TOPICS IN INORGANIC AND ORGANOMETALLIC CHEMISTRY
Chem423 (Winter 2020)

Lectures: Mondays 2:30-3:20 pm
           Tuesdays 4:30-5:20 pm
           Thursdays 3:30-4:20 pm   Location: Kingston 205

Course instructors:
  PART I:                PART II:
  Dr Anne Petitjean      Dr Kevin Stamplecoskie
  Chernoff Hall, room 410 Chernoff Hall, room 505
  anne.petitjean@chem.queensu.ca kevin.stamplecoskie@chem.queensu.ca
  613 533 6587            613 533 2649

Office Hours: Petitjean: Mondays 3:30-4:30 pm, or by appointment.
              Stamplecoskie: Mondays 3:30-4:30 pm, or by appointment.

Course website: this course is supported by an OnQ site associated with course registration. See https://onq.queensu.ca

Intended Student Learning Outcomes for 2020:
(1) The students will be able to apply the principles of organometallic chemistry to analyze and identify the stability and reactivity of organometallic compounds.
(2) The students will be able to design synthetic methods based on cross-coupling reactions for organic compounds.
(3) The students will be able to elucidate the electronic structures and bonding of organometallic compounds and design effective molecules for catalysis.
(4) The students will be able to conduct a critical review and assessment on a topic in current literature and research trend related to organometallics and communicate effectively the finding in the form of oral presentations to the class.
(5) The students will gain understanding of the electronic structure and optical activity of inorganic compounds and materials, especially as it pertains to catalysis.

Course outline: See end of this document.

Textbooks (not required):
- ‘Organometallics, A Concise Introduction’ by Ch. Elschenbroich, A. Salzer [on reserve]
- ‘The Organometallic Chemistry of the Transition Metals’, by Robert Crabtree
- ‘Advanced Inorganic Chemistry’, by F. A. Cotton
- ‘Physical Methods in Chemistry’ by R. S. Drago

Grading Scheme
2 Assignments  2x7.5 %
Midterm examination  35%  Tentatively Thursday February 13th, 2020, 3:30-5:30 pm
Final examination  35%  Scheduled by the exams office
Literature presentation (groups of 2) 15%  Spread during the term

Grading Method: All components of this course will receive numerical percentage marks. The final grade you receive for the course will be derived by converting your numerical course average to a letter grade according to Queen’s Official Grade Conversion Scale:
Queen’s Official Grade Conversion Scale

<table>
<thead>
<tr>
<th>Grade</th>
<th>Numerical Course Average (Range)</th>
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<tbody>
<tr>
<td>A+</td>
<td>90-100</td>
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<tr>
<td>A</td>
<td>85-89</td>
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<tr>
<td>A-</td>
<td>80-84</td>
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<td>B+</td>
<td>77-79</td>
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<tr>
<td>B</td>
<td>73-76</td>
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<tr>
<td>B-</td>
<td>70-72</td>
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<td>C+</td>
<td>67-69</td>
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<tr>
<td>C</td>
<td>63-66</td>
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<tr>
<td>C-</td>
<td>60-62</td>
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<tr>
<td>D+</td>
<td>57-59</td>
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<tr>
<td>D</td>
<td>53-56</td>
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<td>D-</td>
<td>50-52</td>
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<td>F</td>
<td>49 and below</td>
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Calculator Policy: As noted in Academic Regulation 9.2, Calculators acceptable for use during quizzes, tests and examinations are intended to support the basic calculating functions required by most Arts and Science courses. For this purpose, the use of the Casio 991 series calculator is permitted and is the only approved calculator for Arts and Science students. This calculator sells for around $25 at the Queen's Campus Bookstore, Staples and other popular suppliers of school and office supplies.

Academic Integrity: Queen’s students, faculty, administrators and staff all have responsibilities for upholding the fundamental values of academic integrity; honesty, trust, fairness, respect, responsibility and courage (see www.academicintegrity.org). These values are central to the building, nurturing and sustaining of an academic community in which all members of the community will thrive. Adherence to the values expressed through academic integrity forms a foundation for the "freedom of inquiry and exchange of ideas" essential to the intellectual life of the University (see the Senate Report on Principles and Priorities http://www.queensu.ca/secretariat/policies/senate/report-principles-and-priorities).

