The use of ligands with carboxylate groups makes that the first supramolecular association is organized by the effect of OH...O hydrogen bonds. The π...π 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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Keywords: copper complexes; crystal structures; coordination chemistry

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Crystal Structures of Double Oxygen-bridged Tetranauclear and Polyonuclear Metal Complexes.

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The [N,N’-bis(salicylidene) -1,3-propane-diaminate, (SALPD), (C₇H₆N₂O₃)] 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. Various combinations of metal ions are possible. 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 µ-bridges. We report here two new metal atoms. Oxygen, nitrogen, acetate or nitrite anions bridge as well as on the ligand arrangement around the metal 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- bipyramid or square-pyramide was decided on the basis of τ value calculations. φbridge(Cu-N-Cu) = 102.1(3)⁰, φbridge(Cu-O-Cu) = 105.6(2)⁰.

II) [ZnHg(SALPD)(C₇H₆N₂S)]₄, P2₁2₁2₁, a=8.6824(12), b=16.1222(12), c=16.3339(11) Å, Z=4, D=2.01 g.cm⁻³, λ=0.71073 Å, I >2σ 2575, Npar=293, Dmax,Dmin → 0.80, -0.88 e Å⁻³. Doubly oxygen-bridged dinuclear ZnHg complexes are bridged via SCN bridges in an end to end fashion to build a polynuclear chain. The coordination around Zn ion is a distorted square-pyрамide 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)⁰, φbridge(Zn-O-Hg) = 105.5(2)⁰ to 106.5(2)⁰.

Keywords: organometallic crystal structures; metalloorganic structures; coordination compounds

Magnesium(II) phthalocyanine Coordination Compounds with 3,4- and 3,5-lutidines. Vasyl Kinzhylko⁵, Jan Janczak⁶. "Institute of Low Temperature and Structure Research, Polish Academy of Sciences, POBox. 1410, 50-950 Wrocław, Poland E-mail: V.Kinzhylko@int.pan.wroc.pl

Magnesium phthalocyanine (MgPc) and its MgPcL and MgPcL₂ 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:

MgPc + 3,5-lut → MgPc(3,5-lut)₂ + H₂O → MgPc(H₂O)₂ n(3,5-lut)