School of Chemistry

CHEM964: Elucidating Molecular Structure

Subject Outline
Autumn, 2016
On-Campus
Wollongong

Subject Information
Credit Points: 12
Pre-requisite(s): Nil
Co-requisite(s): Nil
Restrictions: Nil
Contact Hours: 33hr Lecture, 24 hr Practical and Tutorial

Subject Contacts
Subject Coordinator/Lecturer

<table>
<thead>
<tr>
<th>Name</th>
<th>Dr Haibo Yu</th>
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<tbody>
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<td>Building 18, Room G26</td>
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</tr>
<tr>
<td>Consultation mode</td>
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Lecturers

<table>
<thead>
<tr>
<th>Name</th>
<th>A/Prof Adam Trevitt</th>
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<tbody>
<tr>
<td>Location</td>
<td>Building 18, Room 224</td>
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<td>Consultation mode</td>
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<tr>
<th>Name</th>
<th>Dr Wilford Le</th>
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<tr>
<td>Location</td>
<td>Building 18., Room G03/ G04</td>
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<td>Consultation mode</td>
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<tr>
<th>Name</th>
<th>Dr Simon Brown</th>
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<tbody>
<tr>
<td>Location</td>
<td>Building 32 Room 230</td>
</tr>
<tr>
<td>Telephone</td>
<td>61 2 4298 1991</td>
</tr>
<tr>
<td>Email</td>
<td><a href="mailto:simon_brown@uow.edu.au">simon_brown@uow.edu.au</a></td>
</tr>
<tr>
<td>Consultation mode</td>
<td>Email for appointment</td>
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<tr>
<td>and times</td>
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Student Support and Advice

For general enquiries please contact StudentHub 41:

Location: 41.138B
Telephone: 61 2 4221 3492
Email: smah-students@uow.edu.au
Student Consultation and Communication

University staff receive many emails each day. In order to enable them to respond to your emails appropriately and in a timely fashion, students are asked to observe basic requirements of professional communication:

Please ensure that you include your full name and student number and identify your practical class or tutorial group in your email so that staff know who they are communicating with and can follow-up personally where appropriate.

Consider what the communication is about
- Is your question addressed elsewhere (e.g. in the subject outline or, on the eLearning site)?
- Is it something that is better discussed in person or by telephone? This may be the case if your query requires a lengthy response or a dialogue in order to address. If so, see consultation times above and/or schedule an appointment.
- Are you addressing your request to the most appropriate person?

Specific email subject title to enable easy identification of issue
- Identify the subject code of the subject you are enquiring about (as staff may be involved in more than one subject) put this in the email subject heading. Add a brief, specific query reference after the subject code where appropriate.

Professional courtesy
- Address the staff member appropriately by name (and formal title if you do not yet know them).
- Use full words (avoid ‘text-speak’ abbreviations), correct grammar and correct spelling.
- Be respectful and courteous.
- Allow 3 – 4 working days for a response before following up. If the matter is legitimately urgent, you may wish to try telephoning the staff member (and leaving a voicemail message if necessary) or inquiring at the School Office.
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Section A: General Information

Subject Learning Outcomes

On successful completion of this subject, students will be able to:

1. To introduce students to the range tools modern chemists use in the determination of molecular structure and provide a working knowledge of the theory & application of these techniques.

2. discuss the core theories behind modern methods of computational chemistry, select an appropriate method for a particular application and interpret the chemical significance of computational data;

3. describe the interaction of light with matter in UV, visible, IR & CD spectroscopies and identify key aspects of such spectra;

4. identify and name the symmetry elements present in a given molecule and discuss their spectroscopic significance;

5. apply modern computational methods to the interpretation of spectroscopic data in the elucidation of molecular structure;

6. explain how a mass spectrometer works and be able to identify molecules based on its mass spectrum; and

7. interpret 1 & 2 dimensional NMR spectra and discuss how they are obtained

Subject Description

Determining the structure of a molecule is the key to unlocking its chemical or biological activity. In the 21st century there are numerous approaches for determining molecular structure. These include: experimental spectroscopic techniques and theoretical predictions, which make use of the increasing power of computers. The combinations of experimental and theoretical techniques are powerful and complementary methods for determining molecular structure and reactivity. CHEM964 is a multi-faceted masters-level subject covering the fundamentals of computational chemistry and spectroscopy and their applications to problems of molecular structure determination. Students will gain experience in conducting and interpreting, electronic structure calculations, optical (infrared, visible & ultraviolet) spectroscopy, mass spectrometry, and nuclear magnetic resonance spectroscopy. A formal treatment of molecular symmetry is also included. Applications of these methods to organic, inorganic, biological and gas-phase systems are covered.

