Crystal Structure of N-picoloylhydrazide and its Binuclear Palladium Complex

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The Ligand N-picoloylhydrazide(Hphz) and its binuclear palladium complex [Pd₂(phz)₂Cl₂] were synthesized and determined by single-crystal X-ray diffraction. They belong to the monoclinic system. Crystal data: Hphz (C₆H₇N₃O), space group C 2/c, a =1.9245(2) nm, b = 0.38927(2) nm, c = 1.8073(2) nm, $\beta = 107.255(2)^{\circ}$, $V = 1.2931(2) \text{ nm}^3$, Z = 8, $Dc = 1.409 \text{ Mg/m}^3$, F(000) = 576, $\mu = 0.102$ mm⁻¹,R = 0.0541 for 1257 observed reflections, wR=0.1762, GOF = 1.124; $[Pd_2(phz)_2Cl_2]$ (C₁₂H₁₂Cl₂N₆O₂Pd₂), space group P 2₁/c, a = 1.48274(9) nm, b = 1.44797(9) nm, c = 0.73951(5) nm, $\beta =$ 92.719(3)°, $V = 1.5860(2) \text{ nm}^3$, Z = 4, $Dc = 2.329 \text{ Mg/m}^3$, F(000) =1072, $\mu = 2.62 \text{ mm}^{-1}$, R = 0.0262 for 2937 observed reflections, wR=0.0555, GOF = 0.959. The palladium(II) ion in the complex [Pd₂(phz)₂Cl₂] is coordinated by two pyridine nitrogen atoms and two diazine nitrogen atoms, forming a distorted square arrangement of four nitrogen donors. The Pd. Pd distance is 0.38111 nm in the complex. There is a one-dimensional chain structure through intermolecular N-H...Cl hydrogen bonds in the crystal. There are π - π interactions between neighboring ligands. ab-initio calculations show that there are intra- and intermolecular Pd...Pd interactions. v(C=O)and v(C=N) are shifted to lower frequencies and v(C-N) are shifted to higher frequencies in the IR spectra. The emission lines (λ_{exc} = 310nm) are shifted to higher frequencies in the fluorescence spectra. Keywords: crystal structure, N-picoloylhydrazide, binuclear palladium complex