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# Chlorido{1-[2-(ethylsulfonyl)phenyldiazenyl]-4-methoxy-2-naphthyl-$\kappa^3C,N,O$}palladium(II) sesquihydrate

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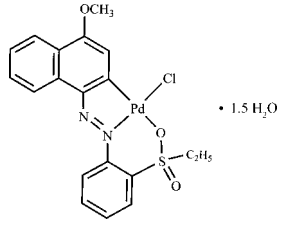
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.031; $wR$ factor = 0.083; data-to-parameter ratio = 14.9.

In the title compound, $[Pd(C_9H_{17}N_2O_3S)Cl]\cdot1.5H_2O$, the Pd atom is tetracoordinated by a naphthyl C, a diazene N, a Cl and a sulfonyl O atom in an approximate square-planar geometry; the asymmetric unit also contains 1.5 molecules of water, one molecule lying on a twofold rotation axis. A hydrophilic environment wrapping the polar portion of the compound is created by an array of water molecules. The crystal packing is stabilized by an intermolecular C—H···O interaction and eight intermolecular $\pi$–$\pi$ interactions; the centroid–centroid distances range from 3.647 (2)–3.8098 (18) Å, with perpendicular interplanar distances between 3.169 and 3.590 Å.

## Related literature

For related literature, see: Bagchi *et al.* (2007); Dupont *et al.* (2005); Neogi *et al.* (2006); Ersanlı, Albayrak, Odabaşoğlu & Kazak (2005); Ghedini *et al.* (1991); Lanfredi *et al.* (1984).




## Experimental

### Crystal data

$[Pd(C_9H_{17}N_2O_3S)Cl]\cdot1.5H_2O$
$M_r$ = 522.31
Monoclinic, $C2/c$
$a$ = 21.1870 (18) Å
$b$ = 17.1097 (14) Å
$c$ = 13.4827 (11) Å
$\beta$ = 124.8240 (10)°
$V$ = 4012.2 (6) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 1.19 mm$^{-1}$
$T$ = 295 (2) K
0.38 × 0.26 × 0.19 mm

### Data collection

Bruker SMART APEX CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.694, $T_{max}$ = 0.799
12258 measured reflections
3904 independent reflections
3503 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.083
$S$ = 1.08
3904 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.07 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.68 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Pd1—C2 | 1.938 (3) | Pd1—O2 | 2.166 (2) |
| Pd1—N2 | 2.018 (2) | Pd1—Cl1 | 2.2895 (8) |
| C2—Pd1—N2 | 80.32 (11) | C2—Pd1—Cl1 | 96.06 (9) |
| N2—Pd1—O2 | 93.58 (9) | O2—Pd1—Cl1 | 90.04 (6) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C3—H3···Cl1 | 0.93 | 2.77 | 3.297 (4) | 117 |
| C13—H13···O3 | 0.93 | 2.41 | 2.841 (5) | 108 |
| C18—H18$A$···O3$^{i}$ | 0.97 | 2.52 | 3.443 (4) | 158 |

Symmetry code: (i) $-x+\frac{1}{2}, -y+\frac{5}{2}, -z+2$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2000); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2462).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2973-m2974 [ **doi:10.1107/S1600536807054815** ]

# Chlorido{1-[2-(ethylsulfonyl)phenyldiazenyl]-4-methoxy-2-naphthyl-$\kappa^3C,N,O$}palladium(II) sesquihydrate

**S. S. Chhetri, A. N. Biswas, P. Das, A. Saha and P. Bandyopadhyay**

## Comment

Cyclopalladated compounds find numerous applications (Dupont *et al.*, 2005) in organic synthesis, catalysis, photochemistry and metallomesogen chemistry. Although a number of cyclometallated complexes of palladium (Dupont *et al.*, 2005 & Neogi *et al.*, 2006) have been reported in literature, the chemistry of cyclopalladates having sulfonyl ligand framework is not explored much. Against this background, we report here the crystal structure of (I).

