

[*N*-Benzyl-*N*-(diphenylphosphanyl-methyl)pyridin-2-amine]chloridomethyl-platinum(II)

Zhi-Wei Wang, Peng Qiao, Zi-Jia Wang and Chong-Qing Wan*

Department of Chemistry, Capital Normal University, Beijing 100048, People's Republic of China

Correspondence e-mail: wanchqing@yahoo.com.cn

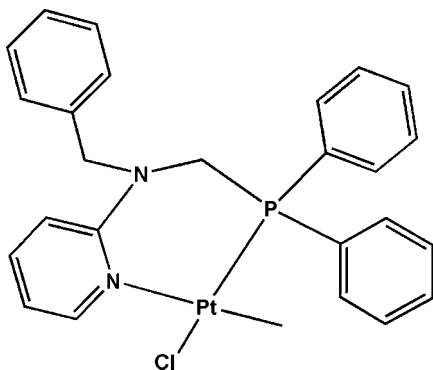
Received 18 November 2010; accepted 28 November 2010

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.020$ Å; R factor = 0.050; wR factor = 0.123; data-to-parameter ratio = 15.0.

In the mononuclear title complex, $[\text{Pt}(\text{CH}_3)\text{Cl}(\text{C}_{25}\text{H}_{23}\text{N}_2\text{P})]$, the *N*-benzyl-*N*-(diphenylphosphanyl-methyl)pyridin-2-amine functions as a bidentate ligand with the pyridyl N atom and the phosphine P atom chelating the Pt^{II} ion, forming a six-membered metalocycle. The Pt^{II} atom adopts a square-planar coordination geometry with one methyl group and one chloride ligand bonding to the metal center in a *cis* relationship. $\text{C}-\text{H}\cdots\pi$ and $\text{C}-\text{H}\cdots\text{Cl}$ interactions help to consolidate the packing.

Related literature

For coordination complexes with hemilabile ligands with PN donor sets, see: Espinet & Soulantica (1999); Song *et al.* (2001); Wang *et al.* (2010). For coordination complexes with the *N*-benzyl-*N*-(diphenylphosphanyl-methyl)pyridin-2-amine ligand, see: Li *et al.* (2003, 2006). For hydrogen bonds, see: Desiraju & Steiner (1999) and for $\text{C}-\text{H}\cdots\pi$ interactions, see: Umezawa *et al.* (1998).



Experimental

Crystal data

$[\text{Pt}(\text{CH}_3)\text{Cl}(\text{C}_{25}\text{H}_{23}\text{N}_2\text{P})]$	$\gamma = 107.266$ (5)°
$M_r = 628.00$	$V = 1197.0$ (6) Å ³
Triclinic, $P\bar{1}$	$Z = 2$
$a = 9.538$ (3) Å	Mo $K\alpha$ radiation
$b = 10.770$ (3) Å	$\mu = 6.06$ mm ⁻¹
$c = 13.125$ (4) Å	$T = 293$ K
$\alpha = 98.367$ (4)°	$0.33 \times 0.24 \times 0.20$ mm
$\beta = 106.256$ (4)°	

Data collection

Bruker APEXII CCD area-detector diffractometer	6265 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2007)	4201 independent reflections
$T_{\text{min}} = 0.675$, $T_{\text{max}} = 1.000$	3270 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.041$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$	281 parameters
$wR(F^2) = 0.123$	H-atom parameters constrained
$S = 1.01$	$\Delta\rho_{\text{max}} = 2.18$ e Å ⁻³
4201 reflections	$\Delta\rho_{\text{min}} = -2.33$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

C_{g1} is the centroid of the C15–C20 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C23-H23\cdots C_{g1}^i$	0.93	3.10	4.001 (2)	154
$C7-H7B\cdots Cl1^{ii}$	0.97	2.72	3.392 (2)	127

Symmetry codes: (i) $-x + 2, -y + 2, -z + 2$; (ii) $x - 1, y, z$.

