

CBMS304

Organic and Biological Chemistry B

S2 Day 2018

Dept of Chemistry & Biomolecular Sciences

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General Information

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Lecturer Fei Liu fei.liu@mq.edu.au

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Lecturer Andrew Piggott andrew.piggott@mq.edu.au 4WW 334 Any time, email first

Tutor, Demonstrator Indrek Pernik indrek.pernik@mq.edu.au none

Credit points 3

Prerequisites 6cp in CBMS units at 200 level including CBMS204 or CBMS203

Corequisites

Co-badged status

Unit description

Biological systems carry out a huge range of complex organic reactions to achieve growth, to reproduce and to compete. This unit, together with CBMS303, examines advanced topics in organic chemistry, relevant to biology and biological systems. This unit has an underlying theme of the structure and reactivity of DNA. Specific topics include: metal-mediated coupling (bond-forming) reactions; aromaticity; heterocyclic chemistry; nucleotides, DNA and RNA; and pericyclic reactions. These topics build upon the foundation of CBMS204, using the same text book supplemented by notes given out in lectures and inexpensive Oxford Chemistry Primers on specialised topics. This unit requires good skills in organic chemistry; a background in other aspects of chemistry and/or biochemistry will be advantageous. The laboratory sessions are aimed at developing skills in organic chemistry, using reactions studied in lectures to reinforce principles and exemplify typical reactions.

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

To distinguish between aromatic, antiaromatic and non-aromatic compounds and to understand the chemical consequences of aromaticity

To identify key bond forming process and building blocks in the synthesis of N-

heteroaromatic molecules such as pyrroles and pyridines

To understanding how metal-ligand interaction affects reactivity and determines reactions outcomes, underlying mechanistic aspects impact catalytic reactions,

To have a detailed understanding of how ligand 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 possess basic laboratory skills necessary for research in Organic and Inorganic Biological Chemistry

Assessment Tasks

Name	Weighting	Hurdle	Due
Practical Pt1	9%	No	E1 31/08; E2 14/9
Practical Pt2	16%	No	E3 19/10; E4 9/11
Mid-semester Test	10%	No	Week 7, Lecture time
Spot tests and work-shops	10%	No	Week 5, 9, 13
Final Examination	55%	No	University Exam Period

Practical Pt1

Due: E1 31/08; E2 14/9 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
- To distinguish between aromatic, antiaromatic and non-aromatic compounds and to understand the chemical consequences of aromaticity
- To identify key bond forming process and building blocks in the synthesis of Nheteroaromatic molecules such as pyrroles and pyridines
- To have a detailed understanding of how ligand coupling processes and heterocyclic chemistry can be used in the synthesis of biologically active molecules and materials
- To possess basic laboratory skills necessary for research in Organic and Inorganic Biological Chemistry

Practical Pt2

Due: **E3 19/10; E4 9/11** 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
- To distinguish between aromatic, antiaromatic and non-aromatic compounds and to understand the chemical consequences of aromaticity
- To understanding how metal-ligand interaction affects reactivity and determines reactions outcomes, underlying mechanistic aspects impact catalytic reactions,
- To have a detailed understanding of how ligand 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 possess basic laboratory skills necessary for research in Organic and Inorganic Biological Chemistry

Mid-semester Test

Due: Week 7, Lecture time Weighting: 10%

There will be a 50 minute test in Week 7, 11am-12 noon, which will cover the first two modules of the unit (*i.e.* heterocyclic chemistry, introduction to organometallic 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
- To distinguish between aromatic, antiaromatic and non-aromatic compounds and to understand the chemical consequences of aromaticity
- To identify key bond forming process and building blocks in the synthesis of Nheteroaromatic molecules such as pyrroles and pyridines
- To understanding how metal-ligand interaction affects reactivity and determines reactions outcomes, underlying mechanistic aspects impact catalytic reactions,
- To have a detailed understanding of how ligand coupling processes and heterocyclic chemistry can be used in the synthesis of biologically active molecules and materials
- To have a detailed chemical understanding of stereoselectivity and chirality in organic reaction processes

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:

- To understand the of the factors affecting reactivity of organic chemicals
- To distinguish between aromatic, antiaromatic and non-aromatic compounds and to understand the chemical consequences of aromaticity
- To identify key bond forming process and building blocks in the synthesis of Nheteroaromatic molecules such as pyrroles and pyridines
- To understanding how metal-ligand interaction affects reactivity and determines reactions outcomes, underlying mechanistic aspects impact catalytic reactions,
- To have a detailed understanding of how ligand 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

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
- To distinguish between aromatic, antiaromatic and non-aromatic compounds and to understand the chemical consequences of aromaticity

- To identify key bond forming process and building blocks in the synthesis of Nheteroaromatic molecules such as pyrroles and pyridines
- To understanding how metal-ligand interaction affects reactivity and determines reactions outcomes, underlying mechanistic aspects impact catalytic reactions,
- To have a detailed understanding of how ligand 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

Delivery and Resources

Classes

CBMS304 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 9th Edition (introductory reading only). QD251.2.M43.

