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cis-[*rac*-1,3-Bis(phenylsulfinyl)propane-*S*,*S*′]-dichloroplatinum(II)

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In the crystal structure of the title compound, [$PtCl_2$($C_{15}H_{16}O_2S_2$)], the central Pt^{II} ion is four-coordinated in a slightly distorted square-planar geometry. The crystal represents the racemate formed by the molecules with the (*R*,*R*) and (*S*,*S*) configurations of the sulfur chiral centres in the chelate ring. The pseudo-torsion angle between two S=O groups (O=S···S=O) is 165.8 (2)° and the dihedral angle formed by the planes of the two phenyl rings is 146.5 (2)°.

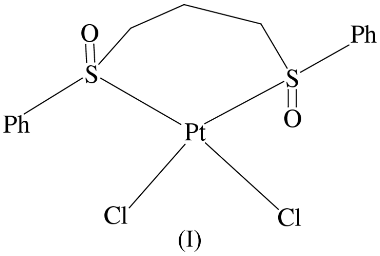
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.014 Å
R factor = 0.047
wR factor = 0.114
Data-to-parameter ratio = 15.4

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

Comment

A number of Pt complexes with monosulfoxide have been isolated and fairly well characterized (Calligaris & Carugo, 1996). It was noted that the sulfoxide group normally coordinates soft metals (Pt, Pd *etc.*) *via* its S atom (Kagan & Ronan, 1992). Pt^{II} usually bonds to bis(sulfoxides) in a *cis*-chelate mode which may potentially produce complexes with antitumor activity. There are, however, just a few examples of the complexes of this type which were structurally characterized (Cattalini *et al.*, 1979). In this paper, we report the crystal structure of a new Pt^{II} complex with the bis(sulfoxide) ligand, namely *cis*-[rac-1,3-bis(phenylsulfinyl)propane-*S*,*S*′]dichloroplatinum(II), (I).



(I)

The crystal represents the racemate formed by the molecules with the (*R*,*R*) and (*S*,*S*) configurations of the sulfur chiral centres in the chelate ring. The central Pt^{II} atom in the title complex, (I), is four-coordinated with two S-donors of the chelate ligand and two terminal Cl ligands, in a slightly distorted square-planar geometry, as shown in Fig. 1. The chelate ring adopts a distorted chair conformation flattened at the platinum end; the displacements of the Pt1 and C2 atoms from the least-squares plane drawn through the S1/C1/S2/C3 atoms (planar to within 0.04 Å) are equal to 0.4836 (4) and −0.771 (3) Å, respectively. The C4 and C10 atoms are displaced from this plane by 1.241 (3) and −1.631 (2) Å. The pseudo-torsion angle between the two S=O groups (O1=S1···S2=O2) is 165.8 (2)° and the dihedral angle formed by the planes of the two phenyl rings is 146.5 (2)°. A number of similar conformational features have been reported

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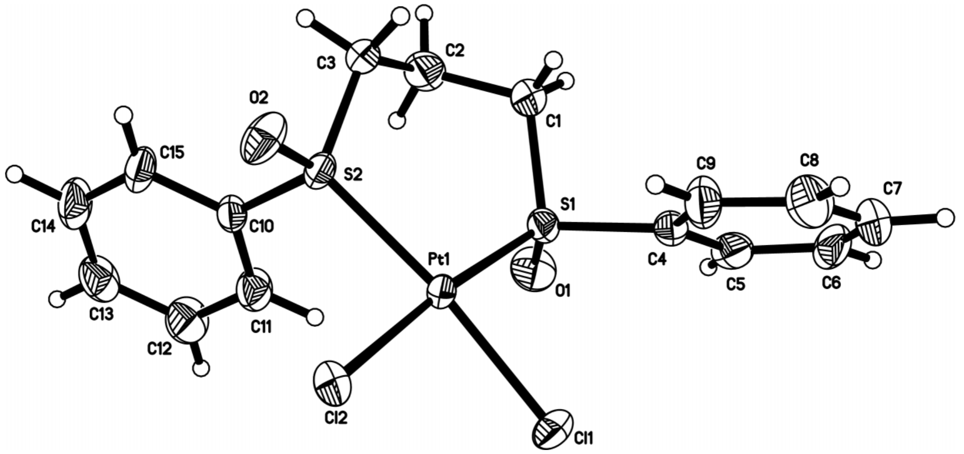