eLearning Space

This subject has materials and activities available via eLearning. To access eLearning you must have a UOW user account name and password, and be enrolled in the subject. eLearning is accessed via SOLS (student online services). Log on to SOLS and then click on the eLearning link in the menu column. For information regarding the eLearning spaces please use the following link: http://uowblogs.com/moodlelab/files/2013/05/Moodle_StudentGuide-1petpo7.pdf

Lecture, Tutorial, Laboratory Times

All timetable information is subject to variation. Check latest timetabling information on the ‘Current Student' webpage on UOW website or log into SOLS to view your personal timetable prior to attending classes.

Readings, References and Materials

Textbooks

The following text(s) will need to be purchased by students enrolled in this class.

PW Atkins & J. de Paula, Physical Chemistry, 10th Ed. (541.3/2)

The subject material from this course is not covered by any single textbook. General physical and analytical texts are useful, supplemented by specific books for each part of the course as listed below (these are available in the library in most cases.)
Prescribed Readings (includes eReadings)
Nil

Materials
 Laboratory Coat
Safety Glasses
UOW Approved Calculator

Recommended Readings
The following references complement the prescribed readings and textbooks:


A Vincent, Molecular Symmetry and Point Group Theory, Wiley 1977. (541.22077/1)


D.O. Hayward, Quantum mechanics for chemists, RSC 2002 (530.12/217)


Recommended readings are not intended as an exhaustive list, students should use the Library catalogue and databases to locate additional resources.

Recent Changes to this Subject
Nil
Laboratory Safety Guidelines

The rules below are general rules that are required in laboratories.

- Before commencing your project you are to ensure that you understand specific procedures for the laboratory in which you work.
- You will need to fill out a risk assessment form before commencing any experiments (confer with your laboratory supervisor).
- Never use any equipment or attempt any experiment without checking the safety implications with your laboratory supervisor or experienced delegated laboratory worker.
- Undergraduate students are not permitted to work after hours unless there is appropriate approval and supervision.

List of Topics Covered

The following are examples of the topics to be covered in this course. This is not an exhaustive list and will be subject to change.

**Computational Chemistry and Molecular Orbital Theory**

- Predicting molecular structure and properties – introduction to GAUSSIAN
- Electrons as waves – the Schrödinger equation
- Molecular orbital theory – linear combinations of atomic orbitals
- Electron Correlation – approaches to the problem
- Molecular Modelling - mechanics approaches to molecular structure
- Theoretical structure prediction and its applications

**Optical Spectroscopy (IR, UV, visible), Symmetry & Group Theory**

- Absorption and emission of light, lasers
- Molecular vibrations, vibrational spectra of small molecules
- Fourier transform infrared (FTIR) spectroscopy, Raman spectroscopy
- Electronic spectra and structure
- Characterisation of molecular symmetry via point groups
- Classification of molecular vibrations using point group tables
- Prediction of infrared spectra based on molecular symmetry

**Mass Spectrometry**

- Introduction to MS, characteristics of mass spectra
- Interpretation of EI mass spectra
- Mass analysers & detectors
- Ionisation methods
- Interpretation of tandem mass spectra, peptide sequencing
- Examples (organic & biological)

**NMR Spectroscopy**

- Principles of NMR, chemical shift, spin-spin splitting
- T1 and T2 relaxation and relaxation mechanisms
- Fourier transform methods of measurement
- Acquisition and processing of NMR spectra
- The nuclear Overhauser effect
- Two-dimensional NMR methods - principles
- Two-dimensional experiments - COSY, NOESY, TOCSY, hetero-correlation experiments
- Polarisation transfer experiments, e.g. DEPT
- Examples
Section B: Assessment

