

# Chemistry 4441B - Inorganic Macromolecules 2018/2019

Instructor: J. F. Corrigan, ChB 16 ext. email: corrigan@uwo.ca

**LECTURES:** 3 lectures each week, MWF 9:30 – 10:20 a. m. in CHB 115

**EVALUATION:** There will be one mid-term test and a final examination. There will also be problem sets assigned (4 in total) Marks will also be assigned for in-class participation as demonstrated when discussing problem sets.

## **DISTRIBUTION OF MARKS:**

2.5 hour Term Test (Part 1 of the course): 35 % (Term test date: Tuesday February 26, 6-8:30 pm, CHB 115)

Participation: 5 % (as demonstrated with discussion of problem sets).

3 Hour Final Examination (Part 2 of the course; not cumulative): 35 % (April; exact date and location to be determined by the Registrar).

Problem Sets 4 x 6.25% each.

## **Chemistry 4441A Course Outline**

The course describes inorganic clusters (Part 1) and the technique of single crystal X-ray diffraction (Part 2), a method of paramount importance for determining the structure of such polymetallic assemblies.

Part 1 will describe bonding models in such polynuclear metal complexes. It will include the application of Wade's Rules and related bonding theories to interpret their formation, structure and reactivity. It will be cemented that many parallels exist when describing the bonding requirements of transition metal clusters to their Main Group element counterparts.

The second Part will detail the technique of single crystal X-ray diffraction for determining molecular structure. This is the "go to" technique for these types of molecules (as well as many others!).

Tentative Course Outline:

PART 1 (approx. 6 weeks)

- **Cluster and Cage Molecules of the p-Block Elements:** electron precise molecules versus PSEP Theory and polyhedra; boranes and carboranes: bonding and reactivity; Zintl ions and related
- **Electron Counting in Organometallic Chemistry and Metal Cluster Chemistry:** review of metal  $d$ -electron configurations and ligand electron

contributions, 18 electron rule; EAN rule, and PSEP Theory; relationships between Main Group and transition metal clusters.

- **The "Isolobal Concept":** cluster fragments as building blocks; cluster construction using isolobal principles. (as time permits)
- **High Nuclearity Clusters:** condensed cluster counting rules and systematics; synthetic strategies for high nuclearity clusters. Structure and bonding in Au-thiolate protected clusters.

PART 2 (approx. 6 weeks)

- **Fundamentals of Single Crystal X-ray Crystallography:** the crystalline state, point symmetry, translational symmetry elements and space groups; diffraction of X-rays by molecules; unit cell geometries and the symmetry elements present; space group assignment.
- **Crystallography in Practice:** measuring diffraction patterns, intensity; "solving" the crystal structure, structure refinement; interpretation and evaluation of the results.

### **Course prerequisite: Chemistry 3371F**

**A Notice from the Registrar:** "Students are responsible for ensuring that their selection of courses is appropriate and accurately recorded and that all course prerequisites have been successfully completed. If the student does not have the requisites for a course, and does not have written special permission from his or her Dean to enroll in the course, the student will be removed from the course and it will be deleted from the student's record. This decision may not be appealed. A student will receive no adjustment to his or her fees in the event that he or she is dropped from a course for failing to have the necessary prerequisites."

**Scholastic offences** are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at the following Web site: <http://www.uwo.ca/univsec/handbook/appeals/scholoff.pdf>

**Plagiarism:** Students must write their essays and assignments in their own words. Whenever students take an idea or a passage from another author, they must acknowledge their debt both by using quotation marks where appropriate and by proper referencing such as footnotes or citations. Plagiarism is a major academic offence (see Scholastic Office Policy in the Western Academic Calendar).

**Course Objectives:** The idea with this course is not to strictly focus on 'memory work' (although some is required!) but instead, in Part 1, to be able to use the tools developed to describe and predict the structures of high nuclearity inorganic complexes and have a thorough understanding of the localized and delocalized bonding descriptions of these molecules and relate the material presented in the lectures to the current literature. In Part

2, the objectives are to be able to demonstrate a level of understanding of single crystal X-ray diffraction so as to be able to interpret, use and critically evaluate the data generated from this experiment.

**Reading and Reference List:** There is no prescribed text for the course. Most textbooks of inorganic chemistry contain useful sections on relevant topics. For example: *Inorganic Chemistry*, by Shriver and Atkins (Freeman), your 2<sup>nd</sup> and 3<sup>rd</sup> year text. Lecture notes will be supplemented with handouts when required.

The following general texts are on reserve in the Taylor library:

*Introduction to Cluster Chemistry* D. M. P. Mingos and D. J. Wales QD921.M645 1990

*Inorganic Chemistry, 4th Edition*, J. E. Huheey, E. A. Keiter and R. L. Keiter QD151.2.H84 1993

*X-ray Crystallography, 2<sup>nd</sup> Edition*, W. Clegg, QD945.C56 2015

**Illness:** If you are unable to meet a course requirement due to illness or other serious circumstances, you must provide valid medical or other supporting documentation to the Dean's office as soon as possible. It is the student's responsibility to contact the course instructor to make alternative arrangements once the accommodation has been approved. In the event of a missed final exam, a "Recommendation of Special Examination" form must be obtained from the Dean's Office immediately. For further information please see:

[http://www.uwo.ca/univsec/handbook/appeals/accommodation\\_medical.pdf](http://www.uwo.ca/univsec/handbook/appeals/accommodation_medical.pdf)

A student requiring academic accommodation due to illness, should use the Student Medical Certificate when visiting an off-campus medical facility or request a Records Release Form (located in the Dean's Office) for visits to Student Health Services. This procedure must also be followed for any missed labs.

The form can be found here:

[https://studentservices.uwo.ca/secure/medical\\_document.pdf](https://studentservices.uwo.ca/secure/medical_document.pdf)

For those students who cannot write the midterm test on the date indicated because of religious or class conflicts see Dr. Corrigan immediately.

**Accessibility Statement:** Please contact the course instructor if you require material in an alternate format or if you require any other arrangements to make this course more accessible to you. You may also wish to contact Services for Students with Disabilities (SSD) at 661-2111 x 82147 for any specific question regarding an accommodation.

**Support Services:** Learning-skills counsellors at the Student Development Centre (<http://www.sdc.uwo.ca>) are ready to help you improve your learning skills. They offer presentations on strategies for improving time management, multiple-choice exam preparation/writing, textbook reading, and more. Individual support is offered throughout the Fall/Winter terms in the drop-in Learning Help Centre, and year-round through individual counselling.

Students who are in emotional/mental distress should refer to Mental Health@Western ([http://www.health.uwo.ca/mental\\_health](http://www.health.uwo.ca/mental_health)) for a complete list of options about how to obtain help.

Additional student-run support services are offered by the USC, <http://westernusc.ca/services>. The website for Registrarial Services is <http://www.registrar.uwo.ca>.