

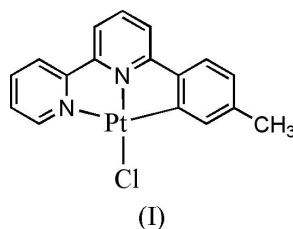
Chloro[2-(2,2'-bipyridyl-6-yl)-5-methylphenyl]-
platinum(II)Qian-Yong Cao,^a Wen-Fu Fu^{b,c,*}
and Xi-Juan Zhao^b^aDepartment of Chemistry, Nanchang University, Nanchang 330047, People's Republic of China, ^bTechnical Institute of Physics and Chemistry, Chinese Academy of Science, Beijing 100101, People's Republic of China, and ^cCollege of Chemistry and Chemical Engineering, Yunnan Normal University, Kunming 650092, People's Republic of China

Correspondence e-mail: fwf@mail.ipc.ac.cn

Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$
 R factor = 0.032
 wR factor = 0.081
Data-to-parameter ratio = 15.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.The title compound, $[\text{Pt}(\text{C}_{17}\text{H}_{13}\text{N}_2)\text{Cl}]$, has a distorted square-planar coordination geometry at the platinum(II) center due to the constraints of the tridentate 6-phenyl-2,2'-bipyridine. No metal–metal interaction was found in the crystal structure.

Comment

Luminescent square-planar platinum(II) complexes with cyclometalated ligands such as 6-phenyl-2,2'-bipyridine have been receiving much attention because of their rich excited states (Lai *et al.*, 2002) and applications as chemical sensors (Che *et al.*, 2003), antitumor agents (Ma & Che, 2003) and organic light-emitting diode (OLED) doping materials (Lu, Mi *et al.*, 2002). In addition, these square-planar complexes often stack to form weak metal–metal interactions in the solid state, with significant variations in their electronic spectra (Lai *et al.*, 2002; Miskowski & Houlding, 1991). However, this metal–metal interaction is highly dependent on the surrounding environment, including the recrystallization medium, counter-ion and inter-ligand steric repulsion, to produce different colors and different crystalline structures (Field *et al.*, 2002; Lu, Mi *et al.*, 2002; Bailey *et al.*, 1995). Recently, we have synthesized a new mononuclear cyclometalated platinum(II) complex, (I), and obtained two crystal forms, their colors being yellow and red, by vapor diffusion of diethyl ether into the $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ solution.The molecular structure of (I) is shown in Fig. 1. The coordination geometry of the Pt atom is distorted square planar. The $\text{N}2-\text{Pt}1-\text{C}16$ and $\text{N}2-\text{Pt}1-\text{N}1$ angles deviate from idealized geometry. This is due to the geometry constraints imposed by the tridentate ligand and is typical for platinum(II) complexes with 6-phenyl-2,2'-bipyridine or terpyridine ligands (Field *et al.*, 2002; Lu, Zhu & Che, 2002; Hofmann *et al.*, 2003). The two Pt–N bond distances are significantly different and comparable with the Pt–N bond in analogous complexes (Lai *et al.*, 1999; Hofmann *et al.*, 2003). In the crystal packing diagram (Fig. 2), the complexes are orientated in a head-to-tail style along the c axis and form a

Received 18 November 2004

Accepted 25 January 2005

Online 5 February 2005

continuous stack with a shortest intermolecular Pt...Pt distance of 6.283 Å.

Experimental

The ligand 6-(4-methylphenyl)-2,2'-bipyridine was prepared according to the literature method of Kröhnke (1976). A mixture of equal amounts of ligand and K₂PtCl₄ in CH₃CN/H₂O (1:1, v/v) was refluxed for 20 h to give a deep-red solution, which was evaporated to dryness. The solid residue was extracted with dichloromethane and then concentrated. A yellow precipitate appeared upon addition of diethyl ether. Recrystallization by vapor diffusion of diethyl ether into a CH₂Cl₂/CH₃CN (1:1, v/v) mixture yielded yellow and red crystals. The yellow crystals were suitable for X-ray crystallography. The red form is very soft and brittle, and is not suitable for X-ray diffraction analysis.

Crystal data

[Pt(C₁₇H₁₃N₂)Cl] D_x = 2.156 Mg m⁻³
 M_r = 475.83 Mo Kα radiation
 Monoclinic, P2₁/n Cell parameters from 942 reflections
 a = 8.418 (3) Å θ = 2.7–26.3°
 b = 11.517 (5) Å μ = 9.75 mm⁻¹
 c = 15.363 (6) Å T = 293 (2) K
 β = 100.250 (7)° Block, yellow
 V = 1465.7 (10) Å³ 0.22 × 0.18 × 0.12 mm
 Z = 4

Data collection

Bruker SMART CCD area-detector diffractometer 2975 independent reflections
 φ and ω scans 2334 reflections with I > 2σ(I)
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996) R_{int} = 0.042
 T_{min} = 0.140, T_{max} = 0.310 θ_{max} = 26.3°
 8203 measured reflections h = -10 → 9
 k = -14 → 13
 l = -13 → 19

Refinement

Refinement on F² H-atom parameters constrained
 R[F² > 2σ(F²)] = 0.032 w = 1/[σ²(F_o²) + (0.0439P)²]
 wR(F²) = 0.081 where P = (F_o² + 2F_c²)/3
 S = 1.01 (Δ/σ)_{max} = 0.003
 2975 reflections Δρ_{max} = 1.48 e Å⁻³
 191 parameters Δρ_{min} = -2.32 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Pt1–N2	1.940 (5)	Pt1–N1	2.107 (5)
N2–Pt1–C16	82.1 (2)	N2–Pt1–N1	79.9 (2)

All H atoms were positioned geometrically and treated as riding [C–H = 0.96 Å for methyl and C–H = 0.93 Å for other H atoms; U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl})]. The highest peak in the final difference map was associated with atom N2 (0.94 Å) and the deepest hole was associated with atom Pt1 (0.87 Å).