Data collection: APEX2 (Bruker, 2007); cell refinement: APEX2 and SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

The authors are grateful for financial support from the Technology Program, Beijing Municipal Education Commission (Ref. No. 09530410099).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2076).

References

- Bruker (2007). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Desiraju, G. R. & Steiner, T. (1999). *The Weak Hydrogen Bond in Structural Chemistry and Biology*. New York: Oxford University Press Inc.
- Espinet, P. & Soulantica, K. (1999). *Coord. Chem. Rev.* **193–195**, 499–566.
- Li, Q.-S., Xu, F.-B., Cui, D.-J., Yu, K., Zeng, X.-S., Leng, X.-B., Song, H.-B. & Zhang, Z.-Z. (2003). *Dalton Trans.* pp. 1551–1557.
- Li, Q.-S., Zhao, Y.-J., Xu, F.-B., Song, H.-B. & Zhang, Z.-Z. (2006). *Acta Cryst.* **E62**, m2366–m2367.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Song, H.-B., Zhang, Z.-Z. & Mak, T. C. W. (2001). *Inorg. Chem.* **40**, 5928–5933.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Umezawa, Y., Tsuboyama, S., Honda, K., Uzawa, J. & Nishio, M. (1998). *Bull. Chem. Soc. Jpn.* **71**, 1202–1213.
- Wang, X. B., Feng, J. Z., Huang, J., Zhang, J. Y., Pan, M. & Su, C. Y. (2010). *CrystEngComm*, **12**, 725–729.

supplementary materials

Acta Cryst. (2011). E67, m36 [doi:10.1107/S1600536810049652]

[*N*-Benzyl-*N*-(diphenylphosphanylmethyl)pyridin-2-amine]chloridomethylplatinum(II)

Z.-W. Wang, P. Qiao, Z.-J. Wang and C.-Q. Wan

Comment

Rigid hemilabile ligands such as (2-diphenylphosphanyl)pyridine (Espinet *et al.*, 1999) and 2,6-bis(diphenylphosphanyl)pyridine (Song *et al.*, 2001; Wang *et al.*, 2010) have extensively been studied, including the fascinating structures and the catalytic properties of their metal complexes. We here report a new complex with the *N*-benzyl-*N*-(diphenylphosphanylmethyl)pyridin-2-amine ligand (abbreviated as *L*), namely Pt(*L*)MeCl.

In the title complex, the pyridyl N atom and the phosphine P atom bond to the square-planar coordinated Pt^{II} ion in relative *cis* sites, generating a six-membered ring similar to the reported Re(*L*)(CO)₃Cl (Li *et al.*, 2006), as shown in Fig. 1. In the crystal structure of the title complex, the main intermolecular non-covalent interactions are C—H(benzene)⋯π (Umezawa *et al.*, 1998) and C—H(methylene)⋯Cl (Desiraju & Steiner, 1999) interactions, which connect the mononuclear units along the *a* direction to form a chain structure. As shown in Fig. 2, the C23ⁱⁱ—H23ⁱⁱ⋯Cg1 contact exhibits a C23⋯Cg1 distance of 4.001 (2) Å and a C23—H23⋯Cg1 bond angle of 154° (Cg1 represents the centroid of the C15—C16—C17—C18—C19—C20 benzene ring [symmetry code: (ii) $-x + 2, -y + 2, -z + 2$]). Regarding the C7—H7B(methylene)⋯Cl1ⁱ contact, the C7⋯Cl1ⁱ distance is 3.392 (2) Å and the C7—H7B⋯Cl1ⁱ angle equals 127° [symmetry code: (i) $x + 1, y, z$].

Experimental

N-benzyl-*N*-(diphenylphosphanylmethyl)pyridin-2-amine (*L*) was obtained by the reaction of *N*-benzylpyridin-2-amine with Ph₂PH and (HCHO)_{*n*}, using a developed method of the Mannich reaction in acidic medium as reported in literature (Li *et al.*, 2003). A mixture of Pt(COD)MeCl (0.210 g, 0.6 mmol) and 0.382 g of *L* (1.0 mmol) in CH₂Cl₂ (20 ml) was stirred at room temperature for 3 h (COD = 1,5-cyclooctadiene). The clear solution was filtered and the solvent was concentrated to a small volume and diethyl ether was subsequently added to give 0.309 g (82%) of the title complex as a white solid, crystals of which were obtained after four days by recrystallization from CH₂Cl₂/*n*-hexane, yield: 0.230 g (61%).

