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(4,4′-Dimethyl-2,2′-bipyridine)(ethynylbenzene)(triphenylphosphine)platinum(II) hexafluoroantimonate

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Key indicators

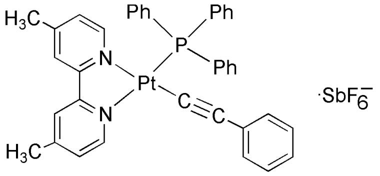
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.013 Å
R factor = 0.041
wR factor = 0.110
Data-to-parameter ratio = 14.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The reaction between the metal diphosphine [Ag(PPh$_3$)$_2$(MeCN)](SbF$_6$) and the metal acetylide compound Pt(dmbpy)(C$_2$Ph)$_2$ (dmbpy is 4,4′-dimethyl-2,2′-bipyridine) gave the title compound, Pt(dmbpy)(C$_2$Ph)·SbF$_6$ or [Pt(C$_8$H$_5$)(C$_{18}$H$_{15}$P)(C$_{12}$H$_{12}$N$_2$)](SbF$_6$). The Pt center is four-coordinated and exhibits a distorted square-planar coordination geometry.

Comment

Transition metal acetylide complexes are of considerable interest because of their potential applications in many fields of materials chemistry, including luminescent materials and conducting polymers (Chan *et al.*, 2001). We are interested in the design of photoluminescent heterometallic cluster complexes by self-assembly between two metal components, one with alkynyl ligands and the other with vacant coordination sites. Thus, the reaction between Pt(dmbpy)(C$_2$Ph)$_2$, with two alkynyl ligands, and [Ag(PPh$_3$)$_2$(MeCN)]$^+$, with a vacant coordination site, was expected to afford a Pt–Ag heteronuclear species. However, the product isolated from the reaction was the title compound, (I). A perspective drawing of the complex with the atomic numbering scheme is depicted in Fig. 1 and selected geometric parameters are presented in Table 1.



(I)

The Pt atom is located in a distorted square-planar coordination geometry. The Pt—P distance is 2.246 (2) Å, which is slightly shorter than that observed in the complex PtCuCl(C$_2$Bu)$_2$(PMe$_2$Ph)$_2$ [2.300 (3) Å; Yamazaki & Deeming, 1993]. The Pt—N distances are 2.068 (6) and 2.094 (6) Å, which are similar to those observed in the complex Pt(1,10-phenanthroline)(C$_9$H$_7$)$_2$ (Hissler *et al.*, 2000).

Experimental

The starting compounds Pt(dmbpy)(C$_2$Ph)$_2$ (Chan *et al.*, 2001) and [Ag(PPh$_3$)$_2$(MeCN)](SbF$_6$) were prepared according to literature procedures (Bachman & Andretta, 1998). Pt(dmbpy)(C$_2$Ph)$_2$ and [Ag(PPh$_3$)$_2$(MeCN)](SbF$_6$) were reacted, in an equimolar ratio, in dichloromethane under anaerobic conditions for 24 h. The solvent was then reduced *in vacuo*. Well-shaped yellow crystals suitable for X-ray diffraction analysis were grown by slow diffusion of diethyl ether into the dichloromethane solution.

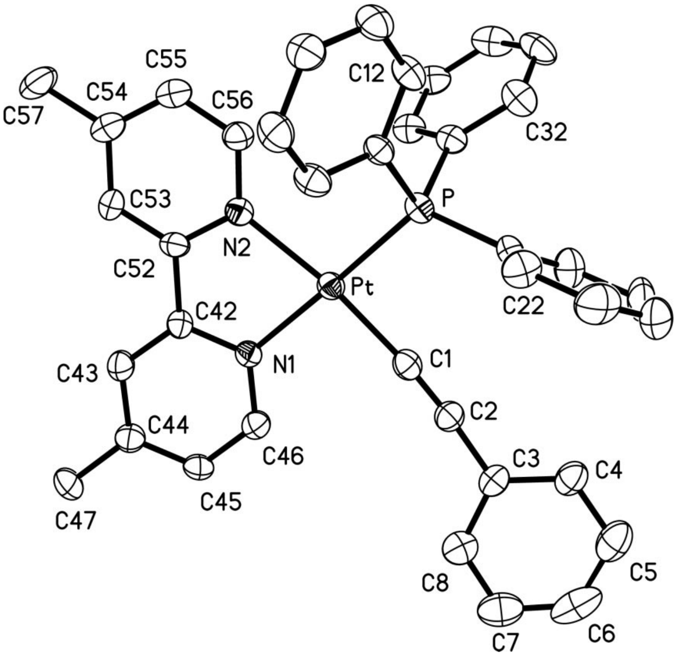


Figure 1
A view of the compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

Crystal data

$[Pt(C_8H_5)(C_{18}H_{15}P)(C_{12}H_{12}N_2)]$-$(SbF_6)$
M_r = 978.47
Monoclinic, $P2_1/n$
a = 14.4131 (4) Å
b = 10.1848 (2) Å
c = 24.7099 (7) Å
β = 98.915 (1)°
V = 3583.46 (16) Å^3
Z = 4
D_x = 1.814 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4988 reflections
θ = 1.5–25.1°
μ = 4.76 mm^{-1}
T = 293 (2) K
Block, yellow
0.50 × 0.30 × 0.25 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.194, T_{max} = 0.304
10524 measured reflections
6291 independent reflections
4473 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.1°
$h = -7 \rightarrow 17$
$k = -9 \rightarrow 12$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.110
S = 1.19
6291 reflections
442 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 9.8193P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt—C1	1.954 (9)	Pt—N2	2.094 (6)
Pt—N1	2.068 (6)	Pt—P	2.246 (2)
C1—Pt—N1	93.0 (3)	C1—Pt—P	88.9 (2)
C1—Pt—N2	171.2 (3)	N1—Pt—P	175.58 (18)
N1—Pt—N2	78.6 (2)	N2—Pt—P	99.68 (18)

All H atoms were included in calculated positions, with C—H distances of 0.93 and 0.96 Å (methyl). They were included in the refinement in riding-motion approximation, with $U_{iso} = 1.2U_{eq}$ ($1.5U_{eq}$ for methyl) of the carrier atom.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SAINT* and *XPREP* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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