Assessment Summary

<table>
<thead>
<tr>
<th>Assessment Item</th>
<th>Form of Assessment</th>
<th>Due Date</th>
<th>Return/Feedback Due Dates</th>
<th>Weighting</th>
</tr>
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<tbody>
<tr>
<td>Assessment 1</td>
<td>Practical Reports &amp; Assignments</td>
<td>Consult Moodle for due-dates</td>
<td>Consult Moodle</td>
<td>25%</td>
</tr>
<tr>
<td>Assessment 2</td>
<td>Mid-Session Quiz</td>
<td>TBA</td>
<td>Consult Moodle</td>
<td>5%</td>
</tr>
<tr>
<td>Assessment 3</td>
<td>Final Exam</td>
<td>During Exam Period</td>
<td>Consult Moodle</td>
<td>35%</td>
</tr>
<tr>
<td>Assessment 4</td>
<td>Research Project</td>
<td>Week 13</td>
<td>Consult Moodle</td>
<td>35%</td>
</tr>
</tbody>
</table>

Total Marks 100%

Details of Assessment Tasks
Assessment tasks will be marked using explicit criteria that will be provided to students prior to submission.

Assessment 1
Practical Reports & Assignments
Due date Consult Moodle for due-dates
Weighting 25%
Submission Submit a hardcopy to your lecturer in class
Type of Collaboration Group Project
Length Varied
Details There are 6 assignments (some involving a laboratory component) to be completed each of which is marked out of 20:
• Computational Chemistry 1 Lab Report
• Molecular Orbital Theory 1 Assignment (no lab component)
• UV spectroscopy 1 Assignment
• NMR spectroscopy 1 Assignment
• Mass spectrometry 1 Assignment
• Symmetry 1 Assignment (no lab component)

Experiments and laboratory demonstrations must be done in groups in order to share expensive pieces of major equipment. You will be assigned to groups of 3-4 students to do each lab exercise, and given experiment notes as required (i.e., there is no single lab manual for this subject). Assignments will be distributed during the session by the appropriate lecturers. Reports which include printouts from computer spreadsheets or word processor documents must have your name written on the printout by the computer program. All assessment material must be submitted with a completed assessment submission form (available from the subject website).

No reports or assignments will be accepted for marking after 5 pm on the Friday of week 13.

Style and format Report
Subject Learning Outcomes 1,2,3,4,5,6,7
Marking Criteria The marking criteria will be made available prior to submission
### Assessment 2

<table>
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<th>Due date</th>
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<tbody>
<tr>
<td>Weighting</td>
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<tr>
<td>Submission</td>
<td>Submit a hardcopy of your assessment to your lecturer in class</td>
</tr>
<tr>
<td>Type of Collaboration</td>
<td>Individual Assessment</td>
</tr>
<tr>
<td>Length</td>
<td>1 hour</td>
</tr>
<tr>
<td>Details</td>
<td>The quiz will be held on in the normal lecture venue. This assessment task will be based on lecture and lab material covered up to that time (see lecture timetable).</td>
</tr>
<tr>
<td>Style and format</td>
<td>In class test</td>
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<td>Subject Learning Outcomes</td>
<td>1,2,3,4,5</td>
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### Assessment 3

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<tbody>
<tr>
<td>Weighting</td>
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</tr>
<tr>
<td>Submission</td>
<td>Exam papers and answers must be submitted at the conclusion of the exam.</td>
</tr>
<tr>
<td>Type of Collaboration</td>
<td>Individual Assessment</td>
</tr>
<tr>
<td>Length</td>
<td>3 hours</td>
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<tr>
<td>Details</td>
<td>The final exam will be based on all lecture material, laboratory work and assignments in so far as they relate to lecture material. Calculators approved for use in exams must be identified by a UOW tamper-evident label. Only approved calculators can be taken into exams.</td>
</tr>
<tr>
<td>Style and format</td>
<td>Final Exam</td>
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<tr>
<td>Subject Learning Outcomes</td>
<td>1,2,3,4,5,6,7</td>
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### Assessment 4

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<th>Due date</th>
<th>Monday Week 13</th>
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<tbody>
<tr>
<td>Weighting</td>
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<tr>
<td>Submission</td>
<td>Submit a hardcopy of your assessment (along with 2 duplicate copies) to your subject coordinator.</td>
</tr>
<tr>
<td>Type of Collaboration</td>
<td>Individual Assessment</td>
</tr>
<tr>
<td>Length</td>
<td>20 pages (see Report Guidelines on Moodle)</td>
</tr>
<tr>
<td>Details</td>
<td>Chem964 students are required to undertake a research project that will involve applying computational chemistry methods to a contemporary problem in chemical research. The research topic and the design of the computational strategy will be decided in consultation with the assigned tutor. Students are required to make an appointment to meet with the Subject Coordinator in Week 4 to be assigned their research project. Assessment is based on a research report written in the style to be submitted on the Monday of week 13. An introduction and a draft of the results and discussion can be submitted to the subject coordinator for comment during the course of the semester. Specific dates for all deadlines related to the Research Report are provided in the Assessment Tasks and Timetable section above details of the report and its assessment are provided below.</td>
</tr>
<tr>
<td>Style and format</td>
<td>Presentation and Report</td>
</tr>
<tr>
<td>Subject Learning Outcomes</td>
<td>1,2,5</td>
</tr>
<tr>
<td>Marking Criteria</td>
<td>The marking criteria will be made available prior to submission</td>
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</table>
Minimum Requirements for a Pass in this Subject

