Crystal structure of *trans*-diiodidobis(4-phenylpyridine-κ*N*)platinum(II), $C_{22}H_{18}I_2N_2Pt$

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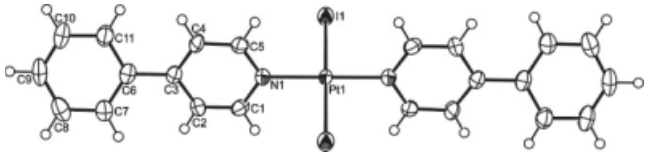

Abstract

$C_{22}H_{18}I_2N_2Pt$, monoclinic, $P2_1/c$ (no. 14), a = 9.072(2) Å, b = 9.158(2) Å, c = 13.169(2) Å, β = 107.281(3)°, V = 1044.8 Å^3, Z = 2, $R_{gt}(F)$ = 0.0319, $wR_{ref}(F^2)$ = 0.0727, T = 200 K.

Table 1. Data collection and handling.

Crystal:	yellow blocks, size 0.09×0.12×0.12 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	96.79 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, φ and ω
$2\theta_{max}$:	52.12°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6220, 2017
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1593
$N(param)_{refined}$:	124
Programs:	SHELX [2], ORTEP-3[3]

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

Atom	Site	x	y	z	U_{iso}
H(1)	4*e*	0.8020	0.2950	0.3366	0.038
H(2)	4*e*	0.7066	0.2734	0.1564	0.041
H(4)	4*e*	0.8961	0.6624	0.1257	0.041
H(5)	4*e*	0.9940	0.6721	0.3063	0.040
H(7)	4*e*	0.5497	0.3126	–0.0053	0.044
H(8)	4*e*	0.4456	0.3095	–0.1882	0.055
H(9)	4*e*	0.5518	0.4514	–0.2942	0.055
H(10)	4*e*	0.7671	0.5919	–0.2181	0.057
H(11)	4*e*	0.8773	0.5977	–0.0364	0.048

Source of material

To a solution of K_2PtCl_4 (0.199 g, 0.478 mmol) in H_2O (20 ml) were added KI (0.719 g, 4.330 mmol) and 4-phenylpyridine (*ppy*; 0.162 g, 1.043 mmol) in EtOH (10 ml) and stirred for 3 h at room temperature. The formed precipitate was separated by filtration, washed with H_2O and EtOH, and dried at 50 °C, to give a yellow powder (0.322 g). Crystals were obtained by slow evaporation from an *N,N*-dimethyl- formamide solution at 60 °C.

Experimental details

Hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms with d(C–H) = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). The highest peak (2.82 e·Å^{-3}) and the deepest hole (–1.08 e·Å^{-3}) in the difference Fourier map are located 1.28 Å and 0.72 Å from the atom I1, respectively.

Discussion

The crystal structure of the related Pt(II) complex, $[PtCl_2(ppy)_2]\cdot H_2O$, has been reported previously [1]. The asymmetric unit of the title crystal structure contains one half of a neutral Pt(II) complex. The central Pt(II) ion has a *trans*-I_2N_2 square-planar coordination defined by two N atoms from two different 4-phenylpyridine ligands and two iodido ligands. The Pt atom is located at an inversion center, and therefore the PtI_2N_2 moiety is exactly planar. The dihedral angle between the PtI_2N_2 plane and the nearly planar pyridine ring is 70.5(2)°. The phenyl ring is inclined to the pyridine ring by 22.1(4)°.

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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)	2*a*	1	$\frac{1}{2}$	$\frac{1}{2}$	0.0244(2)	0.0324(2)	0.0173(2)	–0.0020(2)	0.0051(2)	0.0003(2)
I(1)	4*e*	1.27520(5)	0.45766(5)	0.48279(4)	0.0274(3)	0.0521(3)	0.0266(3)	0.0014(2)	0.0085(2)	–0.0012(2)
N(1)	4*e*	0.9095(7)	0.4860(5)	0.3413(5)	0.028(3)	0.033(3)	0.023(3)	–0.002(2)	0.007(3)	–0.001(2)
C(1)	4*e*	0.8231(8)	0.3703(7)	0.2933(6)	0.038(5)	0.028(4)	0.033(5)	–0.003(3)	0.017(4)	0.001(3)
C(2)	4*e*	0.7652(8)	0.3574(7)	0.1857(6)	0.036(5)	0.041(4)	0.025(4)	–0.008(3)	0.006(4)	–0.007(3)
C(3)	4*e*	0.7902(8)	0.4653(7)	0.1178(6)	0.030(4)	0.033(4)	0.025(4)	0.005(3)	0.009(3)	0.003(3)
C(4)	4*e*	0.8765(8)	0.5842(7)	0.1674(6)	0.042(5)	0.034(4)	0.022(4)	–0.002(3)	0.005(4)	0.009(3)
C(5)	4*e*	0.9335(8)	0.5898(7)	0.2755(6)	0.041(5)	0.032(4)	0.029(5)	–0.012(3)	0.012(4)	–0.003(3)
C(6)	4*e*	0.7259(9)	0.4558(7)	0.0006(6)	0.036(5)	0.032(4)	0.026(4)	0.011(3)	0.011(4)	–0.001(3)
C(7)	4*e*	0.5953(9)	0.3701(8)	–0.0480(6)	0.037(5)	0.041(4)	0.030(5)	0.006(3)	0.007(4)	–0.001(3)
C(8)	4*e*	0.5332(9)	0.3686(9)	–0.1564(7)	0.037(5)	0.056(5)	0.038(5)	0.007(4)	0.002(4)	–0.016(4)
C(9)	4*e*	0.596(1)	0.4519(9)	–0.2191(7)	0.048(6)	0.062(5)	0.022(5)	0.021(4)	0.001(4)	–0.006(4)
C(10)	4*e*	0.723(1)	0.5353(8)	–0.1740(7)	0.061(6)	0.055(5)	0.024(5)	0.012(4)	0.007(4)	0.008(4)
C(11)	4*e*	0.789(1)	0.5388(8)	–0.0663(6)	0.040(5)	0.051(5)	0.028(5)	0.003(3)	0.008(4)	0.003(4)

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