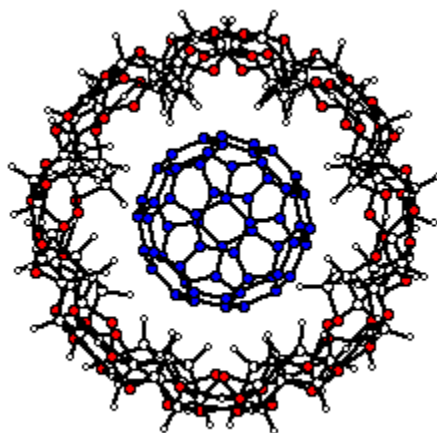


Chemistry Department

400-level Coursebook

2010



Information for B.Sc.(Hons), M.Sc.(Hons) and
P.G.Dip.Sci. students doing CHEM400-480 papers.

General Information

The co-ordinator of fourth year courses in the Chemistry Department is Owen Curnow. Please feel free to see him at any time if you have any queries or concerns about your programme of study.

This booklet contains information about lecture courses and other aspects of fourth year study in Chemistry. The house regulations listed here apply to all students who are doing their research project in the Chemistry Department. If your research project is in another Department or School, then different regulations regarding assessment and grading may apply.

If you are going to be carrying out research work in the Chemistry Department you **MUST** read and sign a Chemistry Department Safety Handbook.

Project work should begin during the week commencing 15 February. Before starting you **MUST** report to Bruce Reid (Room 536). He will provide you with a copy of the Departmental Health and Safety Handbook and other forms relating to photocopy access, keys and your place of research.

All students doing CHEM400 papers should attend a basic first aid course on **Wednesday 17 February at 9 am to 1 pm in Room 533** as well as a briefing session about safety, courses and undergraduate demonstrating on **Wednesday 17 February at 2 pm in room 533**. Lectures begin on 22 February. Most CHEM400 lectures are in room 533.

Demonstrator Training will be on **Friday 19 February at 9 am in Room 533**.

CHEMISTRY MASTERS - PART I and P.G. Dip. Sci. – 2010

Course Structure

Each student must select **eight** papers from CHEM 401–416. Students credited with only 56 points from CHEM 320 and 360 courses will be required to achieve concurrently a satisfactory standard in a further 300-level course as approved by the Head of Department.

Laboratory Work

Students are expected to spend an average of between 12 and 15 hours per week in the laboratory for the first three terms, including at least one week of the April vacation and two weeks of the mid-year recess, and then full time for term four onwards; laboratory work should finish around Friday 5 November, the exact date to be decided by the supervisor. A brief project report (2–4 A4 typed pages) should be submitted to the Head of Department by **Thursday 11 November**.

Part I exams

The exam timetable will be set by the end of term two.

Note that the regulations state that for a student to proceed to M.Sc. Part II, a student must either:

- Pass all eight papers with a grade average of at least C+, or
- Pass six papers with an average of at least B– for the eight papers (with special approval).

Project Talk

At the beginning of the **second** year (Part II) of the M.Sc. all students will be required to give a 15–20 minute presentation to the department outlining the background and aims of their research project, along with a summary of any results obtained in the first year.

B.Sc. Hons 400 Level Project Talks

All M.Sc. Part I students will be required to attend these talks scheduled for the afternoons of (a) March 26 and (b) November 10.

Liaison Committee

There is a small staff-student liaison committee to which a member of the Honours/M.Sc. class belongs.

CHEM 400 - CHEMISTRY HONOURS 400 LEVEL – 2010

Course Structure

Each student must select **eight** papers from CHEM 401–416 along with CHEM 480.

Research Project (CHEM480)

Students are expected to spend an average of between 12 and 15 hours per week in the laboratory for the first three terms, including at least one week of the April vacation and two weeks of the mid-year recess, and then full time for term four onwards; laboratory work should not be carried out beyond **22 October** without the permission of the 400-level coordinator.

Research Project Proposal

A written research proposal (≤ 3 A4 pages, double-spaced) should be submitted to the departmental secretary (Room 534) by **Thursday 2 April**. **This proposal will not be graded in any way**, but advice may be given by academic staff, both during its preparation and after submission. Supervisors are expected to provide verbal feedback on the proposal.

Research Report

The research report should take no longer than 35 hours for its preparation, and should be as short as convenient, and no longer than 4000 words, excluding the experimental section, diagrams, tables, graphs and references. An experimental section must be included. The report must be written using the RSC style, for which guidelines can be found at: <http://www.rsc.org/Publishing/ReSource/AuthorGuidelines/index.asp>. Four copies (which may be double-sided) of the completed research report should be handed to the departmental secretary by **Monday 1 November**, and an electronic copy should be sent to Owen Curnow.