Refinement

The hydrogen atoms were placed in idealized positions and allowed to ride on the relevant carbon atoms, with C—H = 0.93 Å and $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ for aromatic H atoms, with C—H = 0.97 Å and $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ for methylene H atoms, and with C—H = 0.96 Å and $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

Figures

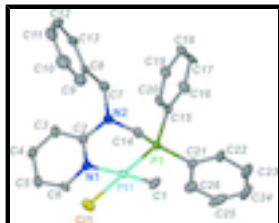


Fig. 1. The atom-numbering scheme of the title complex. Displacement ellipsoids are drawn at the 30% probability level and H atoms are omitted for clarity.

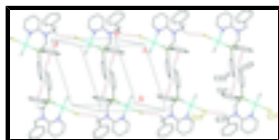


Fig. 2. The C—H(benzene)⋯ π and C—H(methylene)⋯Cl interactions between the mononuclear units arranged along the a direction. The Cg1 represents the centroid of the C15—C16—C17—C18—C19—C20 ring (benzene). Symmetry codes: (i) $x + 1, y, z$; (ii) $-x + 2, -y + 2, -z + 2$.

[N-Benzyl-N-(diphenylphosphanylmethyl)pyridin-2-amine]chloridomethylplatinum(II)

Crystal data

[Pt(CH₃)Cl(C₂₅H₂₃N₂P)]

$M_r = 628.00$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 9.538$ (3) Å

$b = 10.770$ (3) Å

$c = 13.125$ (4) Å

$\alpha = 98.367$ (4)°

$\beta = 106.256$ (4)°

$\gamma = 107.266$ (5)°

$V = 1197.0$ (6) Å³

$Z = 2$

$F(000) = 612$

$D_x = 1.742$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

$\mu = 6.06$ mm⁻¹

$T = 293$ K

Block, colourless

$0.33 \times 0.24 \times 0.20$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2007)

$T_{\min} = 0.675, T_{\max} = 1.000$

6265 measured reflections

4201 independent reflections

3270 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

$\theta_{\text{max}} = 25.0^\circ, \theta_{\text{min}} = 2.3^\circ$

$h = -11 \rightarrow 6$

$k = -12 \rightarrow 12$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$$wR(F^2) = 0.123$$

$$S = 1.01$$

4201 reflections

281 parameters

0 restraints

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.065P)^2] \quad P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 2.18 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -2.33 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pt1	0.99999 (4)	0.54883 (4)	0.70540 (3)	0.03520 (15)
Cl1	1.1825 (3)	0.4495 (3)	0.6820 (3)	0.0641 (8)
P1	0.8409 (3)	0.6473 (2)	0.73503 (19)	0.0340 (5)
N1	0.8123 (9)	0.3822 (8)	0.5717 (6)	0.0402 (19)
N2	0.6167 (9)	0.4091 (8)	0.6379 (7)	0.048 (2)
C1	1.1828 (11)	0.6965 (10)	0.8263 (9)	0.051 (3)
H1A	1.2417	0.7576	0.7941	0.077*
H1B	1.2489	0.6572	0.8691	0.077*
H1C	1.1438	0.7442	0.8726	0.077*
C2	0.6662 (11)	0.3300 (10)	0.5714 (8)	0.043 (2)
C3	0.5668 (12)	0.2033 (10)	0.5068 (8)	0.053 (3)
H3	0.4691	0.1650	0.5125	0.063*
C4	0.6138 (14)	0.1358 (11)	0.4352 (9)	0.057 (3)
H4	0.5499	0.0500	0.3922	0.069*
C5	0.7594 (14)	0.1978 (11)	0.4276 (9)	0.057 (3)
H5	0.7920	0.1568	0.3759	0.068*
C6	0.8527 (12)	0.3189 (11)	0.4967 (8)	0.045 (2)
H6	0.9502	0.3596	0.4913	0.054*
C7	0.4833 (11)	0.3477 (11)	0.6713 (9)	0.054 (3)
H7A	0.3919	0.3019	0.6060	0.064*
H7B	0.4630	0.4184	0.7128	0.064*
C8	0.5046 (12)	0.2502 (10)	0.7386 (8)	0.046 (3)
C9	0.6496 (15)	0.2476 (13)	0.7969 (10)	0.066 (3)
H9	0.7407	0.3058	0.7926	0.080*
C10	0.656 (2)	0.1572 (17)	0.8612 (12)	0.090 (5)
H10	0.7536	0.1558	0.8997	0.109*
C11	0.527 (3)	0.0706 (16)	0.8707 (13)	0.098 (6)

