

General Course Information

CHEM 212 / BCHM 212 Chemical Reactivity

0.1250 EFTS 15 Points
First Semester 2023

Description

This course runs in semester one. It counts 15 points towards a Bachelor of Science degree. It is required to major in chemistry and biochemistry and preferably it is taken in conjunction with other 200-level chemistry and/or biochemistry courses.

The topics covered in this course are: foundational principles of organic and biochemical reaction chemistry; and bioinorganic chemistry and electrochemistry.

Timetable

Lectures & Workshops: Three hours of lectures/workshops per week. Details to be confirmed on 'My Timetable' and the web.

Tutorials: There will be problem-solving workshops held approximately fortnightly during the normal lecture slots. Additional tutorial sessions may be organised as necessary, especially for students needing further assistance.

Students should note that in the Science Faculty that the average student is responsible for approximately 3.2 hours of additional study for each hour of lecture/workshop contact time at the 200-level.

Course Co-ordinator

Professor Rudi Marquez, School of Physical and Chemical Sciences
Room West822, ext 90162, Email: rudi.marquez@canterbury.ac.nz

Email me if you have any queries about the course.

Assessment

In order, with course component indicated:

- Test 40%
- Final Examination 60%

Examination and Formal Tests

Test: 90 min – in person test – time and date to be advised on MyTimetable

Exam: 3 hours, details to be advised.

Textbooks

The general textbook for the course is:

A. Burrows, J. Holman, A. Parsons, G. Pilling and G. Price, *Chemistry*³, Second Edition OUP, 2013.

Additional information may be taken from - Clayden, Greeves, Warren and Wothers, *Organic Chemistry*, Oxford University Press, 2012 (2nd edn.).

These textbooks will be available in the Engineering & Physical Sciences Library, where copies will be on reserve.

Prerequisites/Restrictions

P: CHEM112 R: BCHM205, CHEM232, ENCH241

Web-based resources: Various learning resources (lecture material, reference links, quizzes, discussion forums etc.) for this course are available via the University of Canterbury's *Learn* web site -- <http://learn.canterbury.ac.nz/>. This site will also be used regularly as a means of communication and information distribution for all of your Canterbury courses. You should familiarise yourself with *Learn* as soon as possible.

Goal of the Course

Develop an understanding of fundamental principles of structure and chemical reactivity relevant to organic and biological chemistry that builds on foundational principles from first year chemistry and provides a solid foundation for further study in chemistry and biochemistry.

Learning Outcomes (see also detailed Learning Objectives after Course Content, below)

- Develop the ability to apply scientific principles and concepts
- Develop problem-solving and numeracy skills in the context of organic and bioinorganic chemistry and electrochemistry
- Understand, evaluate, access and critically review new chemical information
- Demonstrate the ability to think independently about chemical concepts
- Develop a more in-depth knowledge of chemical reactivity in the areas of organic reactions, electrochemistry and bioinorganic chemistry
- Effectively access and use information relevant to chemistry and biochemistry
- Communicate effectively in written English

Summary of the Course Content

BLOCK 1: 12 Lectures/Problem sessions

Structures and properties of organic and biological molecules

Three-dimensional structure of organic and biological molecules and the importance of functional groups within molecules.

- Review of basic concepts of organic bonding: molecular orbital and valence bond representations. Three-dimensional structural issues: molecular representations; conformational analysis of simple acyclic and cyclic molecules; isomerism and stereoisomerism; chirality, enantiomers and diastereoisomers with examples taken from biomolecules.
- Common functional groups; nucleophiles and electrophiles; resonance and tautomerism; acidity and basicity of organic molecules.
- Biochemically relevant properties of biomolecules

Lecturer: Professor Rudi Marquez, Room West 822, ext 90162, rudi.marquez@canterbury.ac.nz

BLOCK 2: 6 Lectures/Problem sessions

Thermodynamics and Kinetics in action

Thermodynamic and Kinetic considerations are vitally important for all reactions in Organic Chemistry and Biochemistry. We will introduce these concepts and use them to predict the outcome of reactions.