Grading of the Research Project

The research project (CHEM480) is given a weighting equivalent to **two** written papers and the mark will be determined from four components:

| | |
|-------------------------------------|-----|
| Examination Panel's Project Mark | 30% |
| Supervisor's Project Mark | 30% |
| Research Project Talk (Term 4 only) | 15% |
| Oral Interview | 25% |

The supervisor and examination panel will take into account (i) the experimental ability of the student, (ii) the approach and initiative of the student to the research project, (iii) the level of understanding displayed by the student, and (iv) the ability of the student to produce a written report on the research project. It is anticipated that the supervisor will provide assistance in the preparation of the research report. Mid-year feedback will be provided by your supervisor with respect to areas (i)–(iii).

Research Project Talks

To give Chemistry Honours students experience in presenting brief scientific talks, and to allow academic staff to advise students on presentation techniques, each student will give a 5-minute talk on the aims of the research project. These practice talks will be presented to the Honours/Masters Part I class and the individual student's supervisor(s) on the afternoon of **Friday 26 March**. **These practice talks will not be graded in any way.** Feedback will also be provided.

The mark for the Research Project Talk will be awarded on the basis of a 10-minute presentation by the student to the Chemistry Honours/Chemistry Masters Part I class. These presentations will be scheduled for **Wednesday 10 November**. All students are expected to attend. The grades for these Research Project Talks will be determined by an examination panel, and judged as a verbal scientific presentation, and **NOT** on the extent of the research results.

Interview

An interview of approximately 30 minutes will be held with each student on **Thursday 11 November**. The interview will be worth 25% of the CHEM480 grade and will assess your understanding of the project.

Liaison Committee

There is a small staff-student liaison committee to which a member of the Honours/M.Sc. class belongs.

Other commitments

The 4th year Chemistry programme is a full-time commitment. In addition to lectures (average 5 per week) and project work (average 16–20 hours per week), there are a number of other demands on your time:

First Year Demonstrating

All students (B.Sc(Hons), M.Sc. and P.G.DipSci) doing research projects in the Chemistry Department are expected to demonstrate in the First Year Laboratory Course (for which you are paid). This involves 3 hours in the lab per week, along with marking of the lab books and attendance at the weekly demonstrators' instruction meeting (Monday 12 noon in room 533).

Seminars

Fourth year students are expected to attend ALL Departmental Seminars. These are talks by visiting or local chemists on a diverse range of chemistry-related topics and take place on most Mondays at 11.00 am in room 531. Occasionally, additional seminars are scheduled for other times during the week.

Research group meetings

Most research students will belong to a group that has regular (weekly) meetings to report the latest research results, discuss literature results or solve research problems.

Study

Adding up the above times results in a rather full programme, and this is without doing any study for the final exams which account for 70–80% of your Honours grade. Most papers require significant extra reading of the chemical literature in order to understand the topics covered. The exam timetable will be set by the end of term two taking into account the courses taken by individual students.

CHEMISTRY 400 Course Content 2010

CHEM 401 Inorganic Chemistry

15 lectures. Assessment: Final exam: 100%

Dr. Owen J. Curnow (8 lectures) — Metal clusters: from molecules to metallic lattices

Clusters represent the transition from molecule to nanoparticle and metallic lattice. Their structures can be understood via an extension of Skeletal Electron Pair Theory (SEPT) in addition to other methods such as Topological Electron Counting (TEC) theory and Effective Atomic Number (EAN) rules. We will first look at Main Group clusters and Zintl ions before addressing transition metal, mixed metal clusters, and mega clusters. We will finish with a discussion on the applications of cluster chemistry towards an understanding the heterogeneous catalytic process of hydrodesulfurisation (HDS).

Dr. Richard Hartshorn (7 lectures) — Reactions of coordinated ligands

To achieve a detailed understanding of some of the ways in which the chemistry of small molecules changes on binding to metal ions. The course will focus principally on amine, imine, and amino acid ligands. The chemistry of these systems will be approached by considering concepts such as nucleophilicity, electrophilicity, acidity and basicity. Coordination to metal ions also leads to additional configurational complexity that can be exploited in synthetic reactions.

