

Structure of Dichloro(tetrahydrogenethylenediaminetetra-acetato)palladium(II) Pentahydrate, an Example of a Hexafunctional Ligand behaving as a Bidentate

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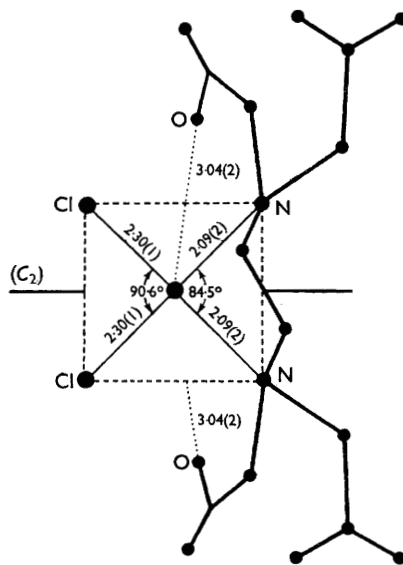
ETHYLENEDIAMINETETRA-ACETIC ACID (EDTA) behaves as a pentadentate or hexadentate ligand in a number of structures.¹ The prediction of Busch and Bailar² that this ligand may chelate as a bidentate had been confirmed in the X-ray structure determination of dichloro(tetrahydrogenethylenediaminetetra-acetato)palladium(II) pentahydrate, $[\text{PdH}_4, \text{EDTA}, \text{Cl}_2], 5\text{H}_2\text{O}$, the golden-brown octahedral crystals of which were prepared using the method of Busch and Bailar.²

Crystal data: $\text{C}_{10}\text{H}_{26}\text{Cl}_2\text{N}_2\text{O}_{13}\text{Pd}$; $M = 559.6$; tetragonal; $a = 10.19 \pm 0.02$; $c = 21.02 \pm 0.03$ Å; $U = 2183$; $D_m = 1.70$ (by flotation); $Z = 4$; $D_c = 1.70$; $F(000) = 1136$; space group $P4_12_12$ (D_4^1) or $P4_32_12$ (D_4^3), Cu- K_α radiation, nickel-filtered, single-crystal oscillation and Weissenberg photographs. 1067 non-zero reflections were recorded from seven levels ($0kl$ to $6kl$), on multiple-film Weissenberg photographs.

Palladium atomic co-ordinates were obtained from a three-dimensional Patterson synthesis. All other atoms, except for hydrogen, were located in subsequent Fourier syntheses. Six cycles of full-matrix least-squares refinement, in the space group $P4_12_12$, using individual isotropic temperature factors, gave an R value of 0.12.

The palladium atom has a square planar environment made up of two chlorine atoms, and two nitrogens from the ethylenediamine part of the EDTA with the carboxyl groups uncomplexed.

Consequently this is an example of a hexafunctional ligand behaving as a bidentate. The



FIGURE

molecule, $[\text{PdH}_4, \text{EDTA}, \text{Cl}_2]$, possesses crystallographically imposed C_2 symmetry (Figure).

The molecules are held together by hydrogen

bonding between carboxyl oxygens and water molecules which are arranged in a three-dimensional array. Although the analytical values indicate the presence of five water molecules per complex, six water molecules are found with four having high temperature factors ($13\text{--}14 \text{ \AA}^2$) compared to the carboxyl oxygens ($5\text{--}8 \text{ \AA}^2$). These results suggest that the water molecules are disordered.

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¹ C. H. L. Kennard, *Inorg. Chim. Acta*, 1967, **1**, in the press.

² D. H. Bush and J. C. Bailar, *J. Amer. Chem. Soc.*, 1956, **78**, 716.