
CHEM964: Elucidating Molecular Structure

Subject Outline

12 credit points

Subject Information

Autumn, 2025, Wollongong
On Campus

On-Campus Delivery This subject is delivered in-person and includes on-campus or other location-based learning activities that cannot be undertaken by students studying Online/Distance. Students unable to attend campus or any other nominated physical delivery location should not enrol in this subject.

Subjects with a delivery mode of On Campus and/or Flexible with International Student enrolments will be delivered in accordance with the ESOS National Code. That is, online learning experiences (such as lectures, tuition, and resources) will be supplementary to in-person learning experiences such as scheduled classes and/or scheduled contact hours.

UOW may need to change teaching locations, teaching delivery and/or assessment delivery at short notice to ensure the safety and well-being of students and staff in response to the COVID-19 pandemic or other public health requirements.

The Faculty of Science, Medicine and Health

The Faculty of Science, Medicine and Health offers a range of undergraduate and postgraduate programs designed to meet the needs of a diverse student population. We carry out world-leading research which is strongly aligned with our teaching program

As a student of our faculty, you will be actively engaged in learning with extensive clinical experiences, use of advanced educational technologies and opportunities for enriching work experience. More information about the Faculty of Science, Medicine and Health and our School is available on our web pages:

<https://www.uow.edu.au/science-medicine-health/>

Teaching Staff

Teaching Role	Name	Telephone	Email	Room	Consultation Times
Coordinator	Professor Haibo Yu	+61 2 4221 4235	hyu@uow.edu.au	42.112	Wednesday 13:30 - 15:30 (appointment required)
Lecturer	Associate Professor Shane Ellis	+61 2 4221 5748	sellis@uow.edu.au	42.214	Email for an appointment
Lecturer	Dr Celine Kelso	+61 2 4221 3501	celine@uow.edu.au	18.104	Email for an appointment
Lecturer	Professor Adam Trevitt	+61 2 4221 5545	adamt@uow.edu.au	42.213	Email for an appointment
Lecturer	Associate Professor Nicholas Deutscher	+61 2 4221 4104	ndeutsch@uow.edu.au	18.224	Email for an appointment
Lecturer	Dr Alan Maccarone	+61 2 4239 4282	alanmac@uow.edu.au	18.104	Email for an appointment
Lecturer	Dr Boris Ucur		bucur@uow.edu.au	42.216	Email for an appointment
Lecturer	Dr Qiang Zhu		qiangzhu@uow.edu.au	42.116	Email for an appointment

Expectations of Students

UOW values are intellectual openness, excellence and dedication, empowerment and academic freedom, mutual respect and diversity, recognition and performance. We will provide a safe, equitable and orderly environment for the University community, and expect each member of our community to behave responsibly and ethically ([Student Conduct Rules](#)).

We expect that students demonstrate these values and professional behaviour, both face to face and online, making genuine efforts to complete their studies successfully, arriving on time to class, taking part constructively in class discussions and activities, demonstrating appropriate professional and ethical conduct in all communication with UOW staff and community members, and submitting assignments on time (or completing a request for Academic Consideration in advance if needed).

Guiding Communication Principles for Students

Moodle Announcements will be the primary platform for communication of general information to students

- Students should ensure they regularly check the main announcements forum at the top of each subject's Moodle site.
- It is the student's responsibility to check all subject Moodle sites regularly for information and notifications.

SOLS messages will be used for all central communication relating to the following:

- Administrative matters relating to student enrolment
- Critical information relating to course or subject, e.g. Changes to assignments, policy updates, class cancellations or changes
- Timetable information
- Security and emergency information
- Students are encouraged to check SOLS messages daily as these messages are often of high priority

SOLS and Moodle announcements can NOT be responded to.

Email

- Communication to UOW staff by students should only be via a UOW email account
- If you have a question of a general nature in relation to assessment questions, Moodle assignment forums should be used rather than email

Remember to use the same principles when communicating online as you would face-to-face. Be clear and respectful and communicate with the same consideration you would expect from others.

Related Policies

- Online and email etiquette <https://tr.uow.edu.au/uow/file/976ffde2-b892-42cf-b20b-5c7a65bc08cc/1/Overview%20of%20Online%20and%20Email%20Etiquette.pdf>
- Using UOWmail <https://www.uow.edu.au/student/support-services/academic-skills/>
- Inclusive language guideline <https://documents.uow.edu.au/about/policy/students/UOW140611.html>
- The Student Charter <https://www.uow.edu.au/student/charter/>

Appropriate Online Behaviour

The University is committed to providing a safe, respectful, equitable and orderly environment for the University community, and expects each member of that community to behave responsibly and ethically. Students must comply with the University's [Student Conduct Rules](#) and related policies including the [IT Acceptable Use Policy](#) and [Bullying Prevention Policy](#), whether undertaking their studies face-to-face, online.

For more information on appropriate communication and etiquette in the online environment please refer to the guide [Online and Email Etiquette](#).

Related Policies

Using UOWmail <https://www.uow.edu.au/student/support-services/academic-skills/>

Inclusive language guideline <https://policies.uow.edu.au/document/view-current.php?id=239>

Copyright

Commonwealth of Australia

Copyright Regulations 1969

© 2025 University of Wollongong

The original material prepared for this guide is covered by copyright. Apart from fair dealing for the purposes of private study, research, criticism or review, as permitted under the Copyright Act, no part may be reproduced by any process without written permission.

