

**s9.m1.p7** Synthesis, Crystal Structure and Magnetic Properties of a ( $\mu$ -Hydroxo)( $\mu$ -Pyrazolato) Dicopper(II) Complex. Y. Elerman<sup>1</sup>, H. Kara<sup>1</sup>, K. Prout<sup>2</sup>, <sup>1</sup>Department of Engineering Physics, Faculty of Sciences, University of Ankara, 06100 Besevler-Ankara, Turkey. <sup>2</sup>Chemical Crystallography Laboratory, University of Oxford, 9 Parks Road, OXFORD OX1 3PD, England  
Keywords: binuclear copper(II) complex, super-exchange interactions, antiferromagnetic coupling.

Preparation and magnetic properties of a 3,5-dimethylpyrazolate bridged binuclear copper(II) complex [Cu<sub>2</sub>(L)(3,5-pyz)] (L=1,3-Bis(2-Hydroxy-1-naphthylideneamino)propan-2-ol) is reported. The crystal structure of the complex was determined at 200K: [C<sub>30</sub>H<sub>26</sub>N<sub>4</sub>O<sub>3</sub>Cu<sub>2</sub>], monoclinic, space group P2<sub>1</sub>/n, a=7.782(2), b=15.672(2), c=20.788(3) Å,  $\beta$ =96.144(2)°, V=2520.7(8)Å<sup>3</sup>, Z=4. The coordination sphere is four-coordinated, planar with an N<sub>2</sub>O<sub>2</sub> donor set. There are significant intermolecular interactions between neighbouring binuclear entities. The shortest intermolecular Cu ... Cu<sup>1</sup> distance is 3.399(1) Å and Cu-O<sup>1</sup> distance is 2.722(1) Å (i= -x, -y, 1-z). In the structure, the dihedral angle between the two coordination planes is 165.04°. The variable-temperature magnetic susceptibility measurement for a powdered sample of the complex was carried out in the temperature range 5-350 K and analysed to obtain values of the parameter J in the exchange Hamiltonian  $H = -2JS_{Cu}S_{Cu}$ ; J=-222 cm<sup>-1</sup>. The magnetic moment at 300 K is about 2.75 $\mu_B$  while 0.3 $\mu_B$  at 5 K. The nature of the magnetic super-exchange interaction of the title compound is compared with similar dinuclear Cu(II) complexes<sup>1,2,3</sup>. The strong antiferromagnetism of the present complex is reasonably explained in terms of the orbital complementary effect based on Hoffmann's theory for superexchange interaction.

**s9.m1.p8** Synthesis, Crystal Structure and Magnetic Properties of a Novel [Gd<sup>III</sup>-Cu<sup>II</sup>] Heterodinuclear Complex. H. Kara<sup>1</sup>, Y. Elerman<sup>1</sup>, K. Prout<sup>2</sup>, <sup>1</sup>Department of Engineering Physics, Faculty of Sciences, University of Ankara, 06100 Besevler-Ankara, Turkey. <sup>2</sup>Chemical Crystallography Laboratory, University of Oxford, 9 Parks Road, OXFORD OX1 3PD, England  
Keywords: heterodinuclear complex, super-exchange interactions, lanthanides.

Preparation and magnetic properties of heterodinuclear complex, namely LCu(Me<sub>2</sub>CO)Gd(NO<sub>3</sub>)<sub>3</sub> (L being (N,N'-bis(3-methoxysalicylidene)propane-1,2-diamine) and (Me<sub>2</sub>CO standing for acetone) is reported. The crystal structure of the complex was determined at 200K: [(C<sub>19</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub>)Cu(C<sub>3</sub>H<sub>6</sub>O)Gd(NO<sub>3</sub>)<sub>3</sub>] the compound crystallizes in the monoclinic space group P $\bar{1}$ , with a=9.795(9), b=18.763(13), c=15.579(13) Å,  $\beta$ =95.30(7)° and Z=4. The X-ray structure show that the Cu(II) ion adopts a square-based [4+1] coordination mode, the equatorial N<sub>2</sub>O<sub>2</sub> donor are from L and the oxygen atom from the coordinated acetone molecule in the apical site. The Gd(III) ion is ten-coordinate. In addition to the two phenolate oxygen atoms, the coordination sphere contains two oxygen from the OMe side arms of L and six oxygen from the three bidentate nitroto ions. The magnetic susceptibility of the complex was measured over the range 5-350 K and the observed data were successfully simulated by the equation based on the spin-hamiltonian operator ( $H = -JS_{Cu}S_{Gd}$ ), giving the exchange integral J(Cu-Gd)=5.6(1) cm<sup>-1</sup>. This indicates a weak ferromagnetic spin exchange interaction between the Cu<sup>II</sup> and Gd<sup>III</sup> ions. The nature of the magnetic super-exchange interaction of the title compound is compared with similar [Gd<sup>III</sup>-Cu<sup>II</sup>] Heterodinuclear complexes<sup>1,2,3</sup>.

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