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

Course Overview

The sections shown on this interface are based on the templates <u>UG OBTL+</u> or <u>PG OBTL+</u>

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	AY2025-2026
Semester/Trimester/Others (specify approx. Start/End date)	Semester 1
	Semester 2
Course Author	Zhong Hongyu, So Cheuk Wai
* Faculty proposing/revising the course	
Course Author Email	hongyu.zhong@ntu.edu.sg; cwso@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)	

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	Describe the relation between metal oxidation state and d-electron count; metal charge, coordination number and coordination geometry; factors dictating metal spin state; periodic trends of transition metals in terms of electronegativity, bond strength and reactivity nature.
ILO 2	Describe the classification of ligands into dative (L-type) or covalent (X-type). Be able to draw bonding interactions (sigma, pi, delta) in metal complexes from the overlap of atomic orbitals; be familiar with ligand denticity, hapticity, bridging ligands and prefixes to describe how ligands coordinate to metals.
ILO 3	Use the "ionic" and "covalent" methods to count valence electrons and work out the formal oxidation state of organometallic complexes. Use the "18-electron rule" to assess the stability of transition metal complexes and know the exceptions.
ILO 4	Describe the bonding interaction between a metal and CO; correlate the IR frequency of CO ligands with the electronic properties and geometry in metal carbonyl complexes. Understand the use of v(CO) as a descriptor in Tolman Electronic Parameter for measuring ligand donor strength; isolobal analogy; ligands isoelectronic to CO.
ILO 5	Describe the bonding interactions between a metal and a phosphine ligand; steric and electronic properties of different phosphines; use of Tolman cone angle in parameterizing steric properties of phosphines; use of 31P NMR spectroscopy for characterization of metal phosphine complexes.
ILO 6	Describe the bonding modes and properties of metal hydrides, dihydrogen complex; sigma-coordinated hydrocarbyl ligands such as alkyl, aryl, vinyl and alkynyl; instability of metal alkyls by beta-hydrogen elimination; agostic interaction; sigma complex of R-H; state the requirements for beta-H elimination and hence illustrate approaches to stabilize transition metal alkyls.
ILO 7	Describe the bonding of metal-alkene complex in the Chatt-Dewar-Duncanson model and metallacyclopropane model; bonding and properties for other pi-coordinated hydrocarbyl ligands such as alkyne, diene and arene. Understand that the coordination of alkene, alkyne or arene to a metal renders them more susceptible to deprotonation and nucleophilic attack.
ILO 8	Describe the bonding and properties of sigma- and pi-coordinated hydrocarbyl ligands such as allyl and cyclopentadienyl; understand hapticity shifts; properties of metallocene and half-sandwich compounds; redox property and reactivity of ferrocene.
ILO 9	Describe the bonding and reactivity nature of Schrock- and Fischer-type metal carbenes; reactions of metal carbenes with olefins and X-H bonds; N-heterocyclic carbene ligands; examples of hybrid of Schrock and Fischer carbene; metal vinylidene; metal carbyne; metal oxo and imido and their reactivity.
ILO 10	Identify different types of elementary reaction that occur on transition metals, explain the factors that control them, and provide the products formed
ILO 11	Provide a mechanism for and discuss the catalytic cycles of selected major industrial homogeneous catalytic processes

ILO 12	Propose a feasible mechanism, built from elementary reactions, for any given transition metal centred transformation of an organic fragment/molecule
ILO 13	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, making sense of organometallic complexes

Carbonyl and phosphine ligands

Hydrides and alkyl ligands

Pi-coordinated ligands

Metal carbenes

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; why study organometallic chemistry? Recap of fundamentals in coordination chemistry; relation between metal oxidation state and d-electron count; metal charge, coordination number and coordination geometry; factors dictating metal spin state; periodic trends of transition metals in terms of electronegativit y, bond strength and reactivity nature.	1	Crabtree Ch 1 Hartwig Ch 1		Supplementa ry questions for Week 1

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
2	Classification of ligands into dative (L-type) or covalent (X-type); bonding interactions (sigma, pi, delta) in metal complexes from the overlap of atomic orbitals; ligand denticity, hapticity, bridging ligands and prefixes to describe how ligands coordinate to metals. The "ionic" and "covalent" methods to count valence electrons and assign formal oxidation state of organometallic complexes; the "18-electron rule" for assessing the stability of transition metal complexes and exceptions.	2-3	Crabtree Ch 2, Hartwig Ch 1		Supplementa ry questions for Week 2
3	Bonding interaction between a metal and CO; experimental evidence for metal-to-ligand pi-back bonding; correlation	4-5	Crabtree Ch 4, Hartwig Ch 2		Supplementa ry questions for Week 3

Week	Topics or Themes	ILO	Readings	Delivery Mode	Activities
or			G	,	
Session					
	between IR				
	frequency of CO				
	ligands with the				
	electronic				
	properties and				
	geometry of				
	metal carbonyl				
	complexes; use				
	of v(CO) as a				
	descriptor in				
	Tolman				
	Electronic				
	Parameter for				
	measuring				
	ligand donor				
	strength;				
	isolobal analogy;				
	ligands				
	isoelectronic to				
	CO. Bonding in				
	metal phosphine				
	complexes;				
	steric and				
	electronic				
	properties of				
	different				
	phosphines; use				
	of Tolman cone				
	angle in				
	parameterizing				
	steric properties				
	of phosphines; use of 31P NMR				
	spectroscopy for				
	characterization				
	of metal				
	phosphine				
	complexes.				
	complexes.				

