CHEM3310 Syllabus 2017.docx
Latest update 09/05/17

Molecular Structure and Energetics I

Autumn 2017
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 11. Last day of classes is Friday, November 17. The Final Exam is scheduled for Saturday, November 18, 8:00 – 9:50 but it probably will move to avoid conflict with a biochemistry 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 available electronically.
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. 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).
http://www.facultybookshelf.org/course/1507 This webpage link provides a one-click access to the course textbook(s), including on-line options and price comparison.
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 homework assignments 20%
Exam #1 20%
Exam #2 20%
Final exam 40%

class	Date	topic	reading
1	M 09/11	Symmetry elements and operations; matrix representations, stereographic projections.	Handout, on Canvas; Housecroft ch. 3; Atkins ch. 5; Carter ch. 1
2	W 09/13	Stereographic projections; multiple operations	Housecroft ch. 3, Carter ch. 1
3	F 09/15	Point groups	Housecroft ch. 3; Carter ch. 2
4	M 09/18	Assigning point groups of molecules	Housecroft ch. 3; Carter ch. 1
5	W 09/20	Multiplication tables and character tables	Housecroft ch. 3; Carter ch. 2
6	F 09/22	Classes of symmetry operations	Carter ch. 2
7	M 09/25	Wave equation, Quantum numbers	Housecroft ch. 1; Atkins ch. 1-2
8	W 09/27	Symmetries of atomic orbitals	Orbital Shapes, on Canvas; Housecroft ch. 1; Atkins ch. 3; Carter ch. 4
9	F 19/29	Combining orbitals on one center – hybrid orbitals	Housecroft ch. 5; Carter ch. 4
10	M 10/2	Combining orbitals on multiple centers – molecular orbitals	Housecroft ch. 5; Carter ch. 4
11	W 10/04	MO's for H_2^+ and H_2 MO's for diatomics	Housecroft ch. 1 Housecroft ch. 2
12	F 10/06	The nature of the chemical bond	
13	M 10/9	No class; combined with class 11	
14	W 10/11	Exam #1	
15	F 10/13	Representations; Use of Symmetry in MO theory; MOs for H_2O	Housecroft ch. 5; Carter ch. 5; Streitwieser on Canvas
16	M 10/16	MOs for H_2O; MOs as representations	Housecroft ch. 5
17	W 10/18	MOs for B_2H_6	Housecroft ch. 5
18	F 10/20	"	
19	M 10/23	Vibrations as representations	Housecroft ch. 3; Carter ch. 6
20	W 10/25	Vibrations of H_2O	Housecroft ch. 3; Carter ch. 6
21	F 10/27	Vibrations of H_2O	Housecroft ch. 3; Carter ch. 6
22	M 10/30	Hückel MO method	Streitwieser
23	W 11/01	"	
24	F 11/03	Determinants, Eigenfunctions, and Eigenenergies	Streitwieser
25	M 11/06	Basis functions as representations	Streitwieser
26	W 11/08	Exam #2	
27	F 11/10	MOs for $B_6H_6^{2-}$	Housecroft ch. 5, 13
28	M 11/13	"	"

29	W 11/15	"	"
30	F 11/17	Review	
	11/18??	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.

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 Canvas

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:

You may have browser problems accessing all feature of some of these sites.
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.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.

http://www.ch.ic.ac.uk/vchemlab/symmetry/
this site needs chime to show modes in action; since chime software is no longer supported, this site may not work for you.

Alternatives accessed 08/23/17 include:

http://www.chemtube3d.com/vibrationsH2O.htm

http://www2.ess.ucla.edu/~schauble/molecular_vibrations.htm

https://www.youtube.com/watch?v=3RqEIr8NtMI this video is a good elementary introduction to vibrations in molecules.

Web sites and software to use them come and go rapidly. If you find better sites, please tell others in the class about them.

Hydrogen probability density plots
http://hyperphysics.phy-astr.gsu.edu/hbase/hydwf.html