

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

Course Overview

The sections shown on this interface are based on the templates [UG OBTL+](#) or [PG OBTL+](#)

If you are revising/duplicating an existing course and do not see the pre-filled contents you expect in the subsequent sections e.g. Course Aims, Intended Learning Outcomes etc. please refer to [Data Transformation Status](#) for more information.

Expected Implementation in Academic Year	AY2022-2023
Semester/Trimester/Others (specify approx. Start/End date)	Semester 1 Semester 2
Course Author * Faculty proposing/revising the course	Leong Weng Kee
Course Author Email	chmlwk@ntu.edu.sg
Course Title	Organometallic Chemistry
Course Code	CM3021
Academic Units	3
Contact Hours	45
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)	CM2031 added as pre-req

Course Aims

The aim of this course is to introduce to you some of the basic concepts in Organometallic Chemistry. You will be introduced to some fundamental ideas that are useful to understanding the subject, including an overview of the various types of ligands, some of their properties, and the reaction mechanisms, that are encountered in organometallic chemistry.

Course's Intended Learning Outcomes (ILOs)

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

ILO 1	Use the “ionic” and “covalent” methods to count valence electrons in organometallic complexes
ILO 2	Work out the formal oxidation state of an organometallic complex
ILO 3	Apply the isolobal analogy to relate or construct related complexes
ILO 4	Use the EAN rule to assess if an organometallic complex is likely to be stable
ILO 5	Construct a qualitative MO diagram for carbon monoxide (CO)
ILO 6	Describe the orbital interactions between the metal atom and CO
ILO 7	Quote experimental evidence for the metal-to-ligand pi-back bonding
ILO 8	Correlate the shift in the CO vibrational frequencies in terms of its bonding mode, electronic properties of the complex, and the geometry
ILO 9	Describe the bonding between the metal atom and a phosphine ligand
ILO 10	Describe the stereoelectronic effects of phosphine ligands in terms of Tolman’s parameters
ILO 11	Extrapolate the bonding descriptions and effects to similar ligands such as CS and CN ⁻
ILO 12	Describe the various bonding modes of a transition metal hydride ligand
ILO 13	Describe the bonding interaction between a metal atom and a dihydrogen ligand (H ₂)
ILO 14	State some of the more useful characterization methods for such ligands, such as, the minimum T ₁ in ¹ H NMR spectroscopy
ILO 15	Describe the primary steps in beta-H elimination and its association with the instability of transition metal alkyls
ILO 16	State the requirements for beta-H elimination and hence illustrate approaches to stable transition metal alkyls
ILO 17	List the characteristics such as ligand type, substituents and nature of the metal centre, of Schrock- and Fischer-type transition metal carbenes

ILO 18	Describe the bonding interactions between the metal atom and the carbene ligand for the two types of transition metal carbenes
ILO 19	Describe the differences between the two types of transition metal carbenes in terms of their reactivity pattern, correlate them with their organic counterparts, and illustrate them with examples
ILO 20	Describe the bonding in N-heterocyclic carbenes (NHC)
ILO 21	Identify pi-electron ligands as open (acyclic) or closed (cyclic), and even (ene) or odd (enyl) number of pi-electron systems
ILO 22	Use simple Hückel theory to describe the molecular orbitals of both open and closed π -systems
ILO 23	Describe the metal-ligand interaction in an open π -system using an example such as an alkene or allyl
ILO 24	Describe the metal-ligand interaction in a closed π -system using an example such as cyclopentadienyl (Cp) or an arene
ILO 25	Describe the effects on the chemistry of these organic ligands on binding to a metal, such as, the change in their susceptibility towards nucleophilic and electrophilic attacks, NMR chemical shifts and steric hindrance
ILO 26	State that ligands such as Cp increases the basicity of the metal centre
ILO 27	Describe hapticity shifts
ILO 28	State the relative stability of ene and enyl ligands
ILO 29	Explain and construct the qualitative MO diagram for the metal-ligand bonding in metallocenes
ILO 30	Describe the chemical behavior and redox properties of ferrocene
ILO 31	Identify different types of elementary reaction that occur on transition metals, explain the factors that control them, and provide the products formed
ILO 32	Provide a mechanism for and discuss the catalytic cycles of selected major industrial homogeneous catalytic processes
ILO 33	Propose a feasible mechanism, built from elementary reactions, for any given transition metal centred transformation of an organic fragment/molecule
ILO 34	Devise a short synthesis for a given organic molecule using organometallic reactions as key steps, including control of some aspects of regioselectivity, chemoselectivity and stereoselectivity