The molecular structure of the title compound, (I), is shown in Fig. 1, with the atom numbering scheme. The palladium atom along with donor set of four atoms lie in a plane. Selected bond lengths and bond angles are listed in Table 1. The packing arrangement of (I) is shown in Fig. 2. The N=N bond length is typical of other cyclopalladated azoarenes (Neogi *et al.*, 2006). A hydrophilic environment wrapping the polar portion of the compound is being created by an array of water molecules. Intramolecular C–H···Cl and C–H···O interactions are also present in (I) (Table 2, Fig. 3). The crystal packing is stabilized by a intermolecular C18–H18A···O3$^{i}$ [Symmetry codes: (i) $-x + 1/2, -y + 5/2, -z + 2$.] interaction (Table 2, Fig. 3) and eight intermolecular π–π interactions (Bagchi *et al.*, 2007); the *Cg3*-*Cg3*$^{ii}$, *Cg3*-*Cg4*$^{ii}$, *Cg3*—*Cg5*$^{iii}$, *Cg4*—*Cg3*$^{ii}$, *Cg4*—*Cg5*$^{iii}$, *Cg5*—*Cg3*$^{iii}$, *Cg5*—*Cg4*$^{iii}$ and *Cg5*—*Cg5*$^{ii}$ [Symmetry codes: (ii) $-x, y, 1/2 - z$; (iii) $-x, -y$, *-z*·*Cg3*, *Cg4* and *Cg5* are the centroids of C1—C10, C5—C9 and C11—C16 rings respectively.] distances are 3.647 (2), 3.6495 (18), 3.8098 (18), 3.6495 (18), 3.740 (2), 3.8098 (18), 3.740 (2) and 3.850 (3) Å (Fig. 4); the corresponding perpendicular distances are 3.396, 3.402, 3.169, 3.464, 3.590, 3.462, 3.434 and 3.480 Å respectively.

## Experimental

The title compound was synthesized by reacting 1-[2-(ethylsulfonyl)phenyldiazenyl]-4-methoxynaphthalene with disodiumtetrachloropalladate in aqueous ethanol medium at room temperature. The product was purified by chromatography. Crystals suitable for X-ray crystallography was obtained by slow diffusion of dichloromethane solution into hexane.

## Refinement

The O-bound H atom was located in a difference Fourier map and its isotropic displacement parameter were freely refined after fixing the coordinates. C-bound H atoms were included at calculated positions as riding atoms with C–H distances of 0.93 Å for aromatic, 0.96 Å for $CH_3$ and 0.97 Å for $CH_2$ H atoms, with $U_{iso}$ (H) =1.2$U_{eq}$ (C) (1.5$U_{eq}$ for methyl groups).

**Figures**

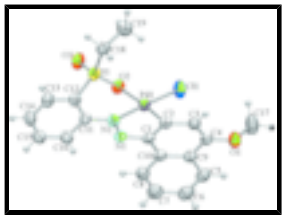


Fig. 1. The asymmetric unit of (I), with displacement ellipsoids drawn at the 50% probability level. Solvent molecules are omited for clarity.

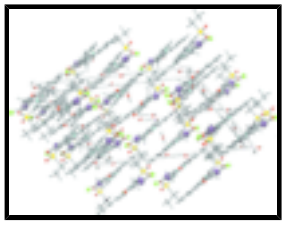


Fig. 2. The molecular arrangement of (I) in the *ac* plane.

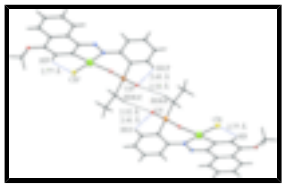


Fig. 3. A representation of the intramolecular C—H···O, C—H···Cl (dotted lines), inter-molecular C—H···O (dashed lines) interactions of (I) [symmetry code: (i) −*x* + 1/2, −*y* + 5/2, −*z* + 2.]. Solvent molecules are omited for clarity.

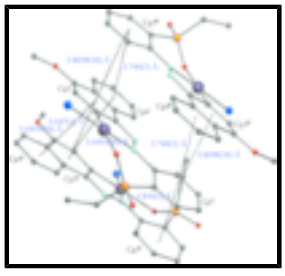


Fig. 4. The inter molecular π—π interaction for (I), indicated by the dotted line. [Symmetry codes: (ii) −*x*, *y*, 1/2 − *z*; (iii) −*x*, −*y*, -*z*. *Cg3*, *Cg4* and *Cg5* are the centroids of C1—C10, C5—C9 and C11—C16 rings, respectively.]

