Crystal structure of diiodido-bis(3-phenylpyridine-κ*N*)platinum(II), $PtI_2(C_{11}H_9N)_2$, $C_{22}H_{18}I_2N_2Pt$

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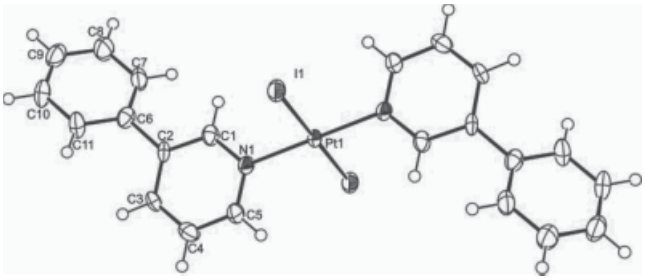

Abstract

$C_{22}H_{18}I_2N_2Pt$, triclinic, $P\overline{1}$ (no. 2), a = 6.498(1) Å, b = 7.154(1) Å, c = 11.750(2) Å, α = 76.864(4)°, β = 82.627(3)°, γ = 82.129(3)°, V = 524.2 Å^3, Z = 1, $R_{gt}(F)$ = 0.0215, $wR_{ref}(F^2)$ = 0.0552, T = 200 K.

Table 1. Data collection and handling.

Crystal:	yellow blocks, size 0.19×0.09×0.08 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	23.27 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, φ and ω
$2\theta_{max}$:	52.1°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3183, 1944
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1759
$N(param)_{refined}$:	124
Programs:	SHELX [2], ORTEP-3 [3], PLATON [4]

Source of material

To a solution of K_2PtCl_4 (0.204 g, 0.49 mmol) and KI (0.717 g, 4.32 mmol) in H_2O (20 ml) was added 3-phenyl- pyridine (*ppy*; 0.173 g, 1.12 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 (0.343 g). Crystals suitable for X-ray diffraction were obtained by slow evaporation from an *N,N*-dimethylformamide 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 (0.76 e·Å^{-3}) and the deepest hole (–1.01 e·Å^{-3}) in the difference Fourier map are located 0.83 Å and 1.01 Å from the Pt1 atom, respectively.

Discussion

The title complex is isomorphous with the previously reported bromido-Pt(II) complex [$PtBr_2$(*ppy*)$_2$] [1]. The central Pt(II) ion has a *trans*-I_2N_2 square-planar coordination geometry defined by two N atoms from two *ppy* ligands and two iodido ligands. The Pt atom is located on an inversion center, and thus the asymmetric unit contains one half of the complex and the PtI_2N_2 moiety is exactly planar. The dihedral angle between the PtI_2N_2 moiety and the nearly planar pyridine ring is 71.8(2)°. In the crystal structure, the dihedral angle between the pyridine and benzene ring planes is 33.0(2)°. The complexes are stacked in columns along [010] with d(Pt···Pt) = 7.154(1) Å (= length of b axis). In the columns, several intermolecular π-π interactions between adjacent six-membered rings are present. For Cg1 (the centroid of ring C6-C11) and Cg1^i (symmetry code i: 1–x,1–y,1–z), the centroid-centroid distance is 4.137(4) Å, the planes are parallel and shifted by 1.928 Å.

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

Atom	Site	x	y	z	U_{iso}
H(1)	2*i*	0.9256	0.0970	0.2371	0.031
H(3)	2*i*	0.3493	0.3815	0.2711	0.034
H(4)	2*i*	0.3048	0.3527	0.0835	0.040
H(5)	2*i*	0.5740	0.2025	–0.0262	0.036
H(7)	2*i*	0.9865	0.2658	0.3738	0.046
H(8)	2*i*	1.0252	0.2664	0.5686	0.057
H(9)	2*i*	0.7399	0.2468	0.7096	0.052
H(10)	2*i*	0.4131	0.2284	0.6557	0.050
H(11)	2*i*	0.3707	0.2250	0.4625	0.045

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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)	1*a*	1	0	0	0.0235(2)	0.0266(2)	0.0167(2)	0.0030(1)	0.0011(1)	–0.0079(1)
I(1)	2*i*	0.91702(6)	–0.32624(5)	0.13694(3)	0.0348(2)	0.0299(2)	0.0244(2)	0.0006(2)	0.0035(2)	–0.0064(2)
N(1)	2*i*	0.7730(7)	0.1372(6)	0.0958(4)	0.027(2)	0.024(2)	0.019(2)	0.000(2)	–0.001(2)	–0.008(2)
C(1)	2*i*	0.7971(9)	0.1500(7)	0.2060(5)	0.031(3)	0.020(3)	0.026(3)	–0.001(2)	0.002(2)	–0.009(2)
C(2)	2*i*	0.6427(8)	0.2371(8)	0.2759(5)	0.025(3)	0.030(3)	0.017(3)	–0.004(2)	0.009(2)	–0.008(2)
C(3)	2*i*	0.4577(8)	0.3167(8)	0.2272(5)	0.023(3)	0.031(3)	0.030(3)	0.007(2)	0.004(2)	–0.013(2)
C(4)	2*i*	0.4323(9)	0.3015(8)	0.1161(6)	0.027(3)	0.033(3)	0.039(4)	0.007(2)	–0.006(3)	–0.009(3)
C(5)	2*i*	0.5924(9)	0.2116(8)	0.0512(5)	0.032(3)	0.030(3)	0.026(3)	0.006(2)	0.001(2)	–0.010(2)
C(6)	2*i*	0.6744(9)	0.2440(8)	0.3991(5)	0.039(3)	0.023(3)	0.024(3)	–0.002(2)	–0.001(2)	–0.009(2)
C(7)	2*i*	0.869(1)	0.257(1)	0.4310(6)	0.029(3)	0.059(4)	0.029(4)	–0.002(3)	0.005(3)	–0.017(3)
C(8)	2*i*	0.891(1)	0.258(1)	0.5470(6)	0.036(4)	0.076(5)	0.034(4)	–0.003(3)	–0.004(3)	–0.021(4)
C(9)	2*i*	0.723(1)	0.247(1)	0.6304(6)	0.059(5)	0.043(4)	0.025(3)	0.004(3)	–0.001(3)	–0.011(3)
C(10)	2*i*	0.531(1)	0.235(1)	0.5984(6)	0.049(4)	0.049(4)	0.028(3)	–0.007(3)	0.013(3)	–0.019(3)
C(11)	2*i*	0.505(1)	0.2335(9)	0.4834(6)	0.034(3)	0.047(4)	0.033(4)	–0.007(3)	0.011(3)	–0.019(3)

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