Hardcopies of this document are considered uncontrolled please refer to your Moodle site for the latest version.

Table of Contents

Section A: General Information	7
Learning Outcomes	7
Subject Learning Outcomes	7
Subject Description	7
Course Handbook	7
Subject Details: Practical Activities, eLearning, Readings and Materials	7
Subject eLearning	7
Safety Guidelines	7
FOUNDATIONAL Work Integrated Learning	8
Additional Subject Details	8
Using Generative Artificial Intelligence (GenAI)	9
Major Text(s)	9
Recommended Readings and Other Resources	9
Additional Materials	10
Lectures, Tutorials and Attendance Requirements	10
Lecture Times *	10
Lecture Program *	10
Additional Lecture Comments	11
Recording of Teaching and Learning Activities	11
Your Privacy - Recording of Teaching and Learning	11
Tutorial/Seminar/Workshop Times	12
Tutorial/Seminar/Workshop Program	12
Recent Improvements to Subject	12
Extraordinary Changes to the Subject Outline	12
Learning Analytics	13
Section B: Assessment	14
Assessment Summary	14
Minimum Requirements to Pass this Subject	16
Hurdle Assessment	16
UOW Grade Descriptors	17
Assessment Learning Outcome Matrix	17
Submission, Retention and Collection of Written Assessment	17
Extensions	17
Late Submission of Assessment Tasks and Penalties	18
Collection	18
Retention	18
Scaling	18
Supplementary Assessment	18
Review and Appeal of Academic Decisions	19
Assessment Quality Cycle	19
Academic Integrity	19
Referencing	19
Section C: General Advice for Students - Policies and Procedures	20
Student Services and Support	20
Student Support Coordinator (SSC)	20
Student Advocacy Service	20
AskUOW	20
Library Services	21
Academic Integrity Policy	21
Code of Practice - Research	21
Honours Policy	21
The Code of Practice - Work Integrated Learning (Professional Experience)	21
Copyright Policy	21
Course Progress Policy	21
Examination Rules and Procedures	21

Ethical Objection by Students to the Use of Animal and Animal Products in Coursework Subjects	22
Coursework Rules	22
Human Research Ethics	22
Inclusive Language Guidelines	22
Intellectual Property Policy.....	22
Review and Appeal of Academic Decisions Policy	22
Student Academic Consideration Policy.....	22
The Student Charter - Your Rights and Responsibilities	22
Student Assignment of Intellectual Property (IP) Policy	22
Student Conduct Rules.....	23
Teaching and Assessment: Assessment and Feedback Policy	23
Teaching and Assessment: Code of Practice - Teaching.....	23
Teaching and Assessment: Subject Delivery Policy	23
Workplace Health & Safety Policy	23

Section A: General Information

Learning Outcomes

Subject Learning Outcomes

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

1. Analyse and synthesize the core theories underpinning modern computational chemistry methods, assess and justify the selection of an appropriate method for specific applications, and interpret the chemical significance of computational data
2. Analyse the symmetry elements present in a given molecule and critically examine their spectroscopic significance
3. Interpret and predict rotational and vibrational spectra of molecules through the consideration of molecular orbitals and symmetry
4. Evaluate a range of mass spectra (including electron ionisation, electrospray ionisation and tandem mass spectra), articulate the methodologies for their acquisition and deduce simple molecules based on their mass spectra
5. Apply modern computational methods to study the structure-activity relationships in molecules of chemical or biological importance through a research project

Subject Description

CHEM964 covers both computational and experimental methods used to determine the structure of molecules and understand their structure-reactivity relationship. We will cover a range of topics, including computational chemistry, symmetry, gas phase spectroscopy and mass spectrometry. Additionally, students will gain hands-on experience in conducting and interpreting computational and experimental studies. Finally, we will apply these methods to a variety of systems of chemical, biological and environmental importance, including organic, inorganic, biological, and gas-phase systems. Students will gain independent research experience in a computational chemistry project by applying the theories covered in this subject. This subject thus will be aligned with the UN Sustainable Development Goals by emphasizing the application of these techniques in the areas of health, sustainable energy, and molecular mass spectrometry environment.

Course Handbook

Information about subject pre-requisites, co-requisites and restrictions as well as course completion requirements and Course Learning Outcomes can be found in the [Course Handbook](#).

Subject Details: Practical Activities, eLearning, Readings and Materials

Subject eLearning

The University uses the eLearning system Moodle to support all coursework subjects. The subject Moodle site can be accessed via your SOLS page.

Safety Guidelines

The rules below are general rules that are required when participating in labs, practicals, fieldwork or simulated fieldwork activities. Before commencing these activities you are to ensure that you understand specific procedures and policy related to safety.

- All first year students undertaking Chemistry (CHEM101/102/104/105) must complete the Moodle WHS Induction (see details below)
- Before commencing lab/practical/fieldwork activity you are to ensure that you understand specific procedures and policy related to safety.

