HIGH-FIELD EPR AND MAGNETIC SUSCEPTIBILITY STUDIES ON A HETEROMETALLIC COMPLEX $[Cu_2CoPbCl_4(HL)_4]_2$ WHERE HL IS 2-(DIMETHYLAMINO)ETHANOL

A. Ozarowski, L.C. Brunel (NHMFL); V.N. Kokozay, (Kiev U., Inorganic Chemistry)

Introduction

In recent years much interest has been focused on synthesis of heterometallic complexes with a variety of bridging ligands. Their role in catalysis, photochemistry and biological systems has been widely examined. The magnetic exchange between different metal ions has become an active field of research in modern coordination chemistry [1,2]. In this work, we have investigated a novel heterotrimetallic complex, $[Cu_2CoPbCl_4(HL)_4]_2$ where HL is 2-(dimethylamino)ethanol.

Experimental

The EPR spectra were taken on the 17 Tesla transmission spectrometer of the EMR facility at the NHMFL. The magnetic susceptibility was measured by using a SQUID magnetometer at the Department of Chemistry, Wroclaw University, Poland.

Results and Discussion

In the EPR spectra no signal was observed that could be attributed to the title compound, most likely because of the fast relaxation processes and line broadening due to the metal-metal interactions in the trinuclear system. The magnetic susceptibility data were interpreted in terms of the spin Hamiltonian

$$\mathbf{H} = J_{Co\text{-}Cu}\,(\mathbf{S}_{Co}\mathbf{S}_{Cu1} + \mathbf{S}_{Co}\mathbf{S}_{Cu2}) + J_{Cu\text{-}Cu}\,\mathbf{S}_{Cu1}\mathbf{S}_{Cu2} + D_{Co}\{\mathbf{S}_z^2{}_{Co} - 1/3\cdot S_{Co}(S_{Co}+1)\} + \mu_B B(g_{Co}\mathbf{S}_{Co} + g_{Cu1}\mathbf{S}_{Cu1} + g_{Cu2}\mathbf{S}_{Cu2})$$

The complex consists of two relatively isolated trinuclear units $CoCu_2$. No interaction between these subunits was assumed. The energies of the 16 levels in the system were calculated by numerical diagonalization of the entire 16x16 spin Hamiltonian matrix. The magnetic susceptibility was then calculated from the formula

$$\chi = -\frac{N}{B}\frac{\sum_{i=1}^{16}\frac{\partial E_i}{\partial B}\exp(-E_i/kT)}{\sum_{i=1}^{16}\exp(-E_i/kT)} + TIP \quad [1]$$

The magnetic data were fitted by using a least-squares procedure based on the Simplex method. The results are shown in Fig. 1.

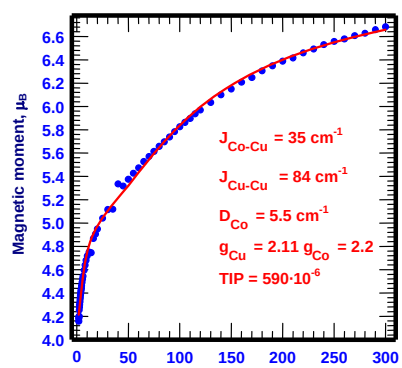

Fig. 1. The temperature dependence of the magnetic moment

Conclusions

The magnetic properties of the title compound are affected by both the antiferromagnetic exchange interactions in the trinuclear $CoCu_2$ system and by the zero-field splitting on the high-spin cobalt(II) ion.

Acknowledgements

This work was supported by INTAS (Ukraine, Project 03-51-4532) and by NHMFL through project 7300-059. NHMFL is funded by the NSF through Grant DMR-0084173 and the state of Florida.

References

[1] Buvaylo, *et al*., Inorganic Chemistry, **44**, 206-216 (2005).
[2] Buvaylo, *et al*., Chemical Communications, **39**, 4976-4978 (2005).