**CHEM 5120: Physical Methods in Chemistry**

**Text:** Russell S. Drago, *Physical Methods for Chemists,* Surfside Scientific Publishers, Gainesville, FL, 1992.

**Grading:** The grade for the course will be determined from;

Two hour exams (100 points each) 50%

Homework assignments (100 points total) 25%

Final exam (100 points) 25%

**Grading** **scale;**

A >90

A- 89-85 C 64-60

B+ 84-80 C- 59-55

B 79-75 D 54-50

 B- 74-70 F <50

C+ 69-65

The course will follow the outline of the text with supplemental readings assigned from the literature. These and the homework assignments will be made at the appropriate times in class. We will cover the first nine chapters, and selected material from chapters 10 and 13 as time permits. Exams will be announced at least two weeks in advance. The class format will be mostly lecture format. However, questions and discussion are encouraged during class and outside of class.

This class explores the use of various spectroscopic techniques in the determination of molecular structures and the application of molecular symmetry to these analyses. We will concentrate on infrared (FTIR), electron absorption (UV-VIS), Fourier Transform nuclear magnetic resonance (FTNMR) and electron paramagnetic resonance (esr or epr) spectroscopies. The emphasis will be on the application of these to problems in Inorganic Chemistry. We will try to balance the underlying theory of these techniques with practical examples of their applications. We will develop in some detail the concepts of molecular symmetry and group theory as many of the techniques depend on knowing the symmetry of the molecule. We will use the results of molecular orbital theory, but will not develop this in depth. An understanding of the concepts of physical chemistry and molecular structure is required for the course.

**References.**

1. F. Albert Cotton, Chemical Applications of Group Theory. 3rd edition, Wiley Interscience, 1990. This is the most authoritative and complete text on symmetry and Group theory. Easily readable. 541.2C829 (1963)

2. R. L. Flurry, Jr., Symmetry Groups: Theory and Chemical Applications. Prentice-Hall, 1980. A more rigorous and mathematically based treatment of symmetry and group theory.

3. William A Guillory, Introduction to Molecular Structure and Spectroscopy Allyn & Bacon, 1977.

4. S. F. A. Kettle, Symmetry and Structure: Readable Group theory for Chemists, 2nd edition, John Wiley, 1995. An easily read text. QD471.K47516

5. M. Orchin and H. H. Jaffee, Symmetry, Orbitals, and Spectra, Wiley-Interscience, 1971. Also an easily read text.

6. E. A. V. Ebsworth, D. W. H. Rankin, and S. Cradock Structural Methods in Inorganic Chemistry, Blackwell Scientific Publications, 1987. A non-mathematical treatment of the subject area of the course. This book focuses more on interpretation of spectra, less rigorously on theory. QD95.E29

7. K. Nakamoto, Infrared Spectra of Inorganic and Coordination Compounds. John Wiley & Sons. I have the 1963 edition, there are later editions. 535.84 N145

8. Chemical Reviews. **2000,** *100,* Number 2. ACS. Dedicated to Computational Transitional Metal Chemistry.

9. Chapters on bonding in inorganic chemistry and structures of inorganic compounds may be found in any current text of inorganic chemistry.