$Bis(bis(\mu_2\text{-dimethylglycine-O,O')-tetrachlorocuprate-dicopper(II))\\ Hydrate$

<u>Manuela Ramos Silva</u>^a, Ana Matos Beja^a, José António Paixão^a, Jesús Martín-Gil^b, ^a*CEMDRX, Physics Department, University of Coimbra.* ^b*ETSII, Paseo del Cauce, SP-47011 Valladolid, Spain.* E-mail: manuela@pollux.fis.uc.pt

The title compound crystallizes in the space group P2₁/c with two symmetry independent tetranuclear Cu(II) complexes. Each complex is centrossymmetric with the Cu(II) ions aligned in a short zigzag chain with sequence Cl-Cu-Cl-Cu-Cl-Cu-Cl. The central Cu ions are 2.7303(8) Å apart and are linked by four dimethylglycine molecules. Each of the central Cu ions is also coordinated by a $[CuCl_4]^{2-}$ ion. The complex has an inversion centre, see ORTEP diagram where the ellipsoids were drawn at the 50% probability level. The polyhedron around Cu1 is quadrangular-pyramidal. The deviation of Cu1 from the L.S. plane of the pyramid base is 0.250(1) Å towards the apical chlorine, so that the distance Cu1-Cl1 is 2.4525(8) Å. Cu2



is coordinated by 4 chlorine atoms in a flattened tetrahedral geometry with distances and angles ranging from 2.2417(9) to 2.2925(8) Å and 96.12(3) to 97.48(4)°. The molecules of dimethylglycine adopt a dipolar zwitterionic form. The Cu(II) complexes seem to crystallize as isolated entities since only intramolecular H-bonds are found.

However two disordered water positions can be found in a Fourier difference map, and two extra oxygen atoms were included in the refinement so that their occupancy adds to unity.

Keywords: x-ray crystallography of coordination compounds, copper coordination compounds, single crystals