University of Guelph, Department of Chemistry
College of Physical and Engineering Science

STRUCTURE AND BONDING: CHEM*2060

Credits: 0.5 CEUs **Fall 2015**

Pre-requisites: CHEM*1050 & [either (MATH*1210(1114) & PHYS*1010) or IPS*1510]
Minimum grade 50%

Undergraduate Calendar Course Description:
This course covers the applications of symmetry, simple crystal structures and principles of bonding. Molecular orbital theory is used to explain the fundamental relationship between electronic and molecular structure. This course provides the elementary quantum background for an understanding of the electronic structures of atoms and molecules.

Course Instructor: Prof. Kathryn Preuss
Office: MACN 335
Phone: x56711
Email: **kpreuss@uoguelph.ca**

Please feel free to drop by my office to see me, but be aware that I may be busy and ask you to come back another time. If it is important that you see me, please **email me for an appointment** so that I can guarantee you adequate time. You may ask questions by email, and I will do my best to answer them in a timely fashion during work hours.

TA/Tutorial Leader: Adam Maahs, Ph.D. candidate
Office: MACN 232
Email: amaahs@uoguelph.ca

Mr. Maahs has office hours on Tuesdays from 2:30pm to 3:30pm. He spends most of his time in the research lab and will be unlikely to accommodate you if you show up outside this allotted time. Please be aware that MACN 232 is shared office space. Please respect the other students in that space.

Lectures: MWF 11:30am – 12:20pm JTP 214
1st class: Friday, September 11th 2015
Mon., Oct. 12th – NO CLASSES – rescheduled to Fri., Dec. 4th

Tutorials: Tues. 1pm – 2:20pm MCKN 120
1st tutorial: Tuesday, September 22nd 2015
(NO TUTORIAL Tues., Oct. 13th – rescheduled to Thur., Dec. 3rd)

Final Exam: Thursday, Dec. 17th 2015, 8:30 – 10:30 am (location TBA)

Course Notes: Available on CourseLink

Evaluation: Students can choose one of two options by which to be evaluated:

OPTION #1

Sapling Learning on-line quizzes	10%	5 Quizzes, each worth 2%
Midterm 1	25%	**Fri. Oct 2nd** – in class
Midterm 2	25%	**Fri. Nov. 6th** – in class
Final Exam	40%	**Thu. Dec. 17th** - 8:30 – 10:30 am - TBA

To choose this option, access Sapling and complete the quizzes online. Your final grade will be calculated both ways (as in Option #1 and #2) and the BETTER GRADE WILL BE ASSIGNED AUTOMATICALLY.

OPTION #2

Midterm 1	30%	**Fri. Oct 2nd** – in class
Midterm 2	30%	**Fri. Nov. 6th** – in class
Final Exam	40%	**Thu. Dec. 17th** - 8:30 – 10:30 am - TBA

This is the default option for those who do not sign up for Sapling.

Course Outline and Objectives:

1. **Structure and Shape** – The properties of a chemical species are often directly related to the structure and the shape of the molecule, fragment, polymer, etc. *X-ray crystallography* is frequently used to determine shapes. Molecular *symmetry* is extremely useful for the elucidation of molecular properties and the creation of simple but powerful models to predict these properties. Molecular symmetry is elegantly expressed by assigning *point groups*. Concepts such as *polarity* and *chirality* clearly rely on shape/symmetry. **Objectives:** Students should be able to explain what is a crystal structure and how is crystallographic data obtained. Students are expected to recall VSEPR theory shape predictions learned in pre-requisite courses. Students should be able to identify and apply symmetry elements and operations to objects and molecular structures, assign point groups to objects/molecules, and identify chirality and polarity in object/molecules. Students should be able to rationalize and explain the concepts related to the above tasks.

2. **Electrostatic Interactions** – *Ionization potentials* are used to probe electrons in bonds. *Electron affinities* are useful for probing reactivity. Chemists especially like to use the concept of *electronegativity* to explain atomic and molecular properties, even though this concept has some flaws. These three properties help elucidate *electronic configurations* and *atomic orbital energies*, and vice versa. *Electronegativity* and *polarizability* are particularly good concepts for understanding electrostatic interactions. **Objectives:** Students should be able to identify, define and explain the concepts, equations and theories presented in this section. In particular, students should be able to rationalize atomic properties using arguments founded on ionization potential, electron affinity and electronegativity. Students should be able to correlate atomic quantum numbers with atomic orbitals and orbital properties. Students should be able to rationalize

atomic properties based on penetration/shielding arguments. Students are expected to recall Coulomb's Law and basic trigonometry from pre-requisite courses and to apply this knowledge to determine/rationalize electrostatic interactions between atoms/molecules/ions. Students should be able to identify/explain H-bonding and rationalize/explain/predict physical properties/trends based on the H-bonding arguments.