supplementary materials

H11	0.5352	0.0092	0.9130	0.117*
C12	0.385 (2)	0.0762 (14)	0.8161 (14)	0.090 (5)
H12	0.2951	0.0215	0.8248	0.108*
C13	0.3726 (14)	0.1606 (12)	0.7495 (11)	0.067 (4)
H13	0.2742	0.1588	0.7101	0.080*
C14	0.6497 (11)	0.5486 (10)	0.6317 (8)	0.042 (2)
H14A	0.5702	0.5802	0.6461	0.051*
H14B	0.6510	0.5567	0.5592	0.051*
C15	0.7980 (11)	0.6491 (9)	0.8610 (8)	0.039 (2)
C16	0.6740 (13)	0.6856 (12)	0.8728 (9)	0.058 (3)
H16	0.6184	0.7164	0.8183	0.069*
C17	0.6329 (15)	0.6761 (14)	0.9664 (11)	0.072 (4)
H17	0.5494	0.7000	0.9733	0.086*
C18	0.7140 (15)	0.6323 (12)	1.0477 (10)	0.063 (3)
H18	0.6868	0.6271	1.1101	0.075*
C19	0.8370 (15)	0.5957 (11)	1.0363 (9)	0.061 (3)
H19	0.8923	0.5640	1.0904	0.073*
C20	0.8774 (13)	0.6066 (10)	0.9431 (8)	0.048 (3)
H20	0.9621	0.5840	0.9370	0.058*
C21	0.8791 (11)	0.8172 (10)	0.7178 (9)	0.044 (2)
C22	0.9235 (16)	0.9260 (11)	0.8040 (12)	0.075 (4)
H22	0.9322	0.9134	0.8738	0.090*
C23	0.955 (2)	1.0538 (16)	0.788 (2)	0.107 (6)
H23	0.9901	1.1264	0.8481	0.129*
C24	0.9375 (19)	1.0761 (16)	0.688 (2)	0.111 (7)
H24	0.9531	1.1622	0.6779	0.133*
C25	0.8956 (16)	0.9686 (19)	0.6016 (16)	0.095 (5)
H25	0.8833	0.9826	0.5318	0.115*
C26	0.8710 (13)	0.8394 (13)	0.6154 (10)	0.062 (3)
H26	0.8493	0.7687	0.5566	0.074*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.0336 (2)	0.0378 (2)	0.0384 (2)	0.01434 (16)	0.01476 (16)	0.01323 (16)
Cl1	0.0534 (16)	0.084 (2)	0.073 (2)	0.0448 (16)	0.0267 (15)	0.0198 (17)
P1	0.0353 (13)	0.0311 (13)	0.0347 (13)	0.0130 (10)	0.0094 (10)	0.0080 (10)
N1	0.046 (5)	0.037 (5)	0.041 (5)	0.014 (4)	0.017 (4)	0.016 (4)
N2	0.034 (4)	0.043 (5)	0.066 (6)	0.012 (4)	0.021 (4)	0.007 (4)
C1	0.044 (6)	0.042 (6)	0.058 (7)	0.007 (5)	0.003 (5)	0.027 (5)
C2	0.036 (5)	0.038 (6)	0.053 (6)	0.015 (5)	0.011 (5)	0.008 (5)
C3	0.048 (6)	0.042 (6)	0.052 (7)	0.008 (5)	0.012 (5)	-0.007 (5)
C4	0.067 (8)	0.037 (6)	0.059 (7)	0.007 (5)	0.024 (6)	0.005 (5)
C5	0.082 (8)	0.039 (6)	0.049 (7)	0.022 (6)	0.026 (6)	0.003 (5)
C6	0.056 (6)	0.054 (7)	0.043 (6)	0.031 (5)	0.031 (5)	0.015 (5)
C7	0.033 (5)	0.052 (7)	0.068 (7)	0.009 (5)	0.020 (5)	-0.001 (6)
C8	0.054 (7)	0.033 (6)	0.046 (6)	0.003 (5)	0.031 (5)	-0.009 (5)
C9	0.061 (8)	0.067 (9)	0.065 (8)	0.016 (7)	0.023 (6)	0.010 (7)

