compounds: Multiple bonding; Carbenes and their heavier analogues; Stable main group radicals. Novel modes of reactivity of main group systems: Frustrated Lewis Pairs; Small molecule activation using singlet carbenes and heavier group 14 carbene analogues; Reactivity of group 14 alkyne analogues. Catalysis using main group systems: Catalysis using Frustrated Lewis Pairs; "Redox" based catalysis using p-block

elements - formal oxidative-additions, reductive eliminations; Catalysis using s-block complexes.

Inorganic Reaction Mechanisms

Ligand substitution reactions in square planar metal complexes (including the trans effect) and in octahedral metal complexes: D, A, 'a, 'd mechanisms, anation and solvolysis reactions. Electron transfer reactions: inner sphere and outer sphere electron transfer. Introduction to Marcus theory: interplay between donor-acceptor overlap, thermodynamic driving force and reorganisation energy. Two-electron transfer and non-complementary reactions.

Organometallic Reaction Mechanisms and Catalysis

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

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.

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 proton NMR spectra: spin decoupling and 2D NMR, ^1H COSY;

Assigning carbon NMR spectra: using carbon-proton spin coupling; spectrum editing (DEPT), 2D NMR- one-bond (HSQC) and multiple-bond (HMBC) ^1H - ^{13}C correlations. Defining molecular stereochemistry using the nuclear Overhauser effect (NOE).

Mass Spectrometry: Principles of hard and soft ionisation methods. 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 and examples.

Organic Synthesis III

This course will cover the strategies and tactics adopted for the controlled and efficient synthesis of organic molecules. It will address aspects of the what, the why and the how of complex molecule synthesis in both academic and industrial settings. A large focus will be on stereocontrol and in particular we will look at the approaches to synthesising compounds as single enantiomers through, for example, classical resolution methods, chiral auxiliary approaches and enantioselective catalytic transformations. The course will cover the discovery and development of various methodologies for effecting stereoselective carbon-carbon, and carbon-heteroatom bond formation, as well as their strategic incorporation as key steps in applied total synthesis. Aspects of retrosynthesis, protecting group chemistry and mechanism will also be covered.

Pericyclic Reactions

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

Transition Metal Catalysis

Introduction to organometallic chemistry of transition metals. Organopalladium chemistry: Suzuki coupling, Heck coupling and related cross couplings. Copper-catalysed cross-coupling reactions. Alkene metathesis.

Curly Arrows of Biology

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

Radical Reactions

Occurrence and structure of free radicals; definitions; characteristic reactions. Free radical substitution reactions; reactivity and regioselectivity. Kinetics and mechanism: addition to multiple bonds; selectivity and chain reactions. Kinetics and mechanism: rearrangement chemistry; kinetic and thermodynamic control. Radicals in synthesis: functional group chemistry; tandem, cascade processes in complexity generation and application for natural product synthesis.

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 - 2018 papers and of Part IB papers in the years up to 2011. Students will be informed about the distribution of topics between the two papers when this has been decided by the examiners.

Magnetic Resonance

A revision of the principles of Nuclear Magnetic Resonance (NMR): magnetic moment, space quantization, the resonance condition, the vector model, populations and bulk magnetization, selection rules, the origin of shielding, diamagnetic and paramagnetic shielding, neighbouring group anisotropy, ring current effects, electronic effects,

intermolecular interactions. J-coupling, multiplet splitting, coupling to spins with I greater than $\frac{1}{2}$, discussion of Fermi contact interaction, an introduction to dipolar coupling. Magnetic resonance spectroscopy of two coupled spin- $\frac{1}{2}$ particles: a quantum mechanical treatment. The rotating frame, linear and circularly polarized fields, NMR as a coherence phenomenon; experimental methods: continuous wave and pulsed NMR, Free Induction Decay (FID) and Fourier Transformation for simple FIDs. Spin relaxation: spin-lattice and spin-spin relaxation, the rotational correlation time and the spectral density function, spin relaxation and the vector model, measurement of relaxation times, the inversion recovery experiment, the spin-echo experiment.

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

Electronic transitions of polyatomic molecules. Beer-Lambert law, selection rules and absorption strength, vibronic transitions, radiative lifetime, Franck-Condon Principle. Fates of excited states: Jablonski diagram, fluorescence and phosphorescence, vibrational relaxation, intersystem crossing and internal conversion, intramolecular vibrational redistribution, dissociation / predissociation.

