CBMS704

Organic and Biological Chemistry B

S2 Day 2016

Dept of Chemistry & Biomolecular Sciences

Contents

General Information

Unit convenor and teaching staff
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Credit points
4

Prerequisites
Admission to MRes

Corequisites

Co-badged status
CBMS804

Unit description
This unit starts with an overview of aromaticity and moves on to the chemistry of heterocyclic compounds. The next section of the course is a detailed treatment of organometallic chemistry, by which we mean metal mediated reaction in organic chemistry. The last part of the unit covers pericyclic (no mechanism) reactions. The laboratory program aims to teach advanced synthetic skills and exemplify the theoretical component through a number of computational workshops involving cutting edge molecular modelling software and ab initio computational packages.

Important Academic Dates

Information about important academic dates including deadlines for withdrawing from units are available at https://www.mq.edu.au/study/calendar-of-dates

Learning Outcomes

On successful completion of this unit, you will be able to:

To understand the of the factors affecting reactivity of organic chemicals including biomolecules

To readily identify key bond forming process and building blocks in the synthesis of N-heteroaromatic molecules such as pyrroles, pyridines, pyrazoles, imidazoles, isoazoles and quinolines

To have a detailed understanding of how liganded coupling processes and heterocyclic chemistry can be used in the synthesis of biologically active molecules and materials

To construct orbital diagrams and orbital symmetry to predict outcomes of pericyclic reactions

To have a detailed chemical understanding of stereoselectivity and chirality in organic reaction processes

To posses high level laboratory skills necessary for research in Organic Biological Chemistry, including the ability to plan synthetic sequences

To have the skills necessary for in-depth literature analysis

Assessment Tasks

Name	Weighting	Due
Practical Pt 1	9%	E1 2/9; E2 16/9
Practical Pt 1	16%	E3 21/10; E4 11/11
Mid-semester Test	10%	Week 7, Lecture time
Spot tests and work-shops	10%	Week 5, 9, 13
Final Examination	55%	University exam period

Practical Pt 1

Due: **E1 2/9; E2 16/9**
Weighting: **9%**

Details on what is expected for assessment of the practical component is provided in the laboratory manual (see the web site at printed notes). The mark will reflect the level of safety and laboratory techniques seen within the laboratory as well as clear presentation, interpretation of results and addressing of specific questions within laboratory reports

On successful completion you will be able to:

- To understand the of the factors affecting reactivity of organic chemicals including biomolecules
- To readily identify key bond forming process and building blocks in the synthesis of N-heteroaromatic molecules such as pyrroles, pyridines, pyrazoles, imidazoles, isoazoles

and quinolines
- To have a detailed understanding of how liganded coupling processes and heterocyclic chemistry can be used in the synthesis of biologically active molecules and materials
- To construct orbital diagrams and orbital symmetry to predict outcomes of pericyclic reactions
- To have a detailed chemical understanding of stereoselectivity and chirality in organic reaction processes
- To posses high level laboratory skills necessary for research in Organic Biological Chemistry, including the ability to plan synthetic sequences
- To have the skills necessary for in-depth literature analysis

Practical Pt 1

Due: **E3 21/10; E4 11/11**
Weighting: **16%**

Details on what is expected for assessment of the practical component is provided in the laboratory manual (see the web site at printed notes). The mark will reflect the level of safety and laboratory techniques seen within the laboratory as well as clear presentation, interpretation of results and addressing of specific questions within laboratory reports

On successful completion you will be able to:
- To understand the of the factors affecting reactivity of organic chemicals including biomolecules
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Mid-semester Test

Due: **Week 7, Lecture time**

Weighting: **10%**

There will be a 50 minute test in Week 7, 8-9 am, which will cover the first two modules of the unit (*i.e.* heterocyclic chemistry and part of the carbohydrate chemistry). This is designed to address specific understanding and application of topics covered up to the end of week 6 lecture material.

On successful completion you will be able to:

- To understand the of the factors affecting reactivity of organic chemicals including biomolecules
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Spot tests and work-shops

Due: **Week 5, 9, 13**
Weighting: **10%**

Spot tests - These may be conducted at any stage within the lectures. They are to encourage continuous learning of the lecture material without the stress of a significant assessment component.

Workshops – The workshops will be run weeks 5, 9 and 13. The mark for the workshops will be based on attendance and participation within the workshops.

