Chemistry 579: Coordination Chemistry Applied to Catalysis
Special Topics in Inorganic Chemistry, Fall 2023, Rutgers University-Newark

Instructor: Prof. Demyan Prokopchuk
Email: demyan.prokopchuk@rutgers.edu
Class Time and Location: Thursdays 6:00 – 8:50 PM, Smith 240
Class Material: Available on Canvas https://canvas.rutgers.edu/
Office Hours: by appointment, please email

Overview
This course will range from classical to modern aspects of coordination chemistry and catalysis using transition metals surrounded by ligands. Fundamental ligand design principles such as coordination number, binding mode, charge, spin state, and steric will be presented. The coordination of different ligand classes to transition metals will be correlated with reactivity trends and catalytic activity. Students are expected to develop a rational approach in assessing the reactivity of metals/ligands using electronic structure and thermodynamic arguments. Particular emphasis will be placed on hydrogenation, small molecule activation, “non-innocent” ligands, and (electro)catalysis.

Class Schedule (Thursdays 6:00-8:50 PM ET)

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<th>Week</th>
<th>Date</th>
<th>Lecture</th>
<th>Topic</th>
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<td>1</td>
<td>Sep 7</td>
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<td>Metals, Ligands, and Bonding</td>
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<td>2</td>
<td>Sep 14</td>
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<td>Important Ligands in Catalysis</td>
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<td>3</td>
<td>Sep 21</td>
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<td>Reaction Mechanisms</td>
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<td>Sep 28</td>
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<td>Reaction Mechanisms; Sterics and Electronics</td>
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<td>5</td>
<td>Oct 5</td>
<td>5</td>
<td>Cross-Coupling and Olefin Metathesis (Assignment 1 Due)</td>
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<td>6</td>
<td>Oct 12</td>
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<td>“Non-Innocent” Ligands</td>
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<td>7</td>
<td>Oct 19</td>
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<td>Hydrogenation of Nonpolar Bonds</td>
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<td>Oct 26</td>
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<td>Hydrogenation of Polar Bonds</td>
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<td>Nov 2</td>
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<td>Thermodynamics of M-H Bonds</td>
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<td>Nov 9</td>
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<td>N₂ Reduction (Assignment 2 Due)</td>
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<td>Nov 16</td>
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<td>Inorganic echem, electrocatalysis (Essay Topic Due)</td>
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<td>12</td>
<td>Nov 21 (Tue)</td>
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<td>Selected Literature Papers; Course Review</td>
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<td>Nov 23-26</td>
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<td>Thanksgiving Break – No Class</td>
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<td>14</td>
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<td>Presentations (All Essays Due)</td>
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<td>15</td>
<td>Dec 7</td>
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<td>Presentations</td>
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<td>Final</td>
<td>Dec 21</td>
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<td>6-9 PM, Smith 240</td>
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Course Objectives
During this course, you will:
- identify major ligand classes coordinated to transition metals
- study transition metal complexes and their reactivity by evaluating a ligand steric, electronic structure, coordination geometry, acidity/basicity, redox potential
- establish general trends of ligand coordination and reactivity across the transition metal series
- identify how ligand(s) affect the product outcome for important reactions catalyzed by homogeneous transition metal complexes
- prepare an essay summarizing an important reaction/process catalyzed by homogeneous transition metal compounds (choosing a suggested essay topic is strongly recommended)
- build your presentation skills by summarizing your essay in a clear and concise manner
- discuss and critique recent literature in the field of coordination chemistry and ligand design

Lectures and Course Material

Everyone is expected to attend lectures at the scheduled class times. If this is not possible due to a situation beyond your control, please notify me as soon as possible. All other course material (assignments, exams, grades) will be managed through Canvas.

Please remember that:
Lectures and materials utilized in this course, including but not limited to videocasts, podcasts, visual presentations, assessments, and assignments, are protected by United States copyright laws as well as Rutgers University policy. As the instructor of this course, I possess sole copyright ownership. You are permitted to take notes for personal use or to provide to a classmate also currently enrolled in this course. Under no other circumstances is distribution of recorded or written materials associated with this course permitted to any internet site or similar information-sharing platform without my express written consent. Doing so is a violation of the university’s Academic Integrity Policy (https://policies.rutgers.edu/sites/default/files/10.2.13%20%20current.pdf). Similarly, these copyright protections extend to original papers you produce for this course. In the event that I seek to share your work further, I will first obtain your written consent to do so.

Required Textbooks (see Reading List on Canvas)
3. Ligand Design in Chemistry: Reactivity and Catalysis; Stradiotto, M.; Lundgren, R. J., Eds.; John Wiley and Sons Inc., 2016 (selected chapters)

Additional Resources (see Reading List on Canvas)
Although not required, this textbook will be useful for the course:
1. Jean, Y. Molecular Orbitals of Transition Metal Complexes; Oxford University Press, 2005. (digital version available)
Grading and Evaluation
Assignments: 30%
Essay: 30%
Presentation: 20%
Final Exam: 20%

Assignments (30%)
Assignments must be hand-written and submitted before the beginning of class on the due date. Assignment questions will broadly cover topics related to coordination chemistry, ligand design, and catalysis taught throughout the course. Late assignments will automatically receive a 10% penalty and you will lose 10% for every 24 h they are overdue (10 days overdue = 0%!).

Essay (30%)
I will provide a list of suggested essay topics in the first couple weeks of class. In the essay, you are expected to:
- identify the unique features of the ligand(s) presented in the essay
- discuss how metal/ligand combinations are suited for the reactions they facilitate
- describe reaction trends with functional group variations, charge, steric, etc.
- show plausible reactions mechanisms for catalyzed reactions and discuss rate-determining step(s), resting state(s), and possible deactivation pathways.