Students are responsible for familiarizing themselves with the regulations concerning academic integrity and for ensuring that their assignments and their behaviour conform to the principles of academic integrity. Information on academic integrity is available in the Arts and Science Calendar (see Academic Regulation 1 http://www.queensu.ca/artsci/academic-calendars/regulations/academic-regulations/regulation-1), on the Arts and Science website (see https://www.queensu.ca/artsci/students-at-queens/academic-integrity), and from the instructor of this course. Departures from academic integrity include plagiarism, use of unauthorized materials, facilitation, forgery and falsification, and are antithetical to the development of an academic community at Queen's. Given the seriousness of these matters, actions which contravene the regulation on academic integrity carry sanctions that can range from a warning or the loss of grades on an assignment to the failure of a course to a requirement to withdraw from the university.

Turnitin Statement: Queen’s University has partnered with the third-party application Turnitin to help maintain our standards of excellence in academic integrity. Turnitin is a suite of tools that
provide instructors with information about the authenticity of submitted work and facilitates the process of grading. Submitted files are compared against an extensive database of content, and Turnitin produces a similarity report and a similarity score for each assignment. A similarity score is the percentage of a document that is similar to content held within the database. Turnitin does not determine if an instance of plagiarism has occurred. Instead, it gives instructors the information they need to determine the authenticity of work as a part of a larger process.

**Copyright of Course Materials:** Course materials created by the course instructor, including all slides, presentations, handouts, tests, exams, and other similar course materials, are the intellectual property of the instructor. It is a departure from academic integrity to distribute, publicly post, sell or otherwise disseminate an instructor’s course materials or to provide an instructor’s course materials to anyone else for distribution, posting, sale or other means of dissemination, without the instructor’s **express consent.** A student who engages in such conduct may be subject to penalty for a departure from academic integrity and may also face adverse legal consequences for infringement of intellectual property rights.

**Accessibility Statement**
Queen’s is committed to an inclusive campus community with accessible goods, services, and facilities that respect the dignity and independence of persons with disabilities. Course materials are available in an accessible format or with appropriate communication supports upon request.

Please contact **Meredith Richards in the Department of Chemistry** in one of the following ways:
  - Email: ugadm@chem.queensu.ca
  - Phone: 613-533-6000 extension 75518
  - In person: Chernoff 200

**Accommodations Statement**
Queen's University is committed to achieving full accessibility for people with disabilities. Part of this commitment includes arranging academic accommodations for students with disabilities to ensure they have an equitable opportunity to participate in all of their academic activities. The Senate Policy for Accommodations for Students with Disabilities was approved at Senate in November 2016 (see [https://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslwwwww/files/files/policies/senateandtrustees/ACADACCOMMPOLICY2016.pdf](https://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslwwwww/files/files/policies/senateandtrustees/ACADACCOMMPOLICY2016.pdf)). If you are a student with a disability and think you may need academic accommodations, you are strongly encouraged to contact the Queen's Student Accessibility Services (QSAS) and register as early as possible. For more information, including important deadlines, please visit the QSAS website at: [http://www.queensu.ca/studentwellness/accessibility-services/](http://www.queensu.ca/studentwellness/accessibility-services/)

**Academic Considerations for Students in Extenuating Circumstances**
Queen’s University is committed to providing academic consideration to students experiencing extenuating circumstances that are beyond their control and are interfering with their ability to complete academic requirements related to a course for a short period of time. The Senate Policy on Academic Consideration for Students in Extenuating Circumstances is available at [http://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslwwwww/files/files/policies/senateandtrustees/Academic%20Considerations%20for%20Extenuating%20Circumstances%20Policy%20Final.pdf](http://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslwwwww/files/files/policies/senateandtrustees/Academic%20Considerations%20for%20Extenuating%20Circumstances%20Policy%20Final.pdf)
Each Faculty has developed a protocol to provide a consistent and equitable approach in dealing with requests for academic consideration for students facing extenuating circumstances. Arts and Science undergraduate students can find the Faculty of Arts and Science protocol and the portal where a request can be submitted at: http://www.queensu.ca/artsci/accommodations. Students in other Faculties and Schools who are enrolled in this course should refer to the protocol for their home Faculty. If you need to request academic consideration for this course, you will be required to provide the name and email address of the instructor/coordinator. Please use the following:

Instructor/Coordinator Name:
Instructor/Coordinator email address:

Location and Timing of Final Examinations: The exam dates for each Term are listed on the Faculty of Arts and Science webpage under “Important Dates.” Student exam schedules for the Winter Term are posted on the Friday before Reading Week. Students should delay finalizing any travel plans until after the examination schedule has been posted. Exams will not be moved or deferred to accommodate employment, travel/holiday plans or flight reservations. Also, as indicated in Academic Regulation 8.3, students must write all final examinations in all on-campus courses on the Kingston campus.

