03.5-5 THE STRUCTURE OF A Hg(II) COMPLEX OF ADENINE N(1)-OXIDE. By M. Damodar Poojarvi and H. Manohar. Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India.

The structure basically consists of a dimeric unit with a centre of symmetry involving two HgO and two adenine N(1)-oxide molecules. Adenine N(1)-oxide acts as a bridging bidentate ligand coordinating through N(7) and O(1). The chloride ions link the two adenine N(1)-oxide molecules.

Crystal data: Hg(C_5Η_4NSO)Cl_2, monoclinic, non-hydrate. The positions of the sulphur atoms were located from a Patterson synthesis and its refinement. The chloride ions link the N(6) atom through a N-H...Cl hydrogen bond.

On the basis of the present structural observations it is suggested that during Hg-DNA complexation, Hg interacts directly with N(6) by releasing a proton at pH 7.0, thus resulting in a chelate. Earlier models, on the other hand, indicated N(3) and O(4) atoms of thymidine as binding sites for Hg in DNA. Interesting features of the structure in relation to Hg-DNA interaction will be discussed.

Crystal data: Hg(C_5Η_4NSO)Cl_2, monoclinic, P_2_1/a, a=8.745(2), b=13.230(8), c=11.728(2), \( \alpha = 94.06(2) \), \( \beta = 95.55(0) \), \( \gamma = 133.54(2) \), D_2 = 1.43, D_2 = 1.42, Mg \( \cdot 0.37 \) mm\(^{-1} \) for HgCl(\( \lambda = 0.7079 \)). The positions of the sulphur atoms were located from a Patterson synthesis and its phases were used to compute a difference Fourier synthesis which enabled the location of the other non-hydrogen atoms. All the hydrogen atoms were located from a subsequent difference Fourier synthesis. The structure was refined by the full-matrix least-squares method to R = 0.055 for 1978 observed reflections [3 > 2(\( F_0 \))] with all hydrogen atom parameters included in the final cycles of refinement.

03.5-6 X-RAY STRUCTURE OF (AQUO)(S')-PHENOPYRIDOXIDENEAMINO-N(3)-AMINO-ADENINE MONOHYDRATE. By S.P. Sudhakara Rao and H. Manohar. Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India and R. S. B. Department of Chemistry, University of Southern California, Los Angeles, California 90089-1062, U.S.A.

The role of metal ions in nonenzymatic pyridoxal-dependent reactions of \( S' \)-amino acids has been examined by a number of studies in solution. Metal-pyridoxideneamino acid complex is an intermediate in such a reaction. The metal serving as a trap for the preformed Schiff base of pyridoxal and amino acid. The title compound crystallizes in space group P1 with a = 8.394, b = 9.819, c = 10.584, \( \alpha = 89.11^\circ \), \( \beta = 112.50^\circ \), and \( \gamma = 100.00^\circ \). The structure was solved by heavy atom method and refined by least squares to R = 0.074 for 1464 observed reflections.

Cu(II) ion has a square pyramidal coordination geometry. Three donor atoms from the terdentate Schiff base ligand (phenolic O, imine N and carboxylate C) and a water O constitute the base (N-L distances: 1.9-2.0A). The axial site is occupied by a sulphate O of a neighbouring molecule (O-w = 2.1A) resulting in a polynuclear structure. Unlike in bis(pyridoxideneconcinate)nickel(II) complex (Rao and Manohar, XV Natl. Seminar on Crystallography, Bangalore, 1984), the ligand is nearly planar. These observations can be correlated with the lower and higher activities of Ni(II) and Cu(II) ions in nonenzymatic reactions.

03.5-7 CRYSTAL AND MOLECULAR STRUCTURE OF 7-(BENZYLAMINO)-2-METHYLMERCAPTO THIAZOLO[5,4-d]PYRIDIMIN. By A. B. Banerjee and P. Roychoudhury, Department of Physics (X-ray Lab.), University College of Science, 92, A.P.C. Road, Calcutta-700009, India.

The crystal structure of the compound has been determined from three dimensional X-ray-diffraction data for 2376 unique reflections, collected on an Enraf-Nonius CAD-4 diffraction meter using graphite monochromatized MoK\( \alpha \) radiation. The structure is nearly planar. These observations can be correlated with the lower and higher activities of Ni(II) and Cu(II) ions in nonenzymatic reactions.

Studies on nucleobases and their derivatives: crystal structures of 1-((S)-2,3-dihydroxypropyl)uracil (structure I) and 1-((S)-2,3-dihydroxypropyl) uracil (structure II) crystallizes in the space group P1 with a = 4.719(1), b = 8.826(1), c = 19.756(3)\( \AA \) and \( \alpha = 97.3^\circ \), \( \beta = 112.6^\circ \), \( \gamma = 100.2^\circ \). The structure has solved by direct method and refined to R = 0.036. S-DMO\( \alpha \), 1-((S)-2,3-dihydroxypropyl) uracil (structure II) crystallizes in the space group P1 with a = 4.719(1), b = 8.367(1), c = 5.205(1)\( \AA \), with R = 0.060. The propyl side chain is extended in these two compounds and the related aliphatic nucleoside analogues - S (1,2,3-dihydroxypropyl) adenosine (SDPA) and \( S, (S'), 3,3-

STUDIES ON NUCLEOBASES AND THEIR DERIVATIVES: CRYSTAL STRUCTURES OF 1-((S)-2,3-

DHIDROXYPROPYL)URACIL (C\( _{11}H\_N\_O\_3 \)), S-DMO\( \alpha \), 1-((S)-2,3-

DHIDROXYPROPYL) URACIL (C\( _{11}H\_N\_O\_3 \)) AND ARAPENOCID (9 - (2-

CLORO-6-

PHELIDROBENZYL) ADENINE, C\( _{11}H\_N\_O\_3 \)) BY

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