Chemistry 6330 **Advanced Inorganic Chemistry – Group Theory**

Autumn Semester 2019, Session 1 MWF 10:20 – 11:15 PM, 2003 Evans Lab

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Principles and Applications of Group Theory in Inorganic Chemistry

Text: F.A. Cotton, "Chemical Applications of Group Theory", 3rd Edition

I. Introduction to groups and group representations (Cotton, Chapters 2 – 4)
   a. Definition and examples of groups
   b. Products of symmetry operations and class structure
   c. Matrix representation of groups
   d. The Great Orthogonality Theorem
   e. Characters and character tables

II. Molecular vibrations (Chapter 10)
   a. Normal modes and fundamental vibrations
   b. Infrared and Raman selection rules
   c. CO stretches in metal carbonyl complexes

III. Applications to π-bonding in organic molecules (Chapter 7)
   a. LCAO and Hückel approximations
   b. Secular equations
   c. Carbocyclic systems and other π-bonded molecules
   d. Electronic transitions

IV. Molecular orbital theory (Chapter 8)
   a. Principles of molecular orbital theory
   b. Symmetry and molecular orbitals
   c. The construction of qualitative MO diagrams
   d. Bonding in σ-donor, π-donor, and π-acceptor complexes
   e. Molecular orbital theory and electronic spectroscopy
   f. Correlation diagrams (Chapter 9)

Additional Course Information

Homework: problem sets will be given in class at a rate of about one per week. These problem sets will not be graded and will not count toward your grade in the course; however, you are strongly urged to understand and solve the assigned problems. Solutions to the homework will be posted on the web at

https://research.cbc.osu.edu/turro.1/graduate-courses/

Office hours: Sean will have office hours at time and days TBD in 4144 Newman-Wolfrom. Profs. Turro and Shafaat will not have specific times set aside for office hours, but time to meet each of them can be arranged via email.

Exams: There will be one midterm exam and a final exam. These will be weighted equally and will cover (approximately) the first and second halves of the course, respectively. We plan to schedule the 2-hour midterm exam on Friday, Sept. 13 in the afternoon or late afternoon (exact time will be decided in class). The 2-hour final exam is scheduled for October 7, 8, or 9 (exact time to be decided in class).

Additional books: In addition to the assigned text, the following books may be useful:

Hall, "Group Theory and Symmetry in Chemistry"

Tinkhan, "Group Theory and Quantum Mechanics"

Ballhausen, "Introduction to Ligand Field Theory"

Orchin, "Symmetry, Orbitals, and Spectra"

Wilson, "Molecular Vibrations"

All students with documented disabilities, who need accommodations, should see the instructor privately to schedule an appointment as early in the quarter as possible. If your disability requires materials in alternative format, please contact the Office for Disability Services at 292-3307, Room 150 Pomerene Hall.