Annexe A: New/Revised Course Content in OBTL+ Format

Course Overview

Expected Implementation in Academic Year	~~AY2022-2023~~ AY2026-2027
Semester/Trimester/Others (specify approx. Start/End date)	Semester 1
Course Author * Faculty proposing/revising the course	Zhong Hongyu, Robin Chi
Course Author Email	hongyu.zhong@ntu.edu.sg; robinchi@ntu.edu.sg
Course Title	STRUCTURAL DETERMINATION
Course Code	CM4012
Academic Units	3
Contact Hours	43
Research Experience Components	Not Applicable

Course Requisites (if applicable)

Pre-requisites	CM3011 and CM3021 or by permission
Co-requisites	
Pre-requisite to	
Mutually exclusive to	CM412S
Replacement course to	
Remarks (if any)	

Course Aims

This course is divided into two parts.

Part I: The aim of this part concerns the use of NMR chemical shifts to elucidate structures of organic molecules. The specific focus is to learn how different (common) functional groups and non-covalent interactions (in organic chemistry) affect the 1H and 13C NMR chemical shifts of molecules.

Part II: This part of the course introduces a few other topics in NMR: aspects of stereochemistry in NMR spectroscopy, vicinal coupling; long-range coupling; virtual coupling; second-order effect; nomenclature and common types of NMR spin systems; other NMR-active nuclei; isotope labeling; two-dimensional NMR experiments; dynamic NMR; the use of NMR for studying organometallic complexes in transition metal catalysis.

Course's Intended Learning Outcomes (ILOs)

Upon the successful completion of this course, you (student) would be able to:

ILO 1	Explain the simplified physics basis of NMR, including nuclear spin states, magnetic field, induced filed, and origin of different chemical shifts for protons present in organic molecules.
ILO 2	List the effects of functional groups on 1H NMR Chemical Shifts, including: (a) how do these functional groups/atoms affect the NMR chemical shifts; what are the other factors that can affect the NMR chemical shifts; and (c) what are the structural information we can get from the NMR chemical shifts. The student should develop understanding on the following specific topics: Electronegativity of neighboring atoms and groups, Magnetic anisotropy, and Electrostatic Interactions
ILO 3	Explain structural equivalence in NMR chemical shift assignments. The students are supposed to figure out how many different sets of proton or carbon chemical shifts can be expected from a molecule. Specific topics include "symmetry of molecules and structure equivalence" and "Chemical Equivalence by Interconversion"
ILO 4	Explain 13C NMR of sp3 carbons, including α-Substituent and Other Effects, β-Substituent Effects, γ-Substituent Effects and other special systems.
ILO 5	Explain 13C NMR of sp2 and sp carbons, including α-Substituent and Other Effects, Effects from other neighboring groups and charges.
ILO 6	Preliminarily integrate the use of NMR for structure determination for modern research especially in the area of synthetic chemistry
ILO 7	Integrate knowledge learned in this course and previous courses to proposed reasonable structures for relatively simple organic molecules, and the ability predict NMR chemical shifts for common functional groups in sophisticated molecules.
ILO 8	Explain influence of stereochemistry on NMR signals. Identify diastereotopic protons; Understand relation between dihedral angle and vicinal coupling constants; Coupling constants of olefinic protons and alkene stereochemistry.
ILO 9	Explain long-range coupling; virtual coupling; second-order coupling; roofing in NMR signals. Understand the nomenclature and common types of NMR spin systems.
ILO 10	Understand the nuclear spin quantum number for atomic nucleus and natural abundance of nuclear isotopes. Understand NMR spectroscopy for other I = 1/2 nuclei, including 31P, 19F and 15N; Understand NMR spectroscopy for quadrupolar nuclei (I > 1/2), including 2H, 11B. Explain the use of isotope labeling in NMR studies.
ILO 11	Understand the use of two-dimensional NMR experiments including COSY, HSQC and HMBC in structural assignments. Understand the use of other NMR techniques including DOSY (Diffusion Ordered Spectroscopy), EXSY (EXchange SpectroscopY), the Nuclear Overhauser effect and NOESY in determining structural and molecular properties.
ILO 12	Explain the use of NMR spectroscopy in studying dynamic molecular processes. Coalescence and variable temperature NMR. Spectral line width analysis and Eyring analysis.

ILO 13	Understand the use of NMR spectroscopy in studying organometallic complexes of transition metals, including NMR mechanistic experiments for asymmetric hydrogenation and hydroformylation using chiral bisphosphine-rhodium catalysts.

Course Content

Part I
- Introduction to NMR (a brief review)
- The effects of functional groups on 1H NMR Chemical Shifts
- Structure equivalence
- A brief overview of 13C NMR
- 13C NMR of sp3 carbons
- 13C NMR of sp2 and sp carbons

Part II

- Stereochemical aspects in NMR

- NMR couplings

- Other NMR-active nuclei

- Two-dimensional NMR

- Dynamic NMR

- NMR in organometallic chemistry

Reading and References (if applicable)

Books

Title: Modern NMR Techniques for Chemistry Research

Authors: Andrew E Derome

Publisher: Pergamon

Call no.: QD96.N8D437

Title: 200 and More NMR Experiments – A Practical Course

Authors: Stefan Berger and Siermar Braun

Publisher: Wiley

Call no.: QD96.N8B496

Title: NMR Spectroscopy in Inorganic Chemistry

Author: Jonathan A. Iggo

Publisher: OUP

Call no.: QD96.N8I24

Websites

Hans Reich collection

https://www.chem.wisc.edu/areas/reich/nmr/

Planned Schedule

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
1	Stereochemical aspects in NMR	8	In-person	In-person lecture	
2	NMR couplings	9	In-person	In-person lecture	
3	Other NMR-active nuclei	10	In-person	In-person lecture	
4	Two-dimensional NMR	11	In-person	In-person lecture	
5	Dynamic NMR	12	In-person	In-person lecture	
6	NMR in organometallic chemistry	13	In-person	In-person lecture	
7	Introduction to NMR (a brief review), The effects of functional groups on 1H NMR Chemical Shifts: Electronegativity of neighboring atoms and groups	1-2,6-7	In-person	In-person lecture	
8	The effects of functional groups on 1H NMR Chemical Shifts: Magnetic anisotropy	1-2, 6-7	In-person	In-person lecture	
9	The effects of functional groups on 1H NMR Chemical Shifts: Electrostatic Interactions	1-2, 6-7	In-person	In-person lecture	