CHEM 402 Organic Chemistry

15 lectures. Assessment: Final exam: 100%

Dr. Antony J. Fairbanks (8 lectures) and Dr. Chris M. Fitchett (7 lectures)

The course is an essential requisite for those interested in continuing their studies of organic chemistry to a higher level. It will also be extremely useful for any student that is interested in, or intends to use, synthetic chemistry more generally. Likewise it will also be valuable to those who have an interest in Chemical Biology. The course is comprised of two distinct sections. The first (8 lectures, AJF) details the synthetic chemistry of carbohydrates, the most structurally diverse set of biomolecules, which play essential roles throughout chemistry and biology. The second section (7 lectures CMF) focuses on recently developed and extremely useful synthetic applications of transition metal catalysts; synthetic methodology that has become an essential part of the armoury of the modern synthetic chemist.

CHEM 403 Chemical Dynamics and Spectroscopy

15 lectures. Assessment: Final exam: 100%

Prof. Peter W. Harland (7 lectures) — Molecular dynamics

Molecular Dynamics or Reaction Dynamics is the study of the mechanisms and energetics of elementary physical and chemical collision processes at the atomic/molecular level (intra- and inter-molecular). Experimental techniques and new concepts will be introduced through reference to the scientific literature and case studies. The course will begin with a comparison of the information determined from macroscopic chemical kinetics *versus* molecular dynamics and parameters used to describe reaction efficiency. The development of methods

for investigating energy disposal in reactive collisions, from flash photolysis in the 1950s to current femtosecond laser photo-fragmentation techniques and ion imaging, will be introduced and the experimental results used to further understand chemical processes at the atomic/molecular level. Energy utilisation in reactive collisions will be discussed in terms of a comparison between initial internal energy and initial translational energy.

Prof. Leon F. Phillips (8 lectures) — Statistical mechanics

Boltzmann statistics for distinguishable particles, partition functions, the heat capacities of Einstein and Debye solids, indistinguishable particles, generalised Pauli exclusion principle, Bose-Einstein and Fermi-Dirac statistics, equilibrium constant calculated from spectroscopic data, statistical theories of chemical reaction rates.

CHEM 404 Analytical and Environmental Chemistry

15 lectures. Assessment: Final exam: 100%

Dr. Sally K. Gaw (8 lectures) — Terrestrial bioavailability

Contaminated soils are a world wide issue as they pose hazards for both humans and ecological receptors. An understanding of the fate and bioavailability of contaminants in soils is necessary for preventing and managing environmental and human health risks associated with contaminated soils. This section of the course will explore the chemical processes that determine the fate of trace elements and organic contaminants in soil, pathways of exposure to contaminants and will introduce methods used to determine the bioavailability of contaminants in soil.

Prof. Ian Shaw (7 lectures) — Toxicology

We will explore the why some chemicals are toxic, their mechanisms of toxicity and how we can assess toxicity and decide whether toxic risk is worth the benefit. Before we can explore the effects of toxic chemicals on cells we must understand how cells work, how they protect themselves against external toxic insults and the physiology and biochemistry of their normal function...then we can look what happens when it all goes wrong! By way of examples, I'll discuss some notorious poisons including 1080, lead, cyanide and mercury, and some others you might not have heard of, but will know their effects - e.g. benzo[A]pyrene the major carcinogen in cigarette smoke.

CHEM 405 (BCHM410) Bioorganic Chemistry

Dr. Andy Pratt and Prof. George Lorimer — Structure-function studies in biological chemistry

The two critical classes of biological macromolecules are proteins and nucleic acids. In this course we will discuss examples of structure-function studies of these key molecules. In one section, we will discuss the details of DNA structure and the way in which synthetic analogues of the individual components (bases, sugars and phosphate linkers) have informed our understanding of nucleic acids and led to technologically useful molecules. The other section of the course will involve a discussion of the chemistry of enzyme catalysis. The properties of RUBISCO (the central enzyme of carbon fixation), will be a key example in revealing aspects of the structure-function relationships of proteins in general and enzymes in particular. This course will use a variety of delivery mechanisms, including lectures, a self-chosen research project, workshops and a student-led poster session.

CHEM 406 Theoretical Chemistry

15 lectures. Assessment: Final exam: 100%

Dr. Deborah Crittenden (7 lectures) — Practical computational chemistry

This course will cover the basics that any practicing research chemist needs to know in order to carry out meaningful computational investigations of their system of interest, and to decipher the existing computational literature. We will ask (and answer) such questions as “Why and when should I use quantum mechanical methods?”, “When are classic dynamics simulations more appropriate?”, “What is Hartree Fock theory?”, “How does DFT work?”, “What is a basis set?”, “What is a force field?”, “How are quantum and classical mechanics related?”. We will also cover the basics of setting up, running and interpreting the output of both quantum calculations and classical MD simulations.

Dr. Robert G. A. R. Maclagan (8 lectures) — Hartree-Fock theory

Details to be announced.