C10	0.119 (13)	0.102 (13)	0.071 (10)	0.055 (11)	0.039 (9)	0.034 (9)
C11	0.182 (19)	0.068 (11)	0.074 (11)	0.050 (12)	0.083 (13)	0.023 (8)
C12	0.111 (13)	0.050 (9)	0.106 (13)	-0.005 (8)	0.073 (11)	0.008 (8)
C13	0.059 (7)	0.052 (8)	0.080 (9)	0.000 (6)	0.045 (7)	-0.011 (7)
C14	0.038 (5)	0.046 (6)	0.048 (6)	0.026 (5)	0.010 (5)	0.011 (5)
C15	0.043 (5)	0.033 (5)	0.040 (5)	0.013 (4)	0.013 (4)	0.004 (4)
C16	0.051 (7)	0.072 (8)	0.054 (7)	0.033 (6)	0.015 (5)	0.007 (6)
C17	0.075 (9)	0.090 (10)	0.074 (9)	0.044 (8)	0.051 (7)	0.004 (8)
C18	0.093 (10)	0.054 (8)	0.058 (8)	0.030 (7)	0.049 (7)	0.012 (6)
C19	0.090 (9)	0.054 (8)	0.058 (7)	0.037 (7)	0.038 (7)	0.021 (6)
C20	0.059 (7)	0.046 (6)	0.046 (6)	0.028 (5)	0.023 (5)	0.003 (5)
C21	0.038 (5)	0.039 (6)	0.060 (7)	0.018 (5)	0.016 (5)	0.019 (5)
C22	0.096 (10)	0.028 (7)	0.107 (11)	0.012 (6)	0.058 (9)	0.012 (7)
C23	0.106 (13)	0.044 (9)	0.18 (2)	0.013 (8)	0.074 (13)	0.024 (11)
C24	0.088 (11)	0.042 (9)	0.23 (3)	0.026 (8)	0.081 (14)	0.056 (13)
C25	0.062 (9)	0.111 (14)	0.143 (15)	0.034 (9)	0.042 (9)	0.100 (13)
C26	0.052 (7)	0.064 (8)	0.070 (8)	0.019 (6)	0.016 (6)	0.030 (7)

Geometric parameters (Å, °)

