

CHM 6680

Spring, 2021

**Characterization of Paramagnetic Molecules  
(Section 22287 3 credits)**

Prof. George Christou

CLB 408A

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**Class Times:** M, W, F: Period 4

**Room:** CCB 221

**Office Hours:** W 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, 1<sup>st</sup> or 2<sup>nd</sup> 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

1. **Other Information: Honor code statement:** see <https://sccr.dso.ufl.edu/policies/student-honor-code-student-conduct-code/>
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