Nickel(II) Metal Complexes as Optically Addressable Molecular Qubits

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INTRODUCTION

What is a qubit?

- A quantum bit, or “qubit” is the basic unit of quantum information
- Quantum information science (QIS) promises advancement across fields like computing, simulation, and sensing. A propitious approach to quantum sensing involves using electronic spins as qubits.

What properties should a qubit have?

- Solid-state defects, like the anionic nitrogen-vacancy defect in diamond, are ideal spin qubits as qubits should be easily initialized, read out, and manipulated.
- Based N centers, like the anionic nitrogen-vacancy defect in diamond, are ideal spin qubits as qubits should be easily initialized, read out, and manipulated.

How can we do this with molecules? Why?

- We want to emulate these properties of the NV center, while benefiting from the tunable, scalable, and portable nature that spin-bearing molecules possess.
- We proposed synthesizing octahedral complexes of biocompatible nickel(II) with strong-field ligands to minimize oxidation state of the metal ion changed.

SYNTHESES

Ligand syntheses

Syntheses of strong field N-heterocyclic carbene (NHC) ligands²

Metalations

Coordination of N-CN³ (CNC=2,6-bis(3-alkylimidazol-2-ylidene)pyridine)) ligands 2:1 to Ni(II)³

Characterization

Characterized [Ni(bpy)²Cl]²⁺ by H-NMR spectroscopy, electronic absorption spectroscopy, single-crystal X-ray diffraction, and magnetometry

RESULTS

Magnetometry

Variable temperature molar magnetic susceptibility experiment

Conclusion

The D value we extracted enables pulse EPR measurements and is smaller than previously reported values for octahedral nickel(II)-complexes with bipyridine ligands (non alkyl-substituted). These results further outline the design of Ni(II) molecules as viable optically addressable qubits, continually expanding the catalogue of qubit materials to air-stable compounds.

Future work

- Preliminary electronic absorption spectra suggests Ni(II) ligands contribute to higher energy excited states. However, the absence of lower energy bumps may suggest that the oxidation state of the metal ion changed.
- Obtaining magnetometry, and X-ray diffraction data on these complexes would be promising.

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References