3. **Ionic Bonding in Molecules and Solids** – The concept of ionic bonding is a natural extension of electrostatic interactions. The *Madelung* constant, *Coulombic* interactions, and *Born-Meyer repulsion* are used to describe ionic bonding. Crystal packing in ionic solids is (somewhat) predictable based on ionic radii. Essentially, this is simple geometry. **Objectives:** Students should be able to recognize, identify and describe the crystal packing motifs covered in the lecture notes. Students should be able to apply the Born-Haber cycle to calculate an experimental lattice enthalpy as well as explain/apply the Born-Mayer (Born-Lande) equation to derive an estimate for the lattice enthalpy. Students should be able to explain/describe the derivation of Madelung constants, to recall specific Madelung constants, and to apply them in appropriate circumstances. Students should be able to use the radius ratio rule to make predictions regarding crystal packing. Students should be able to identify/discuss/describe crystallographic directions and planes.

4. **Introduction to Quantum Concepts in Chemistry** – Atoms and molecules cannot be adequately described by classical physics. *Quantum mechanics* is necessary, even for a simple understanding of non-ionic bonding. Quantum mechanics seems strange (counterintuitive) but the mathematics is actually just *wave mechanics*. The notation takes a bit of getting used to. Once this is understood, the idea of *quantum numbers* to describe electrons seems trivial. **Objectives:** Students should be able to identify/explain/apply the quantum mechanical equations presented in the lecture. Students are expected to recall relevant calculus concepts learned in pre-requisite courses. Students should be able to draw s, p and d atomic orbitals and their radial probability plots, as well as rationalizing atomic properties based on these. Students should be able to derive/apply/explain the "particle-in-a-box" models/equations and the H atom quantum models/equations. Students should be able to recognize/explain the Schrödinger equation and its application.

5. **The Covalent Bond** – There are two equally acceptable quantum mechanical approaches to model covalent bonding: *valence bond (VB) theory* and *molecular orbital (MO) theory*. VB theory relies on the concept of hybridization of local atomic orbitals. The concept of lone pairs and of single/double/triple bonds is more naturally related to VB theory. Molecular orbital theory relies on the mixing of <u>all</u> atomic orbitals to give rise to a complete set of molecular orbitals. MO theory is more naturally suited to explaining electronic and spectroscopic properties. Both theories are significantly simplified by using <u>symmetry</u>. **Objectives:** Students are expected to recall valence bond theory geometry

arguments learned in pre-requisite courses. Students should be able to derive/explain/apply hybridization models/equations covered in lecture. Students should be able to identify/explain molecular orbital theory concepts. Students should be able to sketch molecular orbitals (as linear combinations of atomic orbitals) and molecular orbital (MO) energy level diagrams of simple di- through octa- nuclear linear and cycle molecular structures. Students should be able to fill MO energy level diagrams with the correct number of electrons and make arguments regarding physical/chemical properties based on these MO energy level diagrams. Students should be able to identify/rationalize/sketch bonding, antibonding and nonbonding orbital interactions.

Textbook: There is no mandatory textbook for this course.

Most undergraduate Inorganic Chemistry textbooks cover the topics that are presented in this course. If you want an inexpensive book that covers some of the course material, see:

Chemical Structure and Bonding, by Roger L. DeKock and Harry B. Gray, University Science Books, Sausalito, CA, 1989. (ISBN 0-935702-61-X)

This is available in the bookstore and in the library.

There are a lot of good web resources that cover this material. Wikipedia content is generally very good for this course content and I encourage you to use it.

Molecular Model Kit: Optional. (but highly recommended)

If you've got one already, bring it. If not, there are kits available for purchase in the bookstore: Indigo model 68845NV (1^{st} year) or Indigo model 62053 (org. chem.)

You may find that the some sections of this course (and exams) will be significantly more difficult if you do not have a model kit.

Sapling: Optional.