Pt1—C1	2.039 (10)	C10—H10	0.9300
Pt1—P1	2.178 (2)	C11—C12	1.37 (2)
Pt1—N1	2.219 (8)	C11—H11	0.9300
Pt1—C11	2.361 (3)	C12—C13	1.36 (2)
P1—C15	1.811 (10)	C12—H12	0.9300
P1—C21	1.818 (10)	C13—H13	0.9300
P1—C14	1.828 (10)	C14—H14A	0.9700
N1—C6	1.326 (12)	C14—H14B	0.9700
N1—C2	1.338 (12)	C15—C20	1.355 (13)
N2—C2	1.401 (12)	C15—C16	1.392 (13)
N2—C14	1.461 (12)	C16—C17	1.399 (16)
N2—C7	1.464 (13)	C16—H16	0.9300
C1—H1A	0.9600	C17—C18	1.364 (17)
C1—H1B	0.9600	C17—H17	0.9300
C1—H1C	0.9600	C18—C19	1.382 (15)
C2—C3	1.387 (13)	C18—H18	0.9300
C3—C4	1.357 (14)	C19—C20	1.392 (15)
C3—H3	0.9300	C19—H19	0.9300
C4—C5	1.389 (16)	C20—H20	0.9300
C4—H4	0.9300	C21—C22	1.372 (15)
C5—C6	1.352 (15)	C21—C26	1.385 (15)
C5—H5	0.9300	C22—C23	1.38 (2)
C6—H6	0.9300	C22—H22	0.9300
C7—C8	1.490 (15)	C23—C24	1.34 (2)
C7—H7A	0.9700	C23—H23	0.9300
C7—H7B	0.9700	C24—C25	1.37 (2)
C8—C9	1.391 (16)	C24—H24	0.9300
C8—C13	1.399 (15)	C25—C26	1.388 (19)
C9—C10	1.383 (19)	C25—H25	0.9300

supplementary materials

C9—H9	0.9300	C26—H26	0.9300
C10—C11	1.36 (2)		
C1—Pt1—P1	90.3 (3)	C9—C10—H10	118.6
C1—Pt1—N1	176.2 (4)	C10—C11—C12	118.2 (15)
P1—Pt1—N1	93.5 (2)	C10—C11—H11	120.9
C1—Pt1—C11	86.8 (3)	C12—C11—H11	120.9
P1—Pt1—C11	176.99 (10)	C13—C12—C11	120.7 (14)
N1—Pt1—C11	89.5 (2)	C13—C12—H12	119.6
C15—P1—C21	105.9 (5)	C11—C12—H12	119.6
C15—P1—C14	102.0 (5)	C12—C13—C8	121.7 (13)
C21—P1—C14	104.8 (5)	C12—C13—H13	119.1
C15—P1—Pt1	119.0 (3)	C8—C13—H13	119.1
C21—P1—Pt1	117.2 (3)	N2—C14—P1	107.1 (6)
C14—P1—Pt1	106.0 (3)	N2—C14—H14A	110.3
C6—N1—C2	118.0 (9)	P1—C14—H14A	110.3
C6—N1—Pt1	117.7 (7)	N2—C14—H14B	110.3
C2—N1—Pt1	123.5 (7)	P1—C14—H14B	110.3
C2—N2—C14	116.7 (8)	H14A—C14—H14B	108.5
C2—N2—C7	120.7 (9)	C20—C15—C16	118.0 (9)
C14—N2—C7	117.0 (8)	C20—C15—P1	121.5 (7)
Pt1—C1—H1A	109.5	C16—C15—P1	120.3 (8)
Pt1—C1—H1B	109.5	C15—C16—C17	120.2 (11)
H1A—C1—H1B	109.5	C15—C16—H16	119.9
Pt1—C1—H1C	109.5	C17—C16—H16	119.9
H1A—C1—H1C	109.5	C18—C17—C16	120.8 (11)
H1B—C1—H1C	109.5	C18—C17—H17	119.6
N1—C2—C3	121.4 (9)	C16—C17—H17	119.6
N1—C2—N2	117.4 (9)	C17—C18—C19	119.3 (11)
C3—C2—N2	121.3 (9)	C17—C18—H18	120.4
C4—C3—C2	119.3 (10)	C19—C18—H18	120.4
C4—C3—H3	120.3	C18—C19—C20	119.3 (11)
C2—C3—H3	120.3	C18—C19—H19	120.3
C3—C4—C5	118.5 (11)	C20—C19—H19	120.3
C3—C4—H4	120.8	C15—C20—C19	122.4 (10)
C5—C4—H4	120.8	C15—C20—H20	118.8
C6—C5—C4	118.9 (10)	C19—C20—H20	118.8
C6—C5—H5	120.6	C22—C21—C26	118.4 (11)
C4—C5—H5	120.6	C22—C21—P1	122.4 (9)
N1—C6—C5	123.2 (10)	C26—C21—P1	119.2 (9)
N1—C6—H6	118.4	C21—C22—C23	120.5 (15)
C5—C6—H6	118.4	C21—C22—H22	119.7
N2—C7—C8	114.6 (9)	C23—C22—H22	119.7
N2—C7—H7A	108.6	C24—C23—C22	121.8 (18)
C8—C7—H7A	108.6	C24—C23—H23	119.1
N2—C7—H7B	108.6	C22—C23—H23	119.1
C8—C7—H7B	108.6	C23—C24—C25	118.1 (16)
H7A—C7—H7B	107.6	C23—C24—H24	120.9
C9—C8—C13	117.5 (12)	C25—C24—H24	120.9
C9—C8—C7	123.8 (10)	C24—C25—C26	121.7 (16)