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

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

fluorescence. Intermolecular energy transfer, Electronic energy transfer, long-range (dipolar, FRET) and short-range (exchange) mechanisms, spin correlation rules. Triplet annihilation. Triplet sensitization and delayed fluorescence. Exciplex formation. Chemical reactivity of electronically excited molecules; isomerisation, acidity, redox, orbital character etc. The role of intersections in returning to the ground state.

Geminate recombination, escape probability and recombination timescale. Photoionisation and photoelectron spectroscopy. Ion chemistry, ZEKE.

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

Physical Principles of Solids

Electrons in solids: free electron gas in differing dimensionality, DOS and Fermi energy, electronic heat capacity, Pauli paramagnetism, electrical conductivity, Wiedemann-Franz law, deficiencies in free electron model. Phonons in solids: Einstein theory of heat capacity, deficiencies, Debye model, optical and acoustic phonons, thermal conductivity in insulators.

Defects and disorder in solids: Classification of defects, thermal population of point defects, Schottky heat capacity, theory of the order-disorder transition in alloys. Surfaces: structure of surfaces, types of adsorption, Langmuir and BET isotherms, dissociative and competitive adsorption, heterogeneous catalysis, heat of adsorption.

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 at 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 15 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

Peptide Chemistry. Peptide synthesis: Methods, strategy, factors compromising yields, including loss of stereochemistry, 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 catalysed peptide hydrolysis; importance of hydrolytic enzymes as pharmaceutical targets.

Preparation and applications of chemically modified biopolymers. Functional groups in proteins and nucleic acids. Synthesis of modified nucleic acids. Phosphoramidite reagents and post synthetic modifications. Phosphorothioates, dithioates, PNA and other DNA analogues. Applications of modified oligonucleotides, fluorescent probes – Taqman, Molecular Beacons, Genetic and Forensic analysis of DNA.

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 asides to cover important reactions, reagents, reactivity and strategy principles.

Contemporary Methods in Catalysis for Organic Synthesis

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

Functional Organic Polymers and Materials Chemistry

Dyes- Mauveine, chromophores, commercial dyes, synthesis of azo dyes and cyanines, direct dyes, reactive dyes for cellulose, fluorescence, chemiluminescence, photochromics, photoinduced electron-transfer. Polymers and polymer synthesis- Polymerisation reactions: condensation vs. addition, step-growth vs. chain-growth, DP, Mn,

M_w, polydispersity index, 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 polymerisation will be considered in more detail, including living free-radical polymerisation (nitroxide-mediated polymerization, ATRP and RAFT). Approaches to the synthesis of conjugated polymers will also be discussed: using polyacetylene, polyphenylene vinylene, poly-para-phenylene and polythiophene as examples.

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

Organic Surface Chemistry- Comparison of different techniques for preparing and analysing organic surface functions. Organic Surface Chemistry- Grafting to and grafting from approaches, polymer brushes, applications of organic surface chemistry. Organic Semiconductors Types of organic metals and semiconductors: charge-transfer salts, conjugated polymers, molecular crystals; polyacetylene and poly-para-phenylene: band structure, solitons and bipolarons, synthesis, precursor routes, substituted derivatives, conformation. 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.

Inorganic Molecular Spectroscopy

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

the value of matrix isolation, the use of polarised light and time resolved studies to probe various systems. 3. Applications of NMR spectroscopy including quantitative dynamics and 2D spectra.

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.

Brief review of spin interactions in NMR. Zeeman interaction, chemical shift. J-coupling. Energy levels. Appearance of spectra. Vector model. Magnetization. Rotating frame. Radiofrequency pulses. Free precession. T₁ and T₂ relaxation. Free induction decay. Spin echoes, echo modulation. Fourier transformation, lineshapes. Product operators for one spin. Product operators for two coupled spins. Spin echoes, homonuclear and heteronuclear. INEPT. Polarization transfer. Multiple quantum coherence. Double quantum filter, INADEQUATE. Two-dimensional NMR. COSY. NOESY. HSQC Review of quantum mechanics of spin angular momentum. Spin Hamiltonian. Density matrix. Time-dependent Schrödinger equation. Liouville-von Neumann equation. Pulses and delays. Density matrix description of two-spin systems. Product operator and density matrix calculations in Mathematica.