To receive a clear pass in this subject a total mark of 50% or more must be achieved. In addition, failure to meet any of the minimum performance requirements is grounds for awarding a Technical Fail (TF) in the subject, even where total marks accumulated are greater than 50%.

The minimum performance requirements for this subject are:

- Obtain a final examination mark of >50%
- Submit at least 5 out of 6 practical reports
- Obtain a total combined average of at least 50% in the practical component

Minimum Student Attendance and Participation

It is expected that students will allocate Insert 24 of hrs based on credit points hours per week to this subject, including any required class attendance, completion of prescribed readings and assessment tasks.

Student attendance at tutorials, practicals, seminars and/or simulations is compulsory and students must attend all classes. Absences will require the submission of an application for Academic Consideration via SOLS and the presentation of suitable documentation, for example a Medical Certificate, to Student Central as soon as practical. For further details about applying for academic consideration visit the Student Central webpage:

Scaling

Scaling may occur in this subject at the end of session by the Unit Assessment Committee and/or Faculty Assessment Committee (FAC). Marks will only be scaled to ensure fairness/parity of marking across groups of students. Scaling will not affect any individual student’s rank order within their cohort. For more information refer to Assessment Guidelines – Scaling:

Late Submission

Late submission of an assessment task without an approved extension of the deadline is not acceptable. If you are unable to submit an assessment due to extenuating circumstances (e.g. medical grounds or compassionate grounds), you can make an application of academic consideration. Not all circumstances qualify for academic consideration. For further details about applying for academic consideration visit the Student Central webpage:

Late Submission Penalty – at 5%

Late submission of an assessment task without an approved extension of the deadline is not acceptable. Marks will be deducted for late submission at the rate of 5% of the total possible marks for that particular assessment task per day. This means that if a piece of work is marked out of 100, then the late penalty will be 5 marks per day (5% of 100 possible marks per day). The formula for calculating the late penalty is: the total possible marks x 0.05 x number of days late. For the purposes of this policy a weekend (Saturday and Sunday) will be regarded as two days.

For example:

- Student A submits an assignment which is marked out of 100. The assignment is submitted 7 days late. This means that a late penalty of 35 marks will apply (100 x 0.05 x 7). The assignment is marked as per normal out of 100 and is given a mark of 85/100, and then the late penalty is applied. The result is that the student receives a final mark of 50/100 for the assignment (85 (original mark) – 35 marks (late penalty) = 50/100 (final mark)).
- Student B submits a report which is marked out of 20. The report is submitted three days late. This means that a late penalty of 3 marks will apply ((20 x 0.05 x 3). The report is marked as
per normal out of 20 and is given a mark of 17/20, and then the late penalty is applied. The result is that the student receives a final mark of 14/20 for the report (17 (original mark) – 3 marks (late penalty) = 14/20 (final mark)).

No marks will be awarded for work submitted either after the assessment has been returned to the students or more than two weeks after the due date, whichever is the sooner. This does not apply to situations where a particular assessment task is undertaken by students at different times throughout the session, but where the assessment is based on experiments or case studies specific to a student. In this case no marks will be awarded for work submitted more than two weeks after the due date.

Notwithstanding this, students must complete all assessment tasks to a satisfactory standard and submit them, regardless of lateness or loss of marks, where submission is a condition of satisfactorily completing the subject.

System of Referencing Used for Written Work

Vancouver referencing system: The essay must be structured with sub-headings, can contain figures and tables, and must be fully referenced. Chemistry uses the Vancouver Referencing System. This system is used by Nature, Medical journals and most Chemistry journals. The Vancouver system uses numbers to identify references. Each reference is given a number, starting from 1. This can be above the line like this1, or enclosed in brackets like this (1). If a reference is repeated, you use the original number, not a new one. All the referenced sources are listed continuously together at the end of the essay2,3. While tricky to use initially, the Vancouver system has some advantages4. The titles of books and articles are given minimal capitalisation. Book titles and journal titles are not italicised. Journal titles are highly abbreviated. All authors are listed when there are six or fewer. When there are more than six, only the first three are listed and the expression ‘et al.’ is added. Authors’ initials follow the surnames and are set without full stops or spaces.