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

Miessler, Gary L.; Fischer, Paul J.; Tarr, Donald A.; Inorganic Chemistry, Pearson, 2014. Online access available via the library

Crabtree, Robert H. The Organometallic Chemistry of the Transition Metals, Wiley Interscience, 2005. Online access available via the library

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)

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

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

CBMS304 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 workshops 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 under "Unit Schedule"

Unit Schedule

Lecture Schedule

(Weeks 1-3) AP Lectures

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

Aromaticity and Antiaromaticity

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

Five-membered Heterocycles

- Syntheses
- Reactions
- Incorporation into macrocycles

Six-membered Heterocycles and Bicycles

- Pyridine and quinoline
- Electrophilic and nucleophilic substitution reactions
- DNA bases

(Week 4) KV lectures

This section of the course will provide you with the overview on metal-ligand interactions,

synthesis and reactivity of organometallic complexes.

- Fundamentals of organometallic complexes 18 electron rule, oxidation-state determination, Hard-soft acid base theory, trans effect/ influence
- Synthesis and reactivity of metal-hydride complexes
- Synthesis and reactivity of metal-alkyl, metal aryl, metal-olefin, metal carbene and metal carbyne complexes
- Synthesis and reactivity of metal carbonyl and metal nitrosyl complexes
- Synthesis and reactivity of metal phosphine and metal-N-heterocyclic carbenes complexes

(Week 5) IP lectures

This section of the course will provide you with the overview on mechanistic aspects of specific reactions involved in catalytic cycles

- Oxidative addition, transmetallation, reductive elimination, insertion reactions
- Mechanistic aspects and applications of organometallic complexes in catalysis.

(Weeks 6, 7, 9) 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 cross-coupling reactions from Nature and invented by chemists
- · Key mechanistic aspects of cross-coupling reactions
- Common cross-coupling strategies and reagents
- Chelation control and selectivity models
- Reactions at saturated carbon centres
- Reactions at unsaturated carbon centres
- Examples of applications
- Stereoelectronic principles

(Week 10-13) 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 Br₂ 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 <u>Policy Central (https://staff.m</u> <u>q.edu.au/work/strategy-planning-and-governance/university-policies-and-procedures/policy-centr</u> <u>al</u>). Students should be aware of the following policies in particular with regard to Learning and Teaching:

- Academic Appeals Policy
- Academic Integrity Policy
- Academic Progression Policy
- Assessment Policy
- Fitness to Practice Procedure
- Grade Appeal Policy
- Complaint Management Procedure for Students and Members of the Public
- Special Consideration Policy (Note: The Special Consideration Policy is effective from 4 December 2017 and replaces the Disruption to Studies Policy.)

Undergraduate students seeking more policy resources can visit the <u>Student Policy Gateway</u> (htt ps://students.mq.edu.au/support/study/student-policy-gateway). It is your one-stop-shop for the key policies you need to know about throughout your undergraduate student journey.

If you would like to see all the policies relevant to Learning and Teaching visit Policy Central (http s://staff.mq.edu.au/work/strategy-planning-and-governance/university-policies-and-procedures/p olicy-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/study/getting-started/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 <u>eStudent</u>. For more information visit <u>ask.m</u> <u>q.edu.au</u>.

Student Support

Macquarie University provides a range of support services for students. For details, visit <u>http://stu</u> dents.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 <u>http://www.mq.edu.au/about_us/</u>offices_and_units/information_technology/help/.

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

Graduate Capabilities

Creative and Innovative

Our graduates will also be capable of creative thinking and of creating knowledge. They will be imaginative and open to experience and capable of innovation at work and in the community. We want them to be engaged in applying their critical, creative thinking.

This graduate capability is supported by:

Learning outcomes

- To understand the of the factors affecting reactivity of organic chemicals
- To distinguish between aromatic, antiaromatic and non-aromatic compounds and to understand the chemical consequences of aromaticity
- To identify key bond forming process and building blocks in the synthesis of Nheteroaromatic molecules such as pyrroles and pyridines
- To understanding how metal-ligand interaction affects reactivity and determines reactions outcomes, underlying mechanistic aspects impact catalytic reactions,
- To have a detailed understanding of how ligand 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 possess basic laboratory skills necessary for research in Organic and Inorganic Biological Chemistry

Assessment tasks

- Practical Pt1
- Practical Pt2
- Mid-semester Test
- Spot tests and work-shops
- Final Examination

Capable of Professional and Personal Judgement and Initiative

We want our graduates to have emotional intelligence and sound interpersonal skills and to demonstrate discernment and common sense in their professional and personal judgement. They will exercise initiative as needed. They will be capable of risk assessment, and be able to handle ambiguity and complexity, enabling them to be adaptable in diverse and changing environments.

