Nanyang Technological University
Division of Chemistry and Biological Chemistry

Academic Year	AY2021/2022	**Semester**	1 and 2
Course Coordinator	Ken Lee, Soo Han Sen		
Course Code	CM3011		
Course Title	Chemical Spectroscopy and Applications		
Pre-requisites	CM2021 and CM2031 or by permission		
No of AUs	3		
Contact Hours	Lectures: 39 hours (3 hours per week)		
Proposal Date	22 June 2021		

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.

Intended Learning Outcomes (ILO)

Upon successful completion of this course, you should be able to:

1. Explain the basic principle of mass spectrometry (MS) and discuss advantage and disadvantage of different ionization methods.
2. Analyze EI-MS spectra of organic molecules. Specifically, extract information on molecular mass, structural fragment, and constituent elements through spectral analysis.
3. Explain the basic principle of nuclear magnetic resonance (NMR) spectroscopy and representative nuclei studied by this method.
4. Analyze ^{1}H 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.
5. Analyze ^{13}C NMR spectra of organic molecules. Specifically, extract information on electronic nature of ^{13}C nucleus, number of each type of ^{13}C nuclei, and multiplicity through spectral analysis.
6. Explain the basic principles of infrared (IR) spectroscopy and characteristic functional groups studied by this method.
7. Analyze IR spectra of organic molecules. Specifically, identify the presence (and absence) of characteristic functional groups in the molecule through spectral analysis.
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.
9. Identify the symmetry elements and symmetry operations on molecules.
10. Use group theory to work out the point groups of molecules and generate the irreducible

representations of normal vibrational modes.

11. Employ group theory to predict the expected number and symmetry of IR- and Raman-active vibrational modes.
12. Use basic quantum mechanics to explain the selection rules of electronic transitions.
13. Draw and interpret Jablonski diagrams.
14. Apply the Tanabe-Sugano diagrams to predict the expected number of UV-vis-NIR absorption bands for octahedral complexes.
15. Use the Beer-Lambert law to predict intensities of UV-vis-NIR absorption bands.
16. Explain the nature of fluorescence and phosphorescence.
17. Identify the common forms of electronic transitions.
18. Apply UV-vis-NIR spectroscopy for diagnostic characterisation.
19. Employ UV-vis-NIR spectroscopy in catalysis and kinetics.
20. Use photoluminescence spectroscopy to detect intermediates.
21. Explain the basic principles behind X-ray photoelectron spectroscopy (XPS).
22. Use XPS to determine elemental compositions.
23. Determine oxidation states and quantitate chemical speciation with XPS.
24. Apply XPS for surface and molecular studies.
25. Explain the basic principles behind X-ray absorption spectroscopy (XAS).
26. Use group theory and selection rules to explain the origins behind XAS peaks.
27. Employ XAS for structural studies of compounds and materials that cannot be crystallised.
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 (^{1}H) NMR of organic compounds through examination of chemical shift, integration, and spin-spin coupling.

Analysis of carbon (^{13}C) 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, $^{1}H/^{13}C$ 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.

Assessment (includes both continuous and summative assessment)

Component	Course ILO Tested	Related Programme LO or Graduate Attributes	Weighting	Team/ Individual	Assessment rubrics
1. Midterm Test 1	1-5, 8	Competence, Creativity	20%	Individual	Point-based marking (not rubrics based)

2. Midterm Test 2	9-20	Competence (a-c), creativity (a,b), communication (a), character (a,b), and civic-mindedness (a-c)	20%	Individual	Point-based marking (not rubrics based)
3. Assignment	1-8	Competence, Creativity	10%	Individual	Point-based marking (not rubrics based)
4. Quizzes	9-28	Competence (a-c), creativity (a,b), character (a,b), and civic-mindedness (a-c)	5%	Individual	Point-based marking (not rubrics based)
5. Problem Set (Encouraged to work in groups)	8-12	Competence a-c), creativity (a,b), communication (a,b), character (a,b), and civic-mindedness (a-c)	5%	Individual	Point-based marking (not rubrics based)
6. Final Examination	1-28	Competence (a-c), creativity (a,b), communication (a), character (a,b), and civic-mindedness (a-c)	40%	Individual	Point-based marking (not rubrics based)
Total			100%		

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

Learning and Teaching approach

Approach	How does this approach support students 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.

Reading and References

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, 6^{th} 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, 5^{th} 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.

Course Policies and Student Responsibilities

(1) 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.

(2) 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.

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. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Course Instructors

Instructor	Office Location	Phone	Email
Ken Lee	SPMS-CBC-04-02	6513-2178	ken.lee@ntu.edu.sg
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Planned Weekly Schedule

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

CBC Programme Learning Outcome

The Division of Chemistry and Biological Chemistry (CBC) offers an undergraduate degree major in Chemistry that satisfies the American Chemical Society (ACS) curricular guidelines and equips students with knowledge relevant to the industry. Graduates of the Division of Chemistry and Biological Chemistry should have the following key attributes:

1. Competence
Graduates should be well-versed in the foundational and advanced concepts of chemical science, be able to evaluate chemistry-related information critically and independently, and be able to use complex reasoning to solve emergent chemical problems.

2. Creativity
Graduates should be able to synthesize and integrate multiple ideas across the curriculum, and propose innovative solutions to emergent chemistry-related problems based on their training in chemistry.

3. Communication
Graduates should be able to demonstrate clarity of thought, independent thinking, and sound scientific analysis and reasoning through written and oral reports to audiences with varying technical backgrounds. They should also be able to effectively engage other professional chemists in collaborative endeavours.

4. Character
Graduates should be able to act in responsible ways and uphold the high ethical standards that the society expects of professional chemists.

5. Civic-mindedness
Graduates should be aware of the impact of chemistry on society, and how chemistry can be applied to benefit mankind. They should also be aware of and uphold the best chemical safety practices.