- The application of enthalpy, entropy and Gibbs energy (ΔG) to organic transformations
- Kinetics and stereochemistry as tools to unravel reaction details
- Understanding Transition State structures in reactions – Catalysis, Solvent effects
- methods of monitoring the rates of organic reactions
- enzyme-catalysed reactions and Michaelis-Menten kinetics

Lecturer: Dr Dan Foley, BT323, ext 90479, daniel.foley@canterbury.ac.nz

BLOCK 3: 9 Lectures/Problem sessions

Introduction to Organic Reaction Mechanisms

Understanding mechanism is actually the key to grasping the whole of organic chemistry. This part of the course will consider in detail what can happen when a leaving group is attached to a carbon atom in an organic molecule.

The S_N2 reaction

- mechanism, reaction diagram, and stereochemical consequences
- effect of substrate structure on the rate of S_N2 reactions
- effect of the nature of nucleophile on the rate of S_N2 reactions
- basicity vs nucleophilicity; how to decide what is a good nucleophile and what is a good base
- effects of leaving group and solvent on S_N2 reactions

The S_N1 reaction

- mechanism, reaction diagram, and stereochemical consequences
- effect of substrate structure on the rate of S_N1 reactions
- effect of leaving group, solvent, and the nature of nucleophile on the rate of S_N1 reactions
- the S_Ni reaction
- a comparison of S_N1 vs S_N2 : how to decide which happens

Elimination reactions

- The E2, E1 and E1cB mechanisms
- regiochemistry of elimination: Saytsev and Hofmann elimination
- stereochemistry of elimination: anti vs syn
- comparison of elimination vs substitution – how to decide which occurs: nature of base / nucleophile and effect of temperature.

Lecturer: Professor Antony Fairbanks Room West 801, ext 95217, antony.fairbanks@canterbury.ac.nz

BLOCK 4: 9 Lectures/Problem sessions

Introductory chemistry of the carbonyl group

A thorough grasp of the chemistry of the carbonyl functional group is essential to an understanding of both organic chemistry and biochemistry; the carbonyl group is present in all of the important bio-macromolecules; e.g. amino acids in peptides / proteins, sugars in oligosaccharides, nucleosides in nucleic acids.

This part of the course will focus on examination of the basic reactivity and also the synthetic utility of carbonyl containing compounds. The chemistry of aldehydes, ketones, esters, amides and other carboxylic acid derivatives will be examined in detail.

The structure and reactivity of the of the C=O group

- mode of reactivity by nucleophilic addition
- structural factors affecting reactivity

Nucleophilic addition to aldehydes and ketones

- reversible addition - hemiacetal formation
- irreversible addition: reduction by metal hydrides, addition of organometallics

Nucleophilic substitution of aldehydes and ketones

- acetal formation and hydrolysis
- the formation of imines, oximes and hydrazones
- the formation of enamines
- reductive amination; the synthesis of amines
- amino acid synthesis

Nucleophilic substitution reactions of carboxylic acid derivatives

- explanations of relative reactivity / stability
- inter-conversions of carboxylic acid derivatives
- ester hydrolysis *via* several different mechanisms
- the stability of amides; their hydrolysis under forcing conditions
- the reactions of carboxylic acid derivatives with reducing agents and organometallics.

Lecturer: Professor Antony Fairbanks Room West 801, ext 95217, antony.fairbanks@canterbury.ac.nz

LEARNING OBJECTIVES

BLOCK 1:

At the end of this lecture block you should be able to:

- Draw organic molecules in three dimensions using the appropriate representation.
- Understand the concept of hybridisation and bonding in organic molecules.
- Describe the effect of rotations about carbon-carbon single bonds and assess the relative stabilities of different conformers. Draw the different conformations of cyclohexane and its derivatives.
- Describe the different types of isomerism that are possible for organic molecules.
- Understand the importance of electron delocalisation, resonance, acidity and basicity in organic molecules and their reactions.
- Describe the important functional groups commonly found in organic and biological molecules.
- Understand how the physical properties of biological molecules underpin their role in biochemistry.

