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Key indicators

Single-crystal X-ray study

$T = 293\text{ K}$

Mean $\sigma(\text{C}-\text{C}) = 0.014\text{ \AA}$

R factor = 0.047

wR factor = 0.120

Data-to-parameter ratio = 29.1

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

***trans*-Di- μ -chloro-bis[(dimethyl sulfoxide- κ S)-phenylplatinum(II)]**

The title compound, $[\text{Pt}_2\text{Cl}_2(\text{C}_6\text{H}_5)_2(\text{C}_2\text{H}_6\text{OS})_2]$ or $[\text{Pt}(\mu\text{-Cl})\text{Ph}(\text{dmsO})_2]$ (dmsO is dimethyl sulfoxide), is a dimer with a pseudo square-planar coordination geometry around the Pt atoms, with two bridging Cl ligands creating a four-membered ring at the centre of the dimer. The complex is centrosymmetric, thus necessitating a *trans* configuration, with one dmsO and one phenyl ligand coordinated to each Pt atom. The two Pt—Cl, the Pt—S and the Pt—C distances are 2.366 (2), 2.475 (2), 2.192 (2) and 1.997 (7) Å, respectively.

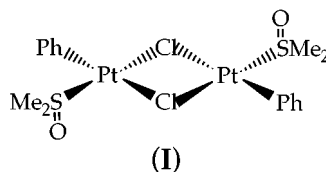
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Comment

Preparation of alkyl-sulfoxide-containing chloro-bridged dimers of platinum(II) was first reported by Annibale *et al.* (1985). The corresponding monomer of the title compound, *cis*-PtPhCl(dmsO)₂, has been prepared by Eaborn *et al.* (1978) and belongs to a group of complexes that has been extensively used to provide convenient routes to alkyl and aryl complexes of platinum(II) with different donor atoms, such as N, P, and As.



The coordination geometry around the Pt atoms in the title complex, (I), is square-planar, with two bridging Cl ligands. This gives rise to a four-membered ring, where the Cl—Pt—Cl and Pt—Cl—Pt angles are 85.02 (7) and 94.98 (7)°, respectively. The greater *trans* influence of the phenyl group

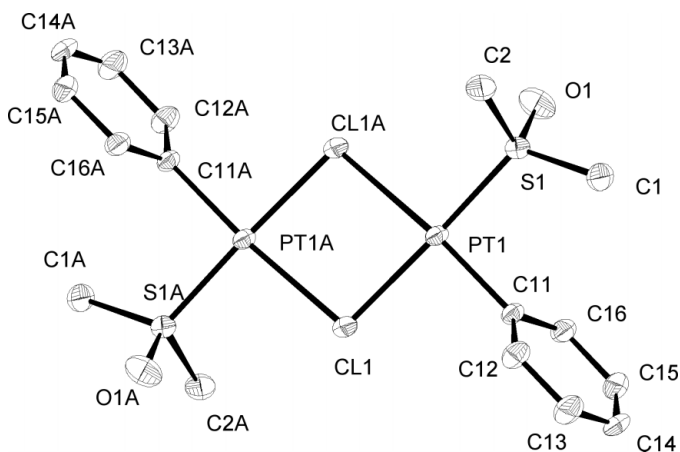


Figure 1

View of the title compound, showing the atom-numbering scheme and displacement ellipsoids at the 30% probability level. H atoms have been omitted for clarity.

compared to the dmsO group is reflected in the longer Pt—Cl bond *trans* to the phenyl ligand. To our knowledge, the Pt—Cl bond distance reported here [2.475 (2) Å] is the longest in a complex of this type. Selected bond lengths and angles are given in Table 1. Previous structure analyses of related dimers show corresponding Pt—Cl bond distances in the range 2.360–2.440 Å (Kukushkin *et al.*, 1991; Watkins, 1970; Boag & Ravetz, 1996; Kazankov *et al.*, 1997).

