

04.6-06 CRYSTAL STRUCTURE OF HYDROGENBIS(PYRIDINE-N-OXIDE) TETRACHLOROAUROATE(III) REVEALING A SHORT HYDROGEN BOND. By M. Sakhawat Hussain, Chemistry Department, University of Petroleum and Minerals, Dhahran Saudi Arabia and E.O. Schlemper, Chemistry Department, University of Missouri Columbia, Mo 65211.

An X-ray diffraction study of the title compound  $[(\text{PyNO})_2\text{H}]^+[\text{AuCl}_4]^-$  was done as part of our program dealing with short intramolecular hydrogen bonds. The compound crystallizes in triclinic space group  $P\bar{1}$  with lattice parameters  $a = 7.276(6)$ ,  $b = 8.631(3)$ ,  $c = 6.799(8)\text{\AA}$ ,  $\alpha = 105.36(2)$ ,  $\beta = 96.38(2)$  and  $\gamma = 67.92(2)^\circ$ . The structure was solved by direct methods as well as by the heavy atom method using the CAD4 SDP system. The final value for  $R(\text{Fo})$  was 0.044 for 1343 reflections. The structure consists of discrete  $[\text{AuCl}_4]^-$  anions and  $[(\text{PyNO})_2\text{H}]^+$  cations with the gold atom and the bridging hydrogen atom at centers of symmetry. The hydrogen bond is symmetric as a result of crystallographic requirements. Two pyridine-N-oxide molecules are hydrogen bonded to form a planar dimeric cation which does not have any hydrogen bonded interactions with any adjacent  $[\text{AuCl}_4]^-$  anions. The results of this structural analysis indicate four-co-ordinated gold similar to the gold in hydrogenbis (NN-dimethylacetamide) tetrachloroaurate(III) reported earlier (Hussain and Schlemper, J.C.S. Dalton (1980), 750). It is further concluded that earlier reports (Ziegler and Stephan, Mikrochim, Acta (1970), 628) about the presence of six co-ordinated gold and nitrogen co-ordinated pyridine-N-oxide are erroneous. The structure of the compound, its comparison with similar structures, its significance and the short intramolecular hydrogen bond will be discussed.

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