- You may need to review a Risk Assessment and complete a Participant Acknowledgement form before commencing any fieldwork/practical work. These materials will be made available by the supervisor/Subject Coordinator.
- You must inform the Subject Coordinator of any medical conditions which may impact upon your ability to participate in these activities before commencing the practical.
- All Reasonable Adjustment cases (Access Plans) must be discussed with the Subject Coordinator prior to commencing the activity.
- Participation in the lab/practical/field/simulation activities may be denied to students who do not abide by these, and other conditions which may be specified by the Subject Coordinator.
- 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.
- For subjects including field trips, students may be required to contribute to costs associated with the provision of field trips that form part of the course of study.

FOUNDATIONAL Work Integrated Learning

This subject contains elements of 'Foundational WIL'. Students in this subject will observe, explore or reflect on possible career pathways or a work-related aspect of their discipline.

Additional Subject Details

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
- Theoretical structure prediction and its applications

Symmetry & Group Theory

- 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

- Principles of instrumentation
- Ionisation methods (MALDI, ESI)
- Tandem MS – principles and selected applications Interpretation of MS/MS spectra of lipids
- Interpretation of MS/MS spectra of simple peptides
- Concepts for quantification by MS/MS

Spectroscopy

- Boltzmann distribution - Calculating relative populations at different energy levels
- Rotational spectroscopy
- Vibrational spectroscopy
- Selection rules for rotational and vibrational spectra
- Quantitatively relating the energies of spectroscopic properties to fundamental molecular characteristics

- Predicting spectra based on fundamental molecular properties
- Predicting how deviation from a rigid rotor will affect spectra

Research Project

- Carry out a mini-research project in computational chemistry

Using Generative Artificial Intelligence (GenAI)

GenAI technology (such as ChatGPT or Microsoft Co-pilot) is reshaping the University experience worldwide. UOW is committed to embracing GenAI as a tool to enhance learning experiences and develop vital work-readiness skills. However, misuse or use of GenAI in assessments where prohibited constitutes academic misconduct (as specified by [University Policy](#)).

It is important that students check if GenAI is permitted for each assessment task and how it is to be used and acknowledged. Please read the [student guidance](#) available on how to use GenAI ethically and critically, equally recognising its capabilities and limitations. For example:

1. **Generative AI is not a substitute for decision-making:** GenAI should complement, not replace, your critical thinking and decision-making skills.
2. **Output quality depends on prompts:** The quality of GenAI outputs is influenced by prompting. Poorly constructed or unclear prompts may generate outputs that are incorrect.
3. **Fact verification is essential:** GenAI outputs can be fabricated, presenting inaccurate information or contain harmful bias. Verify all GenAI outputs against reliable sources.
4. **Protect data and copyright:** Many GenAI technologies collect information in ways that breach privacy and data protection provisions, particularly where the source material is confidential or subject to copyright. Please check the Terms and Conditions of GenAI technologies and if unsure, contact [UOW Copyright Guidance](#). Learn more about how to access UOW secured GenAI tools [here](#).
5. **Transparency in use:** Where required, you must acknowledge GenAI use, including providing prompt histories and detailing how GenAI was utilised.
6. **Thoughtful and appropriate application:** Be mindful of when and how to use GenAI tools. Assess its appropriateness for each use, and refrain from use when not suitable.

If you have any questions, please contact your Subject Coordinator.

Major Text(s)

PW Atkins & J. de Paula, *Physical Chemistry*, 11th Ed. (or earlier versions).

PW Atkins, *Concepts in Physical Chemistry*, <https://books.rsc.org/books/monograph/2194/Concepts-in-Physical-Chemistry>

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).

If there is a textbook available for purchase, you can find the details at University Bookshop <https://unishop.uow.edu.au/>

Recommended Readings and Other Resources

The following references complement the prescribed readings and textbooks:

- F A Cotton, *Chemical Applications of Group Theory*, 3rd Ed. Wiley-Interscience, 1990 (541.22/11)
- A Vincent, *Molecular Symmetry and Point Group Theory*, Wiley 1977. (541.22077/1)
- C N Banwell and E M McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., McGraw Hill 1994. (535.84/6)
- F W McLafferty, *Interpretation of mass spectra*, 4th Ed. University Science Books, 1993 or earlier editions. (547.3085/5)

- J K M Sanders & B K Hunter, Modern NMR spectroscopy: A guide for chemists, OUP 1987 (543.0877/23)
- J K M Sanders, E C Constable & B K Hunter, Modern NMR spectroscopy: A workbook of chemical problems, OUP 1989. (543.0877/22)
- D L Pavia, G M Lampman & G S Kris, Introduction to Spectroscopy: A guide for students of organic chemistry, 3rd Ed., Saunders 2001. (547.30858)
- D A Skoog, F J Holler & T A Nieman, Principles of Instrumental Analysis, 5th Ed., Harcourt, 1998. (543.08/4)
- R M Silverstein, G C Bassler & T C Morrill, Spectrometric identification of organic compounds, 5th Ed., Wiley 1991 (547.346)
- D.O. Hayward, Quantum mechanics for chemists, RSC 2002 (530.12/217)
- J. Foresman & A. Frisch, Exploring Chemistry with Electronic Structure Methods, 2nd Edition, Gaussian 1996

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

This is not an exhaustive list of references. Students should also use the library catalogue and databases to locate additional resources.

