Latest update 09/06/21

Chem 3310, Fall 2021
Molecular Structure and Energetics I

Class Times: MWF 9:00 – 9:50 am, in Olin 103
Instructor: Professor Gareth R. Eaton
Office Hours: Tuesday/Thursday 8:30 am – 10 am, or by appointment, or whenever you see me in the office or lab.

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 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.

We will use some web sites that have good graphics of symmetry. Depending on your learning style, using the on-line video tools may meet your needs. If you learn better with a physical object in your hands, you may want to purchase a molecular model kit. Be sure to select a kit that has "metal atoms" for octahedral and square planar coordination. Kits designed for organic chemistry rarely have these units. One inexpensive kit that is adequate is Molymod MMS-009. This is one of the model kits that I have used in classes.

You will also need to access the Spartan molecular orbital software. The University has a license for this, and you can download it to your personal computer.

Learning goals:
1. 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. Be able to relate the symmetry of a molecule to the shapes of the molecular orbitals and the vibrational modes of the molecule.
3. Learn what it means to 'solve the Schrödinger equation', obtain qualitative pictures of molecular orbitals, and compare with results from the computer program Spartan.

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 class so that time in class can be spent on key points and answering student questions.

Most classes will suggest exercises for your use to increase your mastery of the topics. I encourage you to work together on these exercises. They will not be graded except via exams. If you want feedback on your work you can submit your answers to me.

class	date	topic	reading
1	M 9/13	Symmetry elements and operations; matrix representations, stereographic projections.	Handout, on Canvas; H-S 62-68; C 1-14
2	W 9/15	Stereographic projections; multiple operations	H-S 68-69; C 14-18
3	F 9/17	Point groups	H-S 69-70; C 18-27
4	M 9/20	Assigning point groups of molecules	H-S 70-73; C 28-39
5	W 9/22	Multiplication tables and character tables	H-S 73-74; C 40-46
6	F 9/24	Classes of symmetry operations	C 52-54
7	M 9/27	Reducing representations	C 46-70
8	W 9/29	Vibrations as representations Vibrations of CO_2 and H_2O	H-S 74-76; C 164-179
9	F 10/1	Vibrations of larger molecules	H-S 77-78; C 172-178
10	M 10/4	Vibrations of functional groups of metal complexes	H-S 78-84; C 180-187
11	W 10/6	Wave equation, Quantum numbers	H-S 7-25; S 1-10
12	F 10/8	Exam#1	
13	M 10/11	Symmetries of atomic orbitals	Orbital Shapes, on Canvas; H-S 12-15; C 88-91
14	W 10/13	MO's for H_2^+ and H_2	H-S 32-37
15	F 10/15	MO's for diatomics; Photoelectron spectroscopy	H-S 38-42; S 11-20; H-S 130-131; C 116-117, 124, 130-131
16	M 10/18	heteronuclear diatomics	H-S 130-131; C 116-117, 124, 130-131
17	W 10/20	Combining orbitals on one center – hybrid orbitals	H-S 144-148; C 95-104, 153-156
18	F 10/22	Combining orbitals on multiple centers – molecular orbitals	H-S 149-153; C 104-117, 138-149
19	M 10/25	Representations; Use of Symmetry in MO theory; MOs for H_2O	H-S 153-156; C 138-149; S 79-87
20	W 10/27	MOs for BF_3	H-S 156-168; C 138-149
21	F 10/29	MOs for ethylene (ethene)	H-S 156-168; C 118-126
22	M 11/1	MOs for B_2H_6	H-S 169-171

23	W 11/3	Hückel MO method	S 33-39; C 126-131
24	F 11/5	Exam #2	
25	M 11/8	HMO small organics, electron densities, bond orders, nodes	S 40-44, 48-58
26	W 11/10	HMO continued	S 63-70; 97-106; C 88-89
27	F 11/12	Basis functions as representations; Gaussian	S 65; C 138
28	M 11/15	EPR as illustration of MOs	H-S 121-124; S 50-53
29	W 11/17	Spin density and hyperfine coupling	"
30	F 11/19	Summary and review	
	M 11/23	Final exam	comprehensive

Grading
2 mid-term exams 25% each
Final exam 50%
Final grade also depends on evidence of improvement. A high score on the final exam will be emphasized relative to a low score on the first exam.