1. Go to http://bit.ly/saplinginstructionsCA and follow the instructions to create an account. **Be sure to use your official school email address.**

2. a. If you already have a Sapling Learning account, log in (click on "Canada Higher Ed" on the top right to get to the login page), then skip to step 3.

b. If you have a Facebook account, you can use it to quickly create a Sapling Learning account. Click the blue button with the Facebook symbol on it (to the left of the username field). The form will auto-fill with information from your Facebook account (you may need to log into Facebook in the popup window first). Choose a password and time zone, accept the site policy agreement, and click 'Create my new account'. You can then skip to step 3.

c. Otherwise, click "create account". Supply the requested information (**be sure to use your official school email address**) and click 'Create my new account'. Check your email (and spam filter) for a message from Sapling Learning and click on the link provided in that email.

3. Find your course in the list (listed by subject, term, and instructor) and click the link.

4. Select your payment options and follow the remaining instructions.

5. Work on the Sapling Learning training materials. The activities, videos, and information pages will familiarize you with the Sapling Learning user environment and serve as tutorials for efficiently drawing molecules, stereochemistry, etc. within the Sapling Learning answer modules. These training materials are already accessible in your Sapling Learning course.

Once you have registered and enrolled, you can log in at any time to complete or review your homework assignments.

During sign up - and throughout the term - if you have any technical problems or grading issues, send an email to support@saplinglearning.ca explaining the issue. The Sapling support team is almost always faster and better able to resolve issues than your instructor.

Evaluation of the Professor *"As part of the faculty evaluation process in the Department of Chemistry, students are reminded that written comments on the teaching performance of the lecturer may be sent to the Chair of the department at any time. Such letters must be signed."* – These letters will not be discussed with the professor until grades have been submitted, unless otherwise requested by the student(s).

E-mail Communication:

As per university regulations, all students are required to check their University-issued e-mail account regularly: e-mail is the official route of communication between the University and its students.

When You Cannot Meet a Course Requirement:

When you find yourself unable to meet an in-course requirement because of illness or compassionate reasons, please advise the course instructor (or designated person, such as a teaching assistant) in writing, with your name, id#, and e-mail contact. See the undergraduate calendar for information on regulations and procedures for Academic Consideration:

http://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-ac.shtml

Drop Date:

The last date to drop one-semester courses, without academic penalty, is **Friday, November 6th, 2015**. For regulations and procedures for Dropping Courses, see the Undergraduate Calendar:

http://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-drop.shtml

Copies of out-of-class assignments:

Keep paper and/or other reliable back-up copies of all out-of-class assignments: you may be asked to resubmit work at any time.

Accessibility:

The University of Guelph is committed to creating a barrier-free environment. Providing services for students is a shared responsibility among students, faculty and administrators. This relationship is based on respect of individual rights, the dignity of the individual and the University community's shared commitment to an open and supportive learning environment. Students requiring service or accommodation, whether due to an identified,

ongoing disability or a short-term disability should contact the Centre for Students with Disabilities as soon as possible.
For more information, contact CSD at 519-824-4120 ext. 56208 or email csd@uoguelph.ca or see the website: http://www.csd.uoguelph.ca/csd/

Academic Misconduct:
The University of Guelph is committed to upholding the highest standards of academic integrity and it is the responsibility of all members of the University community – faculty, staff, and students – to be aware of what constitutes academic misconduct and to do as much as possible to prevent academic offences from occurring. University of Guelph students have the responsibility of abiding by the University's policy on academic misconduct regardless of their location of study; faculty, staff and students have the responsibility of supporting an environment that discourages misconduct. Students need to remain aware that instructors have access to and the right to use electronic and other means of detection.

Please note: Whether or not a student intended to commit academic misconduct is not relevant for a finding of guilt. Hurried or careless submission of assignments does not excuse students from responsibility for verifying the academic integrity of their work before submitting it. Students who are in any doubt as to whether an action on their part could be construed as an academic offence should consult with a faculty member or faculty advisor.The Academic Misconduct Policy is detailed in the Undergraduate Calendar:
http://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-amisconduct.shtml

Recording of Materials:
Presentations which are made in relation to course work—including lectures—cannot be recorded or copied without the permission of the presenter, whether the instructor, a classmate or guest lecturer. Material recorded with permission is restricted to use for that course unless further permission is granted.

Resources:
The Academic Calendars are the source of information about the University of Guelph's procedures, policies and regulations which apply to undergraduate, graduate and diploma programs: http://www.uoguelph.ca/registrar/calendars/index.cfm?index