BLOCK 2:

At the end of this lecture block you should be able to:

- Demonstrate a working understanding of the following issues associated with organic reactions by data analysis and problem-solving:
- Mechanism analysing synthetic transformations – relationship of starting material to product; bonds broken and formed
- classification of organic reactions – substitution and elimination/addition
- identification of nucleophiles, electrophiles and leaving groups in organic reactions

- the role of electronic and steric factors in affecting organic reactivity
- curly arrows as a means of keeping track of electron-flow in organic reactions
- the relationship of enthalpy changes and bond dissociation energies
- the role of entropy in controlling the direction of spontaneous reactions
- use of Gibbs energy for understanding the thermodynamics of reversible organic reactions
- use of kinetic data to determine mechanisms
- rate laws for simple organic and enzyme-catalysed transformations
- structure-function relationships - relative reactivity of related chemicals
- solvent effects on reaction rates
- effect of steric and electronic factors on reactivity
- reaction energy diagrams and activation energies
- carbocations and carbanions as reactive intermediates in organic reactions
- Hammond's postulate

BLOCK 3:

At the end of this lecture block you should be able to:

- Appreciate why an understanding of reaction mechanisms is important.
- Be able to represent the bond breaking and bond making processes occurring during nucleophilic substitution and elimination reactions using curly arrows.
- Understand the similarities and differences between bases and nucleophiles; understand what makes a good nucleophile and what makes a good base.
- Understand what makes a good leaving group.
- Understand the S_N2 mechanism for nucleophilic substitution, including the reaction diagram and be able to rationalize the stereochemical consequence; inversion.
- Understand how the rate of an S_N2 reaction depends on the substrate structure, the identity of nucleophile, the solvent, and the leaving group.
- Understand the S_N1 mechanism for nucleophilic substitution including reaction diagram and be able to rationalize the stereochemical consequence; racemisation.
- Understand how the rate of an S_N1 reaction depends on the substrate structure, the identity of nucleophile, the solvent, and the leaving group.
- Appreciate the possibility of an S_Ni reaction.
- Understand that S_N1 and S_N2 reactions are competing processes, and be able to decide which is most likely to happen in a particular case.
- Understand that elimination reactions produce alkenes by removal of a proton and loss of a leaving group.
- Understand the various possible mechanisms for elimination - $E1$, $E2$, $E1_{CB}$ reactions - including being able to draw reaction diagrams for each.
- Understand the stereo- and regiochemical consequences of the different elimination mechanisms; anti vs syn elimination; Saytzeff vs Hoffman elimination.
- Understand that elimination and substitution reactions are competing processes, and be able to decide which is most likely to happen in a particular case.

BLOCK 4:

At the end of this lecture block you should be able to:

- understand the structure of the carbonyl group, why it is reactive, and its principal mode of reactivity.
- understand that structural factors can modulate reactivity of the carbonyl group; e.g. resonance effects.
- understand, and be able to draw mechanisms for reversible nucleophilic addition to aldehydes and ketones; e.g. cyanohydrin formation, hydration and hemiacetal formation.
- understand, and be able to draw mechanisms for irreversible nucleophilic addition to aldehydes and ketones e.g. reduction by metal hydrides, the addition of simple organometallic reagents.
- understand, and be able to draw mechanisms for reversible nucleophilic substitution of aldehydes and ketones; e.g. acetal, imine, oxime, hydrazone and enamine formation.
- be able to explain the pH / rate dependence of reactions of aldehydes and ketones with nitrogen nucleophiles.
- understand, and be able to draw mechanisms for the uses of imines in synthesis: e.g. reductive amination.
- understand and be able to explain the relative reactivity of carboxylic acid derivatives towards nucleophiles.
- understand, and be able to draw mechanisms for nucleophilic substitution reactions of carboxylic acid derivatives by the formation of tetrahedral intermediates, and appreciate the importance of leaving group ability.
- understand how carboxylic acid derivatives can be inter-converted.
- understand, and be able to draw mechanisms for ester hydrolysis by the $B_{AC}2$, $A_{AC}2$, $A_{AL}1$, and $A_{AC}1$ mechanisms.
- understand and be able to draw mechanisms for amide hydrolysis.
- understand and be able to rationalize the reactions of carboxylic acid derivatives with reducing agents
- understand and be able to rationalize the reactions of carboxylic acid derivatives organometallic reagents.

