Magneto-Biological Characterization of New Metal Complexes Containing Nitroimidazole

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Introduction

New complexes of transition metals, like Cu, Ni, Co, Mn, containing in addition to other ligand also the antibiotic molecule 1-(β-hydroxyethyl)-2-methyl-5-nitroimidazole (mnz) were prepared and investigated by HFEPR and other techniques. Structure of the complex $Ni(bba)_2(mnz)_2(H_2O)_2$ (**1**), where bba is 2-bromobenzoic acid is shown in **Fig.1**.

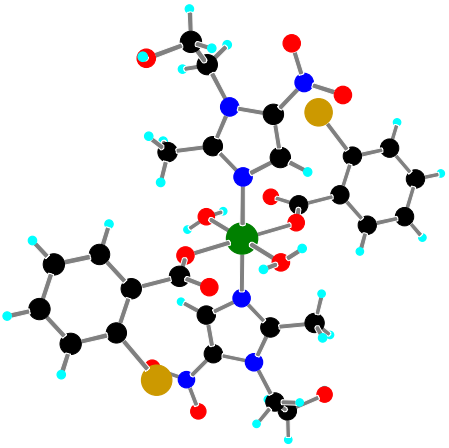

Fig.1 Structure of $Ni(bba)_2(mnz)_2(H_2O)_2$ (**1**)

Experimental

The HFEPR spectra were recorded on the 15/17 T SC magnet and transmission spectrometer of the EMR facility. Other studies, like FT-IR, NIR-Vis-UV and Hirshfeld surface measurements and antimicrobial screening of the complexes were accomplished at the University of Ilorin. Density Functional Theory (DFT) calculations were performed to calculate the exchange integrals in binuclear complexes.

Results and Discussion

Good quality HFEPR spectra were obtained for the mononuclear Ni(II) and Cu(II) complexes as well as for the binuclear Cu(II) complexes. A spectrum of the Ni complex (**1**) is presented in **Fig.2**. Spectra were interpreted using a standard spin Hamiltonian

$$\hat{\boldsymbol{H}} = \mu_B \boldsymbol{B}\{g\}\hat{\boldsymbol{S}} + D\left\{\hat{S}_z^2 - \frac{1}{3}S(S+1)\right\} + E\left(\hat{S}_x^2 - \hat{S}_y^2\right) \qquad [1]$$

with $S = 1$. For **1**, $D = -3.34$ cm^{-1}, $E = -0.59$ cm^{-1} were found from simulation procedures.

One of the studied Cu(II) dimeric complexes has a well-known "paddlewheel" structure with strong antiferromagnetic exchange coupling, and exhibits characteristic EPR spectra [1] with $D = -0.35$ cm^{-1}. The copper ions in the other dimer are very weakly coupled and also the zero-field splitting is very small, $D = -0.023$ cm^{-1}, as it is due to the dipolar interactions only.

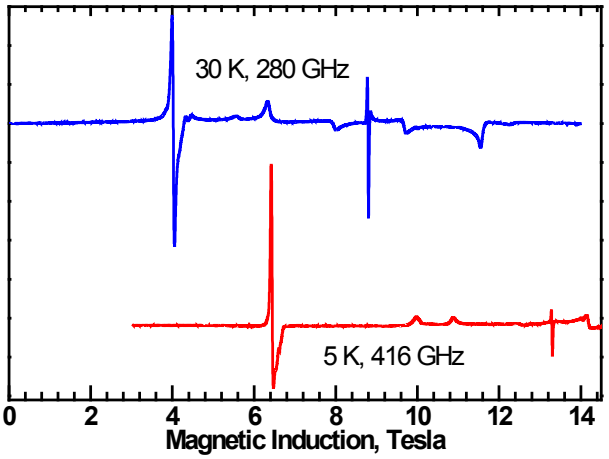

Fig.2 HFEPR spectra of **1**.

Conclusions

Spin Hamiltonian parameters for a variety of transition metal complexes were accurately determined from HFEPR spectra. DFT calculations of the exchange integrals in binuclear copper complexes reproduced reasonably the experimental data. Theoretical calculations of the D parameter in the nickel complex are currently on the way. This research is ongoing.

Acknowledgements

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References

[1] Ozarowski, A., Inorg. Chem., **47**, 9760-9762 (2008).