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Crystal and Molecular Structure of *trans*-dichloro-(η-ethylene)(2,6-dimethylpyridine)platinum(II)

FRANCESCO CARUSO, RICCARDO SPAGNA and LUIGI ZAMBONELLI

Laboratorio di Strutturistica Chimica "Giordano Giacomello", C.N.R., Area della Ricerca, C.P. 10, 00016 Monterotondo Stazione, Roma, Italy

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Complexes of the type *trans*[$PtCl_2(\eta\text{-}C_2H_4)L$] where L is a γ-substituted pyridine allow a systematic study of metal–ligand bonding and ligand–ligand interaction, since the donor–acceptor properties of the pyridine ligand can be varied by an appropriate choice of the γ-substituent [1, 2].

We have recently [3] reported the molecular structure, determined by single crystal X-ray analysis, of two such complexes, with L = 4-methylpyridine and 2,4,6-trimethylpyridine respectively.

Then the complexes containing the unsubstituted pyridine and the 2,6-dimethylpyridine have been prepared to compare them with the complexes containing the electron-releasing CH_3 group in the γ-position of the pyridine ligands. However, many attempts to get single crystals, suitable for X-ray analysis, of the complex containing the unsubstituted pyridine were unsuccessful, therefore only the structural results of the complex with 2,6-dimethylpyridine are reported below.

Experimental

Crystals were obtained from a dichloromethane/n-hexane solution of the compound prepared as previously described [3]. Cell dimensions and intensity data were measured with a Syntex $P2_1$ diffractometer using monochromated Mo-Kα radiation. The crystals of *trans*-[$PtCl_2$(η-ethylene)(2,6-dimethylpyridine)], $C_9H_{14}Cl_2NPt$, are orthorhombic, space group $C222_1$, with a = 8.015(1), b = 16.227(2), c = 9.228(1) Å, $Z = 4, d_c = 2.220, d_m > 2$ g cm^{-3}.

TABLE I. Final Atomic Coordinates. Standard deviations are given in parentheses.

	x	*y*	*z*
Pt	0.5	0.1008(0)	0.25
Cl	0.2143(4)	0.1026(2)	0.2571(15)
N	0.5	0.2292(7)	0.25
C(1)	0.5016(56)	0.2697(6)	0.1238(12)
C(2)	0.4847(67)	0.3559(6)	0.1212(16)
C(3)	0.5	0.3993(8)	0.25
C(4)	0.5205(55)	0.2217(7)	−0.0156(14)
C	0.5259(39)	−0.0252(6)	0.1722(13)

The structure was solved by the heavy atom method and refined by full-matrix least-squares to a final R value of 0.033 for 749 independent reflections having $I > 3\sigma(I)$. The fixed contribution of the hydrogen atoms, geometrically positioned [4], was included in the last cycles of refinement, during which the non-hydrogen atoms were allowed to vibrate anisotropically. The final coordinates of the non-hydrogen atoms of the asymmetric unit (half molecule) are reported in Table I.

Results and Discussion

The molecular geometry of *trans*-[$PtCl_2(\eta\text{-}C_2H_4)(NC_7H_{10})$] which has a crystallographic C_2 point symmetry is shown in Figure 1. Interatomic bond lengths and angles are given in Table II.

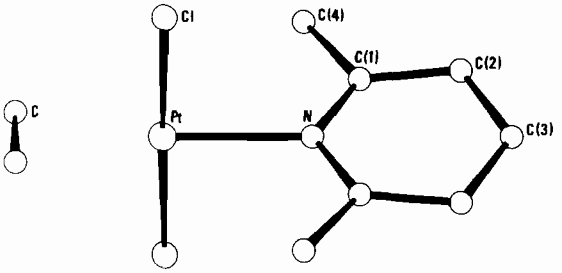

Figure 1. Perspective view of the molecule of *trans*-[$PtCl_2(\eta\text{-}C_2H_4)$(2,6-dimethylpyridine)]. The twofold axis passes through Pt, N and C(3) and bisects the C=C bond.

