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

Course Overview

Expected Implementation in Academic Year	AY2025-2026
Semester/Trimester/Others (specify approx. Start/End date)	Semester 1 Semester 2
Course Author * Faculty proposing/revising the course	Soo Han Sen, Tan Choon Hong
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Course Title	CHEMICAL SPECTROSCOPY & APPLICATIONS
Course Code	CM3011
Academic Units	3
Contact Hours	39
Research Experience Components	Not Applicable

Course Requisites (if applicable)

Pre-requisites	(CM2021 and CM2031) or by permission
Co-requisites	
Pre-requisite to	
Mutually exclusive to	
Replacement course to	
Remarks (if any)	

Course Aims

This course aims to introduce the principles and applications of chemical spectroscopic methods, including mass spectrometry (MS), nuclear magnetic resonance (NMR) spectroscopy, infrared (IR) spectroscopy, Raman spectroscopy, UV-visible-NIR spectroscopy, photoluminescence spectroscopy, X-ray photoelectron spectroscopy, and X-ray absorption spectroscopy as invaluable tools for the structural identification and determination of organic and inorganic compounds as well as for the study of their electronic properties, stabilities and dynamic behaviors at the molecular level. You will learn about the basic principles and techniques of these spectroscopic methods and their applications in the context of organic and inorganic chemistry. Specifically, you will develop the ability to interpret spectra for given molecules, relate their spectral behavior to chemical phenomena/concepts, and to deduce the molecular structure of unknown from given spectra.

Course's Intended Learning Outcomes (ILOs)

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

ILO 1	1. Explain the basic principle of mass spectrometry (MS) and discuss advantage and disadvantage of different ionization methods.
ILO 2	2. Analyze EI-MS spectra of organic molecules. Specifically, extract information on molecular mass, structural fragment, and constituent elements through spectral analysis.
ILO 3	3. Explain the basic principle of nuclear magnetic resonance (NMR) spectroscopy and representative nuclei studied by this method.
ILO 4	4. Analyze 1H NMR spectra of organic molecules. Specifically, extract information on electronic nature of proton, number of each type of protons, and atom connectivity through spectral analysis.
ILO 5	5. Analyze 13C NMR spectra of organic molecules. Specifically, extract information on electronic nature of 13C nucleus, number of each type of 13C nuclei, and multiplicity through spectral analysis.
ILO 6	6. Explain the basic principles of infrared (IR) spectroscopy and characteristic functional groups studied by this method.
ILO 7	7. Analyze IR spectra of organic molecules. Specifically, identify the presence (and absence) of characteristic functional groups in the molecule through spectral analysis.
ILO 8	8. Deduce the molecular structure of unknown compound from given spectra and other relevant information, by combining the skills 2, 4, 5, and/or 7.
ILO 9	9. Identify the symmetry elements and symmetry operations on molecules.
ILO 10	10. Use group theory to work out the point groups of molecules and generate the irreducible representations of normal vibrational modes.
ILO 11	11. Employ group theory to predict the expected number and symmetry of IR- and Raman-active vibrational modes.
ILO 12	12. Use basic quantum mechanics to explain the selection rules of electronic transitions.
ILO 13	13. Draw and interpret Jablonski diagrams.
ILO 14	14. Apply the Tanabe-Sugano diagrams to predict the expected number of UV-vis-NIR absorption bands for octahedral complexes.
ILO 15	15. Use the Beer-Lambert law to predict intensities of UV-vis-NIR absorption bands.
ILO 16	16. Explain the nature of fluorescence and phosphorescence
ILO 17	17. Identify the common forms of electronic transitions.