Experimental

cis-PtPhCl(dmsO)₂ was synthesized according to the literature (Cox *et al.*, 1934; Eaborn *et al.*, 1978). Slow evaporation from CD₂Cl₂ gave the title compound, (I). In the absence of free dmsO, the complex *cis*-PtPhCl(dmsO)₂ dimerizes in solution, as observed in ¹H NMR studies by the appearance of a peak from free dmsO.

Crystal data

[Pt ₂ Cl ₂ (C ₆ H ₅) ₂ (C ₂ H ₆ OS) ₂]	Z = 1
<i>M_r</i> = 771.54	<i>D_x</i> = 2.461 Mg m ⁻³
Triclinic, <i>P</i> $\bar{1}$	Mo <i>K</i> α radiation
<i>a</i> = 5.9625 (12) Å	Cell parameters from 3272 reflections
<i>b</i> = 8.0026 (16) Å	<i>θ</i> = 2.6–30.1°
<i>c</i> = 11.388 (2) Å	<i>μ</i> = 13.89 mm ⁻¹
<i>α</i> = 99.24 (3)°	<i>T</i> = 293 (2) K
<i>β</i> = 102.01 (3)°	Plate, white
<i>γ</i> = 94.91 (3)°	0.14 × 0.10 × 0.06 mm
<i>V</i> = 520.59 (18) Å ³	

Data collection

Bruker SMART CCD diffractometer	3170 independent reflections
<i>ω</i> scans	2621 reflections with <i>I</i> > 2σ(<i>I</i>)
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>R</i> _{int} = 0.053
<i>T</i> _{min} = 0.145, <i>T</i> _{max} = 0.359	<i>θ</i> _{max} = 31.6°
6421 measured reflections	<i>h</i> = -8 → 8
	<i>k</i> = -11 → 11
	<i>l</i> = -16 → 15

Refinement

Refinement on <i>F</i> ²	H-atom parameters constrained
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.047	<i>w</i> = 1/[σ ² (<i>F_o</i> ²) + (0.0771 <i>P</i>) ²]
<i>wR</i> (<i>F</i> ²) = 0.120	where <i>P</i> = (<i>F_o</i> ² + 2 <i>F_c</i> ²)/3
<i>S</i> = 1.00	(Δ/σ) _{max} = 0.001
3170 reflections	Δρ _{max} = 3.63 e Å ⁻³
109 parameters	Δρ _{min} = -2.58 e Å ⁻³

Table 1

Selected geometric parameters (Å, °).

Pt1—C11	1.997 (7)	S1—O1	1.459 (8)
Pt1—S1	2.192 (2)	S1—C2	1.773 (10)
Pt1—Cl1	2.366 (2)	S1—C1	1.784 (11)
Pt1—Cl1 ⁱ	2.475 (2)		
C11—Pt1—S1	92.2 (2)	O1—S1—C2	107.7 (5)
C11—Pt1—Cl1	89.9 (2)	O1—S1—C1	108.5 (7)
S1—Pt1—Cl1	175.98 (8)	C2—S1—C1	100.6 (7)
C11—Pt1—Cl1 ⁱ	174.0 (2)	O1—S1—Pt1	116.7 (4)
S1—Pt1—Cl1 ⁱ	93.10 (8)	C2—S1—Pt1	107.3 (4)
Cl1—Pt1—Cl1 ⁱ	85.02 (7)	C1—S1—Pt1	114.6 (4)
Pt1—Cl1—Pt1 ⁱ	94.98 (7)		

Symmetry code: (i) -*x*, 1 - *y*, 1 - *z*.

The highest residual electron-density peaks are located less than 1.1 Å from atom Pt1, with the deepest hole 0.80 Å from Pt1. H atoms were constrained to parent sites using a riding model.

Data collection: SMART (Siemens, 1995); cell refinement: SAINT (Siemens, 1995); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: DIAMOND (Brandenburg, 1999); software used to prepare material for publication: SHELXL97.

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