Crystal structure of bromido(2-phenylpyridine-κ*N*)[2-(2-pyridyl)phenyl-κ^2*N*,*C*]platinum(II), $C_{22}H_{17}BrN_2Pt$

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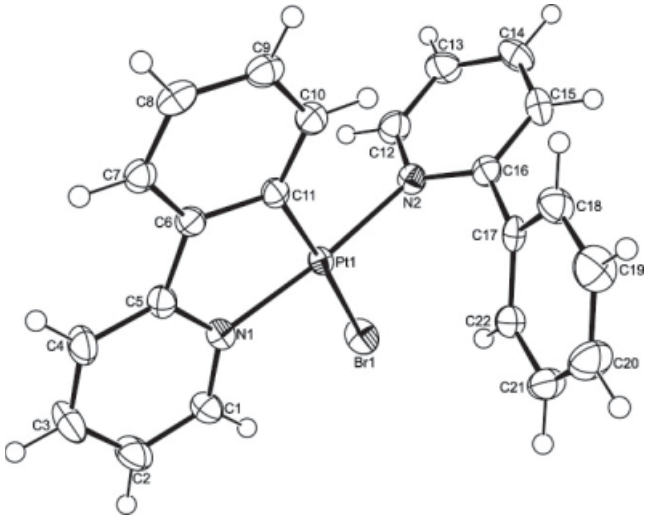
Received December 02, 2012, accepted February 15, 2013, available online May 17, 2013, CCDC no. 1267/3974



Abstract

$C_{22}H_{17}BrN_2Pt$, monoclinic, $P2_1/c$ (no. 14), a = 11.971(1) Å, b = 9.522(1) Å, c = 16.987(2) Å, β = 104.757(2)°, V = 1872.4 Å^3, Z = 4, $R_{gt}(F)$ = 0.0224, $wR_{ref}(F^2)$ = 0.0542, T = 200 K.

Table 1. Data collection and handling.

Crystal:	yellow blocks, size 0.12×0.17×0.27 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	96.36 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, φ and ω
$2\theta_{max}$:	52.1°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	11117, 3583
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2980
$N(param)_{refined}$:	236
Programs:	SHELX [3], ORTEP-3[4], PLATON [5]

Source of material

To a solution of K_2PtBr_4 (0.294 g, 0.497 mmol) in H_2O (30 ml) was added 2-phenylpyridine (0.162 g, 1.046 mmol) in EtOH (20 ml) and refluxed for 7 h. The formed precipitate was separated by filtration, washed with H_2O, and dried at 50 °C to give a yellow powder (0.188 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from a CH_3CN solution.

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) = 1.2 U_{eq}(C). The highest peak (1.19 e·Å^{-3}) and the deepest hole (–1.23 e·Å^{-3}) in the difference Fourier map are located 1.41 Å and 0.87 Å from the atoms H8 and Pt1, respectively.

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Discussion

The title complex is isomorphous with the previously reported Pt(II) complex, $PtCl(C_{11}H_8N)(C_{11}H_9N)$ [1]. The crystal structure of the related *cis*-$PtBr_2(C_{11}H_9N)_2$, which was obtained from the reaction of K_2PtBr_4 with 2-phenylpyridine at room temperature, has been investigated previously [2]. In the title crystal structure, the central Pt(II) ion is four-coordinated by one N and one C atom from the ortho-metalated anionic 2-(2-pyridyl)phenyl ligand, one N atom of 2-phenylpyridine molecule and one bromido ligand in a *trans*-N_2BrC distorted square-planar coordination geometry. The main contribution to the distortion is the tight chelate angle ∠N1–Pt1–C11 = 81.34(16)°, which results in non-linear trans axes (∠N1–Pt1–N2 = 174.25(15)° and ∠C11–Pt1–Br1 = 174.93(12)°). The two Pt–N bond lengths are almost equal (2.022(3) Å and 2.032(4) Å), and slightly longer than the Pt–C bond (1.982(5) Å). In the crystal, the pyridyl and phenyl rings of the chelating ligand are slightly inclined to the least-squares plane of the PtN_2BrC coordination unit (maximum deviation = 0.058(1) Å) at 14.1(2)° and 11.2(2)°, respectively. The dihedral angle between the two ring planes is 11.2(2)°. In contrast, the pyridyl ring of the monodentate neutral ligand is almost perpendicular to the PtN_2BrC plane, with a dihedral angle of 78.2(1)°. The phenyl ring of this ligand is twisted by 48.8(1)° relative to its carrier pyridyl ring. The complex molecules are stacked in columns along [010]. In the columns, numerous inter- and intramolecular π-π interactions between the aromatic rings are present. For Cg1 (the centroid of ring N2-C16) and Cg1^i (symmetry code i: 2-x,1-y,-z), the centroid-centroid distance is 4.246(3) Å, the planes are parallel and shifted by 2.070 Å.