Course Content

Introductory concepts

The carbonyl and phosphine ligands

Hydride, dihydrogen, alkyl and related monohapto ligands

Transition metal carbenes

Ligands employing π -electrons

Elementary Reactions

Cross-Coupling Reactions

Oxidative Functionalization of Alkenes

Catalytic Carbonylation

Catalytic Hydrogenation of Alkenes

Alkene Polymerization and Metathesis

Reading and References (if applicable)

R H Crabtree. The Organometallic Chemistry of the Transition Metals, 5th Ed. 4th edition available as e-book. ISBN: 978-1119465881. Wiley.

D Astruc. Organometallic Chemistry and Catalysis Available as e-book. ISBN 978-3-540-46129-6. Springer.

C Elschenbroich. Organometallics, 3rd Ed. ISBN: 978-3-527-29390-2. Wiley-VCH.

J Hartwig. Organotransition Metal Chemistry – From Bonding to Catalysis. ISBN: 978-1891389535. University Science Books.

A F Hill. Organotransition Metal Chemistry. ISBN: 978-0-85404-622-5. RSC.

Organometallics hypertext: <http://www.ilpi.com/organomet/organometallics.html>

Planned Schedule

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
1	Introductory concepts Revision What are organometallic compounds? Pearson's hard-soft acid-base (HSAB) concept The Effective Atomic Number (EAN) rule The "ionic" and "covalent" models for counting electrons in organometallic chemistry The isolobal analogy	1-4	Astruc Ch 1, 2 Crabtree Ch 1, 2		Videos: HSAB concept; Electron count – ionic and covalent methods; EAN rule; Isolobal analogy

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
2	The carbonyl and phosphine ligands MO diagram for CO The CO ligand in organometallic compounds orbital interactions between the metal atom and CO experimental evidence for metal-to-ligand -back bonding IR spectroscopy of transition metal carbonyls - bonding mode, electronic properties, geometry Phosphine ligands in organometallic compounds bonding between the metal atom and phosphine ligand steric effects electronic effects	5-11	Astruc Ch 7 Crabtree Ch 4		Videos: MO diagram for CO; The M-CO bond; Vibrational spectroscopy of transition metal carbonyls; Phosphine and phosphite ligands

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
3	Hydride, dihydrogen, alkyl and related monohapto ligands The hydride ligand (H) – bonding mode and characterization The dihydrogen ligand (H ₂) – bonding interaction with a metal atom, characterization Alkyl ligands: The reason behind instability of transition metal alkyls – β -H elimination Requirements for β -H elimination and approaches to stable transition metal alkyls	12- 16	Astruc Ch 8 Crabtree Ch 3		Videos Hydride ligand; Dihydrogen ligand; Transition metal alkyls (and β -H elimination)

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
4	Transition metal carbenes Schrock- and Fischer-type transition metal carbenes Bonding description Characteristics such as ligand type, substituents and metal centres Reactivity pattern N- heterocyclic carbenes (NHC) – bonding description and applications	17- 20	Astruc Ch 9 Crabtree Ch 11		Videos: Fischer carbenes; Schrock carbenes
5	Ligands employing π - electrons (I) – acyclic enes and enyls Open, acyclic vs closed, cyclic π -systems molecular orbitals of open π -systems: alkenes, allyls and dienes Description of the metal-ligand interaction for alkene and allyl Hapticity change in metal- allyl Effect of metal binding on reactivity of π - ligands	21- 23, 25, 27, 28	Astruc Ch 10 Crabtree Ch 5		Videos: π - MOs of polyenes and –enyls; open ene and enyl ligands

