



The use of ligands with carboxylate groups makes that the first supramolecular association is organized by the effect of OH...O hydrogen bonds. The  $\pi$ ... $\pi$  stacking interactions between blocking ligands can cooperate in the formation of the whole crystal structure. All of these interactions can link low-dimensional complexes to give high-dimensional supramolecular structures and further stabilize the crystal structures in the solid state.

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[1] D. Braga, *J. Chem. Soc., Dalton Trans.* **2000**, 3705 and references therein.

**Keywords:** copper complexes; crystal structures; coordination chemistry

#### FA4-MS06-P06

##### Crystal Structures of Double Oxygen-bridged Tetranuclear and Polynuclear Metal Complexes.

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The [N,N'-bis(salicylidene)-1,3-propane-diamine, (SALPD), (C<sub>17</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>)] ligand forms different complexes with metal salts in nonaqueous media. These compounds are of interest because of their magnetic super-exchange interactions between bridged metal ions[1]. Various combinations of metal ions are possible[2]. Magnetic interactions depend on the immediate environment of the bridge as well as on the ligand arrangement around the metal atoms. Oxygen, nitrogen, acetate or nitrite anions may constitute the  $\mu$ -bridges. We report here two new structures of this group of compounds:

(I) [Cu<sub>2</sub>(SALPD)(C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>)(N<sub>3</sub>)<sub>2</sub>]<sub>n</sub>, P 2<sub>1</sub>/n, a=11.2922(12), b=15.4136(11), c=13.6107(13) Å,  $\beta$ =97.402(5)°, Z=2, D<sub>x</sub>=1.64 g.cm<sup>-3</sup>,  $\lambda$ =0.71073 Å, I > 2 $\sigma$  2575, N<sub>par</sub>=293, R, R<sub>w</sub>→0.07, 0.16,  $\Delta\rho_{max}$ ,  $\Delta\rho_{min}$ → 1.2, -1.1 e Å<sup>3</sup>. Two doubly oxygen-bridged dinuclear Cu complexes are bridged in a head-on fashion via two azido groups to build a centrosymmetrical tetranuclear complex. The terminal Cu ion has a distorted square-pyramidal coordination,

involving two bridging O and two N atoms from a (SALPD) and one O atom from a dioxane molecule. The inner Cu ions also have an irregular square-pyramidal coordination, consisting of two bridging O atoms from a SALPD ligand, two bridging N atoms from two azido groups, and one N atom from the third azido group. Whether the coordination sphere around the metal atoms is a trigonal-bipyramide or square-pyramide was decided on the basis of  $\tau$  value calculations.  $\phi_{bridge}(Cu-N-Cu) = 102.1(3)^\circ$ ,  $\phi_{bridge}(Cu-O-Cu) = 105.6(2)^\circ$ .

(II) [ZnHg(SALPD)(C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>S<sub>2</sub>)]<sub>n</sub>, P 2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>, a=8.6824(12), b=16.1222(12), c=16.3339(11) Å, Z=4, D<sub>x</sub>=2.01 g.cm<sup>-3</sup>,  $\lambda$ =0.71073 Å, I > 2 $\sigma$  1951, N<sub>par</sub>=276, R, R<sub>w</sub>→0.031, 0.075,  $\Delta\rho_{max}$ ,  $\Delta\rho_{min}$ → 0.80, -0.88 e Å<sup>3</sup>. Doubly oxygen-bridged dinuclear ZnHg complexes are bridged via SCN groups in an end to end fashion to build a polynuclear chain. The coordination around Zn ion is a distorted square-pyramide involving two O and two N atoms from a SALPD and one N atom from a SCN group. The Hg atom has a tetrahedral environment consisting of two O atoms from a (SALPD) and two S atoms from two SCN groups. The S and N atoms of the SCN bridge between the dinuclear ZnHg complexes are coordinated to Hg and Zn atoms, respectively. This results in a polymeric chain structure. The bridging SCN groups are almost linear. S-C-N angle is 176.5(2)°,  $\phi_{bridge}(Zn-O-Hg) = 105.5(2)^\circ$  to 106.5(2)°.

[1] Fukuhara C., Tsuneyoshi K., Matsumoto N., Kida S., Mikuriya M., Mori M. *J.Chem.Soc.Dalton Trans.* **1990**, 3473. [2] Arıcı C., Ülkü D., Tahir M.N., Atakol O. *Acta Cryst.* **2001**, E57,m283-285.

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#### FA4-MS06-P07

##### Magnesium(II) phthalocyanine Coordination Compounds with 3,4- and 3,5-lutidines.

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Magnesium phthalocyanine (MgPc) and its MgPcL and MgPcL<sub>2</sub> coordination complexes (4+1 and 4+2) with N and O donor ligands deserve attention because of similarity with chlorophyll, thus being its synthetic models. Due to their electrochemical properties they find application in solar energy conversion, are used as pigments in optical disks, laser printers, display devices and chemical sensors. As a continuation of the series of works concerned with MgPc coordination with N- and O- donor ligands we present the results of syntheses and structural investigation of a number of coordination compounds of MgPc with 3,5-lutidine (3,5-lut) and 3,4-lutidine (3,4-lut).

All of the compounds were obtained by recrystallization of purified MgPc (Sigma) from solution of the appropriate lutidine. Four compounds were obtained, as presented on the reaction schemes below:

