Crystal structure of *cis*-dichlorobis(5-methylisoxazole)platinum(II), $PtCl_2(C_4H_5NO)_2$

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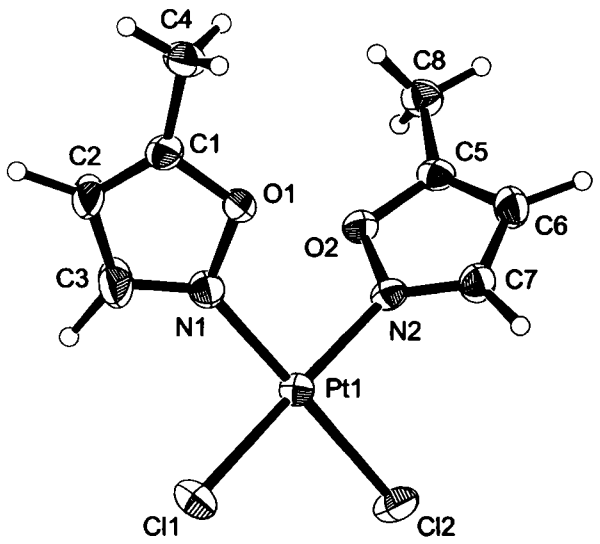

Abstract

$C_8H_{10}Cl_2N_2O_2Pt$, orthorhombic, *Pccn* (no. 56), $a = 8.1012(9)$ Å, $b = 21.113(2)$ Å, $c = 14.014(2)$ Å, $V = 2397.0$ Å^3, $Z = 8$, $R_{gt}(F) = 0.035$, $wR_{ref}(F) = 0.040$, $T = 273$ K.

Source of material

The Pt complex was prepared by mixing a two molar excess of 5-methylisoxazole and K_2PtCl_4 in distilled water at 300 K for 96 h. Transparent yellow crystals of the product were obtained by slow recrystallization from acetone at RT. The crystals decompose in the temperature range 272-300 °C.

Discussion

Heterocyclic compounds containing nitrogen and oxygen atom are very interesting due to their bio-activities. In particular, some isoxazole derivatives have been reported for their bio-activities [1-4]. Furthermore, the respective palladium and platinum complexes with coordinated isoxazole ligands exhibit more bio-activity than isoxazole alone [3]. The ORTEP plot (30% probability ellipsoids) defines the square planar Pt(II) complex as the *cis*-isomer. The atoms Cl1, Cl2, N1, N2 and Pt1 are in the same plane, and the molecule has a non-crystallographic twofold axis of symmetry passing through the metal and the respective midpoints between the chlorine and nitrogen atoms. The dihedral angles between the coordination plane and the two least-square planes defined by the atoms O1-N1-C1-C2-C3 and O2-N2-C5-C6-C7 are 36.7(5)° and 107.8(1)°, respectively, while the latter two planes are inclined by 117.3°. The corresponding bond angles Cl1–Pt1–Cl2, N1–Pt1–N2, Cl1–Pt1–N1 and Cl2–Pt1–N2 are equal to 90.2(1)°, 91.9(4)°, 89.1(3)° and 88.8(3)°, respectively. The two chlorine and nitrogen atoms coordinate to the metal center at the average bonding distances d(Cl—Pt1) = 2.284(3) Å and d(N—Pt1) = 1.999(9) Å. All the other bond distances and angles are also in a normal range.

Table 1. Data collection and handling.

Crystal:	yellow prism, size 0.20 × 0.15 × 0.15 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	120.88 cm^{-1}
Diffractometer, scan mode:	Bruker SMART APEX CCD, ω/φ
$2\theta_{max}$:	56.58°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	14768, 3978
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1929
$N(param)_{refined}$:	136
Programs:	SIR92 [5], SHELXL-97 [6], ORTEP-II [7]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	8*e*	−0.0231	0.2944	0.2716	0.1155
H(2)	8*e*	−0.0266	0.2637	0.0882	0.1149
H(3)	8*e*	0.0028	0.1495	0.4064	0.0758
H(4)	8*e*	0.1900	0.1701	0.3970	0.0758
H(5)	8*e*	0.0545	0.2207	0.4251	0.0758
H(6)	8*e*	0.5170	−0.0385	0.1546	0.0675
H(7)	8*e*	0.2212	−0.0270	0.0734	0.0637
H(8)	8*e*	0.7386	0.0573	0.2059	0.0647
H(9)	8*e*	0.7219	0.1156	0.1354	0.0647
H(10)	8*e*	0.6422	0.1188	0.2384	0.0647

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt(1)	8*e*	0.07308(5)	0.11575(2)	0.02185(3)	0.0355(2)	0.0442(2)	0.0354(2)	−0.0004(2)	0.0025(2)	0.0002(2)
Cl(1)	8*e*	−0.1493(4)	0.1639(2)	−0.0471(2)	0.053(2)	0.071(2)	0.057(2)	0.011(2)	−0.007(2)	0.014(2)
Cl(2)	8*e*	0.1059(4)	0.0537(2)	−0.1103(2)	0.052(2)	0.079(2)	0.051(2)	0.002(2)	−0.005(1)	−0.024(2)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	8*e*	0.078(1)	0.1501(3)	0.2251(5)	0.049(4)	0.044(4)	0.038(4)	0.009(4)	−0.003(4)	0.001(3)
O(2)	8*e*	0.3973(9)	0.1057(3)	0.1147(5)	0.043(4)	0.045(4)	0.045(4)	0.000(4)	−0.007(4)	−0.005(4)
N(1)	8*e*	0.047(1)	0.1728(5)	0.1349(7)	0.060(7)	0.050(5)	0.040(5)	0.009(5)	0.006(5)	0.003(4)
N(2)	8*e*	0.263(1)	0.0706(4)	0.0821(6)	0.038(5)	0.046(5)	0.040(5)	−0.004(4)	−0.004(4)	−0.007(4)
C(1)	8*e*	0.051(2)	0.1978(6)	0.2864(8)	0.050(7)	0.058(7)	0.038(6)	0.009(6)	0.005(6)	−0.008(5)
C(2)	8*e*	0.007(3)	0.2489(8)	0.2412(9)	0.20(2)	0.055(7)	0.037(6)	0.05(1)	−0.00(1)	−0.007(7)
C(3)	8*e*	0.005(3)	0.2321(7)	0.146(1)	0.18(2)	0.055(9)	0.052(8)	0.04(1)	0.01(1)	0.010(7)
C(4)	8*e*	0.077(2)	0.1833(7)	0.3872(9)	0.072(9)	0.075(9)	0.042(7)	0.019(8)	−0.008(7)	−0.001(6)
C(5)	8*e*	0.513(1)	0.0646(6)	0.1470(8)	0.042(6)	0.057(7)	0.029(5)	0.004(5)	0.004(5)	−0.001(5)
C(6)	8*e*	0.456(2)	0.0051(6)	0.135(1)	0.053(8)	0.048(7)	0.068(9)	0.011(6)	−0.004(7)	−0.002(6)
C(7)	8*e*	0.300(2)	0.0119(6)	0.094(1)	0.047(7)	0.044(6)	0.067(9)	−0.003(6)	−0.010(6)	−0.004(6)
C(8)	8*e*	0.667(1)	0.0914(6)	0.1849(9)	0.039(6)	0.065(8)	0.058(7)	0.002(6)	−0.005(6)	−0.002(7)

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