Molecular Reaction Dynamics

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

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

Potential energy surfaces. Origin of the PES, and examples. Inelastic and reactive scattering in terms of classical trajectories on surfaces. Reactive scattering: determining the angular distribution. Crossed molecular beam methods.

Reaction mechanisms: stripping mechanism and the harpoon model; rebound reactions; complex formation.

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

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

Probing the transition state. Half collisions and photodissociation dynamics. Femtochemistry. Photoelectron detachment spectroscopy. Applications of molecular reaction dynamics. Atomic and molecular lasers. Excimer lasers. Energy transfer and the CO₂ laser. Chemical lasers: CO laser. Chemistry in extreme environments: low and high energy collisions.

Molecular Surface Science

Molecular processes at solid surfaces are fundamental to numerous chemical applications of solids, encompassing such fields as catalysis, nanotechnology and energy storage and utilization. The investigation of molecules at surfaces combines the complexity of molecular structure, chemistry and properties with high-performing preparative and analytical methods, which allow for atomic scale insight. Distributed over eight lectures, the course will present the principles of the underlying surface science. The experimental methods employed are introduced, with a focus on atomic scale structural analysis and electronic spectroscopy. With each method, we will look at an application involving molecules at surfaces, underpinned by examples from contemporary research.

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 Catalysts: From Fundamentals to Application

An advanced-level options course that will highlight contemporary organometallic chemistry ranging from fundamental aspects of synthesis, bonding and stoichiometric reactivity to the application of organometallic compounds in catalytic transformations.

Homogeneous olefin polymerisation: Homogeneous vs. heterogeneous olefin polymerisation catalysts; examples of homogeneous transition metal catalysts focussing initially on metallocene-types; co-catalysts: types and mode of operation; polymerisation mechanism: initiation, propagation, termination; α -olefins and control of tacticity. Extension to constrained geometry and post-metallocene systems; brief examination of the use of isoelectronic and isolobal relationships in catalyst design.

Ring Opening Polymerizations to oxygenated polymers Homogeneous catalysts: Ring opening polymerization of lactones: thermodynamic factors and monomer scope; homogeneous catalysts; proposed mechanism for coordination-insertion polymerizations: initiation, propagation, termination, chain exchange reactions, rates of polymerizations, living polymerizations, control of tacticity (stereocontrol) in lactide ring-opening polymerizations – enantiomorphic site control vs. chain end control mechanisms.

Copolymerizations of Oxiranes: alternating copolymerizations: thermodynamics and monomer

scope; metal catalysts for CO₂/epoxide copolymerizations – homogeneous and heterogeneous; catalyst nuclearity – mono- vs. dinuclear complexes; polymerization rates and mechanisms; exemplification of other alternating copolymerizations and block copolymerizations.

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

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

Catalytic functionalisation of organic molecules by borane reagents: Direct borylation of C-H bonds in arenes and alkanes – mechanism, selectivity and synthetic utility.

Solid State Compounds in Technology

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

For example:

1. Materials for Energy applications. Photovoltaics, Battery Materials, Transparent Conductors, Fuel Cell materials, Thermoelectric materials. How do we use our knowledge of Inorganic Chemistry to devise new compounds with particular properties?
2. Superconductivity. Classical and non-BCS superconductors. Factors affecting T_c. Recent developments; superconductors in action.
3. 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 and Medicinal Inorganic Chemistry

This course focuses on supramolecular host-guest chemistry and specific examples of uses of medicinal 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. Anion coordination chemistry: biological importance; exploiting electrostatics, hydrogen bonding, halogen 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. 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 polymetallic cage frameworks. 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. The surface assembly of molecular sensors. Anion sensors, cation sensors, redox and optical sensors including design principles. Molecular machines: introduction, examples, triggering and following molecular motion on surfaces. 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). Multimodality in imaging. Nanoparticles in medical imaging and theranostics.

Theoretical Chemistry

Time-Dependent Quantum Mechanics: Review of time dependence in quantum mechanics; stationary and non-stationary states. Two level system in a rotating field (e.g., ESR/NMR), Rabi oscillations. Perturbation theory: derivation of 1st order amplitudes, application to two-level systems and a continuous final spectrum (Fermi Golden rule rates). Applications of Fermi Golden rule rates to non-radiative processes in molecules, e.g. inter-system crossing and interconversion.

