Syllabus: CHEM 5620.001 and CHEM 4930.001

Selected Topics in Inorganic Chemistry:
Transition Metal Organometallic Chemistry and Catalysis
Spring Semester 2021 (3 credit hours)

Instructor:
Dr. LeGrande M. Slaughter
Chemistry Building Rm. 307E (and Chair's office, 101D)
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Lecture: Tues, Thurs 12:30 am-1:50 pm, CHEM 109.
Delivery Mode: Face-to-Face

Primary Text: *The Organometallic Chemistry of the Transition Metals, 6th Ed.* Robert H. Crabtree, Wiley, 2014. Available as eBook through library: https://onlinelibrary-wiley-com.libproxy.library.unt.edu/doi/book/10.1002/9781118788301

Recommended Text: *Organotransition Metal Chemistry: From Bonding to Catalysis* John Hartwig, University Science Books, 2010.

Office Hours: Monday and Wednesday, 2:00 – 3:00 (other times by request); by appointment only

Prerequisites: Permission of the instructor. CHEM 4610/5560 is recommended but not required. Familiarity with elementary molecular orbital theory is expected.

Learning Outcomes: The course will give students an in-depth overview of the synthesis, structure, bonding, reactivity, and catalytic applications of transition metal organometallic compounds. A primary emphasis of the course will be the fundamental reaction types of organometallic compounds, their mechanisms, methods for studying them, and their relevance to important processes in industrial catalysis and organic synthesis.

Canvas: The instructor will be making limited use of Canvas, an online digital learning platform, to post supplemental materials for this course. Enter your EUID and password at the following Web address to log in:
https://unt.instructure.com/login/ldap

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Topic Outline (subject to adjustments)

		Text Sections
I.	Introduction and Background	
	A. Features of Organometallic Complexes	Ch. 1.1-1.5
	B. Periodic Trends of Transition Metals	Ch. 2.7
	C. Electronic Structure and Bonding	Ch. 1.6-1.11
	D. Electron Counting and the 18 e^- Rule	Ch. 2.1-2.6
II.	Organometallic Complexes & Ligands	
	A. Ligand Types; σ- and π–Bonding	Ch. 3, 4.1-4.3, 5
	B. Metal-Ligand Multiple Bonds	Ch. 11
III.	Fundamental Reactions of Organometallic Compounds	
	A. Ligand Substitution	Ch. 4.4-4.8
	B. Oxidative Addition	Ch. 6.1-6.5
	C. Reductive Elimination	Ch. 6.6
	D. σ-Bond Metathesis	Ch. 6.7, 6.8
	E. Migratory Insertion and Elimination	Ch. 7
	F. Nucleophilic/Electrophilic Attack on Coordinated Ligands	Ch. 8
IV.	Catalysis	
	A. Hydrogenation & Related Reactions	Ch. 9.1-9.3, 9.6, 14.4
	B. Hydroformylation, CO Activation	Ch. 9.4, 12.3
	C. Olefin and Alkyne Metathesis	Ch. 12.1
	D. Olefin Polymerization/Oligomerization	Ch. 12.2
	E. Coupling Reactions	Ch. 9.7,14.1
	F. C-H Activation & Functionalization	Ch. 14.7
	G. Others (as time and interest allow)	

Lecture Materials:

Lectures will be based on a variety of sources, including classic and recent organometallic literature. The goal will be to bridge the gap between basic inorganic/ organometallic concepts and current research. The Crabtree text (eBook) provides a good foundational introduction to key topics in Organometallic Chemistry. The Hartwig text is an excellent supplementary and reference text that covers more reaction types and goes into greater depth. The lectures will draw on these and other sources, but will not follow any one source linearly. Reading the texts is highly recommended but is not a substitute for attending lectures.

Problem Sets:

A total of 10 problem sets will be assigned. These are intended to help you learn the material, and each student should work on them individually. It is acceptable to discuss problems with other students, but sharing or copying answers is unacceptable and may result in penalties. Problem sets will be due at the beginning of class one week after they are assigned. Solutions will be provided after the due date. Three of the problem sets, selected at random, will be comprehensively graded and will be worth 48 points each. The remaining seven problem sets will be checked for completeness and will be worth 8 points each. Altogether, problem sets will count for 20% (200 points) of the final grade.

