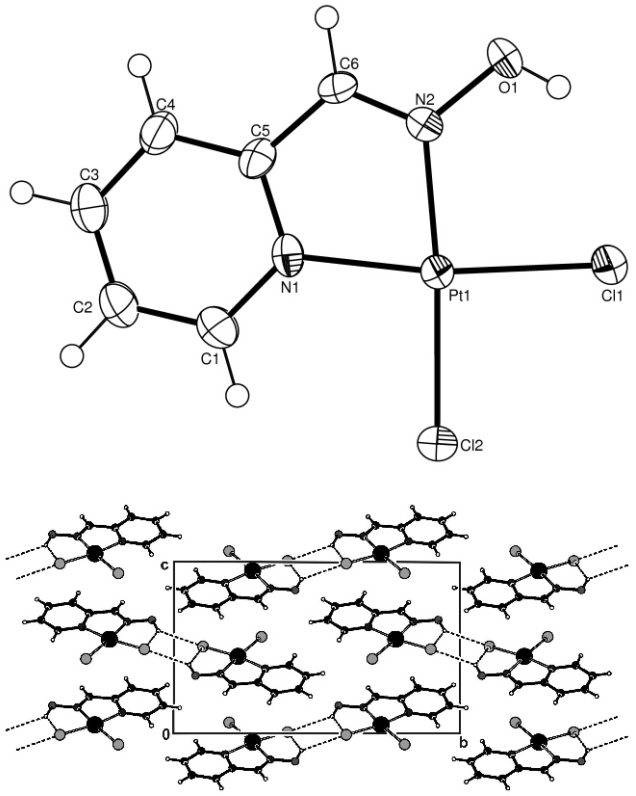
Crystal structure of dichloro(2-pyridinealdoxime-κ^2N,N')platinum(II), $PtCl_2(C_6H_6N_2O)$

Kwang Ha*

Chonnam National University, School of Applied Chemical Engineering, Research Institute of Catalysis, Gwangju 500-757, Republic of Korea

Received April 1, 2011, accepted and available on-line August 24, 2011; CCDC no. 1267/3490



Abstract

$C_6H_6Cl_2N_2OPt$, monoclinic, $P12_1/c1$ (no. 14), a = 5.9133(4) Å, b = 15.881(1) Å, c = 9.6870(7) Å, β = 101.256(1)°, V = 892.2 Å^3, Z = 4, $R_{gt}(F)$ = 0.039, $wR_{ref}(F^2)$ = 0.115, T = 200 K.

Source of material

To a solution of K_2PtCl_4 (0.2074 g, 0.500 mmol) in H_2O (20 ml) was added *syn*-2-pyridinealdoxime (0.1226 g, 1.004 mmol) and stirred for 24 h at room temperature. The formed precipitate was separated by filtration, washed with H_2O and acetone, and dried at 50 °C, to give a red-brown powder (0.1158 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from an acetone solution.

Experimental details

Hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms with d(C—H) = 0.95 Å, d(O—H) = 0.84 Å and U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(O). The highest peak (4.47 e Å^{-3}) and the deepest hole (–1.66 e Å^{-3}) in the difference Fourier map are located 1.98 Å and 1.56 Å from the atoms Pt1 and C6, respectively.

Discussion

In the title complex, the central Pt(II) ion has a distorted square-planar coordination defined by two N atoms of the chelating 2-pyridinealdoxime ligand and two Cl^- anions (figure, top). The compound crystallized in the monoclinic space group $P2_1/c$, whereas the previously reported analogous Hg(II) complex $[HgCl_2(C_6H_6N_2O)]$ crystallized in the triclinic space group $P\bar{1}$ [1]. The main contribution to the distortion is the tight chelate angle ∠N1–Pt1–N2 = 78.8(3)°, which results in non-linear *trans* axes (∠Cl1–Pt1–N1 = 171.1(2)° and ∠Cl2–Pt1–N2 = 175.0(2)°). The Pt—N and Pt—Cl bond lengths are nearly equivalent, d(Pt1—N1$_{pyridine}$) = 2.010(7) Å and d(Pt1—N1$_{oxime}$) = 1.979(8) Å; d(Pt—Cl) = 2.297(2) Å and 2.293(2) Å, respectively. The complex displays weak intermolecular π–π interactions between adjacent pyridine rings. For Cg1 (the centroid of ring N1–C5) and Cg1^i (symmetry code i: 2–x,1–y,1–z), the centroid–centroid distance is 5.519(6) Å, the planes are parallel and shifted for 3.988 Å. In the crystal structure, the complex reveals intramolecular O–H···Cl hydrogen bonding with d(O···Cl) = 3.089(8) Å thus forming a five-membered ring. Dimers of complex molecules are assembled by intermolecular O–H···Cl hydrogen bonds with d(O···Cl) = 3.228(7) Å (figure, bottom).

