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The crystal structure of *trans*-dibromido-bis(pyridine- κN)platinum(II), $C_{10}H_{10}Br_2N_2Pt$

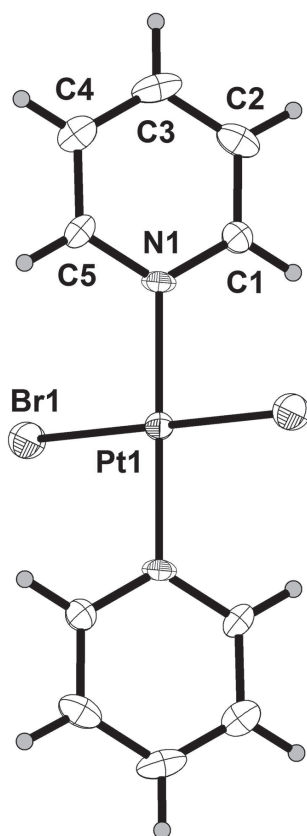


Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.13 × 0.018 × 0.05 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	29.3 cm ⁻¹
Diffractometer, scan mode:	Bruker SMART 1000, φ and ω
$2\theta_{\max}$, completeness:	56.6°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	12659, 1502, 0.107
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1308
$N(\text{param})_{\text{refined}}$:	70
Programs:	Bruker programs [1], SHELX [2], ORTEP [3], PLATON [4]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pt1	0.5000	0.5000	0.5000	0.01933(17)
Br1	0.43957(16)	0.20215(14)	0.71422(11)	0.0319(2)
N1	0.2644(12)	0.6381(10)	0.6493(9)	0.0209(15)
C1	0.0695(14)	0.7216(13)	0.5822(11)	0.0230(18)
H1	0.0460	0.7196	0.4643	0.028*
C2	-0.0962(15)	0.8096(14)	0.6819(13)	0.028(2)
H2	-0.2328	0.8657	0.6332	0.034*
C3	-0.0605(17)	0.8152(15)	0.8543(12)	0.033(2)
H3	-0.1727	0.8741	0.9248	0.039*
C4	0.1418(17)	0.7331(15)	0.9211(12)	0.031(2)
H4	0.1715	0.7381	1.0373	0.038*
C5	0.3007(16)	0.6431(14)	0.8165(11)	0.027(2)
H5	0.4371	0.5843	0.8633	0.032*

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Abstract

$C_{10}H_{10}Br_2N_2Pt$, triclinic, $P\bar{1}$ (no. 2), $a = 5.6590(9)$ Å, $b = 7.0204(12)$ Å, $c = 7.7623(11)$ Å, $\alpha = 79.262(5)^\circ$, $\beta = 84.603(4)^\circ$, $\gamma = 88.928(5)^\circ$, $V = 301.64(8)$ Å³, $Z = 1$, $R_{\text{gt}}(F) = 0.0440$, $wR_{\text{ref}}(F^2) = 0.0946$, $T = 223$ K.

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The molecular structure of the title compound is shown in the figure. Tables 1 and 2 contain details of the measurement

method and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

A pale yellow suspension of dibromido(1,5-cyclooctadiene)platinum(II) (0.2030 g, 0.438 mmol) in pyridine (py; 1 mL) was heated for 30 min at 100 °C. After cooling, the precipitate was separated by filtration, washed with ether, and dried at 50 °C, to give a yellow powder (0.1694 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from a CH₃CN solution.

Experimental details

Hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms with $d(C-H) = 0.94$ Å and

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$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ with the help of the SHELXL program (AFIX 43 option) [2].

Comment

This contribution is part of my continuing interest in the structural chemistry of platinum and palladium complexes containing pyridine [5–7]. The crystal structure of the related complex *cis*-[PtBr₂(py)₂] was previously determined in the monoclinic space group *C2/c* [8].

The title complex *trans*-[PtBr₂(py)₂] is isotypic with the previously reported analogous bromido-Pd complex *trans*-[PdBr₂(py)₂] [6]. In the title complex, the central Pt(II) ion has a *trans*-Br₂N₂ square-planar coordination defined by two N atoms from two distinct pyridine ligands and two Br[−] anions. The complex crystallizes in the triclinic space group *P* $\bar{1}$ and the asymmetric unit contains one half of the complex. Consequently, the Pt atom is located on an inversion center, and therefore the PtBr₂N₂ moiety is exactly planar and the two pyridine rings are parallel (*cf.* the figure). The dihedral angle between the PtBr₂N₂ unit plane and the nearly planar pyridine ring (maximum deviation = 0.01(1) Å) is 58.7(3)°. Bond lengths and angles are in the expected ranges for such Pt(II) complexes [6, 9]. The complexes are stacked in columns along [010] with $d(\text{Pt}\cdots\text{Pt}) = 7.0204(12)$ Å (= length of *b* axis). In the columns, intermolecular very weak π – π interactions between adjacent pyridine rings may be present. For Cg1 (the centroid of ring N1–C5) and Cg1¹ (symmetry code *i*: $-x, 1-y, 2-z$), the centroid-centroid distance is 4.600(5) Å, the planes are parallel and shifted by 2.869 Å [4].

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