Additional Materials

- Laboratory Coat
- Safety Glasses
- UOW Approved Calculator

Lectures, Tutorials and Attendance Requirements

Lecture Times *

UOW may need to change teaching locations, teaching delivery and/or assessment delivery at short notice to ensure the safety and well-being of students and staff in response to the COVID-19 pandemic or other public health requirements.

Up to date timetable and delivery information is located at <http://www.uow.edu.au/student/timetables/index.html>

You can access your personal timetable by logging into SOLS and selecting 'My Timetable'

Lecture Program *

Week	Commencing	Topics Covered
1	07 Mar 2025	Computational Chemistry 1-3
2	14 Mar 2025	Computational Chemistry 4-6
3	21 Mar 2025	Computational Chemistry 7-9
4	28 Mar 2025	Mass Spectrometry 1-3
5	04 Apr 2025	Mass Spectrometry 4-5
6	11 Apr 2025	No Lecture
7	18 Apr 2025	No Lecture (Good Friday)
	21 Apr 2025	Mid-Session Recess
8	02 May 2025	Exam 1
9	09 May 2025	Spectroscopy 1-3

10	16 May 2025	Spectroscopy 4-6
11	23 May 2025	Symmetry and Group Theory 1-3
12	30 May 2025	Symmetry and Group Theory 1-3
13	06 Jun 2025	No Lecture
	09 Jun 2025	Study Recess
	14 Jun 2025	Examinations
	21 Jun 2025	Examinations

* The above times and program may be subject to change. Students will be notified of any change via SOLS.

Additional Lecture Comments

We will have the following Lectorial time for Research Project.

MRes Meeting 1	13:30-15:30 Fri 11 April (Week 6)
MRes Meeting 2	11:00-12:30 Fri 2 May (Week 8)
MRes Meeting 3	11:00-12:30 Fri 23 May (Week 11)
MRes Meeting 4	11:00-12:30 Fri 6 June (Week 13)

Recording of Teaching and Learning Activities

The University of Wollongong supports the recording of UOW educational content as a supplemental study tool, to provide students with equity of access, and as a technology-enriched learning strategy to enhance the student experience.

If you make your own recording of a lecture, class, seminar, workshop or any other educational session provided as part of your course of study you can only do so with the explicit permission of the lecturer and those people who are also being recorded.

You may only use educational content recorded through the delivery of subject or course content, whether they are your own or recorded by the university, for your own educational purposes. Recordings cannot be altered, shared or published on another platform, without permission of the University, and to do so may contravene the University's Copyright Policy, Privacy Policy, Intellectual Property Policy, IT Acceptable Use Policy and Student Conduct Rules. Unauthorised sharing of recordings may also involve a breach of law under the Copyright Act 1969.

Most lectures in this subject will be recorded, when they are scheduled in venues that are equipped with lecture recording technology and made available via the subject Moodle site within 48 hours.

Your Privacy - Recording of Teaching and Learning

In accordance with the Student Privacy & Disclosure Statement, and Lecture Recording Procedures when undertaking our normal teaching and learning activities, the University may collect your personal information. This collection may occur incidentally during the recording of lectures in equipped venues (i.e. when your identity can be ascertained by your image, voice or opinion), or via the delivery of online content therefore the University further advises students that:

- Lecture recordings are made available to students, university staff, and affiliates, securely via the Learning Platform;
- Recordings are made available only for the purpose for which they were recorded, for example, as a supplemental study tool or to support equity and access to educational resources;

If you have any concerns about the use or accuracy of your personal information collected in a lecture recording, you may approach your Subject Coordinator to discuss your particular circumstances.

The University is committed to ensuring your privacy is protected. If you have a concern about how your personal information is being used or managed, please refer to the University's Privacy Policy or consult our Privacy webpage <https://www.uow.edu.au/privacy/>

Tutorial/Seminar/Workshop Times

The Faculty uses the SMP Online Tutorial System and tutorial times and locations can be found at <https://www.uow.edu.au/student/timetables/index.html>. Please note that tutorial times on the timetable are provisional and may change.

Tutorial/Seminar/Workshop Program

Where the restrictions require temporary adjustments for delivery and tutorial/seminar/workshop arrangements, any necessary changes will be advised and provided by your Subject Coordinator. Please check Subject Moodle site regularly

Week	Week Commencing	Topics Covered
1	03 Mar 2025	Computational Chemistry Lab - 1
2	10 Mar 2025	Computational Chemistry Lab - 2
3	17 Mar 2025	Computational Chemistry Lab - 3
4	24 Mar 2025	Computational Chemistry Lab - 4
5	31 Mar 2025	Mass Demo
6	07 Apr 2025	Mass Demo
	21 Apr 2025	Mid-Session Recess
10	12 May 2025	Spectroscopy Tutorial
12	26 May 2025	Symmetry Tutorial
	09 Jun 2025	Study Recess
	14 Jun 2025	Examinations
	21 Jun 2025	Examinations

The above program may be subject to change.

Recent Improvements to Subject

The Faculty of Science, Medicine and Health is committed to continual improvement in teaching and learning and takes into consideration student feedback from many sources including, direct student feedback to tutors and lecturers and responses to the Subject and Course Evaluation Surveys.

