HIGH-FIELD EPR AND MAGNETIC STUDIES ON A HEXA-COPPER COMPLEX $[Cu_3CdI_2(TeaH)_3]_2{\cdot}4DMF$ ($C_{48}H_{106}Cd_2Cu_6I_4N_{10}O_{22}$)

V. Kokozay (Taras Shevchenko University, Kiev, Ukraine); A. Ozarowski, L.C. Brunel (NHMFL)

Introduction

The centro-symmetric compound $[Cu_3CdI_2(TeaH)_3]_2{\cdot}4dmf$ (H_3Tea - triethanolamine) has a peculiar topology with 6 copper atoms joined by bridging O atoms from the ligands to form a zig-zag chain with Cu-Cu separations being 2.937(2) - 2.405(2) A. (Fig. 1)

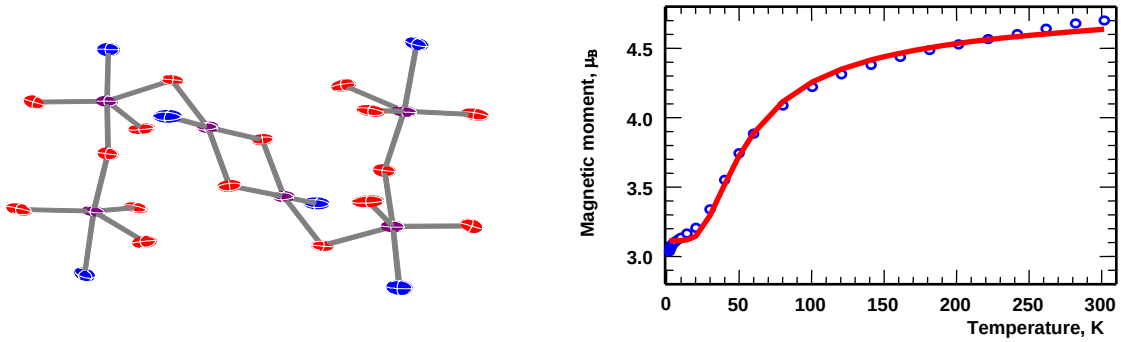

Fig. 1. The structure of the core of $[Cu_3CdI_2(TeaH)_3]_2{\cdot}4dmf$ showing six copper atoms (purple) and the temperature dependence of its magnetic moment (right).

Experimental

The EPR spectra (Fig. 2) were recorded using the 17 Tesla transmission instrument of the EMR facility.

Results and Discussion

The magnetic properties were interpreted with the spin Hamiltonian $H = \sum_i \sum_{j>i} J_{ij} S_i S_j$ The molecular symmetry implies that there are only three pairs of the next-neighbor exchange integrals and other exchange interactions were neglected. The magnetic moments were fitted with $J_{12} = J_{56} = 68$ cm^{-1}, $J_{23} = J_{45} = 20$ cm^{-1}, $J_{34} = -61$ cm^{-1} (Fig. 1). In the high-field, low temperature EPR spectra (Fig. 2) a signal due to the triplet state was observed. The slight discrepancy between the simulated and experimental magnetic moments at the lowest temperatures is likely to be due to the zero-field and Zeeman splitting in the ground triplet state being comparable to kT[1]. The EPR spectrum exhibits effects due to non-coaxiality of the g and zero-field splitting tensors and probably also due to the antisymmetric (Dzialoshinskii-Moriya) exchange interactions that are possible in the copper pairs 1-2, 2-3, 4-5 and 5-6 where the copper atoms are not symmetry-related.

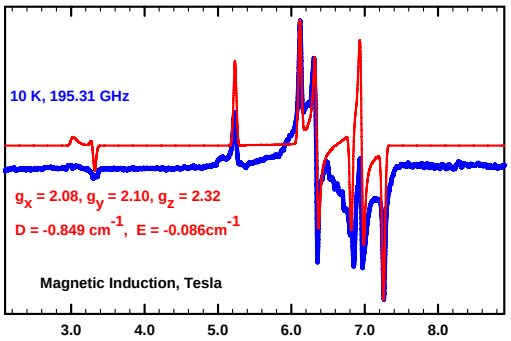

Fig. 2. Spectra of $[Cu_3CdI_2(TeaH)_3]_2{\cdot}4dmf$: Experimental (blue) and the simulated triplet state spectrum (red).

Acknowledgements

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References

[1] Buvaylo, E.A., *et al*., Inorganic Chemistry, **44**, 206-216 (2005).