The interaction of light and matter 1: dipole approximation, derivation of the Einstein A and B coefficients. Derivation of the Einstein A and B coefficients. The interaction of light and matter 2: electric susceptibilities, oscillator strengths, and sum rules. Applications to radiative processes in molecules. Molecular electric susceptibilities, oscillator strengths, sum rules. Statistical Mechanics – Mean-field theory.

Recap of statistical mechanics of non-interacting systems; consequences of interactions; role of theory, models and simulation. Introduction to mean-field theory and concept of molecular field.

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

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

Syllabus for Supplementary Subjects 2019-20

Aromatic and Heterocyclic Pharmaceutical 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-dicarbonyls 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; S_NAr, S_{RN}1, benzyne mechanisms; applications in synthesis. Aromatic rearrangements. Arene metallations and cross couplings.

Heterocyclic Synthesis II

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

Reactions of Heterocycles

C=C versus C=O frameworks. Electrophilic attack easy on pyrroles and pyridines (at nitrogen). Dichotomies of electrophilic substitution mechanisms. Mannich and Vilsmeier in aromatic

and aliphatic systems. Decarboxylation and other ipso substitutions. Easy attack by nucleophiles - sometimes by electrophilic catalysis. Ring opening reactions. Difference from benzene.

Pharmaceutical Chemistry

Key topics of medicinal chemistry will be covered and exemplified with the story of the discovery of ground-breaking medicines: introduction to drug discovery and medicinal chemistry; physicochemical properties of drugs; case study – sildenafil introduction to pharmacology; drug targets; receptors; transporters; case studies – cimetidine and omeprazole introduction to small molecule drug design; drug-protein interactions; structure-based drug discovery; case study – crizotinib introduction to pharmacokinetics; half life, dose, volume of distribution and clearance; case studies – amlodipine and azithromycin. Introduction to drug safety; the central nervous system; drug-drug interactions; case studies – ketoconazole, terfenadine, fexofenadine and maraviroc.

Problem Session

Designing better drugs.

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.
3. Experimental considerations. Structure solutions methods. Parameterisation of structure. Obtaining the best fit of a model to data. Analysis and comparison of crystal structures.

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. Great and Little Orthogonality theorems, including results arising from them. Reduction of representations. Projection formula and SALCs. Direct Product representations, Full Rotation Groups and Russell-Saunders coupling. Symmetry

Properties of integrals and application to selection rules. Application of group theory to electronic transitions and molecular vibrations.

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 H_2^+ , H_2 . 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, Slaters vs Gaussians, Hierachy of basis sets, Beyond the HF approximation, Configuration interaction, Density functional theory, Semi-empirical methods, Hückel and Extended Hückel theory.

Important Dates

Dates of Full Term 2019-20

Michaelmas Term

Sunday 13 October – Saturday 7 December

Hilary Term

Sunday 19 January – Saturday 14 March

Trinity Term

Sunday 26 April – Saturday 20 June

Dates of Extended Term for Part II Candidates in Chemistry 2019-20

Michaelmas Term

Thursday 26 September – Friday 20 December

Hilary Term

Friday 3 January – Wednesday 8 April

Trinity Term

Monday 20 April – Saturday 11 July

Dates of Full Term 2020-21

Michaelmas Term

Sunday 11 October – Saturday 5 December

Hilary Term

Sunday 17 January – Saturday 13 March

Trinity Term

Sunday 25 April – Saturday 19 June

Dates of Extended Term for Part II Candidates in Chemistry 2020-21

Michaelmas Term

Thursday 24 September – Tuesday 22 December

Hilary Term

Tuesday 5 January – Wednesday 31 March

Trinity Term

Monday 12 April – Saturday 10 July

Examination Dates

Examination entries are made through your College, who will advise you of the appropriate deadlines. Detailed dates are not available at the time of publishing this Handbook, but may be found on the [Exams Timetables](#)⁵¹ university web page. Students need to enter for optional examinations only, i.e. Supplementary Subjects. All other entries will take place automatically.