On successful completion you will be able to:

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chemistry can be used in the synthesis of biologically active molecules and materials
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Final Examination

Due: **University exam period**
Weighting: **55%**

The final exam will be 3 hours in length with 10 minutes reading time. It is designed to address specific understanding of all the topics presented within the course and to show that the knowledge obtained can be applied to new problems

On successful completion you will be able to:

- To understand the of the factors affecting reactivity of organic chemicals including biomolecules
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Delivery and Resources

Classes

CBMS704/804 is a traditional Chemistry subject that is organised around lectures and laboratories.

The timetable may be subject to change so please check on the University web site at:

http://students.mq.edu.au/student_admin/timetables

Spot tests will be run in the lecture classes and workshops are also compulsory to attend.

The lab notes, which include safety information and a guide on writing the reports are available from the CBMS304 web page (log in through ilearn.mq.edu.au).

Laboratory Report Due Dates

See the Lab Manual

Required and Recommended Texts and /or Materials

All are in the Reserve section of the library

Required texts

McMurry, John. Organic Chemistry Edition (introductory reading only). QD251.2.M43.

Davies, David T. Aromatic Heterocyclic Chemistry, Oxford University Press. QD400.D38/1992

Fleming, Ian. Pericyclic reactions, Oxford; Oxford University Press, 1999. QD281.R5.F58/1999

Jenkins, Paul. Organometallic Reagents in Synthesis, Oxford; Oxford University Press, 1992. QD411 .J45 1992

Supplementary texts (all on three day loan)

Garrett, R. and Grisham, C.M. Biochemistry, Fort Worth, Saunders College Pub., 1999. QD415.G29/1999

Smith, W.B. Introduction to theoretical organic chemistry and molecular modeling, New York: VCH Publishers, c1996. QD476.S567/1996

Gilchrist, T.L. Heterocyclic Chemistry, Longman Scientific & Technical. QD400.G55/1997

Gilchrist, T.L. Organic reactions and orbital symmetry. New York: Wiley, c1976. QD476.G54/ 1979

Joule J.A. and Mills K. Heterocyclic Chemistry, 4th edition, Oxford, Blackwell Science Ltd, 2000. QD400.J59/2000

Bellamy, Anthony J. An introduction to Conservation of Orbital Symmetry. Longman, 1974. QD476.B363

Fleming, Ian. Frontier Orbitals and Organic Chemical Reactions, Wiley, London 1990, c1978.

QD461.F53/1978

For those that are *really* keen

Entwistle, Norman. Orbital Symmetry Correlations in Organic Chemistry. London: Van Nostrand Reinhold, 1972. QD476.E5

Meijere, de Armin; Diederich, Francois. Metal-catalyzed Cross-coupling Reactions, Wiley-VCH, 2004. QD262.M48 2004, Vol 1

Technology Used and Required

You are expected to access the unit website on a frequent basis and download files for use in class - notes need to added to those provided.

You will need Adobe Acrobat on your computer (can be downloaded at http://get.adobe.com/uk/reader).

Note that information may also be sent to your student email account, so you should be checking that on a daily basis.

Teaching and Learning Strategy

CBMS704/804 is run traditionally with two hours of lectures/week along with 4 hours of laboratories each week (except for weeks 1, 5, 9 and 13). In weeks 5, 9 and 13, workshops will be conducted covering tutorial questions. Lectures will be presented as a combination of formal lectures and interactive tutorial sessions. Some lecture material will be available on the unit web site, while other material will be provided in the lecture class.

Learning is an active process, and as such you MUST engage with the material. This means, at MINIMUM, reading the textbooks (and beyond) before and after the relevant lectures, genuinely attempting the assigned / workshop questions and discussing the concepts with your classmates and the lecturers. Do not be afraid to ask questions as everyone benefits from a robust and open discussion of the topics.

Spot tests (and the mid session test) will also be run in the lecture session. The spot tests will cover material prior to that days lecture (more detail given under assessment), therefore all students are expected to keep up to date with lecture material through revision each week. All laboratory experiments will be conducted individually. The workshops will be run with students in small groups. Some questions relevant to the workshops will be provided (on the web site) prior to the workshop. Additional relevant material will be discussed in the workshops as directed by student questions. Students are expected to bring in all relevant course notes and text books for the workshops and are encouraged to attempt the questions prior to the workshops. All students will be expected to participate in discussions during the workshop and may be required to present some answers to the rest of the class in the workshops.