ILO 18	18. Apply UV-vis-NIR spectroscopy for diagnostic characterisation.
ILO 19	19. Employ UV-vis-NIR spectroscopy in catalysis and kinetics.
ILO 20	20. Use photoluminescence spectroscopy to detect intermediates.
ILO 21	21. Explain the basic principles behind X-ray photoelectron spectroscopy (XPS).
ILO 22	22. Use XPS to determine elemental compositions.
ILO 23	23. Determine oxidation states and quantitate chemical speciation with XPS.
ILO 24	24. Apply XPS for surface and molecular studies.
ILO 25	25. Explain the basic principles behind X-ray absorption spectroscopy (XAS).
ILO 26	26. Use group theory and selection rules to explain the origins behind XAS peaks.
ILO 27	27. Employ XAS for structural studies of compounds and materials that cannot be crystallised.
ILO 28	28. Use XAS to estimate the relative oxidation states of elements in the samples.

Course Content

Basic principles and instrumentation of mass spectrometry (MS).

Analysis of EI-MS spectra of organic compounds through examination of fragmentation reactions and effect of isotopes.

Basic principles and instrumentation of nuclear magnetic resonance (NMR) spectroscopy.

Analysis of proton (1H) NMR of organic compounds through examination of chemical shift, integration, and spin-spin coupling.

Analysis of carbon (13C) NMR of organic compounds through examination of chemical shift, peak counts, and multiplicity.

Basic principles and instrumentation of infrared (IR) spectroscopy.

Analysis of IR spectra of organic compounds through examination of absorption bands of characteristic functional groups.

Structural determination of unknown organic compounds through analysis of MS, 1H/13C NMR, and IR spectra.

Symmetry elements, symmetry operations, and chemical applications of group theory.

Assignments of molecular point groups.

Parts of character tables and its uses for vibrational spectroscopy.

Selection rules and normal mode analyses of Raman-active vibrational modes.

Functional group analyses by vibrational spectroscopy.

Specialised Raman experiments including resonance Raman, Raman microscopy, and surface-enhanced Raman scattering.

Spin and orbital selection rules of UV-vis-NIR spectroscopy.

Jablonski diagrams and photochemistry.

Beer-Lambert law.

Luminescence, fluorescence, and phosphorescence.

Tanabe-Sugano diagrams for d-d transitions.

Applications based on insights from UV-vis-NIR spectroscopy.

Device and biological applications based on photoluminescence spectroscopy.

Principles of photoelectric effect.

Chemical composition by survey spectra.

Determination of relative oxidation states.

Quantitative characterisation of chemical species.

XPS for surface studies.

Selection rules and basic principles of X-ray absorption spectroscopy (XAS).

Applications of XAS for determining the oxidation states and molecular structure within materials and reactive intermediates that cannot be crystallised.

Reading and References (if applicable)

Recommended textbook:

Introduction to Spectroscopy, 5th Ed. (2015), by D. L. Pavia, G. M. Lampman, G. S. Kriz, J. A. Vyvyan, Cengage Learnings; ISBN-13: 978-1-285-46012-3 (paperback);

A Microscale Approach to Organic Laboratory Techniques, 6th Ed. (2018), by D. L. Pavia, G. S. Kriz, G. M. Lampman, R. G. Engel, Cengage Learnings; ISBN: 978-1-305-96834-9 (hardcover);

Inorganic Chemistry (1989), I. S. Butler, J. F. Harrod; ISBN 0-8053-0247-6.

Alan Vincent "Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications" 2013, 2nd edition (available in electronic version from the NTU library), John Wiley & Sons; ISBN: 978-1-118-72338-8.

Daniel C. Harris and Michael D. Bertolucci "Symmetry and Spectroscopy" 1978, Dover Publications; ISBN13: 9780486661445.

F. Albert Cotton "Chemical Applications of Group Theory" 1990, 3rd edition, John Wiley & Sons; ISBN: 978-0-471-51094-9.

Gary L. Miessler, Paul J. Fischer, and Donald A. Tarr "Inorganic Chemistry" 2013, 5th edition (available in reserve from the NTU library), Pearson Education Inc; ISBN-13: 978-1292020754.

Selected current research articles, such as *Organometallics* 2015, 34, 2, 399-407.

