CHEM 443 / 643 – ORGANOMETALLIC CHEMISTRY – 3 CREDITS

1. GENERAL INFORMATION
Course Format  Lectures: 26 75-min sessions  Wed, Fri 08:45–10:00  LOY–CC–314
Instructor  Dr. Xavier Ottenwaelder  SP–201.19  ext. 8934
Office hours: by appointment  dr.x@concordia.ca
There is no laboratory component

2. COURSE DESCRIPTION
This course covers the structure and properties of organometallic compounds, their main reactions and their application in catalysis and organic chemistry.
Prerequisites  CHEM 324: Organic Chemistry III: Organic Reactions
CHEM 341: Inorganic Chemistry III: The Transition Elements

3. OBJECTIVES
This advanced course features in-depth descriptions of organometallic species: molecules containing M–C bonds, where M is an alkali, alkali-earth, main group, or d-block metal or metalloid element. This includes their structure, reactivity and application in catalysis. You will be expected to achieve a high level of analytical and critical thinking. It is highly recommended that you work the material before class. In-class tests throughout the term will evaluate your preparedness by making you apply concepts learned in class to new situations.

4. SCHEDULE (may be subject to change)
See last page for a detailed course content.

5. COURSE MATERIAL
Recommended Textbooks
Didier Astruc, Organometallic Chemistry and Catalysis, 2007 (Springer)
Well organized (by ligand and reaction types) and with a lot of pictures. Lacks insight at times and, being a first edition, contains imprecisions.

John Hartwig, Organotransition Metal Chemistry, 1st ed. 2010 (University Science Books)
Huge, comprehensive book, more adapted for research, does not treat main-group organometallics.

Garry O. Spessard, Gary L. Miessler, Organometallic Chemistry, 2010 (Oxford University Press)
Covers the essential components organometallics with transition metals but lacks a solid description of catalysis. Does not cover alkali and main group.

Well organized (by reaction types) but doesn’t treat main-group organometallics. Lacks pictures.

Christoph Elschenbroich, Organometallics, 3rd ed., 2006 (Wiley-VCH)
More or less complete with a strong emphasis on the main group chemistry. Different organization (by ligand types) but it is relatively easy to locate any information.

6. GRADING
For CHEM 443 students, the final grade will be weighted and calculated as follows:
Assignments / In-Class Tests  60%
Final Exam  40% (in April; scheduled by Exams Office)

A grade ≥ 0%  50.00  53.33  56.67  60.00  63.33  66.67  70.00  73.33  76.67  80.00  85.00  90.00  100%
and <  50.00  53.33  56.67  60.00  63.33  66.67  70.00  73.33  76.67  80.00  85.00  90.00  100%
gets a:  F  D−  D  D+  C−  C  C+  B−  B  B+  A−  A  A+
For **CHEM 643 students**, the final grade will be weighted and calculated as follows:

<table>
<thead>
<tr>
<th>Component</th>
<th>Weightage</th>
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<tr>
<td>Assignments / In-Class Tests</td>
<td>40%</td>
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<tr>
<td>Oral Presentation</td>
<td>20%</td>
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<tr>
<td>Final Exam</td>
<td>40% (in April; scheduled by Exams Office)</td>
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</table>

A grade ≥ 0% 65.00 70.00 73.33 76.67 80.00 85.00 90.00
and < 65.00 70.00 73.33 76.6 80.00 85.00 90.00 100%
gets a: F C B− B B+ A− A A+

In the event of extraordinary circumstances beyond the University’s control, the content and/or evaluation scheme in this course is subject to change.

If absent from an examination or a test, you must produce a written excuse on letterhead paper appropriately signed (e.g., by a doctor or employer) within one week after the exam/test. The Department determines the validity of the absence and necessary arrangements will be made. If no valid excuse is produced, the student will receive a zero grade for the missed work.

**7. ORAL PRESENTATION (CHEM 643 only)**

Every CHEM 643 student is required to present a topic related to the course subject in an oral presentation to the class. The presentation should last about 20 minutes, not exceed 25 minutes, and will be followed by questions from the class. The goal is to cover specific subjects in more detail than will be done during the lectures. You must decide of a topic by **February 17th**. The presentation shall address some aspect of organotransition metal chemistry; some representative topics are provided below. You are welcome to discuss your topic with me and, of course, you are not restricted to the topics listed below. In particular, let me know if you prefer to present a topic related to main-group organometallic chemistry. Included in the presentation should be a brief historical perspective on the area, your own perspective on the significance (or lack thereof) of the topic, and a critical evaluation of the seminal work (rather than a laundry list of all work) in the area. The presentation should also address unresolved issues and your own perspective on new research opportunities in the area. Some possible topics are:

- Transmetallation: Mechanism, Scope and Selectivity
- C–H Activation in Organic Synthesis
- Metathesis Polymerization
- C–C Bond Activation
- Methane Activation and Conversion
- Enantioselective Hydrogenation
- Enantioselective Hydroformylation
- Enantioselective Epoxidation
- Catalytic Aziridination
- Organometallic Electrocatatlysis
- CO₂ Activation
- Catalysis for Fuel Cells
- CO/Olefin Copolymerization
- Catalysis for Fuel Cells
- Catalytic Amination, Etherification (Hartwig / Buchwald Couplings)
- Catalytic Atom Transfer (Amination, Osmylation, Amino-Hydroxylation)

**8. RIGHTS AND RESPONSIBILITIES**

The academic code of conduct can be found in section 17.10 of the academic calendar (http://www.concordia.ca/academics/undergraduate/calendar/current/17-10.html). Any form of unauthorized collaboration, cheating, copying or plagiarism found in this course will be reported and the appropriate sanctions applied. The Department of Chemistry and Biochemistry offers a short seminar on the academic conduct code and the appropriate use of information sources which aims to clarify what practices will be considered unacceptable with regards to work submitted for grading in Chemistry and Biochemistry courses. Attendance at this seminar is highly recommended and represents a clear and fair opportunity to learn what our faculty regards as academic misconduct. Failure to take part in this learning opportunity and thus ignorance of these regulations is no excuse and will not result in a reduced sanction in any case where academic misconduct is observed.
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Lectures
Dr. Xavier OTTENWAELDER
dr.x@concordia.ca
Wed, Fri 08:45–10:00
LOY–CC–314

The following table is a tentative outline of the material covered in this course. The last 5 columns indicate chapters on each topic for the aforementioned books. The end of the books also provide applications that cover several topics at once; we will refer to these sections periodically.

<table>
<thead>
<tr>
<th>glimpse of the lecture content</th>
<th>Spess.</th>
<th>Hartwig</th>
<th>Astruc</th>
<th>Crab.</th>
<th>Elsch.</th>
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<tbody>
<tr>
<td>Introduction</td>
<td>History, classification</td>
<td>1</td>
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<td>Intro</td>
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<tr>
<td>I. Main-group organometallics</td>
<td>Li, Mg, Al, Sn compounds, Zn and Cu groups</td>
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<td>-</td>
<td>12, 13</td>
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<tr>
<td>II. Organo-Transition-Metal Complexes</td>
<td>18-electron rule, structure, bonding, formal oxidation state</td>
<td>2-6, 10</td>
<td>1-4, 13</td>
<td>1, 2, 7-11</td>
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<td>III. Stoichiometric reactions</td>
<td>Ligand substitution</td>
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<td>5</td>
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<td></td>
<td>Oxidative addition, Reductive Elimination</td>
<td>6-8</td>
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<td>6</td>
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<td></td>
<td>Migratory Insertion, Eliminations</td>
<td>8</td>
<td>9-10</td>
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<td>Attack on coordinating ligands</td>
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<td>11-12</td>
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<td>8</td>
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<td>IVa. Introduction to catalysis</td>
<td>Hydrogenation and hydroelementation</td>
<td>12</td>
<td>14</td>
<td>Part 4</td>
<td>9</td>
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<td>IVb. Main reaction types</td>
<td>Hydroformylation</td>
<td>15-16</td>
<td>14</td>
<td>9.2</td>
<td>18.7</td>
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<td>Cross-coupling: Kumada, Suzuki, Heck...</td>
<td>17</td>
<td>14</td>
<td>9.3</td>
<td>18.8</td>
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<td>Olefin polymerization</td>
<td>19</td>
<td>21.3</td>
<td>9.6</td>
<td>18.2</td>
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<td>Reaction of carbenes / metathesis</td>
<td>22</td>
<td>15</td>
<td>12.2</td>
<td>18.11</td>
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<td>Oxidations and C-H functionalization</td>
<td>21</td>
<td>15</td>
<td>11, 12.1, 18.10</td>
<td>14.2</td>
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<td>16, 18</td>
<td>16</td>
<td>14.6</td>
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Notes:
- This schedule is subject to change.
- The schedule of assigned readings will be updated as the term progresses.

\(^a\) Spessar-Miessler 2nd edition. \(^b\) Crabtree 5th edition. \(^c\) Elschenbroich, 3rd edition.