Experimental and Theoretical Studies of a Nickel(II) complex

A. Wojciechowska[a], M. Daszkiewicz[a], Z. Staszak[b], A. Trusz-Zdybek[a], A. Bienko[c], A. Ozarowski[d],

[a] Wrocław University of Technology (Poland), [b] Polish Academy of Science, [c] Wrocław University (Poland), [d] NHMFL

The metal complexes play an important role in regulating biological activities. Many coordination compounds present the activity against tuberculosis, influenza, rheumatism or are suggested as pesticides and fungicides. In this work we present the full X-Ray structure determination, spectroscopic FIR-IR, NIR-Vis-UV, HF EPR and magnetic studies as well as microbiological characterization of a new hexa-coordinated nickel(II) complex containing imidazole and L-tyrosine, of a formula $[Ni(Im)_2(L\text{-}tyr)_2]\cdot 4H_2O$.

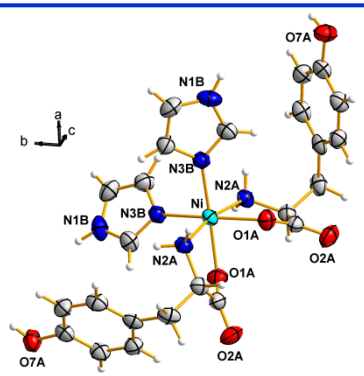
High-field EPR allowed determine the parameters of the spin Hamiltonian

$H = \beta\, B\cdot\mathbf{g}\cdot S + D(S_z^2 - S(S+1)/3) + E(S_x^2 - S_y^2)$

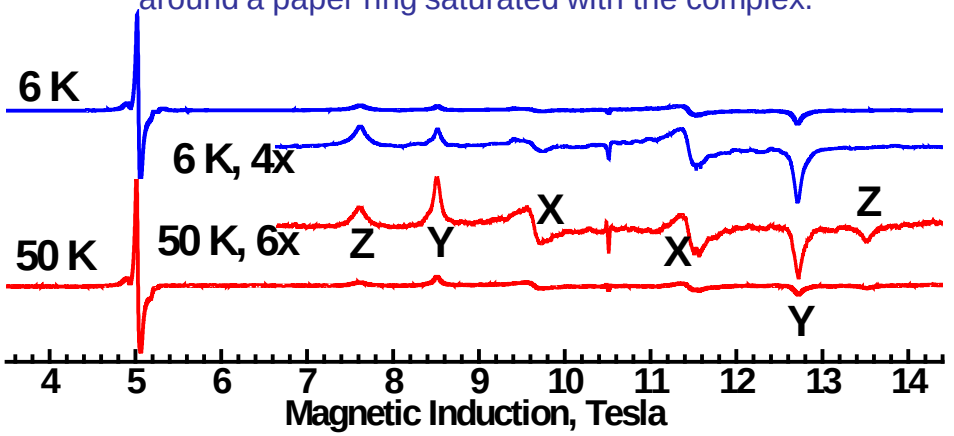
g_x=2.17, g_y=2.17, g_z=2.193, D=-3.010 cm^{-1}, E=-0.4066 cm^{-1}

These results correlated well with the electronic spectroscopy data. Quantum-mechanical calculations (DFT and Unrestricted Hartree-Fock) were also performed to calculate the zero-field splitting parameters D and E, with the UHF method better reproducing the experimental data.

Theoretical interpretation of the zero-field splitting is a topic extensively studied in recent literature and reliable experimental data are needed for continuing progress in that area. Results described above could not be achieved using conventional EPR instrumentation.



Left: The X-Ray structure of $[Ni(Im)_2(L\text{-}tyr)_2]\cdot 4H_2O$. Right: Inhibition of growth of a bacteria colony (Serratia marcescens) around a paper ring saturated with the complex.



High-Field EPR spectra recorded with ν=324 GHz. The molecular orientations for the transitions are labeled by X, Y, Z.

Facilities: EMR.

Acknowledgements : This work was supported by grant DMR 0654118, the DOE, the State of Florida and by the Wrocław U. of Technology

Citation: Wojciechowska, A.; Daszkiewicz, M.; Staszak, Z.; Trusz-Zdybek, A.; Bienko, A. and Ozarowski, A., *Synthesis, Crystal Structure, Spectroscopic, Magnetic, Theoretical, and Microbiological Studies of a Nickel(II) Complex of l-Tyrosine and Imidazole, $[Ni(Im)_2(l\text{-}tyr)_2]\cdot {}_4H_2O$,* **Inorg. Chem.**, **50** (22), 11532-11542 (2011).