## Chlorido{1-[2-(ethylsulfonyl)phenyldiazenyl]-4-methoxy-2-naphthyl- $\kappa^3C,N,O$}palladium(II) sesquihydrate

*Crystal data*

| | |
|---|---|
| $[Pd(C_9H_{17}N_2O_3S)Cl]\cdot 1.5H_2O$ | $F_{000}$ = 2104 |
| $M_r$ = 522.31 | $D_x$ = 1.729 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 3904 reflections |
| *a* = 21.1870 (18) Å | θ = 1.7–25.9º |
| *b* = 17.1097 (14) Å | μ = 1.19 mm$^{-1}$ |
| *c* = 13.4827 (11) Å | *T* = 295 (2) K |
| β = 124.8240 (10)º | Needle, pink |
| *V* = 4012.2 (6) Å$^3$ | 0.38 × 0.26 × 0.19 mm |
| *Z* = 8 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD area detector diffractometer | 3904 independent reflections |
| Radiation source: fine-focus sealed tube | 3503 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.020$ |
| $T = 298(2)$ K | $\theta_{max} = 25.9°$ |
| phi and ω scans | $\theta_{min} = 1.7°$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = -26\rightarrow26$ |
| $T_{min} = 0.694$, $T_{max} = 0.799$ | $k = -20\rightarrow20$ |
| 12258 measured reflections | $l = -16\rightarrow16$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.031$ | H-atom parameters constrained |
| $wR(F^2) = 0.083$ | $w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 5.4842P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.08$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 3904 reflections | $\Delta\rho_{max} = 1.07$ e Å$^{-3}$ |
| 262 parameters | $\Delta\rho_{min} = -0.68$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Pd1 | 0.167430 (12) | 0.985070 (13) | 0.74687 (2) | 0.03443 (9) |
| C2 | 0.09189 (15) | 0.90245 (17) | 0.6922 (2) | 0.0331 (6) |
| S1 | 0.22366 (4) | 1.14847 (5) | 0.85771 (7) | 0.04165 (19) |
| Cl1 | 0.27025 (5) | 0.90451 (5) | 0.81104 (9) | 0.0582 (2) |
| N1 | 0.00874 (14) | 1.01220 (14) | 0.6375 (2) | 0.0354 (5) |