Extraordinary Changes to the Subject Outline

In extraordinary circumstances the provisions stipulated in this Subject Outline may require amendment after the Subject Outline has been distributed. All students enrolled in the subject must be notified and have the opportunity to provide feedback in relation to the amendment, where practicable, prior to the amendment being finalised.

Learning Analytics

Learning Analytics data (such as student engagement with Moodle, access to recorded lectures, University Library usage, task marks, and use of SOLS) may be used by the Subject Coordinator and your faculty's Head of Students to assist in analysing student engagement, and to identify and recommend support to students who may be at risk of failure. If you have questions about the kinds of data the University uses, how we collect it, and how we protect your privacy in the use of this data, please refer to <https://www.uow.edu.au/privacy/>

Section B: Assessment

Assessment Summary

Assessment Item	Form of Assessment	%
Assessment 1	Assignment	40%
Assessment 2	Exam	15%
Assessment 3	Exam	15%
Assessment 4	Project	30%
	TOTAL MARKS	100%

Please note: Copies of student work may be retained by the University in order to facilitate quality assurance of assessment processes.

A formative assessment activity (with written or verbal feedback) will be conducted before census date - please see [UOW Key Dates](#).

Assessment 1: Assignment - Assignments (1 x Presentation & 5 x Report)

Marking Criteria	<ul style="list-style-type: none">• Correctness of response• Logical progression of arguments and explanations• Shows working for calculation based problems• Breadth and depth of knowledge• Overall presentation and clarity
Length	Varied
Weighting	40%
Assessment Due	To Be Announced Final submission time: 11:30pm
Type of Collaboration	Individual assessment and group work
Style and format	Presentation and Report
Assessment submission	Online via Moodle This assessment has been set up to be checked by Turnitin, a tool which helps you check whether you have referenced correctly. You can submit your assessment task to Turnitin prior to the due date and Turnitin will give you an originality report. You may then make any changes that may be required and resubmit your final version by the due date.
Assessment return	Consult Moodle
Detailed information	The five assignments are: <ul style="list-style-type: none">• Computational Chemistry Lab Report (Group work, with Computer Lab; 10%; Report and Presentation)• Molecular Orbital Theory Assignment (no lab component; 6%; Report)• Symmetry Assignment (with Tutorial; 8%; Report)• Spectroscopy Assignment (with Tutorial; 8%; Report)• Mass spectrometry Assignment (with Demo; 8%; Report) Molecular Orbital Theory Assignment, Spectroscopy and Symmetry Assignment are individual work.

	In the Mass Spectrometry demo , 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. However, both assignments have to be completed individually. In the Computational Chemistry Lab Report , 3-4 students will be assigned to a mini project. You are encouraged work collaboratively and the calculated data can be shared within each group. Group members are expected to present a joint oral presentation (not assessed but feedback will be provided by teaching staff). Students shall complete the report individually.
--	---

Assessment 2: Exam - Exam 1

Marking Criteria	<ul style="list-style-type: none"> • Correctness of response • Logical progression of arguments and explanations • Shows working for calculation based problems
Length	2 hours
Weighting	15%
Assessment Due	02 May 2025 (Friday in Session Week 8)
Type of Collaboration	Individual assessment
Style and format	In-class test: 13:30-15:30
Assessment submission	in person exam at the Lecture Theatre.
Assessment return	Consult Moodle
Detailed information	This assessment task will be based on lecture and lab material covered up to that time (see lecture timetable)

Assessment 3: Exam - Exam 2

Marking Criteria	<ul style="list-style-type: none"> • Correctness of response • Logical progression of arguments and explanations • Shows working for calculation based problems
Length	2 hours
Weighting	15%
Assessment Due	The final exam will be held during the UOW exam period, and students should ensure they are available during this period. Students will receive a SOLSmail advising when full details of the delivery format, and date of the final exam are available in the SOLS Exam Timetable.
Type of Collaboration	Individual assessment
Style and format	Exam 2 (final exam) will be an invigilated, on campus exam.
Detailed information	The final exam will be based on the second half of lecture material, laboratory work and assignments. Calculators approved for use in exams must be identified by a UOW tamper-evident label. Only approved calculators can be taken into exams.

Assessment 4: Project - Report

Marking Criteria	The written report will be assessed by up to two members of the academic staff. When arriving at their final mark, the examiners will take into account the number and type of experiments performed by the student, the amount of information derived from those experiments, the degree to which the data is analysed into a coherent story, consistency with respect to formatting and referencing, quality and appropriateness of figures, and whether or not the report has an appropriate structure (e.g. does it have an abstract, list of figures, table of contents, conclusion etc.).
-------------------------	---

Length	20 pages (see Report Guidelines on Moodle)
Weighting	30%
Assessment Due	06 Jun 2025 (Friday in Session Week 13) Final submission time: 11:30pm
Type of Collaboration	Individual assessment and group work
Style and format	Presentation and Report
Assessment submission	Online via Moodle This assessment has been set up to be checked by Turnitin, a tool which helps you check whether you have referenced correctly. You can submit your assessment task to Turnitin prior to the due date and Turnitin will give you an originality report. You may then make any changes that may be required and resubmit your final version by the due date.
Assessment return	UOW Release of Results
Detailed information	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 6 to be assigned their research project. Assessment is based on a research report written in the style to be submitted on the Friday 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.