Prelims

Begin in 7th Week Trinity Term

Part IA

Begin in 8th Week Trinity Term

Part IB

Begin in 6th Week Trinity Term

Part II Thesis

Deadline 12 pm Friday 7th Week Trinity Term

Part II Vivas

Begin 10th Week Trinity Term

Supplementary Subjects (Science)

Begin in 9th Week Hilary Term

Supplementary Subjects (Languages)

Begin in 8th Week Trinity Term

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

⁵¹ <https://www.ox.ac.uk/students/academic/exams/timetables?wssl=1>

Academic Staff List

All staff in the Department of Chemistry can be contacted by e-mail, which is generally the best method of contact. All email addresses end **@chem.ox.ac.uk**.

Name	Section	Office	College	E-mail
Aarts, Prof DGAL	PTC	PTCL	Christ Church	dirk.aarts
Adlington, Prof RM	OC	CRL	Lady Margaret Hall	robert.adlington
Aldridge, Prof S	IC	ICL	Queen's	simon.aldridge
Anderson, Prof E	OC	CRL	Jesus	edward.anderson
Anderson, Prof HL <i>FRS</i>	OC	CRL	Keble	harry.anderson
Armstrong, Prof FA <i>FRS</i>	IC	ICL	St John's	fraser.armstrong
Baldwin, Prof A	PTC	PTCL	Pembroke	andrew.baldwin
Barford, Prof W	PTC	PTCL	Balliol	william.barford
Battle, Prof PD	IC	ICL	St Catherine's	peter.battle
Bayley, Prof JHP <i>FRS</i>	CB	CRL	Hertford	hagan.bayley
Beer, Prof PD	IC	CRL	Wadham	paul.beer
Benesch, Prof JLP	PTC	CRL	University	justin.benesch
Booth, Dr M	OC	CRL	St Hugh's	michael.booth
Bowen, Dr AM	IC	ICL	Jesus	alice.bowen
Brouard, Prof M	PTC	CRL	Jesus	mark.brouard
Brown, Prof T	OC	PTCL		tom.brown
Burt, Dr M	PTC	PTCL		michael.burt
Burton, Prof JW	OC	CRL	Somerville	jonathan.burton
Chippindale, Dr A	IC		Pembroke	ann.chippindale
Claridge, Prof TDW	OC	CRL		tim.claridge
Clarke, Prof SJ	IC	ICL	Exeter	simon.clarke
Clary, Prof Sir DC <i>FRS</i>	PTC	PTCL	Magdalen	david.clary
Compton, Prof RG	PTC	RPB	St John's	richard.compton
Conway, Prof SJ	OC	CRL	St Hugh's	stuart.conway
Cooper, Prof RI	IC	CRL	Pembroke	richard.cooper
David, Prof W <i>FRS</i>	IC	ICL		bill.david
Davies, Prof SG	OC	CRL	Magdalen	steve.davies
Davis, Prof BG <i>FRS</i>	OC	ICL	Pembroke	ben.davis
Davis, Prof JJ	IC	PTCL	Christ Church	jason.davis
Deringer, Prof V	IC	ICL	St Anne's	volker.deringer
Dixon, Prof DJ	OC	CRL	Wadham	darren.dixon
Donohoe, Prof TJ	OC	CRL	Magdalen	timothy.donohoe
Doye, Prof JPK	PTC	PTCL	Queen's	jonathan.doye
Duarte, Prof F	PTC	PTCL	Hertford	fernanda.duartegonzales
Dullens, Prof RPA	PTC	PTCL	Lincoln	roel.dullens
Edwards, Prof PP <i>FRS</i>	IC	ICL	St Catherine's	peter.edwards
Farrer, Dr N	IC	ICL		nicola.farrer
Faulkner, Prof S	IC	ICL	Keble	stephen.faulkner
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Foord, Prof JS	PTC	CRL	St Catherine's	john.foord
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Goodwin, Prof A	IC	ICL		andrew.goodwin
Gouverneur, Prof V <i>FRS</i>	OC	CRL	Merton	veronique.gouverneur
Green, Prof NJB	PTC	ICL		nicholas.green
Harrison, Dr K	IC	PTCL		karl.harrison

