<table>
<thead>
<tr>
<th>Academic Year</th>
<th>AY20/21</th>
<th>Semester</th>
<th>1</th>
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</thead>
<tbody>
<tr>
<td>Course Coordinator</td>
<td>Naohiko Yoshikai, Leung Pak Hing</td>
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<tr>
<td>Course Code</td>
<td>CM3011</td>
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<tr>
<td>Course Title</td>
<td>Chemical Spectroscopy and Applications</td>
<td></td>
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<tr>
<td>Pre-requisites</td>
<td>CM2021 and CM2031 or by permission</td>
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<tr>
<td>No of AUs</td>
<td>3</td>
<td></td>
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<tr>
<td>Contact Hours</td>
<td>Lectures: 39 hours (3 hours per week)</td>
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**Course Aims**

This course aims to introduce the principles and applications of chemical spectroscopic methods, including mass spectrometry (MS), nuclear magnetic resonance (NMR) spectroscopy, and infrared (IR) 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. Correlate the nuclei property of different atoms within the periodic table and select the practically useful nuclei to discover the chemistry of d-block organometallic and inorganic compounds by multi-nuclei NMR spectroscopy.
10. Relate the NMR and magnetic phenomena with different structural features and various oxidation states of the metal complexes with the same central metal ion.
11. Interpret the efficiency and limitations of various nuclei in providing structural information of metal complexes.
12. Differentiate the NMR adsorption and relaxation processes and their employment in coordination chemistry, with emphasis on hydrido and molecular hydrogen complexes.

13. Manipulate the temperature effects on the evaluation of the kinetic and dynamic behavior of metal-ligand bonds by multi-nuclei NMR spectroscopy.


15. Deduce the chelate effects in coordination and organometallic compounds via NMR chemical shifts and coupling constants.

16. Develop mechanistic concepts via NMR spectroscopy in metal complex catalyzed transformations.

17. Correlate the bioinorganic chemistry of f-block metal complexes, particularly as MRI enhancing agents.

**Course Content**

Basic principles and instrumentation of mass spectrometry (MS).

Analysis of El-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.

Selection criteria for appropriate nuclei for investigation of inorganic and organometallic compounds.

Differentiation of thermodynamic and kinetic stabilities of metal-ligand bonds in solution.

Determination of reactivity of coordination and organometallic compounds in solutions.

Designing new metal complexes as catalysts for chemical transformations.

Critique essential steric and electronic factors of metal-ligand bonds in bioinorganic and synthetic chemistry.
### Assessment (includes both continuous and summative assessment)

<table>
<thead>
<tr>
<th>Component</th>
<th>Course ILO Tested</th>
<th>Related Programme LO or Graduate Attributes</th>
<th>Weighting</th>
<th>Team/ Individual</th>
<th>Assessment rubrics</th>
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<tbody>
<tr>
<td>1. Midterm Test 1</td>
<td>1-5, 8</td>
<td>Competence, Creativity</td>
<td>20%</td>
<td>Individual</td>
<td>Point-based marking (not rubrics based)</td>
</tr>
<tr>
<td>2. Midterm Test 2</td>
<td>9-14</td>
<td>Competence, Creativity</td>
<td>20%</td>
<td>Individual</td>
<td>Point-based marking (not rubrics based)</td>
</tr>
<tr>
<td>3. Examination</td>
<td>1-17</td>
<td>Competence, Creativity</td>
<td>60%</td>
<td>Individual</td>
<td>Point-based marking (not rubrics based)</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td>100%</td>
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### Formative feedback

You will be given feedback in four ways:

1. By working through examples provided during lectures
2. By response to postings on the course discussion board
3. By attending consultation hours
4. By studying the comments provided by the instructor after the grading of the midterms

### Learning and Teaching approach

**Lectures**

Face-to-face lectures will be employed to enable you to interact directly with the instructors.

### Reading and References


### 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.

(2) Absenteeism

All the lectures are video-recorded. When you miss a lecture, you are expected to make up for the lost learning activities. 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

<table>
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<tr>
<th>Instructor</th>
<th>Office Location</th>
<th>Phone</th>
<th>Email</th>
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<tbody>
<tr>
<td>Naohiko Yoshikai</td>
<td>SPMS-CBC-05-18</td>
<td>6592-7768</td>
<td><a href="mailto:nyoshikai@ntu.edu.sg">nyoshikai@ntu.edu.sg</a></td>
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Planned Weekly Schedule

<table>
<thead>
<tr>
<th>Week</th>
<th>Topic</th>
<th>Course ILO</th>
<th>Readings/Activities</th>
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<tbody>
<tr>
<td>1</td>
<td>Mass spectrometry: Basic theory and instrumentation, effect of isotopes, fundamental fragmentation reactions in EI-MS.</td>
<td>1, 2</td>
<td>Lecture</td>
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| 2    | Mass spectrometry: EI-MS spectra of different types of organic compounds.  
1H NMR: Basic theory and instrumentation, chemical shift | 2-4, 8     | Lecture             |
| 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             |
| 5    | 1H/13C NMR spectroscopy: Variable-temperature                          | 4–8        | Lecture             |
and two-dimensional techniques
IR spectroscopy: Basic theory and instrumentation, absorption of typical functional groups.

| 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  | Coordination chemistry and multi-nuclei NMR spectroscopy | 9-10 | Lecture |
| 9  | Metal-ligand bonds of d-block complexes | 10-13 | Lecture |
| 10 | Stability, reactivity and ligand effects in solution | 13-15 | Lecture, |
| 11 | Mechanisms involving metal catalyzed transformations | 16 | Lecture |
| 12 | Revision of lecture topics and assessment Midterm test 2 | 1-15 | Class Tutorial assessment |
| 13 | Advanced in metal complexes applications | 16-17 | 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.