Figure 1
*ORTEP*II (Johnson, 1976) view of the title complex with 30% probability displacement ellipsoids.

for the Pt^{II} complex of *rac*-1,2-bis(phenylsulphinyl)ethane with a five-membered chelate ring (Cattalini *et al.*, 1979); the bond distances and angles in the latter complex are also in good agreement with those found for (I).

Experimental

rac-1,3-Bis(phenylsulfinyl)propane (Bpsp) was prepared according to the reported procedure of Zhang *et al.* (1997). To an aqueous solution of K_2PtCl_4 (100 mg, 0.24 mmol) with heating was slowly added a chloroform solution of equimolar Bpsp (70.4 mg, 0.24 mmol) with vigorous stirring. The white complex soon precipitated. Colourless single crystals of the title compound suitable for X-ray diffraction were obtained from a dimethylformamide–methane solution by slow evaporation of the solvent. Yield: 87.4 mg (65%). FT–IR data (KBr pellet, cm^{-1}): 1131 (*s*, S=O). Analysis calculated for the title complex: C 32.26, H 2.89%; found: C 32.18, H 2.88%.

Crystal data

$[PtCl_2(C_{15}H_{16}O_2S_2)]$
$M_r = 558.39$
Monoclinic, $P2_1/n$
$a = 7.5755$ (4) Å
$b = 21.6570$ (12) Å
$c = 11.0354$ (6) Å
$\beta = 103.300$ (1)°
$V = 1761.94$ (17) Å^3
$Z = 4$
$D_x = 2.105$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7023 reflections
$\theta = 2.7$–25.0°
$\mu = 8.51$ mm^{-1}
$T = 298$ (2) K
Prism, colourless
0.30 × 0.25 × 0.25 mm

Data collection

Bruker SMART 1000 diffractometer
ω scans
Absorption correction: multi-scan [*SAINT* (Bruker, 1998) and *SADABS* (Sheldrick, 1997)]
$T_{min} = 0.185$, $T_{max} = 0.225$
7105 measured reflections
3062 independent reflections
2798 reflections with $I > 2\sigma(I)$
$R_{int} = 0.084$
$\theta_{max} = 25.0°$
$h = -8 \rightarrow 9$
$k = -24 \rightarrow 25$
$l = -9 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.114$
$S = 1.04$
3062 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0646P)^2 + 3.6575P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.51$ e Å^{-3}
$\Delta\rho_{min} = -1.94$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt1—S1	2.2412 (18)	S1—C1	1.798 (8)
Pt1—S2	2.2501 (15)	S1—C4	1.798 (8)
Pt1—Cl1	2.3118 (17)	S2—C3	1.795 (9)
Pt1—Cl2	2.3067 (19)	S2—C10	1.778 (7)
S1—O1	1.453 (6)		
S1—Pt1—S2	98.71 (7)	S1—Pt1—Cl1	86.21 (7)
S1—Pt1—Cl2	174.19 (6)	S2—Pt1—Cl1	173.70 (7)
S2—Pt1—Cl2	86.50 (7)	Cl2—Pt1—Cl1	88.42 (7)

The C-bound H atoms were placed in their geometrically calculated positions and included in the final refinement in the riding-model approximation with displacement parameters derived from the atoms to which they were bonded. The U_{iso} for the H atoms were set to be $1.2U_{eq}$ for the parent atom. The highest peak is 1.34 Å from Pt1 and the deepest hole is 0.81 Å from Pt1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Bruker, 1998).

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