| | | | | |
|---|---|---|---|---|
| O2 | 0.24220 (12) | 1.08601 (13) | 0.8039 (2) | 0.0455 (5) |
| O3 | 0.27501 (13) | 1.21410 (14) | 0.9014 (2) | 0.0571 (6) |
| C3 | 0.10189 (16) | 0.82172 (18) | 0.6998 (3) | 0.0379 (6) |
| H3 | 0.1507 | 0.8006 | 0.7355 | 0.046* |
| C1 | 0.01766 (15) | 0.93370 (17) | 0.6381 (2) | 0.0330 (6) |
| N2 | 0.07265 (13) | 1.04999 (14) | 0.6875 (2) | 0.0347 (5) |
| C9 | −0.03752 (16) | 0.80271 (17) | 0.5939 (2) | 0.0354 (6) |
| C10 | −0.04846 (16) | 0.88408 (18) | 0.5863 (2) | 0.0345 (6) |
| O1 | 0.04360 (12) | 0.69462 (13) | 0.6603 (2) | 0.0477 (5) |
| C11 | 0.06450 (17) | 1.13260 (17) | 0.6846 (3) | 0.0362 (6) |
| C4 | 0.03909 (16) | 0.77313 (17) | 0.6542 (3) | 0.0370 (6) |
| C8 | −0.12377 (16) | 0.91331 (19) | 0.5259 (3) | 0.0422 (7) |
| H8 | −0.1318 | 0.9670 | 0.5206 | 0.051* |
| C18 | 0.22294 (19) | 1.1079 (2) | 0.9776 (3) | 0.0491 (8) |
| H18A | 0.2187 | 1.1495 | 1.0224 | 0.059* |
| H18B | 0.1785 | 1.0740 | 0.9450 | 0.059* |
| C5 | −0.10186 (17) | 0.7528 (2) | 0.5393 (3) | 0.0429 (7) |
| H5 | −0.0950 | 0.6989 | 0.5432 | 0.051* |
| C12 | 0.12879 (17) | 1.18202 (18) | 0.7525 (3) | 0.0400 (7) |
| C16 | −0.00722 (18) | 1.16709 (19) | 0.6124 (3) | 0.0419 (7) |
| H16 | −0.0506 | 1.1357 | 0.5675 | 0.050* |
| C6 | −0.17412 (17) | 0.7830 (2) | 0.4809 (3) | 0.0492 (8) |
| H6 | −0.2164 | 0.7497 | 0.4445 | 0.059* |
| C7 | −0.18495 (18) | 0.8641 (2) | 0.4754 (3) | 0.0506 (8) |
| H7 | −0.2344 | 0.8844 | 0.4369 | 0.061* |
| C17 | 0.1169 (2) | 0.6590 (2) | 0.7179 (4) | 0.0663 (11) |
| H17A | 0.1409 | 0.6751 | 0.6786 | 0.099* |
| H17B | 0.1112 | 0.6032 | 0.7129 | 0.099* |
| H17C | 0.1484 | 0.6745 | 0.8012 | 0.099* |
| C13 | 0.1196 (2) | 1.26272 (19) | 0.7420 (3) | 0.0505 (8) |
| H13 | 0.1624 | 1.2950 | 0.7850 | 0.061* |
| C15 | −0.0153 (2) | 1.2474 (2) | 0.6061 (3) | 0.0494 (8) |
| H15 | −0.0642 | 1.2694 | 0.5589 | 0.059* |
| C14 | 0.0481 (2) | 1.2949 (2) | 0.6691 (3) | 0.0549 (9) |
| H14 | 0.0424 | 1.3490 | 0.6621 | 0.066* |
| C19 | 0.2955 (2) | 1.0614 (3) | 1.0621 (4) | 0.0700 (11) |
| H19A | 0.2948 | 1.0145 | 1.0223 | 0.105* |
| H19B | 0.2981 | 1.0479 | 1.1335 | 0.105* |
| H19C | 0.3395 | 1.0922 | 1.0840 | 0.105* |
| O4 | 0.4461 (4) | 1.0023 (4) | 1.0164 (7) | 0.180 (3) |
| O5 | 0.0000 | 0.5318 (7) | 0.7500 | 0.221 (5) |
| H5A | −0.0150 | 0.5680 | 0.6840 | 1.0 (3)* |
| H4B | 0.4840 | 0.9970 | 1.0000 | 0.150* |
| H4A | 0.4280 | 0.9480 | 1.0100 | 0.37 (9)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| Pd1 | 0.02794 (13) | 0.03781 (15) | 0.03805 (15) | −0.00271 (8) | 0.01914 (11) | −0.00357 (9) |
| C2 | 0.0302 (13) | 0.0405 (15) | 0.0278 (13) | −0.0038 (11) | 0.0162 (11) | −0.0027 (11) |
| S1 | 0.0362 (4) | 0.0378 (4) | 0.0512 (4) | −0.0080 (3) | 0.0251 (4) | −0.0050 (3) |
| Cl1 | 0.0369 (4) | 0.0491 (5) | 0.0855 (6) | 0.0040 (3) | 0.0331 (4) | −0.0021 (4) |
| N1 | 0.0319 (12) | 0.0433 (14) | 0.0316 (12) | −0.0012 (10) | 0.0185 (11) | −0.0021 (10) |
