

07-Crystallography of Organometallic and Coordination Compounds

PS-07.04.08 STRUCTURE OF OUTER SPHERE COMPLEXES $M'CuNta(H_2O)$ IN CRYSTALS AND AQUEOUS SOLUTIONS

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We carried out the analysis of structural and spectral characterization of outer sphere complexes $M'[CuNta(H_2O)]$ ($M' = Li^+, Na^+, K^+, Cs^+$)

in the solid state and in aqueous solutions. In crystals M' cations have an "axial-facial" type of coordination that is apparently retained in solutions. The extent of the tetragonal distortion of copper coordinational polyhedron by M' cation in the solid state is changed in the row $Li^+ > Na^+ > K^+ > Cs^+$. The influence of outer sphere cation on the central atom state is effected through the mediation of the donor atoms of ligands, which are bonded with M' . The inversion of the row of copper complex distortion by M' cations in aqueous solution as compared with the solid phase is accounted for by the change of polarizing ability of M' cations as the result of their hydration

compound is solved by direct methods, SHELXS-86, to an R value of 0.057. The stoichiometry of the complex is 1:2. The nickel atom is in an octahedral coordination. The coordination polyhedron is distorted due to the presence of two water molecules. The binding of the thiocyanate group with the metal atom is through the nitrogen atom. The complex does not show any hydrogen bonds or covalent bonds between the metal group and ligand molecule. The packing of the molecules shows a layered arrangement when viewed down b (figure 1).

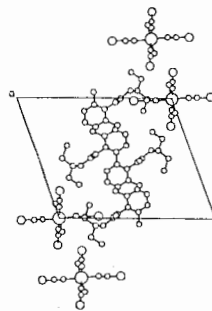


Fig 1. Packing of the molecules down b.

PS-07.04.09 Deformation Density Studies of a Chromium(V)nitrido Complex ($Cr^V(bpb)N$). By Chih-Chieh Wang*, Liang-Kuei Chou, Ming-Chu Cheng, Chi-Ming Che and Yu Wang, Department of Chemistry, National Taiwan University, Taipei, Taiwan

The chromium(V)nitrido complex of bpb ($H_2bpb = 1,2$ -bis(2-pyridine-carboxamido)benzene), $Cr^V(bpb)N$, has been restudied by X-ray diffraction at low temperature (110K). Space group, $P2_1$, $Z=2$, $a=5.977(1)$, $b=13.208(2)$, $c=9.776(1)$ Å, $\beta=90.27(1)^\circ$, $V=771.7(2)$ Å³. MoK α radiation ($\lambda=0.7107$ Å, $\mu=0.75$ mm⁻¹), $R=0.041$ for 5882 reflections. The crystal structure at 110K is the same as that at room temperature. The Cr(V) ion is five coordinated to form N atoms of bpb on equatorial plane and a nitrido N atom at the axial position. The chromium atom is located 0.5142 Å above the equatorial plane and toward nitrido N atom. The Cr-N bond distance is 1.554(2) Å and the average Cr-N(amide) and Cr-N(pyridine) bond distances are 2.082(2) and 1.967(2) Å respectively. The deformation electron-density distribution according to multipole model shows the accumulation of electron density along the Cr-N, Cr-N(amide, pyridine) and C-C, C-N bonds in the ligand. The asphericity in electron density near the transition metal is observed. The parallel theoretical calculated deformation density gives reasonable agreement in comparison. The net atomic charges and d-orbital populations are also going to be presented.

PS-07.04.10 CRYSTAL STRUCTURE OF LIGNOCAINE HYDROCHLORIDE - NICKEL THIOCYANATE COMPLEX. A. Indira, M.A. Sridhar, G. Nagendrappa, J. Shashidhara Prasad*, Department of Studies in Physics, University of Mysore, Manasagangothri, Mysore 570 006, INDIA

The title compound, $Ni_{0.5}S_2C_{16}H_{23}O_2N_4$, crystallizes in the monoclinic space group $P2_1/n$ with $a = 15.062(3)$ Å, $b = 7.829(2)$ Å, $c = 18.527(2)$ Å, $\beta = 110.179(9)^\circ$, $V = 2050.6(7)$ Å³. $Z = 4$. The crystal structure of the title

PS-07.04.11 CRYSTAL STRUCTURE OF LIGNOCAINE HYDROCHLORIDE - PALLADIUM THIOCYANATE COMPLEX. M.A. Sridhar*, A. Indira, G. Nagendrappa, J. Shashidhara Prasad, Department of Studies in Physics, University of Mysore, Manasagangothri, Mysore 570 006, INDIA

The title compound, $Pd_{0.5}S_2C_{16}H_{23}ON$, crystallizes in the monoclinic space group $P2_1/n$ with $a = 9.917(8)$ Å, $b = 15.382(5)$ Å, $c = 13.218(2)$ Å, $\beta = 100.12(3)^\circ$, $V = 1985.00(1)$ Å³, $Z = 4$. The crystal structure of the title compound is solved by direct methods, SHELXS-86, to an R value of 0.048. The stoichiometry of the complex is 1:2. The palladium atom is in a square planar coordination. The coordination polyhedron is undistorted. The binding of the thiocyanate group with the metal atom is through the sulphur atom. The complex does not show any hydrogen bonds or covalent bonds between the metal group and ligand molecule. The packing of the molecules shows a strongly layered arrangement (figure 1).

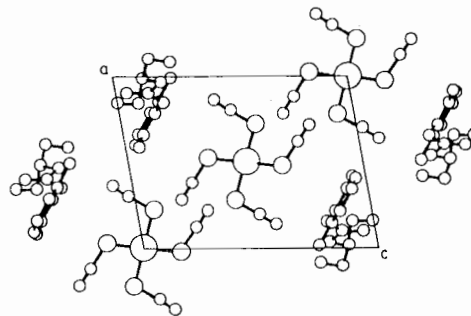


Fig. 1 Packing of the molecules down b.