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
10	Structure equivalence: 3.1: Symmetry of molecules and structure equivalence , 3.2: Chemical Equivalence by Interconversion, A brief overview of 13C NMR	3-7	In-person	In-person lecture	
11	13C NMR of sp3 carbons: 5.1:α-Substituent and Other Effects, 5.2:β-Substituent Effects, 5.3:γ-Substituent Effects and other special systems	4, 6-7	In-person	In-person lecture	
12	13C NMR of sp2 and sp carbons: 6.1: α-Substituent and Other Effects, 6.2: Effects from other neighboring groups and charges	5, 6-7	In-person	In-person lecture	
13	Special Topics in NMR, summary, practice questions, and preparation for mid-term.	1-7	In-person	In-person lecture	

Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?
In-person lectures	In-person lectures with in-class participation component facilitates the class engagement. Lecture materials including lecture slides, problem sets and practice questions, reading materials and quizzes will help with the understanding and application of the knowledge learnt.

Assessment Structure

Assessment Components (includes both continuous and summative assessment)

No.	Component	ILO	Related PLO or Accreditation	Weightage	Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
1	Continuous Assessment (CA): Test/Quiz(Quiz 1)	ILO1-2	Competence, Communication	15		Individual	Holistic	Not Applicable
2	Continuous Assessment (CA): Test/Quiz(Quiz 2)	ILO1-3	Competence, Creativity	15		Individual	Holistic	Not Applicable
3	Continuous Assessment (CA): Test/Quiz(Mid-term Test I)	ILO1-7	Competence, Creativity,	20		Individual	Analytic	Not Applicable
4	Continuous Assessment (CA): Test/Quiz(Mid-term Test II)	ILO 8-10	Competence, Creativity	20		Individual	Analytic	Not Applicable
5	Continuous Assessment (CA): Test/Quiz(Mid-term Test III)	ILO 11-13	Competence, creativity	20		Individual	Analytic	Not Applicable
6	Continuous Assessment (CA): Class Participation()	ILO 8-13	Competence, creativity, communication	10		Individual	Analytic	Not Applicable

Description of Assessment Components (if applicable)

Formative Feedback
8

Part I

Frequent and flexible office hours will be made available for face-to-face discussions on concepts and problems that are challenging to you. For students with excellent performance and the willing to receive deeper trainings, additional study materials will be made available upon request.

Part II

In-class practice problems and quizzes will be used to provide formative assessment on the knowledge learnt and engage class participations. Midterm 1, 2 and 3 will provide more holistic and formal feedback on the understanding and application of lecture concepts.

NTU Graduate Attributes/Competency Mapping

This course intends to develop the following graduate attributes and competencies (maximum 5 most relevant)

Attributes/Competency	Level
Collaboration	Intermediate
Learning Agility	Advanced
Critical Thinking	Advanced

Course Policy

Policy (Academic Integrity)

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values. As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. On the use of technological tools (such as Generative AI tools), different courses / assignments have different intended learning outcomes. Students should refer to the specific assignment instructions on their use and requirements and/or consult your instructors on how you can use these tools to help your learning. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Policy (General)

You are expected to complete all assigned pre-class readings and activities, attend all seminar classes punctually and take all scheduled assignments and tests by due dates. You are expected to take responsibility to follow up with course notes, assignments and course related announcements for seminar sessions they have missed. You are expected to participate in all seminar discussions and activities.

Policy (Absenteeism)

Absence from class without a valid reason will affect your overall course grade. Valid reasons include falling sick supported by a medical certificate and participation in NTU's approved activities supported by an excuse letter from the relevant bodies.

If you miss a lesson, you must inform the course instructor via email prior to the start of the class.

Policy (Others, if applicable)

Diversity and Inclusion policy

Integrating a diverse set of experiences is important for a more comprehensive understanding o science and engineering.

It is our goal to create an inclusive and collaborative learning environment that supports a diversity of perspectives and learning experiences. That honours your identities; including ethnicity, gender, socioeconomic status, sexual orientation, religion or ability.

To help accomplish this:
•   If you are neuroatypical or neurodiverse, have dyslexia or ADHD (for example), or have a social anxiety disorder or social phobia:
•   If you feel your performance in the course is being impacted by your experiences outside of class:
•   If something was said in the course (by anyone, including instructor/supervisor) that made you

uncomfortable.

Please e-mail to your Associate Chair (Undergraduate) at AC-CCEB-UG@ntu.edu.sg about how we can help facilitate your learning experience.

As a participant in course discussions you should also strive to honour the diversity of your classmates. You can do this by; using preferred pronouns and names; being respectful of others opinions and actively making sure all voices are being heard; and refraining from the use of derogatory or demeaning speech or actions.

All members of the course are expected to strictly adhere to the student code of conduct (https://www.ntu.edu.sg/life-at-ntu/student-life/student-conduct) . If you witness something that goes against this or have ny other concerns, please speak to your instructors or a faculty member.

Last Updated Date: 12-03-2026 09:38:08

Last Updated By: Natasha Bhatia (Dr)