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[Ferrocene-1,1′-diylbis(diphenylphosphine-*P*)](toluene-3,4-dithiolato)platinum(II) dichloromethane solvate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.010 Å
R factor = 0.051
wR factor = 0.111
Data-to-parameter ratio = 18.3

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

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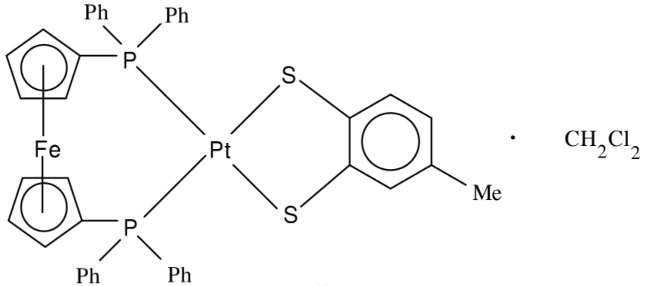
The title compound, [Pt($C_{34}H_{28}FeP_2$)($C_7H_6S_2$)]·CH_2Cl_2, has a distorted square-planar geometry with two sets of *cis* S and P atoms. The Pt—S bonds differ significantly, with bond distances of 2.306 (2) and 2.322 (2) Å. The longer Pt—S distance may be due to the *trans* influence by the shorter Pt—P bond.

Comment

A number of metal complexes containing thiolate ligands are known to absorb SO_2 reversibly, with the SO_2 bound to the S atom of the thiolate ligand (Eller & Kubas, 1977; Mazid *et al.*, 1981; Darensbourg *et al.*, 1994; Shaver & Plouffe, 1992). In some of our recent work, we have investigated SO_2 binding by diphosphinonickel(II)–dithiolate complexes (Darkwa, 1997), but we found no conclusive evidence for the binding site of the SO_2 from spectroscopic data. In pursuing the objective of identifying the binding site for SO_2 adducts in diphosphinometal dithiolates, we reacted the title Pt complex (Maisela, 2001) with sulfur dioxide gas and attempted to grow crystals of this product. UV-vis and ^{1}H NMR spectroscopic data indicate the formation of an SO_2 adduct, but attempts to grow crystals of this adduct under an atmosphere of SO_2 resulted in crystals of (I), whose structure is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1, and selected bond distances and angles are shown in Table 1. The essential features of this molecular structure are similar to that of [Pd($C_{22}H_{36}FeP_2$)(C_6H_5S)$_2$] (Guzei *et al.*, 2000). The coordination geometry around the Pt^{II} ion is square planar, with P and S atoms *cis* to each other. There is a small amount of distortion of the square plane towards a tetrahedron. The Pt atom is displaced slightly at a distance of 0.026 (1) Å from the coordination plane defined by the P1/P2/S1/S2 atoms. The Pt—P and Pt—S distances are typical in similar complexes (Maisela *et al.*, 2001). However, the difference between the two Pt—S distances are significant. The longer Pt—S2 bond than Pt—S1 may be due to the *trans* influence by the shorter Pt—P1 bond than Pt—P2.

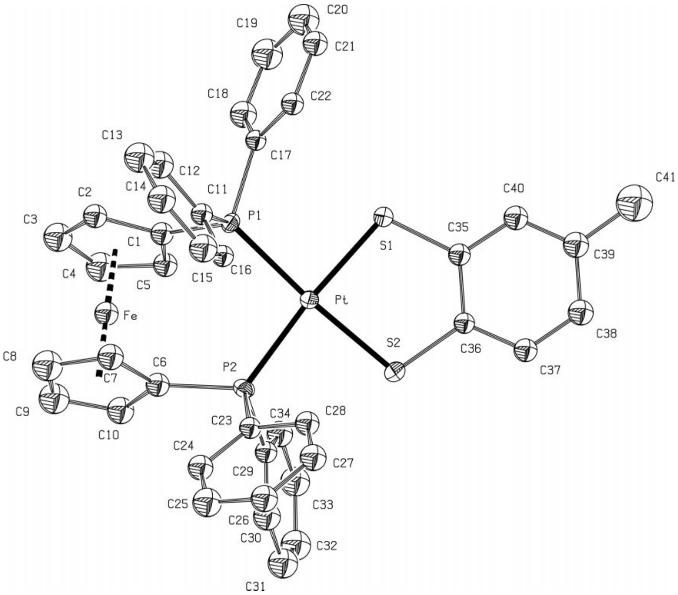


Figure 1
A view of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

The two Fe—*Cp* (*Cp* is the cyclopentadienyl centroid) distances [1.639 (3) and 1.644 (3) Å] of the ferrocene moiety are the same within experimental error. The two Cp rings are staggered with an interplanar distance of 3.283 (4) Å. The dihedral angle of the Cp rings is 4.4 (1)°. The closest distance between the two Cp rings occurs at the C1 and C6 atoms bonded to P, and it is likely that the tilting is due to coordination of P atoms to Pt.

Experimental

The title complex was synthesized by a recently reported procedure (Maisela *et al.*, 2001). Crystals of (I) were grown by layering an SO_2-saturated solution of [Pt(dppf)(SC_6H_3MeS-*o*)] in dichloromethane with SO_2-saturated hexane and allowing the hexane to diffuse slowly into the solution of the platinum compound.

Crystal data

$[Pt(C_{34}H_{28}FeP_2)(C_7H_6S_2)]\cdot CH_2Cl_2$
$M_r = 988.61$
Monoclinic, $P2_1/n$
$a = 14.539$ (1) Å
$b = 14.550$ (1) Å
$c = 17.850$ (1) Å
$\beta = 94.550$ (1)°
$V = 3764.1$ (4) Å^3
$Z = 4$
$D_x = 1.744$ Mg m^{-3}
Mo Kα radiation
Cell parameters from 4233 reflections
$\theta = 2$–27°
$\mu = 4.47$ mm^{-1}
$T = 173$ (2) K
Parallelepiped, orange
0.37 × 0.25 × 0.16 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans with κ offsets
Absorption correction: empirical (*SORTAV*; Blessing, 1995)
$T_{min} = 0.264$, $T_{max} = 0.489$
20 154 measured reflections
8290 independent reflections
5735 reflections with $I > 2\sigma(I)$
$R_{int} = 0.075$
$\theta_{max} = 27.5°$
$h = -18 \rightarrow 13$
$k = -18 \rightarrow 17$
$l = -13 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > (F^2)] = 0.051$
$wR(F^2) = 0.111$
$S = 1.04$
8290 reflections
453 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 1.43$ e Å^{-3}
$\Delta\rho_{min} = -1.93$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt1—P1	2.2835 (16)	Pt1—S1	2.3058 (15)
Pt1—P2	2.2956 (15)	Pt1—S2	2.3217 (16)
P1—Pt1—P2	97.24 (6)	P1—Pt1—S2	175.87 (5)
P1—Pt1—S1	87.92 (6)	P2—Pt1—S2	86.84 (6)
P2—Pt1—S1	174.42 (6)	S1—Pt1—S2	87.98 (6)

H atoms were placed in calculated positions and treated as riding atoms.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1997); software used to prepare material for publication: *PLATON*.

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m110 John Bacsa *et al.* • $[Pt(C_{34}H_{28}FeP_2)(C_7H_6S_2)]\cdot CH_2Cl_2$ *Acta Cryst.* (2001). E**57**, m109–m110