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Key indicators

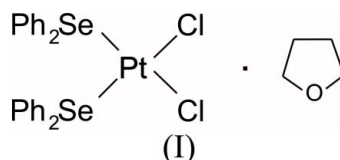
Single-crystal X-ray study
 $T = 120$ K
Mean $\sigma(\text{C}-\text{C}) = 0.008$ Å
 R factor = 0.032
 wR factor = 0.088
Data-to-parameter ratio = 17.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*cis*-Dichlorobis(diphenyl selenide)platinum(II)
tetrahydrofuran solvate

The title compound, $\text{cis}[\text{PtCl}_2(\text{C}_{12}\text{H}_{10}\text{Se})_2] \cdot \text{C}_4\text{H}_8\text{O}$, contains discrete mononuclear platinum complexes and tetrahydrofuran solvent molecules. The Pt atom shows an approximately square-planar *cis*- PtSe_2Cl_2 coordination geometry, with Pt—Se bond lengths of 2.3920 (6) and 2.3948 (6) Å. The complexes form stacks of dimeric units that are linked together through weak C—H···Cl hydrogen bonds. The metal complex interacts with the solvent molecule *via* a C—H···O hydrogen bond.

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Comment

We have recently reported the NMR spectroscopic and single-crystal and powder X-ray diffraction characterization of a series of platinum and palladium complexes containing selenoether and thioether ligands, with the emphasis on the comparison of the isomerism in these analogous systems (Vigo *et al.*, 2006). A single-crystal study of one of these complexes revealed the presence of solvent-free *cis*- $[\text{PtCl}_2(\text{SePh}_2)_2]$, (II) (Vigo *et al.*, 2006). The powder X-ray diffraction pattern of the solid bulk material indicated a 55:45 mixture of *trans*- and *cis*- $[\text{PtCl}_2(\text{SePh}_2)_2]$. Recrystallization from tetrahydrofuran afforded yellow crystals of the title compound, (I) (Fig. 1).



The coordination environment around the Pt atom in (I) is approximately square-planar [the sum of the bond angles about Pt is 360.0°]. The Pt—Se bond lengths of 2.3920 (6) and 2.3948 (6) Å in (I) are consistent with the equivalent values for (II) [2.3900 (8) and 2.3960 (9) Å; Vigo *et al.*, 2006]. The Pt—Cl distances in (I) show typical single-bond values [2.310 (1) and 2.322 (1) Å] and also agree well with the equivalent values of 2.305 (1) and 2.322 (2) Å in (II).

The packing of (I) is compared with that of the solvent-free complex (II) in Fig. 2. The crystal structure of (I) consists of stacks of complexes that are linked into inversion-generated pairs involving two weak C—H···Cl hydrogen bonds (Table 2). By contrast, the complexes in (II) are linked into pairs by a C—H···Cl hydrogen bond ($\text{H} \cdots \text{Cl} = 2.88$ Å) and a C—H···Se interaction ($\text{H} \cdots \text{Se} = 2.99$ Å).

Superficially, the pairing up of the complexes resembles the dimer formation in Pd^{II} complexes containing telluroether ligands (Oilunkaniemi *et al.*, 1998). However, whereas the pairing of the complexes in $[\text{PdCl}_2(\text{TeRR}')_2]$ compounds is due to the interactions between Te and nearby halogen atoms, those between Se and Cl in (I) and (II) are virtually negligible.

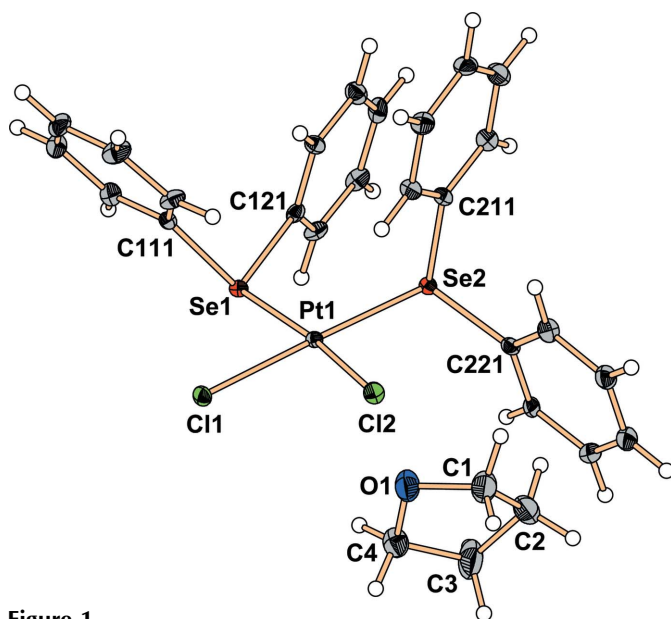


Figure 1
The molecular structure of (I), showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