CHEM 407 Metallosupramolecular Chemistry

15 lectures. Assessment: Final exam: 100%

Prof. Peter J. Steel (8 lectures) — Part A: Discrete assemblies

Metallosupramolecular chemistry involves the use of combinations of bridging organic ligands and metals to prepare discrete or polymeric assemblies. My lectures will focus on discrete species with various architectures, such as polygons, polyhedra, cages, helicates, rotaxanes, catenanes, knots and molecular machines.

Dr. Paul Kruger (7 lectures) — Part B: Infinite assemblies

This series of lectures will build upon the design principles learnt from the metallosupramolecular chemistry of discrete species, and show how they have been applied to the development of extended or infinite coordination polymers and metal-organic framework (MOF) species. A particular emphasis will be given to the study of porous materials from the perspective of synthesis and characterisation, through to their potential applications. Extensive reference to the current literature in this area will be made.

CHEM 408 Reaction Mechanisms

15 lectures. Assessment: Final exam: 100%

Dr. Emily Parker (8 lectures) — Catalysis, reactions and mechanism

In this section we will examine a number of reactions in detail and discuss the methods for determining mechanisms. This will include the study of reaction intermediates, principles of catalysis and the use of kinetic isotope effects for determining mechanism. We will compare and contrast enzymatic and non-enzymatic reaction mechanisms, and consider examples of how detailed understanding of reaction mechanisms has been used for drug design. No background in biological chemistry will be assumed.

Prof. Paul Wyatt (7 lectures) — asymmetric organic synthesis

Details to be announced.

CHEM 409 Rate Processes

Not offered in 2010.

CHEM 410 Nanotechnology

15 lectures. Assessment: Final exam: 100%

Dr. Vladimir B. Golovko (7 lectures) — Nanostructured materials

This is an introductory course aimed at providing foundation-level knowledge as preparation for the next block of lectures. The course will start with a brief reflection on the major stages in development of materials science, which led to the emergence of Nanotechnology. Classification of nano-materials will be introduced and unique properties of nano-sized materials will be discussed. The importance of the development of characterization techniques will be highlighted with several characterization techniques considered in detail. Next, examples of 0-D, 1-D (and, time permitting, 3-D) materials and their applications will be discussed in detail.

Prof. Alison J. Downard (8 lectures) — Nanosensors

These eight lectures begin with general information about sensors (chemical- and biosensors) and a consideration of what constitutes a 'nanosensor'. We then look at methods of surface immobilisation, a common part of nanosensor fabrication, before moving onto specific examples of nanosensors and nanosensing strategies. Examples of sensors based on nanopores, nanowires and nanotubes, and nanoparticles are examined. This part of the course is centred on reports from the recent research literature and also includes background information on the basic principles of the various sensing strategies. No particular prior lecture course or knowledge is assumed for these lectures, but it is assumed that students will have the good general chemistry knowledge acquired over the course of a chemistry degree.

CHEM 411 (BCHM411) Bioinorganic Chemistry

15 lectures. Assessment: Final exam: 100%

Prof. Vicki McKee (10 lectures)

The aim of the lectures will be to develop understanding of why a particular metal ion is used for a given bioinorganic function and how the metal ion properties are tuned to achieve its primary (and sometimes secondary) function. Examples from the major metalloprotein classes will be discussed. Aspects of metal ion transport, storage, regulation and toxicity will also be illustrated.

Dr. Jan Wikaira (5 lectures) — Model Complexes for bio-inorganic molecules

The design strategy for complexes which have been developed as models for biologically important molecules will be considered. Whether these act as either successful structural or functional (or both) models will be investigated.

CHEM 412 (BCHM412) Structural Chemistry and Biology

15 lectures. Assessment: Final exam: 100%

Dr. Chris Fitchett (9 lectures) and Dr. Marie Squire (6 lectures)

The ability to accurately determine chemical structure is one of the bedrocks of modern chemistry and biochemistry. NMR spectroscopy and X-ray crystallography are currently the only techniques capable of determining the structure of molecules with atomic resolution. In addition, it is also possible to study time dependent phenomena with NMR, such as molecular dynamics, reaction kinetics and molecular recognition. X-ray radiation can also be used to determine macroscale information of partially ordered systems, such as the shape, size and

interactions of proteins and macromolecules (SAXS and WAXS), or the local structure of metal atoms in coordination and organometallic compounds including metalloproteins (EXAFS and XANES). This course will take an integrated approach to the practical use of NMR and X-ray techniques, drawing extensively on examples from the literature. This course will be valuable for students expecting to undertake synthetic chemistry projects (organic or inorganic), or those interested in protein structure analysis. No prior background will be assumed, but completion of CHEM381 or BCHM381 is recommended preparation.