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
4	Bonding modes and properties of metal hydrides, dihydrogen complex; sigmacoordinated hydrocarbyl ligands such as alkyl, aryl, vinyl and alkynyl; instability of metal alkyls by beta-hydrogen elimination; agostic interaction; sigma complex of R-H; requirements for beta-H elimination; approaches to stabilize transition metal alkyls.	6	Crabtree Ch 3, Hartwig Ch 3		Supplementa ry questions for Week 4

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
5	Bonding of metal-alkene complex in the Chatt-Dewar-Duncanson model and metallacyclopro pane model; bonding and properties for other picoordinated hydrocarbyl ligands such as alkyne, diene and arene; reactivity of picoordinated ligands. Bonding and properties of sigma- and picoordinated hydrocarbyl ligands such as allyl and cyclopentadieny l; hapticity shifts; properties of metallocene and half-sandwich compounds; redox property and reactivity of ferrocene.	7-8	Crabtree Ch 5, Hartwig Ch 3		Supplementa ry questions for Week 5

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
6	Describe the bonding and reactivity nature of Schrock- and Fischer-type metal carbenes; reactions of metal carbenes with olefins and X-H bonds; N-heterocyclic carbene ligands; examples of hybrid of Schrock and Fischer carbene; metal vinylidene; metal carbyne; metal oxo, metal imido and their reactivity.	9	Crabtree Ch 11, Hartwig Ch 2		Supplementa ry questions for Week 6
7	Review and Mid- term exam I	1-9			Supplementa ry questions for Week 7

Week	Topics or Themes	ILO	Readings	Delivery Mode	Activities
or					
Session					
8	Elementary	10-			Supplementa
	Reactions What	13			ry questions
	is an elementary				for Week 8
	reaction?				
	Ligand				
	substitution:				
	dissociative,				
	associative and				
	interchange				
	mechanisms; the				
	trans effect				
	Oxidative				
	addition and				
	reductive				
	elimination:				
	mechanisms;				
	bite angle				
	dependence s-				
	bond				
	metathesis:				
	occurence 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				
	inserton of				
	alkenes and				
	alkynes,				
	regioselectivity				
	issues;				
	reversibility				

Week	Topics or Themes	ILO	Readings	Delivery Mode	Activities
or					
Session					
9	Cross-Coupling	10-			Supplementa
	Reactions	13			ry questions
	General				for Week 9
	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				
					<u> </u>

Week or Session	-	ILO	Readings	Delivery Mode	Activities
10	Oxidative Functionalizatio n 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	10-13			Supplementa ry questions for Week 10

Week	Topics or Themes	ILO	Readings	Delivery Mode	Activities
or					
Session					
11	Catalytic	10-			Supplementa
	Carbonylation	13			ry questions
	Industrial				for Week 11
	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				
	Hydrocarboxyla				
	tion and				
	hydroesterificati				
	on of olefins:				
	traditional				
	method for				
	producing				
	methyl				
	methacrylate;				
	Lucite Alpha				
	Process				
	Hydroformylatio				
	n: cobalt vs				
	rhodium				
	catalyzed; ligand				
	control of				
	regioselectivity				
	and				
	chemoselectivit				
	У				

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 H2; heterolytic cleavage of H2 Asymmetric hydrogenation; importance; ligand control	10-13			Supplementa ry questions for Week 12

Week	Topics or Themes	ILO	Readings	Delivery Mode	Activities
Session					
	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-	10-13			Supplementa ry questions for Week 13
	term III				

Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?			
Lectur	Core course contents will be delivered via traditional lectures. To allow the students of focus on listening			
es	and learning, rather than note taking, slides will be posted on NTULearn prior to the lectures. The lectures			
	provide an introduction to bonding and 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(Mid-Term Test I)	1-9	Competence, Creativity	20	Individual	Holistic	Not Applicable
2	Continuous Assessment (CA): Test/Quiz(Mid-Term Test II)	10- 13	Competence, Creativity	20	Individual	Holistic	Not Applicable
3	Continuous Assessment (CA): Class Participation()	1- 13	Competence, Creativity	10	Individual	Holistic	Not Applicable
4	Summative Assessment (EXAM): Final exam()	1- 13	Competence, Creativity	50	Individual	Holistic	Not Applicable

Description of Assessment Components (if applicable)					

Formative 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 Al 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 in-class activities, attend all lectures punctually, and take all scheduled assignments and tests. You are expected to take responsibility to follow up with course notes, assignments, and course related announcements for lectures that you have missed.

Policy (Absenteeism)

Attendance at lectures is strongly encouraged. For those absent, you must catch up each week and follow the recorded lectures yourselves. Cramming the night before 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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Last Updated By: Natasha Bhatia (Dr)