Essays must be submitted online before the due date along with a paper copy submitted before class. Late submissions will automatically receive a 10% penalty and an extra 10% for every 24 h they are overdue.


Presentation (20%)
The presentation will be based upon your essay topic (20 min. presentation with 5 min. for questions). You should:
- introduce the field of study (motivation, challenges, goals, etc.) to the audience in a clear and concise manner
- compare and contrast the effects of different variables (metal, charge, spin state, oxidation state, electronics, steric) for the reaction(s) under investigation
- show a general reaction mechanism and highlight important reaction steps (rate determining, selectivity determining, deactivation, etc.)
- select one or two papers from the recent literature (< 5 yrs. old) to inform the class about cutting-edge work in the area
Final (20%)
The final exam will be written in-person. All lecture and/or assignment content will be examinable. Makeup exams will not be allowed unless there is a legitimate written reason in accordance with University Policy.

Important Dates
Last day to drop without “W” Grade: Sep 14th, 2023
Last day to drop course and receive “W” Grade: Oct 30th, 2023

Academic Integrity
As an academic community dedicated to the creation, dissemination, and application of knowledge, Rutgers University is committed to fostering an intellectual and ethical environment based on the principles of academic integrity. Academic integrity is essential to the success of the University’s educational and research missions, and violations of academic integrity constitute serious offenses against the entire academic community. The entire Academic Integrity Policy can be found here: http://academicintegrity.rutgers.edu/academic-integrity-policy/

Your health and well-being matter, and Rutgers has put in place a number of resources that are intended to help students through the challenges that might emerge during these times. Information on many of these resources appears below. Please let us know immediately if you are experiencing circumstances that are negatively impacting your academic performance. We also strongly encourage you to contact your academic advisor.

Accommodation and Support
Rutgers University Newark (RU-N) is committed to the creation of an inclusive and safe learning environment for all students. RU-N has identified the following resources to further the mission of access and support:

· Absences: All students are responsible for timely notification of their instructor regarding any expected absences. The Division of Student Affairs can provide assistant for absences related to religious observance, emergency or unavoidable conflict (illness, personal or family emergency, etc.) Students should refer to the University’s Course Attendance policy (10.2.7), for complete expectations and responsibilities. The office can be contacted at: (973) 353-5063 or deanofstudents@newark.rutgers.edu.

· Disabilities: The Office of Disability Services (ODS) is responsible for the determination of appropriate accommodations for students who encounter barriers due to disability. Once a student has completed the ODS process (registration, initial appointment, and submitted documentation) and reasonable accommodations are determined to be necessary and appropriate, a Letter of Accommodation (LOA) will be provided. The LOA must be given to each course instructor by the student and follow up with a discussion. This should be completed as
early in the semester as possible as accommodations are not retroactive. More information can be found at ods.rutgers.edu. Contact ODS: (973) 353-5375 or ods@newark.rutgers.edu.

·**Temporary Conditions/Injuries:** The Division of Student Affairs can assist students who are experiencing a temporary condition of injury (broken or sprained limbs, concussions, or recovery from surgery). Students experiencing a temporary condition or injury should submit a request for assistance at: https://temporaryconditions.rutgers.edu.

·**Pregnancy:** The Office of Title IX and ADA Compliance is available to assist students with any concerns or potential accommodations related to pregnancy. Students may contact the office at (973) 353-1906 or TitleIX@newark.rutgers.edu.

·**Gender or Sex-Based Discrimination or Harassment:** The Office of Title IX and ADA Compliance can assist students experiencing any form of gender or sex-based discrimination or harassment, including sexual assault, sexual harassment, relationship violence, or stalking. Students can report an incident to the office at: (973) 353-1906 or TitleIX@newark.rutgers.edu. Incidents may also be reported by using the following link: tinyurl.com/RUNReportingForm. For more information, students should refer to the University’s Student Policy Prohibiting Sexual Harassment, Sexual Violence, Relationship Violence, Stalking and Related Misconduct located at: http://compliance.rutgers.edu/title-ix/about-title-ix/title-ix-policies/.

·**Interpersonal Violence:** The Office for Violence Prevention and Victim Assistance can provide any student with confidential support. The office is a confidential resource and does not have a reporting obligation to report information to the University’s Title IX Coordinator. Students can contact the office at: (973) 353-1918 or run.vpva@rutgers.edu. There is also a confidential, text-based line students can text for support: (973) 339-0734.

·**Crisis and Concerns:** The Campus Awareness Response and Education (CARE) Team works with students in crisis to develop a support plan to address personal situations that might impact academic performance. Students may contact the CARE Team at: http://tinyurl.com/RUNCARE or careteam@rutgers.edu.

·**Stress, Worry, or Concerns about Well-Being:** The Counseling Center has confidential therapists available to support students. To schedule an appointment: counseling@newark.rutgers.edu or (973) 353-5805. If a student is not quite ready to make an appointment with a therapist but is interested in self-help, check out TAO at Rutgers-Newark for an easy, web-based approach to self-care and support: https://tinyurl.com/RUN-TAO.

·**Emergencies:** Call 911 or contact Rutgers University Police Department (RUPD) at (973) 353-5111.

**Learning Resources:**

·**Rutgers Learning Center (tutoring services)**
  (973) 353-5608
https://sasn.rutgers.edu/student-support/tutoring-academic-support/learning-center

· Writing Center (tutoring and writing workshops)
  (973) 353-5847
  nwc@rutgers.edu
  https://sasn.rutgers.edu/student-support/tutoring-academic-support/writing-center