CHEM3310 Syllabus.doc
Latest update 10/09/07

Molecular Structure and Energetics I

Autumn 2007
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 10.
Last day of classes is Friday, November 16.
Exam period November 19-21.

Texts

C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, 2nd ed., 2005, Pearson/Prentice Hall, Publisher. This text will be used in both CHEM3310 and CHEM3120
The chapters on HMO in Streitwieser will be available on electronic reserve
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).

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%

Very tentative outline of classes; this will be updated from time-to-time during the Quarter.

class	date	topic	reading
1	M 09/10	Wave equation, Quantum numbers	Housecroft chapter 1; Atkins chapters 1-2
2	W 09/12	Shapes of atomic orbitals	Handout, on Blackboard; Housecroft chapter 1; Atkins chapter 3
3	F 09/14	Combining orbitals on one center – hybrid orbitals	Housecroft chapter 4
4	M 09/17	Combining orbitals on multiple centers – molecular orbitals	Housecroft chapter 4
5	T 09/18	MO's for H_2^+ and H_2	Housecroft chapter 1
6	W 09/19	The nature of the chemical bond	
7	M 09 24	MO's for diatomics	Housecroft chapter 1
8	W 09/26	Symmetry elements and operations; matrix representations, stereographic projections.	Handout, on Blackboard; Housecroft chapter 3; Atkins chapter 5; Hall
9	F 09/28	Stereographic projections; multiple operations	Housecroft Ch. 3, other texts on symmetry and group theory
10	M 10/01	Group; Point groups	Housecroft chapter 3
11	W 10/03	Assigning point groups of molecules	Housecroft chapter 3
12	F 10/05	Multiplication tables and character tables	Housecroft chapter 3
13	M 10/08	Symmetries of atomic orbitals	
14	W 10/10	Exam #1	
15	F 10/12	Classes of symmetry operations	
16	M 10/15	Representations; Use of Symmetry in MO theory; MOs for H_2O	Housecroft chapter 4; Streitwieser electronic reserve
17	W 10/17	MOs for H_2O; MOs as representations	
18	F 10/19	MOs for B_2H_6	
19	M 10/22	"	
20	W 10/24	Vibrations as representations	Housecroft chapter 3
21	F 10/26	Vibrations of H_2O	
22	M 10/29	"	
23	W 10/31	Exam #2	
24	F 11/02	Hückel MO method	
25	M 11/05	"	
26	W 11/07	Determinants, Eigenfunctions, and Eigenenergies	
27	F 11/09	Basis functions as representations	
28	M 11/12	MOs for $B_6H_6^{2-}$	Housecroft chapter 12
29	W 11/14	"	
30	F 11/16	Review	
	11/17?	Final exam	

The final exam is scheduled for Saturday, 11/17, from 10-12 am, but it might change in order to ensure that the exams in the three graduate core courses are on different days.

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.
R. L. Carter, Molecular Symmetry and Group Theory. QD461.C32 1998. Many students find this an accessible introduction to symmetry.
L. H. Hall, Group Theory and Symmetry in Chemistry. McGraw-Hill, 1969 QD461.H17. This is text I like best for 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.
Shriver and Atkins, Inorganic Chemistry, 4th ed. QD151.5.S57 2006 The 3rd ed. is QD151.5.S57 1999 (shelved in the oversize section).
A. Streitwieser, Molecular Orbital Theory for Organic Chemists. Wiley, 1961. QD255.S88 The assigned chapters are on e reserve.
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.