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

Atom	Site	x	y	z	U_{iso}
H(1)	4*e*	0.4876	0.6549	0.0801	0.034
H(2)	4*e*	0.3418	0.7545	0.1299	0.043
H(3)	4*e*	0.3734	0.7926	0.2696	0.047
H(4)	4*e*	0.5432	0.7117	0.3573	0.039
H(7)	4*e*	0.7003	0.5985	0.4315	0.030
H(8)	4*e*	0.8634	0.4690	0.4987	0.032
H(9)	4*e*	0.9754	0.3591	0.4232	0.034
H(10)	4*e*	0.9329	0.3815	0.2830	0.031
H(12)	4*e*	0.9413	0.6635	0.1234	0.037
H(13)	4*e*	1.1214	0.6052	0.1088	0.040
H(14)	4*e*	1.1700	0.3678	0.1016	0.041
H(15)	4*e*	1.0335	0.1979	0.1090	0.036
H(18)	4*e*	0.9246	0.0960	0.2036	0.037
H(19)	4*e*	0.7930	–0.0885	0.1950	0.049
H(20)	4*e*	0.6105	–0.0740	0.1051	0.049
H(21)	4*e*	0.5554	0.1276	0.0283	0.039
H(22)	4*e*	0.6842	0.3128	0.0365	0.032

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*	0.73359(2)	0.54300(2)	0.15150(1)	0.0197(1)	0.0190(1)	0.0189(1)	0.00132(8)	0.00697(7)	0.00030(7)
Br(1)	4*e*	0.66350(4)	0.61681(5)	0.00412(3)	0.0368(3)	0.0381(3)	0.0232(3)	0.0073(2)	0.0108(2)	0.0084(2)
N(1)	4*e*	0.5979(3)	0.6221(4)	0.1876(2)	0.023(2)	0.020(2)	0.025(2)	0.001(2)	0.009(2)	0.002(2)
C(1)	4*e*	0.4988(4)	0.6659(5)	0.1372(3)	0.025(3)	0.030(3)	0.030(3)	0.004(2)	0.006(2)	0.002(2)
C(2)	4*e*	0.4125(4)	0.7267(5)	0.1663(3)	0.028(3)	0.042(3)	0.037(3)	0.013(3)	0.004(2)	0.005(3)
C(3)	4*e*	0.4301(5)	0.7467(5)	0.2487(3)	0.034(3)	0.046(3)	0.042(3)	0.016(3)	0.019(3)	0.002(3)
C(4)	4*e*	0.5305(4)	0.6996(5)	0.3002(3)	0.035(3)	0.039(3)	0.026(3)	0.008(3)	0.013(2)	–0.004(2)
C(5)	4*e*	0.6140(4)	0.6340(5)	0.2689(3)	0.025(3)	0.022(2)	0.027(3)	–0.003(2)	0.012(2)	–0.002(2)
C(6)	4*e*	0.7193(4)	0.5665(4)	0.3165(3)	0.020(3)	0.025(2)	0.021(3)	–0.003(2)	0.007(2)	–0.001(2)
C(7)	4*e*	0.7472(4)	0.5543(5)	0.4012(3)	0.025(3)	0.025(2)	0.026(3)	–0.004(2)	0.008(2)	–0.003(2)
C(8)	4*e*	0.8435(4)	0.4774(5)	0.4411(3)	0.031(3)	0.029(2)	0.019(3)	–0.009(2)	0.004(2)	0.002(2)
C(9)	4*e*	0.9103(4)	0.4132(5)	0.3960(3)	0.027(3)	0.024(2)	0.029(3)	–0.003(2)	0.001(2)	0.000(2)
C(10)	4*e*	0.8846(4)	0.4258(5)	0.3121(3)	0.025(3)	0.027(2)	0.026(3)	–0.001(2)	0.007(2)	–0.002(2)
C(11)	4*e*	0.7885(4)	0.5030(4)	0.2696(3)	0.021(3)	0.016(2)	0.026(3)	–0.002(2)	0.008(2)	–0.002(2)
N(2)	4*e*	0.8801(3)	0.4698(4)	0.1262(2)	0.024(2)	0.024(2)	0.020(2)	–0.001(2)	0.010(2)	0.000(2)
C(12)	4*e*	0.9604(4)	0.5671(5)	0.1208(3)	0.030(3)	0.030(3)	0.034(3)	–0.007(2)	0.012(2)	–0.004(2)
C(13)	4*e*	1.0675(4)	0.5335(5)	0.1119(3)	0.024(3)	0.035(3)	0.043(3)	–0.007(2)	0.011(2)	0.000(2)
C(14)	4*e*	1.0961(4)	0.3943(5)	0.1075(3)	0.022(3)	0.043(3)	0.041(3)	0.005(3)	0.016(2)	0.002(3)
C(15)	4*e*	1.0149(4)	0.2945(5)	0.1119(3)	0.035(3)	0.026(2)	0.033(3)	0.007(2)	0.013(2)	–0.003(2)
C(16)	4*e*	0.9061(4)	0.3315(5)	0.1204(3)	0.027(3)	0.027(2)	0.015(2)	0.003(2)	0.004(2)	0.000(2)
C(17)	4*e*	0.8183(4)	0.2234(4)	0.1205(3)	0.031(3)	0.017(2)	0.022(3)	0.000(2)	0.014(2)	–0.004(2)
C(18)	4*e*	0.8497(4)	0.1029(5)	0.1677(3)	0.031(3)	0.029(3)	0.031(3)	0.005(2)	0.005(2)	0.004(2)
C(19)	4*e*	0.7716(5)	–0.0071(5)	0.1624(4)	0.045(4)	0.027(3)	0.052(4)	0.000(3)	0.016(3)	0.009(3)
C(20)	4*e*	0.6631(5)	0.0022(6)	0.1097(4)	0.037(3)	0.035(3)	0.049(4)	–0.014(3)	0.011(3)	–0.004(3)
C(21)	4*e*	0.6308(4)	0.1211(5)	0.0637(3)	0.025(3)	0.039(3)	0.034(3)	–0.006(2)	0.005(2)	–0.007(3)
C(22)	4*e*	0.7072(4)	0.2311(5)	0.0686(3)	0.025(3)	0.030(2)	0.025(3)	0.001(2)	0.007(2)	–0.005(2)

Acknowledgments. 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 (2009-0094055). The author thanks the KBSI, Jeonju Center, for the X-ray data collection.

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