The reference list at the end of the essay would look something like this:

References


Dale JW. Molecular genetics of bacteria. 2nd ed. Chichester, West Sussex: Wiley & Sons Ltd; 1994.

Shaffer RA. Advances in chemistry are starting to unlock mysteries of the brain: How the messengers work. Wall Street Journal 1977 Aug 12;1 (col. 1), 10(col. 1).

For further information on the formatting used in the Vancouver Referencing System see one of the following websites:

Use of Internet Sources

Students are able to use the Internet to access the most current information on relevant topics and information. Internet sources should only be used after careful critical analysis of the currency of the information, the role and standing of the sponsoring institution, reputation and credentials of the author, the clarity of the information and the extent to which the information can be supported or ratified by other authoritative sources.
Plagiarism
The full policy on Academic Integrity and Plagiarism is found in the Policy Directory on the UOW website.

“The University's Academic Integrity and Plagiarism Policy, Faculty Handbooks and subject guides clearly set out the University's expectation that students submit only their own original work for assessment and avoid plagiarising the work of others or cheating. Re-using any of your own work (either in part or in full) which you have submitted previously for assessment is not permitted without appropriate acknowledgement. Plagiarism can be detected and has led to students being expelled from the University.

The use by students of any website that provides access to essays or other assessment items (sometimes marketed as ‘resources’), is extremely unwise. Students who provide an assessment item (or provide access to an assessment item) to others, either directly or indirectly (for example by uploading an assessment item to a website) are considered by the university to be intentionally or recklessly helping other students to cheat. This is considered academic misconduct and students place themselves at risk of being expelled from the University.”

Submission of Assessments
Refer to the submission requirements under the details of the individual assessments. Students should ensure that they receive a receipt acknowledging submission. Students will be required to produce this in the event that an assessment task is considered to be lost. Students are also expected to keep a copy of all their submitted assessments in the event that re-submission is required.

Assessment Return
Students will be notified when they can collect or view their marked assessment. In accordance with University Policy marked assessments will usually only be held for 21 days after the declaration of marks for that assessment.
Section C: General Advice

Students should refer to the Faculty of Science, Medicine and Health website for information on policies, learning and support services and other general advice.

University Policies

Students should be familiar with the following University policies:

a. Code of Practice – Teaching and Assessment

b. Code of Practice – Research, where relevant

c. Code of Practice – Honours, where relevant

d. Student Charter

e. Code of Practice – Student Professional Experience, where relevant

f. Academic Integrity and Plagiarism Policy

g. Student Academic Consideration Policy

h. Course Progress Policy

i. Graduate Qualities Policy

j. Academic Complaints Policy (Coursework and Honours Students)

k. Policy and Guidelines on Non-Discriminatory Language Practice and Presentation

l. Workplace Health and Safety, where relevant

m. Intellectual Property Policy

n. IP Student Assessment of Intellectual Property Policy, where relevant

o. Policy on Ethical Objection by Students to the Use of Animal and Animal Products in Coursework Subjects, where relevant

p. Human Research Ethics Guidelines, where relevant

q. Animal Research Guidelines, where relevant
r. Student Conduct Rules and accompanying Procedures or Research Misconduct Policy for research students

Student Support Services and Facilities
Students can access information on student support services and facilities at the following link. This includes information on “Academic Support”, “Starting at University”, “Help at University” as well as information and support on “Career’s and Jobs”. http://www.uow.edu.au/student/services/index.html

Student Etiquette
Guidelines on the use of email to contact teaching staff, mobile phone use in class and information on the university guide to eLearning ‘Netiquette’ can be found at http://www.uow.edu.au/student/elearning/netiquette/index.html

Version Control Table

<table>
<thead>
<tr>
<th>Version Control</th>
<th>Release Date</th>
<th>Author/Reviewer</th>
<th>Approved By</th>
<th>Amendment</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>20151112</td>
<td>Dr Haibo Yu</td>
<td>Mrs Sonia Losinno – ADE Nominee</td>
<td>FINAL CHEM964 Autumn 2016 Subject Outline</td>
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</table>