

CHM 6680

Spring, 2016

**Characterization of Paramagnetic Molecules
(Section 1A24 3 credits)**

Prof. George Christou

CLB 408A

Email: christou@chem.ufl.edu

Class Times: T, R: Period 4/5

Room: CLB 414

Office Hours: T 2.00-4.00, and
by appointment

Description: Metal-containing paramagnetic molecules are commonly encountered in chemistry and biochemistry, in fields ranging from inorganic chemistry to the active sites of metalloproteins and metalloenzymes. In all these areas, the presence of the unpaired electron(s) has a major impact on the observed physical and spectroscopic properties. Many chemical and biochemical systems contain mononuclear metal ions, whereas others contain polynuclear sites comprising two or more interacting metal ions. The course will therefore cover the qualitative and quantitative tools and theories needed to understand the magnetic and spectroscopic properties of molecular metal compounds (both mononuclear and multinuclear) possessing unpaired electrons.

Outline: Basic concepts and definitions in magnetism
Magnetization and magnetic susceptibility
Spin and orbital angular momentum
The van Vleck equation
Transition metals vs lanthanides
Zero-field splitting in mononuclear metal compounds
High-spin/low-spin equilibrium, and spin crossover
Polynuclear compounds and intramolecular exchange interactions
Mechanisms of antiferromagnetic and ferromagnetic interactions
Spin frustration in polynuclear compounds
Single-molecule magnets (molecular nanomagnets)
NMR of paramagnetic molecules
EPR of mononuclear paramagnetic metal complexes (time permitting)

Grade: The course grade will be determined by two exams during the semester (30% each) and a Final Exam (40%).

Reference Texts (no required text):

1. *Molecular Magnetism*, O. Kahn, VCH Publishers, Mannheim, 1993
2. C. J. O'Connor, *Prog. Inorg. Chem.* **1982**, 29, 203
3. *Physical Methods in Chemistry*, R. S. Drago, 1st or 2nd Edition
4. *Magnetochemistry*, R. L. Carlin, Springer-Verlag, Berlin, 1986
5. *Magnetism and Transition Metal Complexes*, F.E. Mabbs and D.J. Machin, Dover Publications, New York, 2008

Other Information:

Honor code statement: see <http://www.chem.ufl.edu/~itl/honor.html>

Students with disabilities: see <http://www.chem.ufl.edu/~itl/disabilities.html>

Counseling and Health Care: see <http://www.chem.ufl.edu/~itl/counseling.html>