C13—C8—C7	118.6 (11)	C24—C25—H25	119.2
C10—C9—C8	119.0 (13)	C26—C25—H25	119.2
C10—C9—H9	120.5	C21—C26—C25	119.2 (14)
C8—C9—H9	120.5	C21—C26—H26	120.4
C11—C10—C9	122.9 (16)	C25—C26—H26	120.4
C11—C10—H10	118.6		
C1—Pt1—P1—C15	-69.7 (5)	C10—C11—C12—C13	4(2)
N1—Pt1—P1—C15	110.5 (4)	C11—C12—C13—C8	-4(2)
Cl1—Pt1—P1—C15	-57 (2)	C9—C8—C13—C12	1.5 (16)
C1—Pt1—P1—C21	59.9 (5)	C7—C8—C13—C12	-175.0 (11)
N1—Pt1—P1—C21	-119.9 (4)	C2—N2—C14—P1	-90.2 (9)
Cl1—Pt1—P1—C21	73 (2)	C7—N2—C14—P1	115.7 (8)
C1—Pt1—P1—C14	176.3 (5)	C15—P1—C14—N2	-72.7 (7)
N1—Pt1—P1—C14	-3.5 (4)	C21—P1—C14—N2	177.1 (6)
Cl1—Pt1—P1—C14	-171 (2)	Pt1—P1—C14—N2	52.5 (7)
C1—Pt1—N1—C6	-22 (5)	C21—P1—C15—C20	-125.7 (9)
P1—Pt1—N1—C6	154.9 (7)	C14—P1—C15—C20	125.0 (9)
Cl1—Pt1—N1—C6	-25.8 (7)	Pt1—P1—C15—C20	8.8 (10)
C1—Pt1—N1—C2	148 (5)	C21—P1—C15—C16	58.9 (9)
P1—Pt1—N1—C2	-35.2 (8)	C14—P1—C15—C16	-50.5 (9)
Cl1—Pt1—N1—C2	144.2 (8)	Pt1—P1—C15—C16	-166.7 (7)
C6—N1—C2—C3	10.0 (15)	C20—C15—C16—C17	-1.0 (16)
Pt1—N1—C2—C3	-159.9 (8)	P1—C15—C16—C17	174.6 (10)
C6—N1—C2—N2	-169.3 (9)	C15—C16—C17—C18	1(2)
Pt1—N1—C2—N2	20.8 (13)	C16—C17—C18—C19	-1(2)
C14—N2—C2—N1	47.3 (12)	C17—C18—C19—C20	1.2 (18)
C7—N2—C2—N1	-159.6 (10)	C16—C15—C20—C19	1.6 (16)
C14—N2—C2—C3	-132.0 (10)	P1—C15—C20—C19	-174.0 (9)
C7—N2—C2—C3	21.1 (15)	C18—C19—C20—C15	-1.7 (18)
N1—C2—C3—C4	-6.0 (16)	C15—P1—C21—C22	21.9 (11)
N2—C2—C3—C4	173.3 (10)	C14—P1—C21—C22	129.3 (10)
C2—C3—C4—C5	-1.3 (17)	Pt1—P1—C21—C22	-113.6 (9)
C3—C4—C5—C6	4.3 (18)	C15—P1—C21—C26	-161.4 (8)
C2—N1—C6—C5	-7.0 (15)	C14—P1—C21—C26	-54.0 (9)
Pt1—N1—C6—C5	163.6 (8)	Pt1—P1—C21—C26	63.1 (9)
C4—C5—C6—N1	-0.2 (17)	C26—C21—C22—C23	1.6 (19)
C2—N2—C7—C8	61.9 (13)	P1—C21—C22—C23	178.3 (11)
C14—N2—C7—C8	-145.1 (9)	C21—C22—C23—C24	3(2)
N2—C7—C8—C9	20.8 (15)	C22—C23—C24—C25	-4(3)
N2—C7—C8—C13	-162.9 (9)	C23—C24—C25—C26	0(2)
C13—C8—C9—C10	0.5 (16)	C22—C21—C26—C25	-5.1 (16)
C7—C8—C9—C10	176.7 (11)	P1—C21—C26—C25	178.1 (9)
C8—C9—C10—C11	0(2)	C24—C25—C26—C21	4(2)
C9—C10—C11—C12	-2(2)		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 is the centroid of the C15–C20 benzene ring.