Hayward, Prof MA	IC	ICL	Somerville	michael.hayward
Heazlewood, Dr B	PTC	PTCL		brianna.heazlewood
Hodgson, Prof DM	OC	CRL	Oriel	david.hodgson
Hore, Prof PJ	PTC	PTCL	Corpus Christi	peter.hore
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Jenkinson, Dr SF	OC	CRL	Wadham/Hertford	sarah.jenkinson
Kawamura, Dr A	OC	CRL		akane.kawamura
Krishnan, Prof M	PTC	PTCL	Merton	madhavi.krishnan
Kukura, Prof P	PTC	PTCL	Exeter	philipp.kukura
Laidlaw, Dr WM	IC	CRL	Jesus	michael.laidlaw
Lee, Dr V	OC	CRL	Oriel	victor.lee
Langton, Dr M	IC	CRL		matthew.langton
Logan, Prof DE	PTC	PTCL	University	david.logan
Mackenzie, Prof S	PTC	PTCL	Magdalen	stuart.mackenzie
Manolopoulos, Prof DE <i>FRS</i>	PTC	PTCL	St Edmund Hall	david.manolopoulos
McCullagh, Prof J	OC	CRL		james.mccullagh
McGrady, Prof J	IC	PTCL	New College	john.mcgrady
Mohammed, Prof S	CB	BioChem		shabaz.mohammed
Moloney, Prof MG	OC	CRL	St Peter's	mark.moloney
Mountford, Prof P	IC	CRL	St Edmund Hall	philip.mountford
Myers, Dr W	IC	ICL		william.myers
O'Hare, Prof DM	IC	CRL	Balliol	dermot.ohare
O'Neill, Dr M	IC	ICL	Queen's	michael.oneill
Penfold, Dr R	PTC	PTCL		robert.penfold
Perkin, Prof S	PTC	PTCL	Trinity	susan.perkin
Quarrell, Dr REL	OC		Balliol	rachel.quarrell
Rauschenbach, Prof S	PTC	CRL	Wadham	stephan.rauschenbach
Rees, Dr NH	IC	CRL		nick.rees
Ritchie, Prof GAD	PTC	PTCL	Worcester	grant.ritchie
Roberts, Dr PM	OC	CRL	Exeter	paul.roberts
Robertson, Prof J	OC	CRL	Brasenose	jeremy.robertson
Robinson, Prof Dame CV <i>FRS</i>	PTC	PTCL	Exeter	carol.robinson
Russell, Prof A	OC	CRL	St John's	angela.russell
Schofield, Prof CJ <i>FRS</i>	OC/CB	CRL	Hertford	christopher.schofield
Sheppard, Dr D	PTC	PTCL	Magdalen/Merton	dean.sheppard
Smith, Prof LJ	CB	ICL	St Hilda's	lorna.smith
Smith, Prof MD	OC	CRL	University	martin.smith
Stewart, Dr MI	OC	CTL	St Hugh's	malcolm.stewart
Thompson, Dr AL	IC	CRL		amber.thompson
Thomson, Dr JE	OC	CRL	St Catherine's	james.thomson
Timmel, Prof CR	IC	ICL	New College	christiane.timmel
Tsang, Prof SCE	IC	ICL	University	edman.tsang
Vallance, Prof C	PTC	CRL	Hertford	claire.vallance
Vincent, Prof K	IC	ICL	Jesus	kylie.vincent
Weller, Prof AS	IC	CRL	Magdalen	andrew.weller
Williams, Prof CK	IC	CRL	Trinity	charlotte.williams
Willis, Prof MC	OC	CRL	Lincoln	michael.willis
Wilson, Prof M	PTC	PTCL	Brasenose	mark.wilson
Wong, Prof LL	IC	ICL	St Hugh's	luet.wong
Worrall, Dr A	OC	CTL		andrew.worrall
Xiao, Dr T	IC	ICL		xiao.tiancun
Zhao, Dr P	IC	ICL		pu.zhao

Principal Officials

Head of MPLS	Prof. S. Howison	sam.howison@mpls
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	Prof. JHP Bayley (CB)	hagan.bayley@chem
Associate Head of Department (Teaching)	Prof. NJB Green	nicholas.green@chem
Director of Studies	Prof. NJB Green	nicholas.green@chem
Deputy Director of Studies	Dr. MR Galpin	martin.galpin@chem
Chair of Chemistry Teaching Committee	Prof. NJB Green	nicholas.green@chem
Chair of Chemists' Joint Consultative Committee	Dr. MR Galpin	martin.galpin@chem
Director of Teaching Laboratory	Dr. MI Stewart	malcolm.stewart@chem
Deputy Director of Teaching Laboratory	Dr. A Worrall	andrew.worrall@chem
Undergraduate Studies Administrator	Miss L Fenwick	undergraduate.studies@chem
Undergraduate Administrative Assistant	Mr. M Shott	mike.shott@chem