GENERAL INFORMATION | TE KIMI MŌHIOHIO 2023

Policy on 'Dishonest Practice' / Ngā Takahitanga me ngā Tinihanga

The University has strict guidelines regarding 'dishonest practice' and 'breach of instructions' in relation to the completion and submission of examinable material. In cases where dishonest practice is involved in tests or other work submitted for credit, a department may choose to not mark such work – see the online guidelines in relation to ['Academic Integrity'](#).

The School of Physical and Chemical Sciences upholds this policy. It considers plagiarism, collusion, copying and ghost writing – all detailed below – to be unacceptable and dishonest practices:

- **Plagiarism | Tārua Whānako** is the presentation of any material (text, data or figures, on any medium including computer files) from any other source without clear and adequate acknowledgement of the source. Note that the use of **AI generative tools such as ChatGPT** for assessment work is *strictly forbidden*, except where the lecturer concerned has specifically granted approval.
- **Collusion** is the presentation of work performed in whole, or in part, in conjunction with another person or persons, but submitted as if it has been completed by the named author alone. This interpretation is not intended to discourage students from having discussions about how to approach an assigned task and incorporating general ideas that come from those discussions into their own individual submissions, but acknowledgement is necessary.
- **Copying** is the use of material (in any medium, including computer files) produced by another person or persons with or without their knowledge and approval. **This includes copying of the lab reports (raw data may be shared within the group if permitted or required by the experiment) – data analysis and interpretation of obtained results MUST be performed individually.**
- **Ghost writing** is the use of other person(s) (whether with or without payment) to prepare all or part of an item of work submitted for assessment.

Special consideration of assessment | Ngā Pairuri Motuhake

['Special Consideration'](#) (previously termed 'Aegrotat Application') for an item of assessment is for students who have covered the work involved but have been prevented from demonstrating their knowledge or skills at the time of the assessment due to unforeseen circumstances, whether illness, injury, bereavement, car crash or any other extenuating circumstance *beyond one's control*. Special Consideration for a test/exam may be because a student has not sat it or has done so with impaired performance. Applications can be submitted via the above link and must be made **no later than five working days after the assessment due date**. Note that special consideration is **not available for items worth less than 10% of the overall course mark**. In the case of illness or injury, medical consultation should normally have taken place either shortly before or within 24 hours after the due date for the required work or test/examination.

Note that you may be required to sit a special exam or your grade may not be changed if there is insufficient evidence of your performance from other invigilated assessment items in the course. **You have the right to appeal any decision.**

It is important to understand that Special Consideration is only available *where course work has been covered*, and the inability to demonstrate this fully is both *no longer possible* AND is due to *unexpected circumstances beyond one's control*. Thus Special Consideration is **NOT available for**:

- essays, assignments or quizzes where an extension of time is available to complete the assessment item (see below for the process to involved);
- missed lectures during the semester;
- experiencing examination anxiety;
- having several examinations or assessments close together;
- known impairment, such as chronic illness (medical or psychological), injury or disability unless medical evidence confirms that the circumstances were exacerbated, despite appropriate management, at the time of assessment;
- mistaking the date or time of an examination (this is a circumstance one can control!);
- failing to turn up to an examination or test because of sleeping in (a circumstance as above!);
- where applications are repeatedly made for the same or similar reason, then the application may be declined on the grounds that the reason is not unexpected;
- where the application is made at the time of the assessment but the supporting documentation is received significantly after this date or after the date results are released; or
- the application is made following the release of results (unless under exceptional circumstances).

