

CHM 6680

Spring, 2023

Characterization of Paramagnetic Molecules

Section: 19501 Credits: 3

Instructor: Prof. George Christou

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Class Times: T, R: Periods 3-4 (Class will be 10.00 – 11.15 am) **Room:** CLB 414

Office Hours: W 2.00 - 4.00 pm, 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%).

Final Exam: 3:00 - 5:00 pm on May 1, 2023

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

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