Abbreviations

OC = Organic Chemistry

CB = Chemical Biology

IC = Inorganic Chemistry

PTC = Physical & Theoretical Chemistry

CRL = Chemistry Research Laboratory

ICL = Inorganic Chemistry Laboratory

PTCL = Physical & Theoretical Chemistry Laboratory

DP = Dyson Perrins Building

RPB = Rodney Porter Building

CTL = Chemistry Teaching Laboratory

MPLS = Mathematical, Physical and Life Sciences Division

Policies & Resources

Policies

The University has a wide range of regulations and policies that apply to students. These are easily accessible through the [A-Z of University regulations and policies](#)⁵².

- [Intellectual property](#)⁵³
- [Plagiarism](#)⁵⁴
- [Equality & Diversity](#)⁵⁵
- [Disability](#)⁵⁶
- [Harassment](#)⁵⁷
- [Health and safety](#)⁵⁸
- [Chemistry Department safety](#)⁵⁹
- [Recording lectures and other teaching sessions](#)⁶⁰
- [Examination regulations](#)⁶¹
- [Compliance](#)⁶² (Data Protection)

Other Useful Resources

- [University Careers Service](#)⁶³
- [University IT Services](#)⁶⁴
- [Oxford Life](#)⁶⁵ (University resources)
- [Health & Welfare](#)⁶⁶ (University resources)
- [Enterprising Oxford](#)⁶⁷
- [Undergraduate News](#)⁶⁸ (Chemistry website)
- [Undergraduate Part II News](#)⁶⁹ (Chemistry website)

Mental Health & Wellbeing Resources

- Your GP
- Your College Tutor or Supervisor
- College Staff Welfare Officer (may have a slightly different title depending on the college)
- College Student Welfare Officer (probably on your JCR committee)
- [University Counselling Service](#)⁷⁰
- [Oxford Nightline](#)⁷¹
- [Samaritans](#)⁷²
- [Students Against Depression](#)⁷³
- [Student Minds](#)⁷⁴
- [Mind](#)⁷⁵

⁵²

<https://www.ox.ac.uk/students/academic/regulations?wssl=1>

⁵³ <https://researchsupport.admin.ox.ac.uk/innovation/ip>

⁵⁴

<https://www.ox.ac.uk/students/academic/guidance/skills/plagiarism?wssl=1>

⁵⁵ <https://edu.admin.ox.ac.uk/home>

⁵⁶ <https://www.ox.ac.uk/students/welfare/disability?wssl=1>

⁵⁷ <https://edu.admin.ox.ac.uk/harassmentadvice>

⁵⁸ <http://www.admin.ox.ac.uk/safety/hs-mgmt-policy/>

⁵⁹ <http://safety.chem.ox.ac.uk/>

⁶⁰ <https://academic.admin.ox.ac.uk/policies/recording-lectures-other-teaching-sessions>

⁶¹ <http://www.admin.ox.ac.uk/examregs/>

⁶² <https://compliance.admin.ox.ac.uk/>

⁶³ <https://www.careers.ox.ac.uk/>

⁶⁴ <https://www.it.ox.ac.uk/do>

⁶⁵ <https://www.ox.ac.uk/students/life?wssl=1>

⁶⁶ <https://www.ox.ac.uk/students/welfare?wssl=1>

⁶⁷ <https://www.eship.ox.ac.uk/>

⁶⁸ <http://ugnews.chem.ox.ac.uk/home>

⁶⁹ <http://ugnews.chem.ox.ac.uk/part-ii-students.aspx>

⁷⁰ <https://www.ox.ac.uk/students/welfare/counselling?wssl=1>

⁷¹ <https://oxfordnightline.org/>

⁷² <https://www.samaritans.org/>

⁷³ <https://www.studentsagainstdepression.org/>

⁷⁴ <https://www.studentminds.org.uk/>

⁷⁵ <https://www.mind.org.uk/>