The staff in this unit will regularly update the web site to provide further information relevant to the unit. All students are expected to visit the web site on a regular basis and enter in web-based discussions.

A week-by-week list of the topics to be covered in this unit is provided below:

Lecture Schedule

(Weeks 1-4) AT lectures

This section of the course will provide you with an overview of heterocyclic chemistry.

Week 1: Aromaticity and Antiaromaticity

- Delocalisation and the 4n+2 rule
- Bond lengths, ring currents
- Aromatic heterocycles
- Contributing and non-contributing lone pairs

Week 2: Simple Five-membered Heterocycles

- Reactions
- Syntheses
- Examples of incorporation into macrocycles

Week 3 & 4: Six-membered Heterocycles and Bicycles

- Pyridine - electrophilic and nucleophilic substitution reactions
- Quinoline

Week 4: DNA

- The DNA bases
- H-bonding and complementarity

(Weeks 5-8) FL lectures

This section of the course will provide you with an overview of coupling reactions with important applications.

- Introduction to Coupling reactions
- Principle of atom economy
- General classes of coupling reactions from Nature and invented by chemists
- Key mechanistic aspects of coupling reactions
- Common coupling strategies and reagents
- Chelation control and selectivity models
- Reactions at saturated carbon centres
- Reactions at unsaturated carbon centres
- Examples of applications
- Ligand effects
- Stereoelectronic principles
- Special reactivities by higher coordination
- Redox cycles

- Sigma- and pi-complexes
- Metallocycles and transmetallation

Week 9-12: Pericyclic Reactions (PK Lectures)

This section of the course will provide you with an overview of pericylic reactions. This includes:

Lecture Notes and Practice Problems that can be found at these web sites:

http://www.ch.ic.ac.uk/local/organic/pericyclic/

Introduction to molecular orbitals

A quiz will be completed at the start of the class. It does not count toward your final mark but should be a guide to whether some remedial work is required.

- Valence bond model and why it does not work
- FMO theory
- Orbital symmetry

Concerted reactions

- S_N1 vs S_N2
- Addition of Br_2 to a double bond
- Examples of concerted reactions

Orbital symmetry

- Construction of a MO energy diagram
- Symmetry rules OK?
- Secondary effects

Examples

- Regioselectivity
- Stereoselectivity
- cycloadditions, sigmatropic shifts, electrocyclisation

Policies and Procedures

Macquarie University policies and procedures are accessible from Policy Central. Students should be aware of the following policies in particular with regard to Learning and Teaching:

Academic Honesty Policy http://mq.edu.au/policy/docs/academic_honesty/policy.html

New Assessment Policy in effect from Session 2 2016 http://mq.edu.au/policy/docs/assessment/policy_2016.html. For more information visit http://students.mq.edu.au/events/2016/07/19/new_assessment_policy_in_place_from_session_2/

Assessment Policy prior to Session 2 2016 http://mq.edu.au/policy/docs/assessment/policy.html

Grading Policy prior to Session 2 2016 http://mq.edu.au/policy/docs/grading/policy.html

Grade Appeal Policy http://mq.edu.au/policy/docs/gradeappeal/policy.html

Complaint Management Procedure for Students and Members of the Public http://www.mq.edu.au/policy/docs/complaint_management/procedure.html

Disruption to Studies Policy http://www.mq.edu.au/policy/docs/disruption_studies/policy.html *The Disruption to Studies Policy is effective from March 3 2014 and replaces the Special Consideration Policy.*

In addition, a number of other policies can be found in the Learning and Teaching Category of Policy Central.

Student Code of Conduct

Macquarie University students have a responsibility to be familiar with the Student Code of Conduct: https://students.mq.edu.au/support/student_conduct/

Results

Results shown in *iLearn*, or released directly by your Unit Convenor, are not confirmed as they are subject to final approval by the University. Once approved, final results will be sent to your student email address and will be made available in eStudent. For more information visit ask.mq.edu.au.

Student Support

Macquarie University provides a range of support services for students. For details, visit http://students.mq.edu.au/support/

Learning Skills

Learning Skills (mq.edu.au/learningskills) provides academic writing resources and study strategies to improve your marks and take control of your study.