BCHM403 Protein Science

Assessment: Assignments: 60% Final exam (in September): 40%

Prof. Juliet Gerrard (Rm 464 Biology): Tutorials 1 and 6–8

Dr. Andy Pratt: Tutorials 2, 3 and 8

Prof. George Lorimer: Tutorials 4, 5 and 8

CHEM 413–416 Special Topics

In special circumstances, and by arrangement with the Head of Department and fourth-year coordinator, a special course of study may be designed to meet the needs of a particular student and examined under these paper designations.

CHEM 400 Lecture Timetable First semester

| | | | 22/2 | 1/3 | 8/3 | 15/3 | 22/3 | 29/3 | 2/4-25/4 | 26/4 | 3/5 | 10/5 | 17/5 | 24/5 | 31/5 |
|----|----|---------|------|-----|-----|------|------|------|----------|------|-----|------|------|------|------|
| | | | 1 | 2 | 3 | 4 | 5 | 6 | Break | 7 | 8 | 9 | 10 | 11 | 12 |
| M | 9 | CHEM405 | | | | | AJP | AJP | | AJP | AJP | GL | GL | | |
| M | 10 | CHEM403 | LFP | LFP | LFP | LFP | PWH | PWH | | PWH | PWH | | | | |
| M | 10 | CHEM406 | | | | | | | | | | | | RGM | RGM |
| | | | | | | | | | | | | | | | |
| Tu | 9 | CHEM406 | | | | | | | | | | | | RGM | RGM |
| Tu | 10 | CHEM401 | | | RMH | RMH | RMH | RMH | | OJC | OJC | OJC | OJC | | |
| Tu | 10 | CHEM402 | | | | | | | | | | | | AJF | AJF |
| Tu | 11 | CHEM408 | | | EJP | EJP | EJP | EJP | | PW | PW | PW | PW | PW | |
| Tu | 12 | CHEM411 | | | | | | | | VM | VM | VM | VM | VM | JLW |
| | | | | | | | | | | | | | | | |
| W | 9 | CHEM404 | | | | | | | | | | SKG | SKG | SKG | SKG |
| W | 10 | CHEM402 | | | | | | | | | | | | AJF | AJF |
| W | 10 | CHEM403 | LFP | LFP | LFP | LFP | PWH | PWH | | PWH | | | | | |
| W | 10 | CHEM407 | | | | | | | | | | PJS | PJS | | |
| W | 11 | CHEM407 | | | | | | | | | | | | PJS | PJS |
| W | 11 | CHEM412 | | | CMF | CMF | CMF | CMF | | MAS | MAS | MAS | MAS | | |
| W | 12 | CHEM411 | | | | | | | | VM | VM | VM | VM | VM | JLW |
| | | | | | | | | | | | | | | | |
| Th | 9 | CHEM404 | | | | | | | | | | SKG | SKG | SKG | SKG |
| Th | 9 | CHEM408 | | | EJP | EJP | EJP | EJP | | PW | PW | | | | |
| Th | 10 | CHEM410 | | | VBG | VBG | VBG | VBG | | AJD | AJD | AJD | AJD | | |
| Th | 11 | CHEM412 | | | CMF | CMF | CMF | CMF | | MAS | MAS | MAS | | | |
| Th | 12 | CHEM407 | | | | | | | | | | PJS | PJS | PJS | PJS |
| | | | | | | | | | | | | | | | |
| F | 9 | CHEM405 | | | | AJP | AJP | | | AJP | AJP | GL | GL | GL | GL |
| F | 10 | CHEM410 | | | VBG | VBG | VBG | | | AJD | AJD | AJD | AJD | | |
| F | 11 | CHEM401 | | | RMH | RMH | RMH | | | OJC | OJC | OJC | OJC | | |

CHEM400 Important Dates

| | |
|--------------|--|
| 15 February | Research Project begins (week before lectures begin) |
| 17 February | First aid course (9–11 am) and orientation (2 pm) |
| 19 February | Demonstrator training (9:30 am) |
| 22 February | Lectures begin |
| 22 February | Library information seminar (11 am in 531) |
| 26 March | BSc(Hons) practise talks |
| 1 April | Written Proposals due |
| 30 April | MSc(part 2) seminars |
| 2 June | 400-level liaison meeting |
| 30/8 to 13/9 | EXAM period |
| 22 October | Complete experimental |
| 1 November | BSc(Hons) project reports due |
| 10 November | BSc(Hons) project talks |
| 11 November | BSc(Hons) interviews |
| 11 November | MSc(part 1) reports due |
