Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

{2-[(Benzylmethylamino)methyl]ferrocene-κ^2N,C^1}-chloro(dimethyl sulfoxide-κS)platinum(II)

Hong-Xing Wang,* Hong-Fei Wu, Feng-Ying Geng, Ren-Qing Gao and Hui-Chao Zhou

Department of Chemistry, College of Sciences, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail:
hongxing_wang@hotmail.com

Received 15 December 2005
Accepted 22 December 2005
Online 7 January 2006

In the title compound, [PtCl{Fe(C_5H_5)($C_{14}H_{14}NO$)}(C_2H_6SO)] or [FePt(C_5H_5)($C_{14}H_{15}N$)Cl(C_2H_6OS)], the Pt^{II} atom is in a slightly distorted square-planar environment. The substituted cyclopentadienyl plane is nearly perpendicular to the plane of the benzene ring [dihedral angle = 84.6 (1)°].

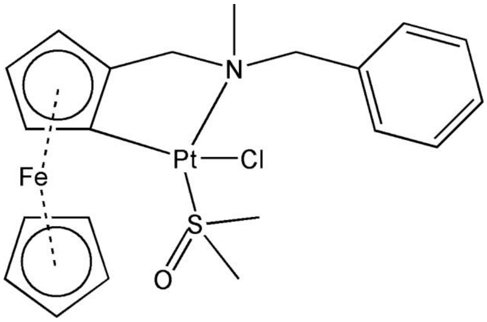
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.019
wR factor = 0.047
Data-to-parameter ratio = 15.7

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

Comment

There is an increasing interest in cycloplatination reactions due to their applications in organic synthesis (Fossy & Richards, 1999), but only a few cycloplatinated complexes with *N*-donor ligands have been reported (Ryabov *et al.*, 2002). As a part of our ongoing investigations of *N*-methyl-*N*-ferrocenylmethylbenzyamines (Wang *et al.*, 2006), a new compound, (I), has been prepared and we report its crystal structure here.



(I)

In the compound (I), atom Pt1 is in a slightly distorted square-planar environment (Fig. 1 and Table 1). Atoms Pt1, N1, Cl1, C1 and S1 deviate from the mean plane through them by −0.0334 (9), −0.0770 (11), 0.0790 (11), 0.0983 (13) and −0.0658 (10) Å, respectively. Atoms N1 and C11 deviate from the mean plane through the Pt1—N1—C11—C2—C1 ring by 0.156 (1) and −0.168 (2) Å, respectively. The substituted cyclopentadienyl and benzene ring planes are nearly perpendicular to each other, with a dihedral angle of 84.6 (1)°. The crystal packing is stabilized by C—H···O and C—H···Cl hydrogen bonds (Table 2).

Experimental

cis-[Pt(DMSO)$_2$Cl$_2$] (30 mg, 0.5 mmol) was added to a stirred solution of {[(*N*-methyl-*N*-benzyl)amino]methyl}ferrocene (160 mg, 0.5 mmol) in methanol (20 ml). The resulting mixture was refluxed for 30 min under a nitrogen atmosphere. The mixture was cooled to room temperature and the solvent was removed *in vacuo*. The solid was purified by column chromatography to afford compound (I)

(Yield: 56%). ^{1}H NMR ($CDCl_3$, δ, p.p.m.): 7.94 (*m*, 2H), 7.04 (*m*, 3H), 4.22 (*m*, 1H), 4.13 (*s*, 5H), 4.11 (*d*, 2H), 3.57 (*s*, 3H), 3.54 (*s*, 3H), 2.83 (*m*, 4H), 1.55 (*s*, 3H). Analysis calculated for $C_{21}H_{26}ClFeNOPtS$: C 40.24, H 4.18, N 2.23%; found: C 40.19, H 4.16, N 2.18%.