| O2 | 0.0379 (11) | 0.0475 (13) | 0.0556 (13) | −0.0094 (9) | 0.0295 (11) | −0.0069 (10) |
| O3 | 0.0456 (13) | 0.0448 (13) | 0.0768 (17) | −0.0139 (10) | 0.0326 (13) | −0.0100 (12) |
| C3 | 0.0291 (14) | 0.0435 (16) | 0.0364 (15) | −0.0001 (12) | 0.0158 (12) | −0.0026 (12) |
| C1 | 0.0307 (13) | 0.0403 (16) | 0.0291 (14) | −0.0028 (12) | 0.0177 (12) | −0.0037 (11) |
| N2 | 0.0313 (12) | 0.0391 (13) | 0.0345 (12) | −0.0007 (10) | 0.0193 (10) | −0.0010 (10) |
| C9 | 0.0327 (14) | 0.0425 (16) | 0.0321 (14) | −0.0028 (12) | 0.0191 (12) | −0.0032 (12) |
| C10 | 0.0304 (13) | 0.0448 (16) | 0.0275 (13) | −0.0021 (12) | 0.0161 (11) | −0.0051 (12) |
| O1 | 0.0374 (11) | 0.0386 (12) | 0.0606 (14) | 0.0006 (9) | 0.0242 (11) | −0.0002 (10) |
| C11 | 0.0405 (15) | 0.0392 (16) | 0.0358 (15) | 0.0003 (12) | 0.0259 (13) | −0.0016 (12) |
| C4 | 0.0349 (14) | 0.0399 (16) | 0.0341 (15) | −0.0012 (12) | 0.0185 (13) | −0.0025 (12) |
| C8 | 0.0329 (15) | 0.0470 (18) | 0.0415 (16) | 0.0034 (13) | 0.0181 (13) | −0.0056 (13) |
| C18 | 0.0490 (18) | 0.0493 (19) | 0.0474 (19) | −0.0071 (15) | 0.0266 (16) | −0.0062 (15) |
| C5 | 0.0373 (15) | 0.0453 (18) | 0.0444 (17) | −0.0080 (13) | 0.0223 (14) | −0.0081 (14) |
| C12 | 0.0395 (15) | 0.0385 (16) | 0.0462 (17) | −0.0020 (13) | 0.0269 (14) | 0.0002 (13) |
| C16 | 0.0420 (16) | 0.0467 (18) | 0.0387 (16) | 0.0039 (13) | 0.0240 (14) | 0.0023 (13) |
| C6 | 0.0330 (16) | 0.058 (2) | 0.0501 (19) | −0.0119 (14) | 0.0200 (15) | −0.0139 (16) |
| C7 | 0.0279 (15) | 0.063 (2) | 0.0506 (19) | −0.0002 (14) | 0.0161 (14) | −0.0092 (16) |
| C17 | 0.0419 (19) | 0.045 (2) | 0.097 (3) | 0.0077 (16) | 0.031 (2) | 0.006 (2) |
| C13 | 0.0541 (19) | 0.0381 (17) | 0.061 (2) | −0.0064 (15) | 0.0336 (18) | −0.0025 (15) |
| C15 | 0.0516 (19) | 0.052 (2) | 0.0458 (18) | 0.0125 (16) | 0.0286 (16) | 0.0072 (15) |
| C14 | 0.069 (2) | 0.0399 (18) | 0.061 (2) | 0.0086 (17) | 0.040 (2) | 0.0069 (16) |
| C19 | 0.076 (3) | 0.066 (3) | 0.054 (2) | 0.008 (2) | 0.029 (2) | 0.0016 (19) |
| O4 | 0.146 (5) | 0.171 (6) | 0.165 (6) | −0.029 (4) | 0.054 (5) | 0.013 (4) |
| O5 | 0.143 (7) | 0.224 (10) | 0.341 (15) | 0.000 | 0.166 (10) | 0.000 |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Pd1—C2 | 1.938 (3) | C18—C19 | 1.514 (5) |
| Pd1—N2 | 2.018 (2) | C18—H18A | 0.9700 |
| Pd1—O2 | 2.166 (2) | C18—H18B | 0.9700 |
| Pd1—Cl1 | 2.2895 (8) | C5—C6 | 1.362 (4) |
| C2—C3 | 1.392 (4) | C5—H5 | 0.9300 |
| C2—C1 | 1.408 (4) | C12—C13 | 1.390 (5) |
| S1—O3 | 1.435 (2) | C16—C15 | 1.381 (5) |
| S1—O2 | 1.466 (2) | C16—H16 | 0.9300 |
| S1—C18 | 1.768 (3) | C6—C7 | 1.402 (5) |
| S1—C12 | 1.768 (3) | C6—H6 | 0.9300 |
| N1—N2 | 1.290 (3) | C7—H7 | 0.9300 |
| N1—C1 | 1.356 (4) | C17—H17A | 0.9600 |
| C3—C4 | 1.380 (4) | C17—H17B | 0.9600 |
| C3—H3 | 0.9300 | C17—H17C | 0.9600 |
| C1—C10 | 1.433 (4) | C13—C14 | 1.365 (5) |
| N2—C11 | 1.422 (4) | C13—H13 | 0.9300 |
| C9—C10 | 1.405 (4) | C15—C14 | 1.374 (5) |