Course Outline (tentative):
Note that you are responsible for, and will be tested on, in-class material. If you miss a class, please make an effort to get copies of the notes from that day. Some information for the lectures will be posted on OnQ but not complete lecture notes (available upon request).

PART I:

Introduction: Classification; Electronegativity; Metals/Main group.

Chapter 1: Main Group Organometallics
1.1 Alkali Metals
   Focus on organolithium compounds (synthesis, properties, applications)
1.2 Alkaline-Earth metals
   Focus on organomagnesium compounds (synthesis, properties, applications)

Chapter 2: Examples of Organoelements of the Carbon and Nitrogen Groups
2.1 Silicon Organyls
2.2 A Short Incursion into Phosphorus-C bonds (complement on Wittig reactions)

Chapter 3: Organometallic Compounds of the Transition Metals
3.1 Introduction
   (18 valence electron rule, elementary steps)
3.2 σ-Donor ligands
   e.g., M-Alkyl, M-aryl
   Application to bio-inorganic catalysis (Vit B_{12})
3.3 σ-Donor and π-Acceptor Ligands
   e.g., CO
3.4 σ and π-Donors, π-Acceptor Ligands
   e.g., Olefins, Cp, arenes
PART II

Chapter 4: Photocatalysis
4.1 Energetics & Jablonski Diagrams
4.2 Classic examples of photocatalysts
   – i.e. Ru(bpy)$_3^{2+}$
   - Iridium photocatalysts – water splitting
4.3 Photovoltaics – a subclass of photocatalysts
4.4 Light Emitting Devices

Chapter 5: Bonding and Band Theory
5.1 Introduction to Materials
   - inorganic complexes
   - can we describe “large” ordered materials the same way
   - examples like methyl ammonium lead halide
5.2 – Band Theory for large ordered materials
   Bloch Functions
   LCAO - MO theory
5.3 – Band Theory for Nanomaterials
   - unique properties of nanomaterials

Chapter 6: Metal Nanomaterials
6.1 – noble metals – definition
   - plasmons in metals, bulk and nanomaterials
6.2 – clusters – the missing link
6.3 – the Au-S bond revisited
6.4 – metal clusters as a new class of catalyst/photocatalysts

Chapter 7: Semiconductor Nanomaterials
7.1 – Band structure of semiconductor nanomaterials – quantum dots
7.2 – Photovoltaics with quantum dots
7.3 – semiconductor ‘clusters’

Proposed list of presentation topics:

<table>
<thead>
<tr>
<th>Topic #</th>
<th>Topic</th>
</tr>
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<tbody>
<tr>
<td># 1</td>
<td>Suzuki-Miyaura cross-coupling reactions</td>
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<tr>
<td># 2</td>
<td>Sonogashira cross-coupling reactions</td>
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<tr>
<td># 3</td>
<td>Copper-catalyzed azide-alkyne cycloaddition (a member of the ‘Click’ reactions)</td>
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<tr>
<td># 4</td>
<td>C-H activation in organometallic catalysis</td>
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<tr>
<td># 5</td>
<td>Photophysics/Photochemistry of B-N bridged Charge-Transfer Complexes</td>
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<tr>
<td># 6</td>
<td>Pt(II) Compounds for Light Emitting Diodes</td>
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<tr>
<td># 7</td>
<td>Carbene – Au Self-Assembled Monolayers</td>
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<tr>
<td># 8</td>
<td>Ultrafast Spectroscopy</td>
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</tbody>
</table>

Each topic presentation includes 10 minutes of speech and 3-5 minutes of questions (both will be assessed). It is anticipated that 3 groups will present per class session of 50 minutes. Topics 1-4 will tentatively be presented in week 6, and topics 5-8 in week 12.