Table 1. Data collection and handling.

Crystal:	red-brown stick, size 0.11 × 0.12 × 0.30 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	162.75 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, φ/ω
$2\theta_{max}$:	56.56°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6276, 2147
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1720
$N(param)_{refined}$:	110
Programs:	SHELXS-97, SHELXL-97 [2], ORTEP-3 [3]

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

Atom	Site	x	y	z	U_{iso}
H(1O)	4*e*	0.6456	0.0540	0.4002	0.061
H(1)	4*e*	0.5271	0.4225	0.4542	0.047
H(2)	4*e*	0.7296	0.5209	0.3509	0.050
H(3)	4*e*	0.9927	0.4776	0.2171	0.051
H(4)	4*e*	1.0431	0.3334	0.1804	0.042
H(6)	4*e*	0.9303	0.1793	0.2341	0.034

* e-mail: hakwang@chonnam.ac.kr

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)	4*e*	0.48926(6)	0.22464(2)	0.44981(3)	0.0242(2)	0.0200(2)	0.0277(2)	0.0001(1)	0.0079(2)	0.0005(1)
Cl(1)	4*e*	0.3213(5)	0.1026(1)	0.5078(3)	0.040(2)	0.023(1)	0.053(2)	–0.0015(9)	0.023(1)	0.001(1)
Cl(2)	4*e*	0.2652(4)	0.3065(1)	0.5646(2)	0.037(1)	0.027(1)	0.036(1)	0.002(1)	0.016(1)	–0.0031(9)
O(1)	4*e*	0.706(1)	0.0761(4)	0.3373(8)	0.052(5)	0.017(3)	0.060(5)	0.000(3)	0.028(4)	0.000(3)
N(1)	4*e*	0.657(1)	0.3203(4)	0.3782(8)	0.033(5)	0.022(4)	0.031(4)	–0.003(3)	0.007(3)	0.006(3)
N(2)	4*e*	0.697(1)	0.1630(4)	0.3479(8)	0.032(5)	0.021(4)	0.037(4)	0.003(3)	0.013(3)	0.000(3)
C(1)	4*e*	0.631(2)	0.4039(6)	0.398(1)	0.047(7)	0.025(5)	0.049(6)	0.006(4)	0.017(5)	0.004(4)
C(2)	4*e*	0.753(2)	0.4626(6)	0.337(1)	0.046(7)	0.023(5)	0.057(7)	0.001(4)	0.015(5)	0.004(4)
C(3)	4*e*	0.907(2)	0.4372(6)	0.258(1)	0.054(7)	0.026(5)	0.051(6)	–0.003(5)	0.019(5)	0.011(4)
C(4)	4*e*	0.937(2)	0.3522(6)	0.236(1)	0.031(6)	0.035(5)	0.042(5)	–0.001(4)	0.014(4)	0.008(4)
C(5)	4*e*	0.810(2)	0.2952(6)	0.2975(9)	0.014(5)	0.033(5)	0.029(4)	0.001(4)	0.001(3)	0.007(4)
C(6)	4*e*	0.828(2)	0.2052(6)	0.286(1)	0.021(5)	0.029(5)	0.038(5)	0.005(4)	0.013(4)	0.001(4)

Acknowledgment. This work was supported by Priority Research Centers Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (grant no. 2010-0029626).

References

1. Torabi, A. A.; Kian, R.; Souldozi, A.; Welter, R: Crystal structure of dichloro(pyridine-2-aldoxime-*N*,*N*′)mercury(II), $HgCl_2(NC_5H_4CHNOH)$. Z. Kristallogr. NCS **220** (2005) 613-614.
2. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.
3. Farrugia, L. J.: ORTEP-3 for Windows - a version of ORTEP-III with a Graphical User Interface (GUI) J. Appl. Crystallogr. **30** (1997) 565.