Minimum Requirements to Pass 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:

- Meet the minimum attendance and participation requirements set out below

Minimum Student Attendance and Participation

Attendance at all practicals and demonstrations is compulsory and should be met to successfully complete the subject. If attendance is affected due to compassionate, compelling, or extenuating circumstances, an academic consideration application should be lodged via SOLS and supporting documentation, for example a Medical Certificate, presented to Student Central. For further details about applying for academic consideration visit the Student Central webpage: <http://www.uow.edu.au/student/central/academicconsideration/index.html>

Hurdle Assessment

Subjects may include a hurdle assessment. A hurdle assessment is an assessment that requires a minimum level of performance as a condition for passing the subject. Examples include, achievement of a pass grade or above in a skills-based assessment or final examination. Hurdle assessments are applied to subjects to ensure students:

1. meet learning outcomes
2. demonstrate you can complete a task safely and/or meet professional standards.

For more on hurdle assessments see the Assessment and Feedback Policy [Section 8: Hurdle Assessments \(50-51-52\)](#).

Should this subject contain a hurdle assessment, it will be stated under the specific assessment in Section B: Assessments.

UOW Grade Descriptors

The UOW Grade Descriptors are general statements that communicate what our grades represent, in terms of standards of performance, and provide a frame of reference to ensure that assessment practice across the University is appropriate, consistent and fair. Grade Descriptors are expressed in general terms so that they are applicable to a broad range of disciplines. Grade Descriptors are available here <https://www.uow.edu.au/student/exams/results/>. For more information on the UOW grade descriptors refer to the Teaching and Assessment: Assessment and Feedback Policy: [Teaching and Assessment: Assessment and Feedback Policy](#)

Assessment Learning Outcome Matrix

Learning Outcomes	Measures - Assessment weighting			
	Assignments (1 x Presentation & 5 x Report)	Exam 1	Exam 2	Project
	(40%)	(15%)	(15%)	(30%)
Analyse and synthesize the core theories underpinning modern computational chemistry methods, assess and justify the selection of an appropriate method for specific applications, and interpret the chemical significance of computational data	✓	✓		
Analyse the symmetry elements present in a given molecule and critically examine their spectroscopic significance	✓	✓		
Interpret and predict rotational and vibrational spectra of molecules through the consideration of molecular orbitals and symmetry	✓		✓	
Evaluate a range of mass spectra (including electron ionisation, electrospray ionisation and tandem mass spectra), articulate the methodologies for their acquisition and deduce simple molecules based on their mass spectra	✓		✓	
Apply modern computational methods to study the structure-activity relationships in molecules of chemical or biological importance through a research project				✓

Submission, Retention and Collection of Written Assessment

Assessed work must be handed in by the date and time listed under each assessment task. All assessment tasks must represent the enrolled student's own ORIGINAL work and must not have been previously submitted for assessment in any formal course of study.

Extensions

Students requesting an extension of time to submit an assessment task, deferred exam or exemption of a compulsory attendance requirement, must apply using Academic Consideration through SOLS. Students must apply before, or on the assessment/s due date and where evidence is required, students must provide evidence no later than three working days after the assessable item's due date for their request to be considered. **For information on the Academic Consideration Policy, eligibility requirements and how to apply, see:** <https://www.uow.edu.au/student/admin/academic-consideration/>

Late Submission of Assessment Tasks and Penalties

Assessed work must be submitted in by the date and time given. If an assessment is submitted late, it will be marked in the normal way, and a penalty will then be applied.

In the absence of an approved request for Academic Consideration in the form of an extension, assessment tasks must be submitted in line with the assessment instructions.

- An assessment task that is submitted late will receive a penalty of 5% of the total possible marks for each 24-hour period, or part thereof, that it is late.
- Work submitted after seven calendar days will not be marked and will be given a mark of 0.
- No assessment task can be handed in for a mark once the assessment task has been returned to students.
- Penalties accrue on each day that the assessment task is late, including Saturday, Sunday and public holidays

Note: Assessments must still be submitted to meet minimum performance requirements even though no mark is to be awarded.

Quiz Completion

Where there is a quiz component, any student who has not attempted and submitted a quiz within the specified timeframe will receive 0 (zero) marks for this assessment type. The quiz will not be reopened, and no alternative assessment will be set without extenuating circumstances and an approved academic consideration application. Late penalties do not apply to quizzes. If a student attempts a quiz but for technical issues is not able to submit the quiz, students must show evidence and apply for an academic consideration to sit a supplementary quiz.

Collection

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.

Retention

The university may retain copies of student work in order to facilitate quality assurance of assessment processes, in support of the continuous improvement of assessment design, assessment marking and for the review of the subject. The University retains records of students' academic work in accordance with the University Records Management Policy and the State Records Act 1988 and uses these records in accordance with the University Privacy Policy and the Privacy and Personal Information Protection Act 1998.