- Workshops
- StudyWise
- Academic Integrity Module for Students
- Ask a Learning Adviser

Student Services and Support

Students with a disability are encouraged to contact the Disability Service who can provide appropriate help with any issues that arise during their studies.

Student Enquiries

For all student enquiries, visit Student Connect at ask.mq.edu.au

IT Help

For help with University computer systems and technology, visit http://www.mq.edu.au/about_us/offices_and_units/information_technology/help/.

When using the University's IT, you must adhere to the Acceptable Use of IT Resources Policy. The policy applies to all who connect to the MQ network including students.

Graduate Capabilities

PG - Capable of Professional and Personal Judgment and Initiative

Our postgraduates will demonstrate a high standard of discernment and common sense in their professional and personal judgment. They will have the ability to make informed choices and decisions that reflect both the nature of their professional work and their personal perspectives.

This graduate capability is supported by:

Assessment tasks

- Practical Pt 1
- Practical Pt 1

PG - Discipline Knowledge and Skills

Our postgraduates will be able to demonstrate a significantly enhanced depth and breadth of knowledge, scholarly understanding, and specific subject content knowledge in their chosen fields.

This graduate capability is supported by:

Learning outcomes

- To understand the of the factors affecting reactivity of organic chemicals including biomolecules
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- To have a detailed chemical understanding of stereoselectivity and chirality in organic reaction processes
- To posses high level laboratory skills necessary for research in Organic Biological

Chemistry, including the ability to plan synthetic sequences
- To have the skills necessary for in-depth literature analysis

Assessment tasks

- Practical Pt 1
- Practical Pt 1
- Mid-semester Test
- Spot tests and work-shops
- Final Examination

PG - Critical, Analytical and Integrative Thinking

Our postgraduates will be capable of utilising and reflecting on prior knowledge and experience, of applying higher level critical thinking skills, and of integrating and synthesising learning and knowledge from a range of sources and environments. A characteristic of this form of thinking is the generation of new, professionally oriented knowledge through personal or group-based critique of practice and theory.

This graduate capability is supported by:

Learning outcomes

- To understand the of the factors affecting reactivity of organic chemicals including biomolecules
- To readily identify key bond forming process and building blocks in the synthesis of N-heteroaromatic molecules such as pyrroles, pyridines, pyrazoles, imidazoles, isoazoles and quinolines
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- To have the skills necessary for in-depth literature analysis

Assessment tasks

- Practical Pt 1
- Practical Pt 1
- Mid-semester Test

- Spot tests and work-shops
- Final Examination

PG - Research and Problem Solving Capability

Our postgraduates will be capable of systematic enquiry; able to use research skills to create new knowledge that can be applied to real world issues, or contribute to a field of study or practice to enhance society. They will be capable of creative questioning, problem finding and problem solving.

This graduate capability is supported by:

Learning outcomes

- To understand the of the factors affecting reactivity of organic chemicals including biomolecules
- To readily identify key bond forming process and building blocks in the synthesis of N-heteroaromatic molecules such as pyrroles, pyridines, pyrazoles, imidazoles, isoazoles and quinolines
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Assessment tasks

- Practical Pt 1
- Practical Pt 1
- Mid-semester Test
- Spot tests and work-shops
- Final Examination

PG - Effective Communication

Our postgraduates will be able to communicate effectively and convey their views to different social, cultural, and professional audiences. They will be able to use a variety of technologically supported media to communicate with empathy using a range of written, spoken or visual formats.

This graduate capability is supported by:

Learning outcomes

- To understand the of the factors affecting reactivity of organic chemicals including biomolecules
- To have a detailed understanding of how liganded coupling processes and heterocyclic chemistry can be used in the synthesis of biologically active molecules and materials

Assessment tasks

- Practical Pt 1
- Practical Pt 1
- Mid-semester Test
- Spot tests and work-shops
- Final Examination

PG - Engaged and Responsible, Active and Ethical Citizens

Our postgraduates will be ethically aware and capable of confident transformative action in relation to their professional responsibilities and the wider community. They will have a sense of connectedness with others and country and have a sense of mutual obligation. They will be able to appreciate the impact of their professional roles for social justice and inclusion related to national and global issues

This graduate capability is supported by:

Assessment tasks

- Practical Pt 1
- Practical Pt 1