

Chem 5050
Physical Inorganic Chemistry
Fall 2024

Instructor: Aaron Sadow, 2101B Hach Hall, Email: sadow@iastate.edu; phone: 4-8069
Class Hours: Monday, Wednesday, Friday 8:50 – 9:40 am in 1114 Gilman Hall
Office Hours: MWF 9:40 am or by appointment
Required Texts: F. A. Cotton, *Chemical Applications of Group Theory*, Wiley, 1990 and Harris and Bertolucci, *Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy*, Dover Books

Class Goals: Learn about chemical models for molecular spectroscopy and bonding particularly of inorganic complexes; become comfortable with anticipating molecules' structures, analyzing bonding and electronic properties in molecules, and interpreting some spectra with respect to structure and bonding.

In Class Activities: We will primarily work on answering questions in problem sets in class. Prior to class, you will need to read assigned content and work on problem sets.

Topics:

- (1) VSEPR, electron counting, electronic structure
- (2) Chapter 2: Properties of Groups
- (3) Chapter 3: Symmetry Operations and Point Groups
- (4) Chapter 4: Representation of Groups
- (5) Chapter 5: Group Theory and Quantum Mechanics
- (6) Chapter 6: Symmetry Adapted Linear Combinations
- (7) Chapter 10: Molecular Vibrations
- (8) Chapter 7: MO Theory in Organic Chemistry
- (9) Chapter 8: MO Inorganic and Organometallics
- (10) Chapter 9: Ligand Field Theory and Electronic Spectroscopy
- (11) NMR spectroscopy
- (12) EPR spectroscopy

Success in the course: Group theory and its applications in molecular orbital theory and spectroscopy require significant study efforts to understand both theoretical/abstract concepts be able to perform practical applications in analysis.

We have high standards for the class

Reading materials and practice problems should be studied prior to class.

Engage in class activities - ask questions and come prepared.

Communicate in appropriate style and language.

Punctually attend class. Tardiness and unexcused absences create embarrassment.

Do not cheat. Academic misconduct will not be tolerated.

Supplementary Literature: It is often useful to read a number of perspectives describing a topic for better understanding, and these supplementary literature are useful for that purpose.

- 1) *Molecular Symmetry and Group Theory*, Robert L. Carter, Wiley 1998
- 2) *Physical Methods in Chemistry*, R. Drago
- 3) *Introduction to Ligand Field Theory*, B. N. Figgis
- 4) *Elementary Linear Algebra*, Howard Anton

Electronic Tools and Software

ChemDraw is available for free. Install and use, with Drawing Settings "ACS Style"

Mathematica and/or MatLab may be used for a number of computations. Also freely available.

Course Grading:	Two exams:	2 × 100 points	TBD
	Final	150 points	
	In class participation	150 points	

Content Expectations:

- (1) VSEPR. Be able to use the VSEPR approach to quickly identify simple molecular geometries as a starting point for more detailed analysis. Know how to use the periodic table to count valence shell electrons, and then apply the VSEPR scheme.
- (2) Properties of Groups: Understand what makes a Group. Matrix manipulations, multiplication rules and other operations, orders of groups, Abelian groups, classes
- (3) Symmetry Operations: Operations (identity, rotation, reflection), their representations, multiplication, point groups, assigning molecules to point groups
- (4) Orthogonality and character tables; derivation, reducing representations, projection operators
- (5) Group theory and vibrational spectroscopy. Application of projection operators to determine normal modes. Force constant analysis. Spectral analysis.
- (6) Quantum mechanics, understand how quantum mechanics is simplified by group theory. perturbation theory.
- (7) Molecular Orbital Theory: group theory and other bonding models; symmetry of the secular determinant, organic and inorganic molecular orbital diagrams.
- (8) Apply Crystal Field Theory and Ligand Field theory to understanding electronic spectra of transition metal compounds.
- (9) Other topics: Jahn-Teller Effects, crystallographic symmetry, NMR spectroscopy, EPR spectroscopy

Schedule for Chem 5050

Week 1: 26, 28, 30 August

Classify molecules electronic structure and shape

Assignments. Read Parkin *J. Chem. Ed.* **2006**, Burdett "Molecular Shapes" Chapter 3

Install and begin to use Chemdraw and Mathematica

Problem Sets 1 and 2.

Week 2: 4, 6 September

Properties of Groups

Assignment. Read Cotton Chapter 2: Definitions and Theorems of Group Theory

Read Harris, Section 1.1-1.3

Problem Set 3.

Week 3: 9, 11, 13 September

Symmetry operations

Assignments. Read Cotton Chapter 3: Molecular symmetry and the symmetry groups

Read Harris, Chapter 1.4-1.5

Problem Set 4.

Week 4: 16, 18, 20 September

Representations

Assignments. Read Cotton Chapter 4. Matrix algebra in Appendix I;

Harris 1-6-1.7

Problem Set 5. Matrix operations on a single point. Matrix multiplication is easier using Mathematica (or MatLab). You may wish to bring your computer to do the matrix math.

Problem Set 6. Reducible representations.

Week 5: 23, 25, 27 September

Group Theory and Quantum Mechanics

Assignments. Read Cotton Chapter 5.

Harris, Secs. 1-8 and Chapter 2

Problem Set 7. Direct Products

Week 6: Friday 30 September; 2 October, **4 October: Exam 1 covers through Chapter 5**

Begin Projection operators and functions

Assignments. Read Cotton Chapter 6.

Problem Set 8. Projection operators to generate SALCS

Week 7: 7, 9, 11 October

Symmetry adapted linear combinations (SALCS)

Assignments. Read Cotton Chapter 6 and Sannigrahi

Week 8: 14 October (Maybe MWR ACS), 16, 18 October

Molecular Vibrations.

Assignments. Read Cotton Chapter 10, Harris, Chapter 3

Problem Set 9.

Week 9: 21, 23, 25 October

Molecular Vibrations Continued

Problem Set 10.

Week 10: 28, 30 October, **Exam 2: 1 November Chapters 6 and 10 (SALCs and Vibrations)**

MO Theory in Organic Chemistry

Assignments. Read Cotton, Chapter 7;

Woodward and Hoffman

Harris Chapter 4

Problem Set 11.

Week 11: 4, 6, 8 November
MO Theory in Inorganic and Organometallic Chemistry
Assignments. Read Cotton. Chapter 8
Problem Set 12.

Week 12: 11, 13, 15 November
Ligand Field Theory and Electronic Spectroscopy
Assignment. Read Cotton Chapter 9
Harris Chapter 5

Week 13: 18, 20, 22 November
18, 20 November Guest Lectures (TBD)
NMR

Week 14: 2, 4, 6 December
EPR

Week 15: 9, 11, 13 December
Catch Up, Review, and Presentations

Finals Week: 16-20 December

Syllabus Statements

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