Scaling

Marks awarded for any assessment task or part of any assessment task, including an examination may be subject to scaling at the end of the session. Marks will be scaled only when unpredicted circumstances occur and in order to ensure fairness of marking across groups of students. The method of scaling will depend on the type of scaling required by the circumstances. When scaling is deemed necessary, it will follow a detailed consideration by the Unit Assessment Committee and/or the Faculty Assessment Committee of the marks of the group of students concerned. Scaling will not affect any individual student's rank order within their cohort. For more information please refer to [Finalisation of Student Results Policy](#) for details.

Supplementary Assessment

Supplementary assessment may be offered to students whose performance in this subject is close to that required to pass the subject, and are otherwise identified as meriting an offer of a supplementary assessment. For information about eligibility criteria and the form and timing of supplementary assessments see the [Supplementary Assessment Procedure](#)

Review and Appeal of Academic Decisions

A student may request an explanation of a mark for an assessment task or a final grade for a subject consistent with the student's right to appropriate and useful feedback on their performance in an assessment task. A student may also seek further explanation for other academic decisions such as Academic Consideration, Supplementary Assessment or Credit for Prior Learning. If a student is not satisfied with the explanation, or have further concerns, they may have grounds for a formal review. For further information refer to [Review and Appeal of Academic Decisions Policy](#)

Assessment Quality Cycle

The UOW Assessment Quality Cycle provides a level of assurance that assessment practices across the University are appropriate, consistent and fair. Quality assurance activities are undertaken to support the continuous improvement of assessment and promote good practices in relation to assessment design, marking and review of the subject prior to subsequent delivery.

Academic Integrity

The University's Academic Integrity Policy, faculty handbook 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. Uploading an assessment task, subject outline or other course materials without express permission of the University is considered academic misconduct and students place themselves at risk of being expelled from the University.

Students should visit the following University website and become familiar with the University's policy on plagiarism [Academic Integrity Policy](#)

Referencing

The Author-Date (Harvard) referencing system should, unless otherwise specified for a particular assessment (check Details of Assessment Tasks), be utilised. A summary of the Harvard system can be accessed on the Library website at: <http://uow.libguides.com/refcite>

Section C: General Advice for Students - Policies and Procedures

Student Services and Support

There are a range of services available to students that are provided free of charge. A good place to get to know services that may be of use to you is the [Get Started @ UOW](#) or search for "Get Started @ UOW". Services available include:

Service	Link to information about the service
Aboriginal & Torres Strait Islander	https://www.uow.edu.au/about/services/woolyungah-indigenous-centre/about-us/
Careers advice	https://www.uow.edu.au/student/careers/
Counselling	https://www.uow.edu.au/student/support-services/counselling/
Student Accessibility and Inclusion (SAI)	https://www.uow.edu.au/student/support-services/sai/
Information Tech.	https://www.uow.edu.au/its/index.html?ssSourceSiteId=getstarted
Study Skills	https://www.uow.edu.au/student/support-services/academic-skills/

Student Support Coordinator (SSC)

If you have a temporary or ongoing issue or a problem that is affecting your study, including issues that are related to belonging to an equity group, then the Student Support Coordinators may be able to help. There are Student Support Coordinators available to assist students who are studying at all UOW Campuses and in all UOW Faculties. Contact details can be found on the UOW website: <https://www.uow.edu.au/student/support-services/coordinators/>

Student Advocacy Service

The Student Advocacy Service (SAS) is free, confidential and independent service for all UOW students. The SAS provides advocacy and referral for a range of academic, procedural and administrative issues. For more information visit: <https://www.uow.edu.au/student/support-services/advocacy/>

AskUOW

AskUOW is your primary administrative and information contact during your studies.

Our purpose is to ensure students have access to the information they need, at the time they need it. We can help with a wide range of enquiries, including key topics such as:

- Applying for [academic consideration](#)
- Fees and scholarships
- Official documentation and student letter requests
- Student forms such as course transfer and leave of absence applications
- Student ID card issuance and replacement
- Subject enrolment
- Transport concession cards and Opal cards
- Updating personal details

Get instant answers 24/7 online using [AskUOW](#). Log in with your UOW username and password.

For further support contact askuow@uow.edu.au or call on 1300 275 869 (1300 ASK UOW) or +61 2 4221 3927.

Library Services

Save yourself time and enhance your studies: connect with information specialists and resources anytime, anywhere.

- For Library support connect with [Live Chat](#) or [contact the Library](#).
- For self-help see [Frequently Asked Questions](#) or browse [Library guides](#) to find information, databases and skills tutorials.
- [Research consultations](#) are available to UOW Postgraduate, Honours and Deans Scholar students.

Academic Integrity Policy

Academic integrity involves upholding ethical standards in all aspects of academic work, including learning, teaching and research. It involves acting with the principles of honesty, fairness, trust and responsibility and requires respect for knowledge and its development. The Policy can be found at:

<https://policies.uow.edu.au/document/view-current.php?id=26>

Code of Practice - Research

This Code mandates the current policy and best practice relating to procedures for responsible research. The Code can be found at: <https://policies.uow.edu.au/document/view-current.php?id=11>

Honours Policy

This policy sets out the responsibilities of all parties involved in managing students undertaking Honours Programs. The Code can be found at: <https://policies.uow.edu.au/document/view-current.php?id=36>

The Code of Practice - Work Integrated Learning (Professional Experience)

The Code of Practice - Work Integrated Learning (Professional Experience) sets out what is expected from students, the University and Host Organisations in providing work integrated learning professional experience programs. It applies to professional experience programs that form the whole or part of a subject or course offered at the University. The Code assists in promoting a productive work integrated learning experience for students and in promoting relevant UOW Work Integrated Learning Design Principles.