Midterm Examinations:

Two midterm exams will be given during regular class hours (tentatively February 18 and April 1; 80 min each). Exams will be closed book, i.e. no notes or textbooks may be used. Students will receive excused absences exams only for University-approved reasons that can be documented (e.g. death in the family, illness requiring medical treatment, religious holidays). If you must miss an exam for a University-approved reason, please see the instructor to discuss accommodations.

Final Examination:

The final exam will take place on Thursday, April 29 from 10:30 am - 12:30 pm. The final will be a cumulative, closed book examination. Students missing the final exam who notify the instructor of the reasons for their absence by noon of the day following the scheduled time for the exam will receive a grade of incomplete ("I") for the course and must arrange a time for a make-up examination with the instructor (before the end of the first week of classes of the Summer I term). If there is no valid excuse for the absence, there will be a fifteen-percent penalty on the final exam. Students who miss the final exam and do not notify the professor of the reason by noon of the following day will receive a score of zero on the exam.

Grades (for 5620):

Problem sets:	200 points (see above for details)
Examination #1:	250
Examination #2:	250
Final Examination:	300
	1000 points

Letter grade scale:

A	880-1000 points
B	750-879
C	620-749
D	500-619
F	0-500

Grading Scheme for 4930:
For students enrolled in CHEM 4930, the class will use a slightly different grading scheme. The maximum point total for the class is 750 points. You have the option of either 1) dropping one of the midterm exams, or 2) submitting written summary of a paper in the area of organometallic chemistry in lieu of the Final Exam (to count up to 50 points). The above letter grade scheme will apply, with the point total determined as [(points earned)/(750)]*1000.

Attendance:
There is no grade for attendance, but you are expected to attend all lectures. Given the large amount of material to be covered, it will negatively impact your preparation for exams and assignments if you miss lectures. If you must miss a lecture, please inform the instructor in advance. Make arrangements to pick up handouts for the class you missed, and ask a classmate to share notes with you.

Academic Integrity:
Students are responsible for honoring UNT's Academic Integrity Policies (https://vpaa.unt.edu/fs/resources/academic/integrity) and the *Code of Student Conduct* (https://deanofstudents.unt.edu/conduct). There will zero tolerance for any form of academic misconduct, including copying assignments, in this course. Any instances of academic misconduct may result in a grade of zero for all parties involved. Repeated violations may lead to a grade of F for the course.

Special Accommodations for Students: If you feel that you have a disability or any other circumstances requiring special accommodation, please contact the Office of Disability Access (Sage Hall Suite 167, Phone 565-4323). If possible, please meet with the instructor during the first week of classes to discuss any needed arrangements. The instructor is committing to ensuring that all students have an equal opportunity to succeed in this course.

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Suggested Supplemental Reading

Organometallic Reference Text

Elschenbroich, Ch.; *Organometallics,* 3rd Ed.; Wiley-VCH: Weinheim, Germany, 2005.
Comprehensive survey of synthesis, structure, bonding, and reactivity, including both main group and transition metal organometallics.

Applications in Organic Synthesis

Hegedus, L. S.; Söderberg, B. C. G. *Transition Metals in the Synthesis of Complex Organic Molecules*; University Science Books: Mill Valley, CA, 2009.

Kinetics and Mechanism

Jordan, R. B. *Reaction Mechanisms of Inorganic and Organometallic Systems,* 2nd Ed.*;* Oxford Univ. Press: New York, 1998.**
(eBook of newer, 2007 edition also available through UNT Libraries)

NMR Spectroscopy

Pregosin, P. S. *NMR in Organometallic Chemistry;* Wiley-VCH: Weinheim, Germany, 2012. (An eBook version *may* be available through UNT Libraries)

General Inorganic Chemistry: Concepts

Miessler, G. L.; Tarr, D. A. *Inorganic Chemistry*, 3rd Ed.; Pearson: Upper Saddle River, NJ, 2004.** (Newer versions available for purchase)

General Inorganic Chemistry: Reference

Cotton, F. A.; Wilkinson, G.; Murillo, C. A.; Bochmann, M. *Advanced Inorganic Chemistry*, 6th Ed.; Wiley: New York, 1999.**