| | | | |
|---|---|---|---|
| C9—C5 | 1.408 (4) | C15—H15 | 0.9300 |
| C9—C4 | 1.430 (4) | C14—H14 | 0.9300 |
| C10—C8 | 1.405 (4) | C19—H19A | 0.9600 |
| O1—C4 | 1.346 (4) | C19—H19B | 0.9600 |
| O1—C17 | 1.418 (4) | C19—H19C | 0.9600 |
| C11—C16 | 1.384 (4) | O4—H4B | 0.9500 |
| C11—C12 | 1.409 (4) | O4—H4A | 0.9900 |
| C8—C7 | 1.358 (4) | O5—H5A | 0.9800 |
| C8—H8 | 0.9300 | | |
| C2—Pd1—N2 | 80.32 (11) | C19—C18—H18A | 109.4 |
| C2—Pd1—O2 | 173.86 (10) | S1—C18—H18A | 109.4 |
| N2—Pd1—O2 | 93.58 (9) | C19—C18—H18B | 109.4 |
| C2—Pd1—Cl1 | 96.06 (9) | S1—C18—H18B | 109.4 |
| N2—Pd1—Cl1 | 176.38 (7) | H18A—C18—H18B | 108.0 |
| O2—Pd1—Cl1 | 90.04 (6) | C6—C5—C9 | 120.3 (3) |
| C3—C2—C1 | 119.5 (2) | C6—C5—H5 | 119.8 |
| C3—C2—Pd1 | 129.6 (2) | C9—C5—H5 | 119.8 |
| C1—C2—Pd1 | 110.8 (2) | C13—C12—C11 | 120.2 (3) |
| O3—S1—O2 | 114.78 (14) | C13—C12—S1 | 115.7 (2) |
| O3—S1—C18 | 109.40 (16) | C11—C12—S1 | 124.1 (2) |
| O2—S1—C18 | 108.13 (15) | C15—C16—C11 | 121.0 (3) |
| O3—S1—C12 | 108.86 (15) | C15—C16—H16 | 119.5 |
| O2—S1—C12 | 110.03 (14) | C11—C16—H16 | 119.5 |
| C18—S1—C12 | 105.20 (15) | C5—C6—C7 | 120.2 (3) |
| N2—N1—C1 | 113.1 (2) | C5—C6—H6 | 119.9 |
| S1—O2—Pd1 | 114.10 (11) | C7—C6—H6 | 119.9 |
| C4—C3—C2 | 119.8 (3) | C8—C7—C6 | 120.4 (3) |
| C4—C3—H3 | 120.1 | C8—C7—H7 | 119.8 |
| C2—C3—H3 | 120.1 | C6—C7—H7 | 119.8 |
| N1—C1—C2 | 119.3 (2) | O1—C17—H17A | 109.5 |
| N1—C1—C10 | 119.3 (2) | O1—C17—H17B | 109.5 |
| C2—C1—C10 | 121.3 (3) | H17A—C17—H17B | 109.5 |
| N1—N2—C11 | 114.2 (2) | O1—C17—H17C | 109.5 |
| N1—N2—Pd1 | 116.19 (19) | H17A—C17—H17C | 109.5 |
| C11—N2—Pd1 | 129.48 (19) | H17B—C17—H17C | 109.5 |
| C10—C9—C5 | 119.5 (3) | C14—C13—C12 | 120.5 (3) |
| C10—C9—C4 | 118.6 (3) | C14—C13—H13 | 119.7 |
| C5—C9—C4 | 121.9 (3) | C12—C13—H13 | 119.7 |
| C9—C10—C8 | 118.7 (3) | C14—C15—C16 | 120.5 (3) |
| C9—C10—C1 | 118.5 (2) | C14—C15—H15 | 119.7 |
| C8—C10—C1 | 122.8 (3) | C16—C15—H15 | 119.7 |
| C4—O1—C17 | 118.7 (2) | C13—C14—C15 | 119.8 (3) |
| C16—C11—C12 | 117.8 (3) | C13—C14—H14 | 120.1 |
| C16—C11—N2 | 120.7 (3) | C15—C14—H14 | 120.1 |
| C12—C11—N2 | 121.4 (3) | C18—C19—H19A | 109.5 |
| O1—C4—C3 | 123.9 (3) | C18—C19—H19B | 109.5 |
| O1—C4—C9 | 113.9 (2) | H19A—C19—H19B | 109.5 |
| C3—C4—C9 | 122.2 (3) | C18—C19—H19C | 109.5 |
| C7—C8—C10 | 120.8 (3) | H19A—C19—H19C | 109.5 |

