Chem 3310, Fall 2018
Molecular Structure and Energetics I

Updated 09/11/2018

Class Times: MWF 9:00 – 9:50 am, Olin 103
Instructor: Sandra S. Eaton
Office: Olin 202
Office Hours: Tuesday/Thursday 8:30 am – 10 am, or by appointment

Texts:
R. L. Carter, *Molecular Symmetry and Group Theory*, Wiley, 1998 (denoted as **C** in the reading assignments.)
C. E. Housecroft and A. G. Sharp, *Inorganic Chemistry*, 5th ed., Pearson/Prentice Hall (this text will also be used in Chem 3120) (denoted as **H-S** in reading and homework assignments.)
Ch. 1-3 of A. Streitweiser, Jr., *Molecular Orbital Theory for Organic Chemists* can be accessed via the Canvas page for the class. (denoted as **S** in the reading assignments.)
Students should have available an undergraduate physical chemistry text for background review. Whichever one you used as an undergraduate is fine.

Learning goals:
1. Students should become familiar with the use of symmetry to characterize compounds and simplify chemical problems, and learn that orbitals and molecular vibrations are representations of point groups.
2. A student should be able to relate the symmetry of a molecule to the shapes of the molecular orbitals and the vibrational modes of the molecule.
3. Students should learn what it means to 'solve the Schroedinger equation' and obtain energy levels and coefficients for molecular orbitals by the Huckel method.

This course is a prerequisite for Chem 3320 (Molecular Structure and Energetics II) and Chem 3120 (Chemical Systems II).

Students are expected to do the assigned reading before coming to class so that time in class can be spent on key points and answering student questions.

Updated versions of the syllabus, including homework assignments and literature presentation assignments, will be posted on the Blackboard page for this class.

Tentative Course Outline

Date	Topic	Reading	Homework due
Sept. 10	Symmetry elements and operations	**C**: 1-14; **H-S**: 62 - 68	
12	Matrix representations, products of operations, stereographic projections	**C**: 14-18; **H-S**: 68 - 69; handout on stereographic projections	
14	Point groups	**C**: 18-27; **H-S**: 69 - 70	
17	Assigning molecules to point groups	**C**: 28-34; **H-S**: 70 - 73	**H-S:** 3.3, 3.4, 3.8, 3.10, 3.12
19	Character tables and representations	**C**: 40-46; **H-S**: 73 - 74	
21	"	**C**: 46 - 52	
24	Irreducible and reducible representations	**C**: 61-64, 66-70	
26	Vibrations of CO_2	**H-S:** 74 - 76	
28	Vibrations of H_2O, SO_2, selection	**C:** 164 – 185; **H-S**: 77 -	

	rules for vibrational spectroscopy	78	
Oct. 1	Selection rules for vibrational spectroscopy	**C:**180–190	
3	The wave equation and quantum numbers	**H-S**: 7-25; **S**: 1-10	
5	Exam #1		
8	Symmetries of atomic orbitals	**C**: 88-91; **H-S**: 12-15	
10	MOs for H_2^+ and H_2	**H-S**: 32-37	
12	MOs for diatomics	**H-S:** 38-42; **S**: 11-20	
15	Photoelectron spectroscopy and heteronuclear diatomics	**C**: 94-104; **H-S**: 130-131	
17	Combining orbitals on one center to form hybrid orbitals	**C**: 104-117; **H-S**: 144 - 148	
19	Use of symmetry in MO theory, formation of symmetry adapted combinations: C_2H_4	**C**: 138-149; **H-S**: 149 - 150	
22	MO's of H_2O	**H-S**: 151 - 156	
24	MO's of BH_3, BF_3 and CO_2	**H-S**: 156 - 165	
26	MO's of B_2H_6	**H-S**: 167 - 171	
29	Huckel MO method, variation method	**S**: 33 - 39	
31	Huckel MO's – small organics	**S**: 40 - 44	
Nov. 2	Exam #2		
5	Electron densities, bond orders, nodes	**S**:48 - 59	
7	Huckel MO's of larger organics	handout	
9	Comparison of HMO spin densities and EPR hyperfine couplings	handout	
12	Breaking symmetry by adding substituents	handout	
14	Student presentations – applications		
16	Student presentations - applications		
Tues. 20	Final exam (comprehensive)		

Examinations and Homework

There will be two exams during the quarter and a final exam.

Answers to homework and exams will be provided on Canvas.

Note that final was moved from Saturday Nov. 17 to Tues. Nov. 20th to have it on different day than the final for Advanced Proteins.

Grading

Homework:	12%
Presentation:	8%
2 mid-term exams	25%, each
Final exam:	30%