** These books will be available for 2 hour loan at the Willis Library Reserve Desk. Bring your ID and give the passcode **omcatalysis**

Recommended Journals and Electronic Resources

Journals: General/High Impact

Journal of the American Chemical Society
Angewandte Chemie, International Edition
Chemical Science
Chemical Communications

Journals: Specialized

Organometallics
ACS Catalysis
Dalton Transactions
Organic Letters

Databases

SciFinder Scholar

Available from www.library.unt.edu under "Databases"
Many searching options (chemical structure, formula, keyword, author, etc.).
Includes most articles ever published (including old and out-of-print journals)

Web of Science

Available from www.library.unt.edu under "Databases"
Good for searching citations to a given article. However, only covers articles published since 1995.

Cambridge Structural Database

Contains every X-ray crystal structure ever published for non-biological molecules containing at least one C-H bond (including organic and organometallic compounds).

Excellent for searching metal-ligand complexes and analyzing structural features (e.g. metal-carbon bond lengths, bond angles in ligands).

Web-based version (WebCSD; can only be accessed from on-campus computers): http://webcsd.ccdc.cam.ac.uk/

Full version available for installation on UNT research computers (contact Dave Hrovat; Dave.Hrovat@unt.edu)

Important Dates

January 25	Last day to drop a course without a grade
February 18	Midterm Exam #1 (tentative)
April 1	Midterm Exam #2 (tentative)
April 2	Last day to drop course with a grade of "W"
April 22	Last Class Day
April 29	Final Examination 10:30 am - 12:30 pm.

COVID-19-RELATED POLICIES

Face Covering Requirement:
Masks or other approved face coverings are required in all UNT facilities. Students are expected to wear face coverings during all in-person meetings for this class. If you are unable to wear a face covering due to a disability, please contact the Office of Disability Access to request an accommodation. UNT face covering requirements are subject to change due to community health guidelines. Any changes will be communicated via the instructor. See this link for details of UNT's face covering policy.

Social Distancing Requirements:
Sit only in seats that do not have "Do Not Perch Here" stickers. The seat you occupy on the first day of class will be assigned to you for the remainder of the semester. When entering CHEM 109, use only the right entrance, closer to the Chemistry Main Office. Exit the room through the other door, on the right as you face the front of the classroom. When entering or exiting, and during class, maintain a distance of 6 feet (2 meters) from other people at all times.

Disinfection Requirements:
Custodial Services will be cleaning all classrooms nightly, but students will be responsible for disinfecting their seat and desk before each class. There will be a green plastic "camouflage" bucket in the classroom with disinfectant spray and paper towels. We should also have a pump bottle of hand sanitizer in the classroom, and there will be sanitizer stations in the hallways. Please wash your hands and use hand sanitizer frequently throughout the day to help avoid spreading the coronavirus.

Class Materials for Remote Instruction:
A switch to remote instruction may be necessary if community health conditions change or you need to self-isolate or quarantine due to COVID-19. Students will need access to reliable internet and speakers, possibly a microphone and webcam, to participate in fully remote portions of the class. Additional required classroom materials for remote learning include: Zoom software either on a desktop/laptop or cell phone. Information on how to be successful in a remote learning environment can be found at https://online.unt.edu/learn.

Class Recordings:
Some live sessions in the course may be recorded and/or streamed via Zoom to provide access for students who cannot attend for COVID-related reasons. Recordings will be available for all students to access via Canvas throughout the semester. Class recordings are the intellectual property of the University or instructor and are reserved for use only by students in this class and only for educational purposes. Students may not post or share the recording outside the class, or outside the Canvas system, in any form. Doing so could lead to disciplinary action.

COVID-19 EMERGENCY INFORMATION

If you experience any symptoms of COVID-19—such as fever, shortness of breath, or coughing—or if you had close contact with an individual who tested positive for COVID-19, contact the UNT COVID hotline immediately using the phone number or email address below.

COVID@unt.edu
(844) 366-5892

If you contact the hotline, UNT personnel will provide you information about testing and self-isolation procedures that you may be required to follow. ***Please do not hesitate to contact the hotline if you believe you may have been exposed to COVID-19. It is very important to prevent the virus from spreading throughout the UNT community, and your responsible behavior is an important part of this effort.***