Synthetic Tuning of Ligand field for Precise Control of Molecular Zero-Field Splitting

Wesley J. Transue

Motivation

- Molecules are highly tunable and compact, making them highly promising for quantum sensing applications
- Realization of this goal will require precise control of the magnetic properties that control the relevant quantum states

Project Description

- We will pursue the synthesis of new titanium(II) transition metal complexes
- Restriction to trigonal symmetry will enable comparisons with nitrogen vacancy centers of diamond
- We aim to allow for optical initialization of the quantum states

Context

- The use of molecules is currently limited by their generally poor coherence properties and their ESR addressability
- Control of spin Hamiltonian parameters is necessary to enable use of pulsed magnetic resonance techniques

University of Pittsburgh

Tuning of **Magnetic Properties** of Early Transition Metal Complexes Towards **Molecular Quantum Sensors**

Project Deliverables

- Synthesis of trigonally-symmetric titanium(II) transition metal complexes
- Characterization of their ground and excited states through magnetic circular dichroism (MCD) spectroscopy
- Assignments of excited states through ligand field theory and computational techniques (density functional theory, multireference post-Hartree–Fock methods)
- Insight into molecular coherence properties through measurement of T_1/T_2 times with electron spin resonance spectroscopy

Potential Impact

- We aim to identify ways to design the molecular ligand sphere to enable precise control of the zero-field splitting and g matrix that control the molecular magnetism
- Through control of the identities and energetic spacings of electronic excited states, we will give insight into the ways that optical excitation may be used to deliver spin polarized ground states

References and/or Acknowledgements

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