Crystal data

$[FePt(C_5H_5)(C_{14}H_{15}N)Cl(C_2H_6OS)]$
$M_r = 626.88$
Monoclinic, $P2_1/c$
$a = 12.3198\ (12)$ Å
$b = 9.7102\ (9)$ Å
$c = 18.3096\ (18)$ Å
$\beta = 90.842\ (1)^\circ$
$V = 2190.1\ (4)$ Å^3
$Z = 4$
$D_x = 1.901$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7216 reflections
$\theta = 2.4$–27.8°
$\mu = 7.27$ mm^{-1}
$T = 293\ (2)$ K
Block, red
$0.38 \times 0.20 \times 0.16$ mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.135$, $T_{max} = 0.312$
11498 measured reflections
3872 independent reflections
3560 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0^\circ$
$h = -14 \rightarrow 14$
$k = -11 \rightarrow 11$
$l = -21 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.047$
$S = 1.05$
3872 reflections
247 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0219P)^2 + 0.9438P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt1—C1	1.981 (3)	Pt1—S1	2.1879 (8)
Pt1—N1	2.132 (3)	Pt1—Cl1	2.3998 (8)
C1—Pt1—N1	82.14 (11)	C1—Pt1—Cl1	171.17 (9)
C1—Pt1—S1	96.69 (9)	N1—Pt1—Cl1	92.09 (7)
N1—Pt1—S1	177.64 (7)	S1—Pt1—Cl1	89.31 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1	0.98	2.42	3.057 (5)	122
C13—H13*A*···Cl1	0.97	2.71	3.326 (4)	122
C15—H15···Cl1	0.93	2.66	3.479 (4)	148
C20—H20*A*···O1^i	0.96	2.54	3.407 (5)	151
C21—H21*B*···Cl1	0.96	2.65	3.314 (4)	126
C21—H21*C*···O1^i	0.96	2.45	3.341 (5)	154

Symmetry code: (i) $-x, -y, -z + 2$.

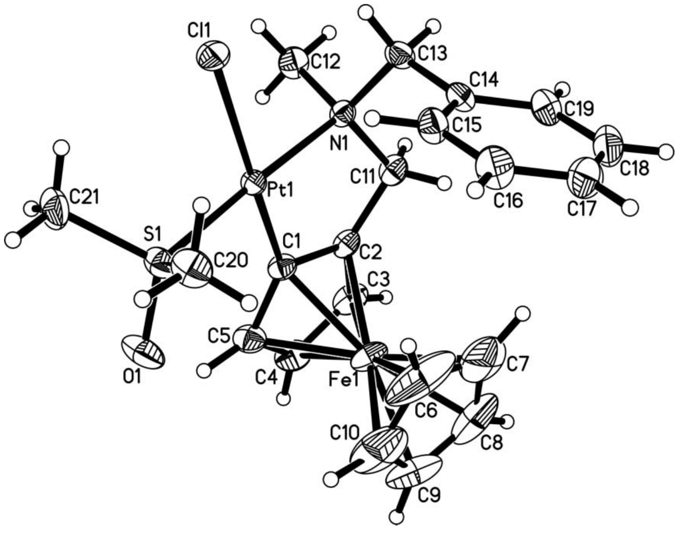


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size.

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry with C—H distances of 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); 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*.

The authors acknowledge the Natural Science Foundation of Tianjin City, People's Republic of China, for financial support (grant No. 033609011).

References

Bruker (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fossy, J. S. & Richards, C. J. (1999). *Organometallics*, **18**, 2116–2124.
Ryabov, A. D., Panyashkina, I. M., Polyakov, V. A. & Fischer, A. (2002). *Organometallics*, **21**, 1633–1636.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, H.-X., Wu, H.-F., Geng, F.-Y., Gao R.-Q. & Zhou, H.-C. (2006). *Acta Cryst.* E**62**, m14–m15.

Acta Cryst. (2006). E**62**, m192–m193 Wang *et al.* • $[FePt(C_5H_5)(C_{14}H_{15}N)Cl(C_2H_6OS)]$ **m193**

]