The internet.

Planned Schedule

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
1	Mass spectrometry: Basic theory and instrumentation, effect of isotopes, fundamental fragmentation reactions in EI-MS.	1, 2	Lectures		
2	Mass spectrometry: EI-MS spectra of different types of organic compounds. 1H NMR: Basic theory and instrumentation, chemical shift	2-4, 8	Lectures		
3	1H NMR spectroscopy: Chemical equivalence and integration, spin-spin coupling	4, 8	Lecture		
4	1H NMR spectroscopy: Spin-spin coupling (cont'd) 13C NMR spectroscopy: Chemical shift, signal count, multiplicity	4, 5, 8	Lecture		

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
5	1H/13C NMR spectroscopy: Variable-temperature and two-dimensional techniques IR spectroscopy: Basic theory and instrumentation, absorption of typical functional groups.	4–8	Lecture		
6	IR spectroscopy: Absorption of typical functional groups (cont'd). Midterm test 1	7, 8	Lecture, assessment		
7	Review and exercises	1-8	Lecture		
8	Symmetry elements, symmetry operations, chemical applications of group theory, and assignments of molecular point groups	9	Lecture, Harris & Bertolucci; Chapter 1-1 – 1-5; Miessler, Fischer, & Tarr Chapter 4.1, 4.2; Vincent; Programmes 1 and 2		
9	Parts of character tables and its uses for vibrational spectroscopy	10	Lecture. Open-book, open-notes Quiz 1 on NTULearn. Harris & Bertolucci; Chapter 1-7, 1-8, 3-5, 3-7, 3-8, 4-3; Miessler, Fischer, & Tarr Chapter 4.3, 4.4; Vincent; Programmes 3, 5, and 7		

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
10	Selection rules, normal mode analyses of Raman-active vibrational modes, functional group analyses by vibrational spectroscopy, and specialised Raman experiments including resonance Raman, Raman microscopy, and surface-enhanced Raman scattering	11	Lecture. Open-book, open-notes Quiz 2 on NTULearn. Harris & Bertolucci; Chapter 3-1, 3-2, 3-6 – 3-11, 4-3; Cotton Chapter 10; Vincent; Programme 7		
11	Spin and orbital selection rules of UV-vis-NIR spectroscopy, Jablonski diagrams and photochemistry, Beer-Lambert law, luminescence, fluorescence, and phosphorescence, Tanabe-Sugano diagrams for d-d transitions, applications based on insights from UV-vis-NIR spectroscopy, and device and biological applications based on photoluminescence spectroscopy	12-20	Lecture, Harris & Bertolucci; Chapter 5-4, 5-6, 5-7, 5-9; Cotton Chapter 9.4 – 9.6		

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
12	Principles of photoelectric effect, chemical composition by survey spectra, determination of relative oxidation states, quantitative characterisation of chemical species, and XPS for surface studies	21-24	Lecture, Open-book, open notes Midterm 2		
13	Selection rules and basic principles of X-ray absorption spectroscopy (XAS); applications of XAS for determining the oxidation states and molecular structure within materials and reactive intermediates that cannot be crystallised	25-28	Lectures		

Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?
Lectures (in class or online) with incomplete notes and hand-written examples	This encourages students to remain engaged by taking notes and working on problems at the pace they should try to achieve. This gives them practice and a better idea about how long it takes to draw chemical structures and answer questions. They are also less likely to sit back, relax, and watch a performance while understanding nothing.
Video clips of (potentially dangerous) experiments relevant to the class or applications of the chemistry	Helps to break the monotony and keep them engaged. Some of the experiments are visually more impactful so they can understand the chemistry without being exposed to potential hazards. The applications also expose them to the practical aspects of the chemistry that they learn, and hopefully will help students become more aware of chemistry in their daily lives
In-lecture tutorials (where possible, subject to prevailing regulations)	To provide students a familiar, stress-free environment to acquire confidence in public speaking and presentations. Chemistry students do not have sufficient opportunities at publics speaking and need to build up confidence for their future careers
Open-book, open notes assessments	Helps them to think and explain concepts critically. The questions are designed so that they apply concepts instead of just regurgitating information. Information is freely available online nowadays. But our students need to be able to critically analyse information and explain things in their own words instead of reproducing information
Online quizzes	Partly the same as above. In addition, online quizzes give students the flexibility to take the assessment under a stress-free environment at a convenient time that they choose
Clickers	Clickers provide me with instant feedback about the level of understanding. I can gauge whether the concept is easy or difficult and adjust my pace. It also gives students the opportunity to compare themselves with their peers anonymously. I hope that weaker students can recognise their lack of understanding and approach me separately for consultation.
Problem set	The students are encouraged to work in teams to arrive at answers for the problem sets. In addition, some of the questions require students to look for chemistry in their daily lives.

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(Midterm 1)	1-14	Competence, Creativity	20		Individual	Analytic	Relational
2	Continuous Assessment (CA): Test/Quiz(Midterm 2)	23-26	Competence (a-c), creativity (a,b), communication (a), character (a,b), and civic-mindedness (a-c)	15		Individual	Analytic	Relational
3	Continuous Assessment (CA): Test/Quiz(Quizzes)	1-22	Competence (a-c), creativity (a,b), character (a,b), and civic-mindedness (a-c)	5		Individual	Analytic	Multistructural
4	Continuous Assessment (CA): Others(Problem Set (Encouraged to work in groups))	1-6	Competence (a-c), creativity (a,b), character (a,b), and civic-mindedness (a-c)	5		Individual	Analytic	Multistructural
5	Continuous Assessment (CA): Assignment()	23-26	Competence a-c), creativity (a,b), communication (a,b), character (a,b), and civic-mindedness (a-c)	15		Individual	Analytic	Multistructural

No.	Component	ILO	Related PLO or Accreditation	Weightage	Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
6	Continuous Assessment (CA): Class Participation()	1-28	Competence (a-c), creativity (a,b), character (a,b), and civic-mindedness (a-c)	5		Individual	Analytic	Multistructural
7	Summative Assessment (EXAM): Final exam()	1-28	Competence (a-c), creativity (a,b), communication (a), character (a,b), and civic-mindedness (a-c)	35		Individual	Analytic	Extended Abstract

Description of Assessment Components (if applicable)

Formative Feedback

You will be given feedback in six ways:

1. By working through examples provided during lectures
2. By participating in the live polling questions during lectures
3. By response to postings on the course discussion board
4. By attending consultation hours
5. By studying the comments provided by the instructor after the grading of the midterms, quizzes, and problem set
6. By reviewing the answer key of all the graded assessments

NTU Graduate Attributes/Competency Mapping

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

Attributes/Competency	Level
Adaptability	Advanced
Care for Environment	Intermediate
Collaboration	Basic
Communication	Basic
Information Literacy	Basic

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 read the lecture materials prior to the lecture session in question. This will help you to learn much more efficiently as you will already have an impression on the topics to be covered. You should also read the textbook and to attempt the exercises provided in the problem sets. You should take all the scheduled assignments and tests by the due dates. You are expected to take responsibility to follow up with course notes, assignments, and course related announcements for lectures that they have missed.

Policy (Absenteeism)

All the lectures are video-recorded. Attendance of classes is strongly encouraged, when safe, to participate in TurningPoint Cloud and in-class practice. When you miss a lecture, you are expected to make up for the lost learning activities yourself. If you miss any mid-term tests due to valid reasons, the overall grading will be based on other test that you have attended or the final exam score.

Policy (Others, if applicable)

Diversity and Inclusion Policy
Integrating a diverse set of experiences is important for a more comprehensive understanding of 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 (Students & Continuing Education) at ac-cceb-stud@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 any other concerns, please speak to your instructors or a faculty member.

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