CHEM3310 Syllabus 2014.docx

Latest update 09/06/14

**Molecular Structure and Energetics I**

Autumn 2014

Professor G. R. Eaton

**Goals**

Students should become facile with the use of symmetry to characterize compounds and simplify problems, and learn that atomic and molecular orbitals and molecular vibrations are representations of groups. Qualitative approaches to constructing molecular orbitals of polyatomic molecules, and the simplifications made possible by the use of molecular symmetry will be emphasized. Students should learn what it means to “solve the Schrodinger equation,” and obtain energy levels and coefficients for the molecular orbitals of a molecule.

This course is required background for CHEM3320 and CHEM3120.

**Calendar**

Classes begin Monday, September 8. Last day of classes is Friday, November 14. Note that a review is scheduled for Friday, 11/14.

The Final Exam is scheduled for Wednesday, November 19, 8:00 – 9:50 but it may move to avoid conflict with another course.

Office hours are Tuesday, Wednesday, and Thursday 5-6 pm, or by appointment.

**Texts**

C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, 4th ed., Pearson/Prentice Hall.

R. L. Carter, Molecular Symmetry and Group Theory. Wiley, 1998

These texts will be used in both CHEM3310 and CHEM3120

The chapters on HMO in Streitwieser are on Blackboard.

It will be useful to have a molecular model set that includes 6-coordinate atoms.

An introduction to symmetry and a discussion of shapes of atomic orbitals are available as electronic files on Blackboard. See also <http://www.orbitals.com/orb/>

Students should have available an undergraduate physical chemistry text for some background review (it does not matter which text you have).

The computer program Spartan will also be useful. Find it on Pioneer Web>Resources>Software download>Spartan

**Cooperative Learning Groups**

Students will be assigned to Cooperative Learning Groups. See separate documents on Cooperative Learning Groups.

**Grading**

Group projects 20%

Exam #1 20%

Exam #2 20%

Final exam 40%

|  |  |  |  |
| --- | --- | --- | --- |
| **class** | **date** | **topic** | **reading** |
| 1 | M 09/08 | Symmetry elements and operations; matrix representations, stereographic projections. | Handout, on Blackboard; Housecroft ch. 3; Atkins ch. 5; Carter ch. 1 |
| 2 | W 09/10 | Stereographic projections; multiple operations | Housecroft ch. 3, Carter ch. 1 |
| 3 | F 09/12 | Point groups | Housecroft ch. 3; Carter ch. 2 |
| 4 | M 09/15 | Assigning point groups of molecules | Housecroft ch. 3; Carter ch. 1 |
| 5 | W 09/17 | Multiplication tables and character tables | Housecroft ch. 3; Carter ch. 2 |
| 6 | F 09/19 | Classes of symmetry operations | Carter ch. 2 |
| 7 | M 09/22 | Wave equation, Quantum numbers | Housecroft ch. 1; Atkins ch. 1-2 |
| 8 | W 09/24 | Symmetries of atomic orbitals | Orbital Shapes, on Blackboard; Housecroft ch. 1; Atkins ch. 3; Carter ch. 4 |
| 9 | F 9/26 | Combining orbitals on one center – hybrid orbitals | Housecroft ch. 5; Carter ch. 4 |
| 10 | M 9/29 | Combining orbitals on multiple centers – molecular orbitals | Housecroft ch. 5; Carter ch. 4 |
| 11 | W 10/01 | MO’s for H2+ and H2 | Housecroft ch. 1 |
| 12 | F 10/03 | The nature of the chemical bond |  |
| 13 | M 10/06 | Exam #1 |  |
| 14 | W 10/08 | MO’s for diatomics | Housecroft ch. 1 |
| 15 | F 10/10 | Representations; Use of Symmetry in MO theory; MOs for H2O | Housecroft ch. 5; Carter ch. 5; Streitwieser electronic reserve |
| 16 | M 10/13 | MOs for H2O; MOs as representations |  |
| 17 | W 10/15 | MOs for B2H6 |  |
| 18 | F 10/17 | “ |  |
| 19 | M 10/20 | Vibrations as representations | Housecroft ch. 3; Carter ch. 6 |
| 20 | W 10/22 | Vibrations of H2O |  |
| 21 | F 10/24 | “ |  |
| 22 | M 10/27 | Hückel MO method | Streitwieser |
| 23 | W 10/29 | “ |  |
| 24 | F 10/31 | Determinants, Eigenfunctions, and Eigenenergies | Streitwieser |
| 25 | M 11/03 | Exam #2 |  |
| 26 | W 11/05 | Basis functions as representations |  |
| 27 | F 11/07 | MOs for B6H62- | Housecroft ch. 5, 13 |
| 28 | M 11/10 | “ |  |
| 29 | W 11/12 | “ |  |
| 30 | F 11/14 | Review |  |
|  | W 11/19 | Final exam |  |

This very tentative outline of classes will be updated from time-to-time during the Quarter, but my intent is to follow this outline within ±one class meeting.

The final exam is scheduled for Wednesday, 11/29, from 8:00-9:50 am, in Olin 103, but it might change in order to ensure that the exams in the three graduate core courses are on different days. A review class will be scheduled consistent with other time commitments of the class.

**Other potentially useful books:**

Atkins’ Physical Chemistry, P. Atkins and J. DePaula, 8th ed., Freeman, 2006; also published as a 2-volume paperback. Chapter and page references are to volume 2 of the paperback edition, as “Atkins chapter 1” etc.

L. H. Hall, Group Theory and Symmetry in Chemistry. McGraw-Hill, 1969 QD461.H17. This is the text that I like best for showing all of the details.

F. A. Cotton, Chemical Applications of Group Theory, 3rd ed. QD461.C65 1990. This is the classic text on symmetry and group theory in chemistry.

Shriver and Atkins, Inorganic Chemistry, 5th ed. QD151.5.S57 2010, 4th ed. QD151.5.S57 2006.

A. Streitwieser, Molecular Orbital Theory for Organic Chemists. Wiley,1961. QD255.S88 The assigned chapters are on Blackboard

John G. Verkade, A pictorial approach to molecular bonding and vibrations, 2nd ed.

H. E. Zimmerman, Quantum Mechanics for Organic Chemists, Academic Press, 1975

A. Rauk, Orbital Interaction Theory of Organic Chemistry, 2nd ed., Wiley-Interscience, 2001. QD461.R33 2001

S. M. Bachrach, Computational Organic Chemistry, Wiley-Interscience, 2007. QD255.5.M35.B33 2007. Chapter 1 is an overview of methods. Many chapters contain interesting interviews with major figures in computational organic chemistry.

**Useful web sites for learning symmetry:**

<http://symmetry.otterbein.edu/gallery/index.html>

<http://www.staff.ncl.ac.uk/j.p.goss/symmetry/>

this site gives pictures that rotate so the molecules can be seen from many directions, and some nice pictures of stereographic projections with molecules

<http://www.ch.ic.ac.uk/vchemlab/symmetry/>

this site needs chime to show modes in action

<http://www.reciprocalnet.org/edumodules/symmetry/>

this site has a good tutorial with pictures of planes and axes, etc.

<http://csi.chemie.tu-darmstadt.de/ak/immel/index.html> click on tutorials, which include symmetry, atomic orbitals, chirality, and other topics.

See Journal of Chemical Education, November 2005, page1736 and 1741. These articles tell of using Jmol and WebWare for learning molecular symmetry.