This graduate capability is supported by:

Assessment tasks

- Practical Pt1
- Practical Pt2
- Spot tests and work-shops

Discipline Specific Knowledge and Skills

Our graduates will take with them the intellectual development, depth and breadth of knowledge, scholarly understanding, and specific subject content in their chosen fields to make them competent and confident in their subject or profession. They will be able to demonstrate, where relevant, professional technical competence and meet professional standards. They will be able to articulate the structure of knowledge of their discipline, be able to adapt discipline-specific knowledge to novel situations, and be able to contribute from their discipline to inter-disciplinary solutions to problems.

This graduate capability is supported by:

Learning outcomes

- To understand the of the factors affecting reactivity of organic chemicals
- To distinguish between aromatic, antiaromatic and non-aromatic compounds and to understand the chemical consequences of aromaticity
- To identify key bond forming process and building blocks in the synthesis of Nheteroaromatic molecules such as pyrroles and pyridines
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Assessment tasks

- Practical Pt1
- Practical Pt2
- Mid-semester Test
- · Spot tests and work-shops

• Final Examination

Critical, Analytical and Integrative Thinking

We want our graduates to be capable of reasoning, questioning and analysing, and to integrate and synthesise learning and knowledge from a range of sources and environments; to be able to critique constraints, assumptions and limitations; to be able to think independently and systemically in relation to scholarly activity, in the workplace, and in the world. We want them to have a level of scientific and information technology literacy.

This graduate capability is supported by:

Learning outcomes

- To understand the of the factors affecting reactivity of organic chemicals
- To distinguish between aromatic, antiaromatic and non-aromatic compounds and to understand the chemical consequences of aromaticity
- To identify key bond forming process and building blocks in the synthesis of Nheteroaromatic molecules such as pyrroles and pyridines
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Assessment tasks

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- Final Examination

Problem Solving and Research Capability

Our graduates should be capable of researching; of analysing, and interpreting and assessing data and information in various forms; of drawing connections across fields of knowledge; and they should be able to relate their knowledge to complex situations at work or in the world, in order to diagnose and solve problems. We want them to have the confidence to take the initiative

in doing so, within an awareness of their own limitations.

This graduate capability is supported by:

Learning outcomes

- To understand the of the factors affecting reactivity of organic chemicals
- To distinguish between aromatic, antiaromatic and non-aromatic compounds and to understand the chemical consequences of aromaticity
- To identify key bond forming process and building blocks in the synthesis of Nheteroaromatic molecules such as pyrroles and pyridines
- To understanding how metal-ligand interaction affects reactivity and determines reactions outcomes, underlying mechanistic aspects impact catalytic reactions,
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- To possess basic laboratory skills necessary for research in Organic and Inorganic Biological Chemistry

Assessment tasks

- Practical Pt1
- Practical Pt2
- Mid-semester Test
- Spot tests and work-shops
- Final Examination

Effective Communication

We want to develop in our students the ability to communicate and convey their views in forms effective with different audiences. We want our graduates to take with them the capability to read, listen, question, gather and evaluate information resources in a variety of formats, assess, write clearly, speak effectively, and to use visual communication and communication technologies as appropriate.

This graduate capability is supported by:

Learning outcomes

- To understand the of the factors affecting reactivity of organic chemicals
- To distinguish between aromatic, antiaromatic and non-aromatic compounds and to

understand the chemical consequences of aromaticity

 To identify key bond forming process and building blocks in the synthesis of Nheteroaromatic molecules such as pyrroles and pyridines

Assessment tasks

- Practical Pt1
- Practical Pt2
- Mid-semester Test
- Final Examination

Socially and Environmentally Active and Responsible

We want our graduates to be aware of and have respect for self and others; to be able to work with others as a leader and a team player; to have a sense of connectedness with others and country; and to have a sense of mutual obligation. Our graduates should be informed and active participants in moving society towards sustainability.

This graduate capability is supported by:

Learning outcome

 To possess basic laboratory skills necessary for research in Organic and Inorganic Biological Chemistry

Changes from Previous Offering

Dr Andrew Piggott will replace A/Prof. Andrew Try teaching the aromaticity and heterocyclic synthesis section of the unit. Dr Indrek Pernik will provide an introduction to mechanistic aspects of specific reactions involved in catalytic cycles. A/Prof. Koushik Venkatesan will provide an overview of metal-ligand interactions, synthesis and reactivity of organometallic complexes.