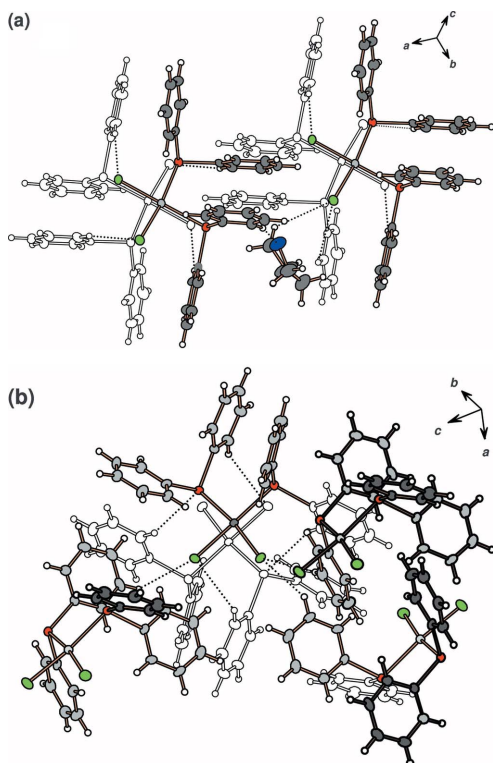


Figure 2
Comparison of the hydrogen bonds (dotted lines) in (a) (I) and (b) (II). [(II) redrawn from Vigo *et al.* (2006)].

In the solvent-free crystal structure, the shortest Se...Cl distance is 3.833 (2) Å (Vigo *et al.*, 2006), and in (I) the closest two Se...Cl distances are 3.869 (2) and 3.701 (1) Å. These are all significantly larger than the sum of the van der Waals radii of 3.65 Å for Se and Cl atoms (Bondi, 1964).

Each metal complex in (I) is linked to a nearby solvent molecule *via* a C—H...O interaction. In the case of (II), the

dimeric pairs are linked by C—H...Cl hydrogen bonds, with H...Cl = 2.75 or 2.82 Å.

Experimental

The reaction of [PtCl₂(NCPH)₂] with SePh₂ in a molar ratio of 1:2 in dichloromethane precipitates a mixture of *cis*- and *trans*-isomers of [PtCl₂(SePh₂)₂] (Vigo *et al.*, 2006). Recrystallization of the precipitate from tetrahydrofuran by slow evaporation of the solvent at room temperature gave yellow crystals of (I) suitable for single-crystal X-ray analysis.

Crystal data

[PtCl₂(C₁₂H₁₀Se)₂]·C₄H₈O
M_r = 804.41
 Monoclinic, *P*2₁/*n*
a = 10.461 (2) Å
b = 14.671 (3) Å
c = 18.059 (4) Å
 β = 102.96 (3)°
V = 2701.0 (10) Å³

Z = 4
D_x = 1.978 Mg m⁻³
 Mo *K*α radiation
 μ = 8.11 mm⁻¹
T = 120 (2) K
 Block, yellow
 0.20 × 0.20 × 0.15 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
 φ scans, and ω scans with κ offsets
 Absorption correction: multi-scan (XPREP in SHELXTL; Bruker, 2001)
T_{min} = 0.232, *T_{max}* = 0.297

17438 measured reflections
 5232 independent reflections
 4817 reflections with *I* > 2σ(*I*)
R_{int} = 0.057
 θ_{\max} = 26.0°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.032
wR (*F*²) = 0.088
S = 1.05
 5232 reflections
 308 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2 + 4.3298P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.16 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -1.34 \text{ e } \text{Å}^{-3}$
 Extinction correction: SHELXL97 (Sheldrick, 1997)
 Extinction coefficient: 0.00214 (19)

Table 1

Selected geometric parameters (Å, °).

Pt1—Cl2	2.3096 (12)	Pt1—Se1	2.3920 (6)
Pt1—Cl1	2.3220 (11)	Pt1—Se2	2.3949 (6)
Cl2—Pt1—Cl1	89.70 (4)	Cl2—Pt1—Se2	93.37 (3)
Cl2—Pt1—Se1	173.04 (3)	Cl1—Pt1—Se2	175.00 (3)
Cl1—Pt1—Se1	83.49 (3)	Se1—Pt1—Se2	93.52 (2)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C216—H216...O1 ⁱ	0.95	2.47	3.384 (7)	163
C226—H226...Cl1 ⁱⁱ	0.95	2.77	3.667 (5)	158

Symmetry codes: (i) *x* − 1, *y*, *z*; (ii) −*x*, −*y*, −*z*.

H atoms were positioned geometrically and treated as riding, with C—H = 0.95–0.99 Å and with *U_{iso}*(H) = 1.2–1.5*U_{eq}*(C). The deepest hole is located 0.99 Å from atom Pt1 and the highest peak is located 0.93 Å from atom Pt1.

Data collection: *KappaCCD Server Software* (Bruker Nonius, 2002); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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