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

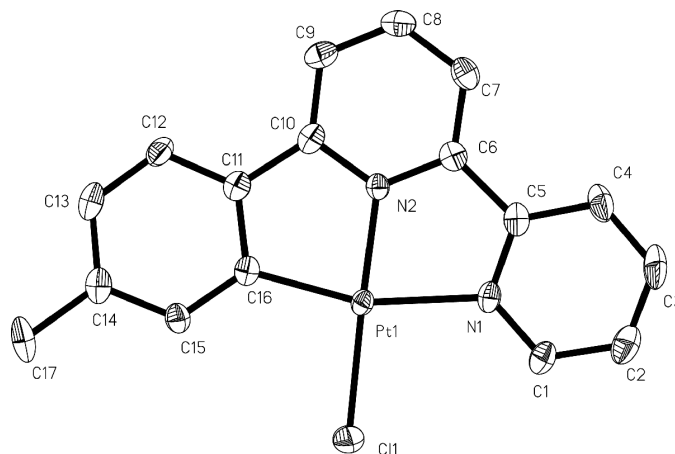


Figure 1 Perspective view of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and all H atoms have been omitted for clarity.

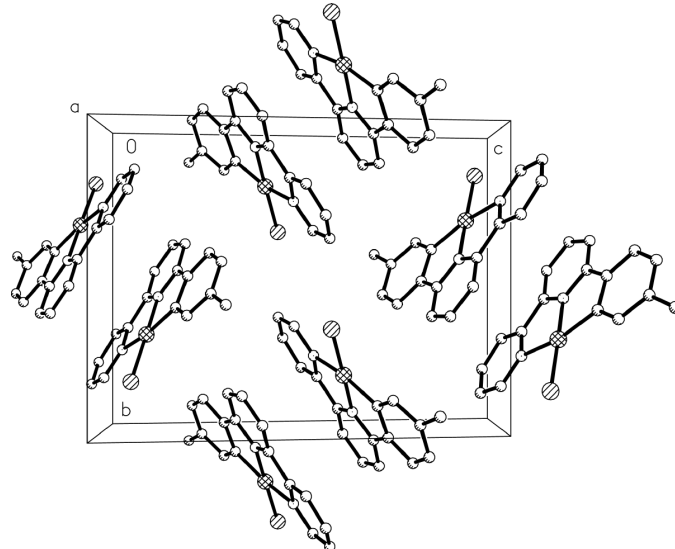


Figure 2 The crystal packing of (I). H atoms have been omitted.

This work was supported by the National Natural Science Foundation of China (Nos 50273045 and 90210033). We thank the Chinese Government for support of the Chinese Academy of Science Hundred Talents and the Foundation (No. 2001E0005Z) for Key Project of Yunnan Provincial Science and Technology Commission.

References

Bailey, J. A., Hill, M. G., Marsh, R. E., Miskowski, V. M., Schaefer, W. P. & Gray, H. B. (1995). *Inorg. Chem.* **34**, 4591–4599.
 Bruker (1998). *SHELXTL* (Version 5.10), *SAIN*T (Version 4.00) and *SMART* (Version 5.0). Bruker AXS Inc., Madison, Wisconsin, USA.
 Che, C.-M., Fu, W.-F., Lai, S.-W., Hou, Y.-J. & Lu, Y.-L. (2003). *Chem. Commun.* pp. 118–119.
 Field, J. S., Haines, R. J., McMillin, D. R. & Summerton, G. C. (2002). *J. Chem. Soc. Dalton Trans.* pp. 1369–1376.
 Hofmann, A., Dahlenburg, L. & Eldik, R. V. (2003). *Inorg. Chem.* **42**, 6528–6538.
 Kröhnke, F. (1976). *Synthesis*, pp. 1–24.
 Lai, S.-W., Chan, M. C., Cheung, T.-C., Peng, S.-M. & Che, C.-M. (1999). *Inorg. Chem.* **38**, 4046–4055.

- Lai, S.-L., Lam, H.-W., Lu, W., Cheung, K.-K. & Che, C.-M. (2002). *Organometallics*, **21**, 226–234.
- Lu, W., Mi, B.-X., Chan, M. C. W., Hui, Z., Zhu, N., Lee, S.-T. & Che, C.-M. (2002). *Chem. Commun.* pp. 206–207.
- Lu, W., Zhu, N. & Che, C.-M. (2002). *Chem. Commun.* pp. 900–901.
- Ma, D.-L. & Che, C.-M. (2003). *Chem. Eur. J.* **9**, 6133–6144.
- Miskowski, V. M. & Houlding, V. H. (1991). *Inorg. Chem.* **30**, 4446–4452.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.