03.5-5 THE STRUCTURE OF A Hg(II) COMPLEX OF ADENINE (N(1))-OXIDE. By M. Damodara Rao 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 $\text{HgCl}_2$ and two adenine $N(1)$-oxide molecules. adenine $N(1)$-oxide acts as a bridging bidentate ligand coordinating to $N(7)$ and $O(1)$. The chloride ions link up metal ions to give a polymeric structure. Mercury has a distorted square-pyramidal coordination geometry with $O(1)$ occupying the axial position. Three chloride ions and $N(7)$ atom constitute the basal plane. The metal serves as a trap for the preformed hydrogen bond.

On the basis of the present structural results it is suggested that during Hg-DNA complexation, Hg interacts directly with N(6) by releasing a proton at pH ~9.0, thus resulting in a chelate. Earlier models, on the other hand, have linked to the $N(6)$ atom through a N-H hydrogen bond.

Crystal data: $\text{Hg(C}_5\text{H}_5\text{N}_2\text{O})\text{Cl}_2$, monoclinic, $\text{P2}_1/n$, $\text{a}=8.745(2),\text{b}=13.230(8),\text{c}=11.728(2)\text{Å},\beta=94.06(2)^\circ,\text{V}=1353.5\text{Å}^3,\text{Z}=4,\rho=1.43\text{g cm}^{-3}$. The crystal data are: $\text{C}_5\text{H}_5\text{N}_2\text{O}_2\text{Cl}_2$, monoclinic, $\text{space group P2}_1\text{/a},\text{a}=8.745(2),\text{b}=13.230(8),\text{c}=11.728(2)\text{Å},\beta=94.06(2)^\circ,\text{V}=1353.5\text{Å}^3,\text{Z}=4,\rho=1.43\text{g cm}^{-3}$.

03.5-6 X-RAY STRUCTURE OF (AQUO)($\text{S'}$-PHOS-PHOPROPYRIDOXILIDENE)NICKEL(II) HYDRATE. By S.P. Sudhakara Rao and H. Manohar, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India and R.Bau, Department of Chemistry, University of Southern California, Los Angeles, California 90089-1062, U.S.A.

The role of metal ions in nucemolytic reactions of $\text{S'-amino}$ acid has been examined by a number of studies in solution. Metal-pyridoxylideneamino acid complex is an intermediate in such a reaction. The metal serves as a trap for the preformed Schiff base of pyridoxal and amino acid. The title compound crystallizes in space group $\text{P1}$ with $a=8.294, b=9.819, c=10.844, \alpha=97.3^\circ, \beta=112.60^\circ$ and $\gamma=90^\circ$. The structure was solved by heavy atom method and refined by least squares to $R=0.064$ 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 $O$) and a water $O$ constitute the base ($X$-y distances: 1.9-2.0 Å). The axial site is occupied by a phosphate $O$ of a neighbouring molecule ($X=2.31Å$) resulting in a polymeric structure. Unlike in bis(pyridoxylidenechloro)nickel(II) complex (Rao and Manohar, X 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 nucemolytic reactions.

03.5-7 CRYSTAL AND MOLECULAR STRUCTURE OF 7-BENZYLAMINO-2-METHYLMERCAPTO THIOLACTO[5,4-d] PYRIMIDIN-4-YL 2,3-DIHYDROXYPROPYL URACIL (structure I) and 1-(S)-2,3-DIHYDROXYPROPYL URACIL (structure II). By T. Thomas Luthraiah and S.K. Mazumdar, Crystallography Division, Saha Institute of Nuclear Physics, Jadavpur, Calcutta-700032, India.

The crystal structure of the compound has been determined from three dimensional X-ray diffraction data for 2470 unique reflections, collected on an Enraf–Nonius CAD-4 diffractometer using graphite monochromated MoKα radiation with a crystal of dimensions 0.100X0.280X0.13 mm. The crystal data are: $C_{13}H_{12}N_4O_2S_2$, $M_r=288.39$, monoclinic, space group $\text{P2}_1/n$, $a=8.394, b=9.819, c=10.884, \alpha=89.15^\circ, \beta=94.06(2)^\circ, \gamma=97.3^\circ, \text{V}=1001\text{Å}^3, \text{Z}=4, \rho=1.43\text{g cm}^{-3}$.

The positions of the sulphur atoms were located from a Patterson synthesis and its hydrogen atoms were located from a subsequent difference Fourier synthesis. The structure was refined by the full-matrix least-squares (Busing, Martin and Levy, 1962) to a $R$ of 0.035 for 1988 observed reflections ($l > 2\sigma(l)$) with all hydrogen atom parameters included in the final cycles of refinement.