Extensions of deadlines | Tononga Wā Āpiti

Where an extension may be granted for an assessment item, this will be decided by application to the course co-ordinator and/or the lecturer concerned.

Late withdrawal from a course

If you are prevented by extenuating circumstances from completing the course after the final date for withdrawing from the course, you may apply for special consideration for late discontinuation. For details on special consideration, or to make an application, refer to the Examinations Office website <http://www.canterbury.ac.nz/exams/>. Applications must be submitted **within five days** of the end of the main examination period for the semester.

Missing of tests | Te Matangaro i ngā Whakamātautau

In rare cases a student will not be able to sit a test. In such cases, the student should consult with the course co-ordinator to arrange alternative procedures. **This must be done well in advance of the set date for the test.**

Past tests and exams

Past tests can be found on our [Chemistry Undergraduate](#) website. Past exams can be found on the [Library website](#).

Submission of reports and assignments

Reports (including lab reports) and assignments should be handed in on time. Extensions will be granted only in exceptional circumstances (such as illness or bereavement). If an extension is required, as early as possible you should request it from the lecturer concerned.

Note: If you do not submit an assignment for assessment, you will be allotted zero marks, which will affect your final result. You should ensure that you pick up marked assignments and keep them until the end of the course as evidence that the work was completed and marked in the case that either is disputed. To guard against accidental loss, it would be prudent to keep photocopies or electronic copies of anything submitted.

Late Work

Acceptance of late work for assessment will be at the discretion of the course coordinator and/or the lecturer concerned. If your assessment is likely to be late, please contact the relevant of these people **before the assessment is due**. Never assume that an extension will be automatically granted – some courses have the policy of no late work being accepted. A commonly exercised policy is to deduct 10% of the total marks for each day that the work is late, where weekends and public holidays also count as such days.

Marks and Grades | Taumata Ako

The following numbers should be considered as a guide to the expected grades under normal circumstances. The School reserves the right to adjust mark/grade conversions, if necessary.

Please note that for all invigilated assessments (tests and exams) worth 33% and above, failure to obtain a mark of at least 40% will result in a final grade no higher than an R at 100 and 200 level; in general this requirement will not be applied at 300 level, but if it is then the course coordinator will inform the class and it will result in a final grade no higher than a C-.

Grade:	A+	A	A-	B+	B	B-	C+	C	C-	D	E
Minimum mark %:	90	85	80	75	70	65	60	55	50	40	0

Reconsideration of Grades

Students should, in the first instance, speak to the course co-ordinator about their marks. If they cannot reach an agreeable solution, or have questions about their grade in a course, students should then speak to the Director of Undergraduate Studies, [Assoc Prof Greg Russell](#). Students can appeal any decision made on their final grade. You can apply at the Registry for reconsideration of the final grade within four weeks of the date of publication of final results. Be aware that there are time limits for each step of the appeals process.

Students with Disabilities | Te Whaikaha

Students with disabilities should speak with someone at [Equity and Disability Service](#), phone: 369 3334 (or ext. 93334), email: eds@canterbury.ac.nz).

Academic Advice

[Assoc Prof Greg Russell](#) is the coordinator of undergraduate chemistry courses. His interest is in the academic performance and well-being of all such students. Anyone experiencing problems with their chemistry courses or requiring guidance about their B.Sc. in Chemistry should get in contact with Greg.

Staff-Class Rep Liaison

[Assoc Prof Greg Russell](#) is in charge of liaison with students in chemistry courses. Your class will appoint a student representative to the liaison committee at the start of the semester. Please feel free to talk to the Academic Liaison or the student rep about any problems or concerns that you might have.

Greg Russell (greg.russell@canterbury.ac.nz, tel. 369 5129)
Director of Undergraduate Studies
School of Physical and Chemical Sciences
2023