<https://policies.uow.edu.au/document/view-current.php?id=12>

Copyright Policy

The purpose of this Policy is to outline responsibilities and procedures regarding the use of third party copyright material, with the objectives of reducing staff and UOW exposure to the risks associated with the use of third party copyright material, assisting staff to make full legal use of the materials at their disposal by clearly identifying responsibilities and promoting copyright compliance. The Policy can be found at:

<https://policies.uow.edu.au/document/view-current.php?id=135>

Course Progress Policy

The Course Progress Policy establishes the requirements, definitions and procedures to be used in determining the standards of acceptable course progress. The Policy can be found at:

<https://policies.uow.edu.au/document/view-current.php?id=30>

Examination Rules and Procedures

The UOW rules and procedures outline exam conditions, student conduct in exams, and the procedures for exam management. Further information can be found here: <https://www.uow.edu.au/student/exams/>

Ethical Objection by Students to the Use of Animal and Animal Products in Coursework Subjects

This policy provides a framework for recognition of and responses to students' ethical or religious objection to animal use in coursework subjects at the University of Wollongong. For the purpose of this policy, animal use includes killing of animals in experimental work, dissection of animals that are already dead, use of animal tissues, use of animal-derived products (such as sera). These uses are relevant to teaching and assessment. Further information about this policy can be found here: <https://policies.uow.edu.au/document/view-current.php?id=154>

Coursework Rules

The Coursework Rules (hereafter the Rules) govern the admission, enrolment, progression through, and qualification for a coursework award offered by the University. Further information can be found here: <https://policies.uow.edu.au/document/view-current.php?id=4>

Human Research Ethics

The Human Research Ethics Committee protects the welfare and rights of the participants in research activities. Further information can be found here: <https://www.uow.edu.au/research-and-innovation/researcher-support/ethics/human-ethics/>

Inclusive Language Guidelines

UOW endorses a policy of non-discriminatory language practice in all academic and administrative activities of the University. Further information is available from: <https://policies.uow.edu.au/document/view-current.php?id=239>

Intellectual Property Policy

UOW's IP Intellectual Property Policy provides guidance on the approach taken to Intellectual Property (IP), including its ownership, protection and exploitation. Further information about the management of IP is available at <https://policies.uow.edu.au/document/view-current.php?id=146>

Review and Appeal of Academic Decisions Policy

UOW aims to provide a transparent and consistent process for resolving a student concern about an academic decision that has affected their academic progress, including a mark or grade. Further information is available at: <https://policies.uow.edu.au/document/view-current.php?id=40>

Student Academic Consideration Policy

The purpose of the Student Academic Consideration Policy is to enable student requests for academic consideration for assessable components of a subject to be evaluated in a fair, reasonable, timely and consistent manner throughout the University. **For information on the Policy, eligibility and how to apply see:** <https://www.uow.edu.au/student/admin/academic-consideration/>

The Student Charter - Your Rights and Responsibilities

The Student Charter is based on principles that guide all members of the University and that promote responsible partnerships within and beyond the University community. <https://www.uow.edu.au/student/charter/>

Student Assignment of Intellectual Property (IP) Policy

This policy applies to all Students (under-graduate and post-graduate) of the University of Wollongong (UOW). It may also apply to other persons by agreement. This policy sets out the approach taken by UOW in relation to

Student assignment of intellectual property. Further information about this policy can be found here: <https://policies.uow.edu.au/document/view-current.php?id=146>

Student Conduct Rules

These Rules outline the required conduct of students of UOW, and direct staff and students to University Rules, standards, codes, policies, guidelines, procedures and other requirements which specify acceptable and unacceptable student conduct, and the management of alleged student misconduct. <https://policies.uow.edu.au/document/view-current.php?id=6>

Teaching and Assessment: Assessment and Feedback Policy

The purpose of this Policy is to set out the University of Wollongong's approach to effective learning, teaching and assessment, including the principles and minimum standards underlying teaching and assessment practice. The Policy can be found at: <https://policies.uow.edu.au/document/view-current.php?id=38>

Teaching and Assessment: Code of Practice - Teaching

This Code is a key document in implementing the University's Teaching and Assessment Policy and sets out the specific responsibilities of parties affected in relation to learning, teaching and assessment, as well as procedures for teaching staff. The Code can be found at: <https://policies.uow.edu.au/document/view-current.php?id=9>

Teaching and Assessment: Subject Delivery Policy

This Policy sets out specific requirements in relation to the delivery of Subjects. The policy can be found at: <https://policies.uow.edu.au/document/view-current.php?id=39>

Workplace Health & Safety Policy

The Workplace Health and Safety (WHS) unit at UOW aims to provide structures, system and support to ensure the health, safety and welfare of all at the campus. Further information is available from: <https://policies.uow.edu.au/document/view-current.php?id=177>