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
6	Ligands employing pi-electrons (II) – aromatic systems pi molecular orbitals of closed - systems: cyclobutadiene, cyclopentadienyl and benzene Description of the metal-ligand interaction for closed - systems Relative stability of ene and enyl ligands Half-sandwich complexes - hapticity change, basicity of metal centre Effect of metal binding on benzene - susceptibility to nucleophilic and electrophilic attacks, NMR chemical shifts, steric hindrance Metallocenes - Description of the bonding Chemical and redox properties of ferrocene	21, 22, 24, 25-30	Astruc Ch 11 Crabtree Ch 5		Videos: Cyclopentadienyl and arene ligands
7	Mid-term I and review	1-30			Administering and review of mid-term

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
8	Elementary Reactions What is an elementary reaction? Ligand substitution: dissociative, associative and interchange mechanisms; the trans effect Oxidative addition and reductive elimination: mechanisms; bite angle dependence s-bond metathesis: occurrence and stereochemistry External attack on ligands: electrophilic vs nucleophilic; nucleophilic addition to CO, alkenes and alkynes; regioselectivity for alkenes Migratory Insertion and Elimination: 1,1-migratory insertion of CO; 1,2-migratory insertion of alkenes and alkynes, regioselectivity issues; reversibility	1-31			Supplementary questions for Week 8

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
9	Cross-Coupling Reactions General mechanistic features: oxidative addition; transmetallation ; reductive elimination; side reactions; influence of ligands Prominent C-C coupling reactions and their features: Kumada, Negishi, Stille, Suzuki and Sonogashira Coupling Buchwald-Hartwig Reaction: arylation of amines; other heteroatoms Mizoroki-Heck Reaction: mechanism; reactivity trends; predicting geometry and stereoselectivity ; regioselectivity patterns	1-34			Supplementary questions for Week 9

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
10	Oxidative Functionalization of Alkenes Wacker Process: catalytic cycle; mechanistic details Wacker-Tsuji Oxidation of Alkenes: mechanism; regioselectivity Alternative nucleophiles: vinyl acetate production; amines and alcohols 1,3-diene substrates: mechanism; control of stereochemistry Mid-term II	1-34			Supplementary questions for Week 10

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
11	Catalytic Carbonylation Industrial production and use of CO: generation of Syngas; conversion of Syngas to methanol Carbonylation of methanol: Monsanto and Cativa Processes; Tennessee Eastman Acetic Anhydride Process Hydrocarboxylation and hydroesterification of olefins: traditional method for producing methyl methacrylate; Lucite Alpha Process Hydroformylation: cobalt vs rhodium catalyzed; ligand control of regioselectivity and chemoselectivity	1-34			Supplementary questions for Week 11

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
12	Catalytic Hydrogenation of Alkenes Dihydride complexes: hydride mechanism; alkene mechanism; reactivity trends Monohydride complexes: oxidative addition of H ₂ ; heterolytic cleavage of H ₂ Asymmetric hydrogenation; importance; ligand control	1-34			Supplementary questions for Week 12

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
13	Alkene Polymerization and Metathesis Ziegler-Natta vs single-site catalysts Cossee-Arlman Mechanism: initiation; chain growth; termination Control of polymer architecture: chain length; chain branching; tacticity Alkene and alkyne metathesis: types of reaction; mechanism; general catalytic cycle Mid-term III	1-34			Supplementary questions for Week 13

Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?
Directed self-learning (~6 hours)	This course involves directed self-learning and peer learning. The first component will involve a list of the concepts to be learned on your own each week. The supporting material available include: Bite-sized videos – these are about 5-10 min long each. A list of the currently available ones for each week's lesson is provided, and they have also been set up in a LAMS environment on NTULearn. You can watch any of them at any time and for any number of times. Each presentation is on one or a couple of concepts. They are not meant to cover everything that you can learn about a topic or concept, but as a springboard for you to explore your books and the internet for more. Internet and ebooks. List of recommended textbooks Concept questions – these are meant to prompt you on what you will need to learn. We will go through them during the key points sessions.
Key point lectures (5 hours)	During these sessions, we will begin with (a) feedback from the previous reflections session, (b) revision of the key points for the previous week's lesson, together with (c) some clicker-based questions. The concept question for the week will then be discussed, using clicker-based questions. This is followed by the key points to be learned for the week, reinforced with another series of clicker-based questions. Reproductions of the Powerpoint slides for the lectures are already available from NTULearn so that you can focus on learning rather than on copying things down.
Tutorials (6 hours)	The tutorial sessions provide a peer teaching and learning environment. You will have already been provided with a list of tutorial questions, one for each tutorial session. The tutorial class sizes are kept small (<25) deliberately, in order that it will not inhibit discussion. All tutorial classes will be facilitated by the lecturer. In each tutorial session, you will self-assemble into groups of up to six to discuss the tutorial question which you already have on hand. This will be followed by a class-level discussion. After that, a second tutorial question will be provided to the class for discussion.
Reflections (5 hours)	During these sessions, you will be given a set of questions based primarily on the concepts to be learned for the week. This is to allow you to ponder over the concepts and allow you to determine if you have understood the lesson or not. It is also a chance for you to explore connected ideas, and perhaps come up with new queries, all of which can be jotted down. The lecturer will go through all the reflection papers and any misconception, etc., from the class will be noted and discussed at the next key point lecture session.
Lectures (18 hours)	Core course content for the second half of the course will be delivered via traditional lectures. To allow the students to focus on listening and learning, rather than note taking, slides will be posted on NTULearn prior to the lectures. This half of the course provides an introduction to reactivity of organometallic complexes via consideration of industrially relevant homogeneous catalysis. Thus, it focusses on real-world examples.

Assessment Structure

Assessment Components (includes both continuous and summative assessment)

No.	Component	ILO	Related PLO or Accreditation	Weightage	Team/Individual	Rubrics	Level of Understanding
1	Continuous Assessment (CA): Test/Quiz(Mini-quiz and tutorial questions)	1-30	Competence, Communication	10	Individual	Holistic	Not Applicable
2	Continuous Assessment (CA): Others(Reflections)	1-30	Competence, Communication, Creativity	10	Individual	Holistic	Not Applicable
3	Continuous Assessment (CA): Others(Concept Question)	1-30	Competence, Creativity	5	Individual	Holistic	Not Applicable
4	Continuous Assessment (CA): Test/Quiz(Mid-Term Test I)	1-34	Competence, Creativity	25	Individual	Holistic	Not Applicable
5	Continuous Assessment (CA): Test/Quiz(Mid-Term Test II)	1-34	Competence, Creativity	25	Individual	Holistic	Not Applicable
6	Continuous Assessment (CA): Test/Quiz(Mid-Term Test III)	1-34	Competence, Creativity	25	Individual	Holistic	Not Applicable

Description of Assessment Components (if applicable)

Formative Feedback

Formative feedback: The online quizzes will allow you to monitor your learning of the concepts on a weekly basis. During the weekly workshop sessions, there will also be clicker-type questions to allow you to assess your understanding although it will not be formally assessed. Through the weekly reflections, you will be able to test your own learning. The lecturer will have read through your reflections and offer a summative feedback to the class weekly. Tutorial classes provide another avenue for you to assess the status of your learning. Along with regular consultation hours, tutorial classes also provide a point of contact with the lecturers. Model answers are provided throughout.

Summative Feedback: Summative feedback will be in the form of the mid-term which will also be reviewed in class.

NTU Graduate Attributes/Competency Mapping

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

Attributes/Competency	Level
Curiosity	Basic
Learning Agility	Basic
Problem Solving	Basic
Critical Thinking	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)

Your learning is your own responsibility; what has been set up is aids and an environment conducive for that. You are expected to complete all assigned pre-class readings and activities, attend all lectures punctually, and take all 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 you have missed. You are expected to participate in all tutorial discussions and activities.

Policy (Absenteeism)

Attendance at lectures, reflection sessions and tutorial classes is strongly encouraged. For those absent, you must catch up each week and follow the recorded lectures and tutorials yourselves. Cramming the night before quizzes and mid-terms to catch up is not recommended.

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 our 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, 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 has any other concerns, please speak to your instructors or a faculty member.

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