D—H \cdots A

D—H

H \cdots A

D \cdots A

D—H \cdots A

supplementary materials

C23—H23…Cg1 ⁱ	0.93	3.10	4.001 (2)	154
C7—H7B…C11 ⁱⁱ	0.97	2.72	3.392 (2)	127

Symmetry codes: (i) $-x+2, -y+2, -z+2$; (ii) $x-1, y, z$.

Fig. 1

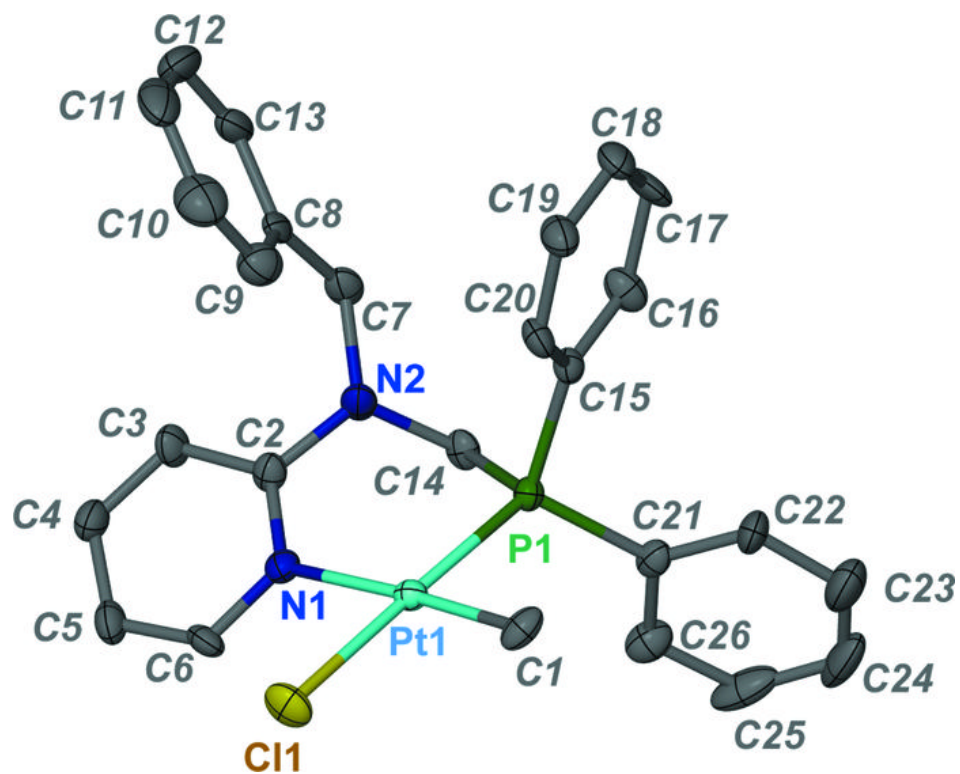


Fig. 2