TABLE II. Bond Lengths and Angles. Estimated standard deviations are given in parentheses.[a]

Pt–Cl	2.291(3) Å	Cl–Pt–Cl′	178.5(1)°
Pt–N	2.084(11)	Cl–Pt–N	89.3(1)
Pt–C	2.177(11)	Cl–Pt–M	90.7
Pt–M	2.05	N–Pt–M	180.0
C–C′	1.494(21)	C–Pt–C′	40.2(5)
N–C(1)	1.338(12)	Pt–N–C(1)	119.5(6)
C(1)–C(2)	1.404(15)	C(1)–N–C′(1)	121.0(10)
C(2)–C(3)	1.387(16)	N–C(1)–C(2)	120.3(11)
C(1)–C(4)	1.511(18)	N–C(1)–C(4)	119.2(9)
		C(2)–C(1)–C(4)	120.6(11)
		C(1)–C(2)–C(3)	118.8(14)
		C(2)–C(3)–C′(2)	119.0(12)

[a] M is the midpoint of the coordinated double bond. Primed and unprimed symbols refer to atoms related by the twofold axis.

The platinum atom has the expected square planar coordination, with the pyridine ligand in *trans* position to the η-coordinated ethylene. As a consequence of the imposed C_2 point symmetry the ligand atoms

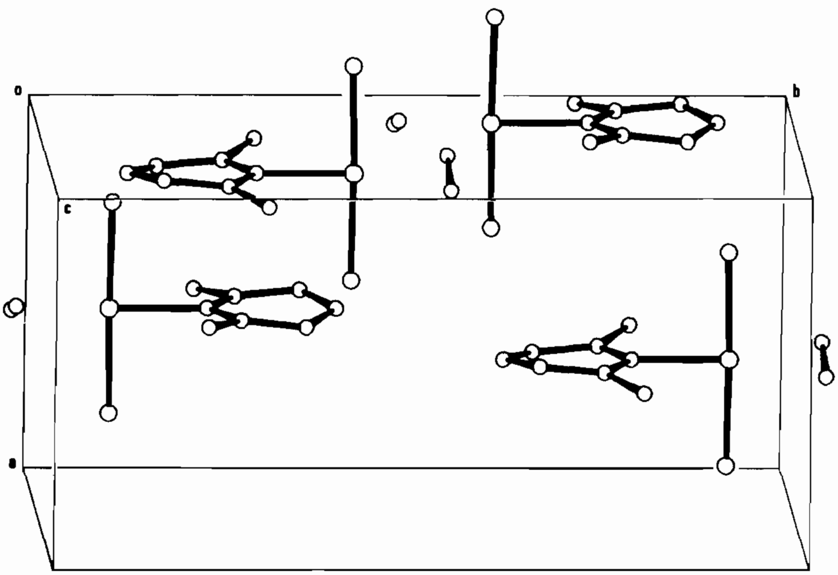

Figure 2. Packing of the molecules.

are exactly coplanar with the platinum atom, and the coordination plane defined by Pt, Cl, Cl′ and N contains the midpoint M of the coordinated ethylene. The pyridine ligand lies in a plane which is almost perpendicular (91.1°) to the coordination plane. The coordinated double bond of the ethylene deviates strongly from the direction perpendicular to the coordination plane, the angle between the direction of the coordinated double bond and the coordination plane being 72.2°. Since the carbon atoms of the ethylene are equidistant from the platinum atom, for the imposed C_2 symmetry, such deviation is only due to a tilt of the ethylene around the Pt–double bond direction.

Bond lengths and angles in the coordination sphere of the platinum are regular and compare well with the corresponding values found in the analogous complexes containing 4-methylpyridine and 2,4,6-trimethylpyridine [3]. In particular the structure of *trans*-[$PtCl_2(C_2H_4)$(2,6-dimethylpyridine)] compares strictly with that of *trans*-[$PtCl_2(C_2H_4)$(2,4,6-trimethylpyridine)] : the Pt–N bond has the same length in the two complexes and the presence of the *alpha* methyl groups in the two pyridine ligands determines the same arrangement of these ligands with respect to the $(C_2H_4)PtCl_2$ moiety.

The more significant difference between the two structures concerns the arrangement of the ethylene which is strongly tilted in the present case.

The shortest intermolecular contact (3.28 Å) is between two carbon atoms of two different ethylene molecules. The packing of the structure is shown in Figure 2.

References

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3 F. Caruso, R. Spagna and L. Zambonelli, *J. Cryst. Mol. Structure,* in press.

4 C–H = 1.0 Å, C–C–H = 120° (sp^2), H–C–H = 109.5° (sp^3); each hydrogen atom was assigned the isotropic thermal parameter of the carbon atom to which it is attached. The positions of the atoms were readjusted after each cycle of refinement.