| | | | |
|---|---|---|---|
| C7—C8—H8 | 119.6 | H19B—C19—H19C | 109.5 |
| C10—C8—H8 | 119.6 | H4B—O4—H4A | 103.0 |
| C19—C18—S1 | 111.0 (3) | | |
| N2—Pd1—C2—C3 | −176.2 (3) | C17—O1—C4—C3 | 0.7 (5) |
| Cl1—Pd1—C2—C3 | 3.6 (3) | C17—O1—C4—C9 | 179.8 (3) |
| N2—Pd1—C2—C1 | 3.79 (18) | C2—C3—C4—O1 | −178.2 (3) |
| Cl1—Pd1—C2—C1 | −176.32 (18) | C2—C3—C4—C9 | 2.7 (4) |
| O3—S1—O2—Pd1 | 177.03 (14) | C10—C9—C4—O1 | 177.8 (2) |
| C18—S1—O2—Pd1 | 54.61 (17) | C5—C9—C4—O1 | −4.2 (4) |
| C12—S1—O2—Pd1 | −59.78 (17) | C10—C9—C4—C3 | −3.1 (4) |
| N2—Pd1—O2—S1 | 38.00 (15) | C5—C9—C4—C3 | 175.0 (3) |
| Cl1—Pd1—O2—S1 | −141.84 (13) | C9—C10—C8—C7 | −0.3 (4) |
| C1—C2—C3—C4 | 0.1 (4) | C1—C10—C8—C7 | 178.3 (3) |
| Pd1—C2—C3—C4 | −179.9 (2) | O3—S1—C18—C19 | −75.3 (3) |
| N2—N1—C1—C2 | 1.0 (4) | O2—S1—C18—C19 | 50.3 (3) |
| N2—N1—C1—C10 | 179.6 (2) | C12—S1—C18—C19 | 167.9 (3) |
| C3—C2—C1—N1 | 176.1 (2) | C10—C9—C5—C6 | −0.9 (4) |
| Pd1—C2—C1—N1 | −4.0 (3) | C4—C9—C5—C6 | −178.9 (3) |
| C3—C2—C1—C10 | −2.5 (4) | C16—C11—C12—C13 | −2.7 (4) |
| Pd1—C2—C1—C10 | 177.5 (2) | N2—C11—C12—C13 | 176.0 (3) |
| C1—N1—N2—C11 | 178.1 (2) | C16—C11—C12—S1 | 175.1 (2) |
| C1—N1—N2—Pd1 | 2.4 (3) | N2—C11—C12—S1 | −6.2 (4) |
| C2—Pd1—N2—N1 | −3.68 (19) | O3—S1—C12—C13 | −7.3 (3) |
| O2—Pd1—N2—N1 | 176.99 (19) | O2—S1—C12—C13 | −133.9 (2) |
| C2—Pd1—N2—C11 | −178.6 (2) | C18—S1—C12—C13 | 109.8 (3) |
| O2—Pd1—N2—C11 | 2.1 (2) | O3—S1—C12—C11 | 174.8 (2) |
| C5—C9—C10—C8 | 1.2 (4) | O2—S1—C12—C11 | 48.2 (3) |
| C4—C9—C10—C8 | 179.3 (3) | C18—S1—C12—C11 | −68.1 (3) |
| C5—C9—C10—C1 | −177.4 (3) | C12—C11—C16—C15 | 0.8 (4) |
| C4—C9—C10—C1 | 0.6 (4) | N2—C11—C16—C15 | −177.9 (3) |
| N1—C1—C10—C9 | −176.4 (2) | C9—C5—C6—C7 | −0.5 (5) |
| C2—C1—C10—C9 | 2.1 (4) | C10—C8—C7—C6 | −1.0 (5) |
| N1—C1—C10—C8 | 4.9 (4) | C5—C6—C7—C8 | 1.4 (5) |
| C2—C1—C10—C8 | −176.6 (3) | C11—C12—C13—C14 | 2.1 (5) |
| N1—N2—C11—C16 | −12.3 (4) | S1—C12—C13—C14 | −175.8 (3) |
| Pd1—N2—C11—C16 | 162.7 (2) | C11—C16—C15—C14 | 1.8 (5) |
| N1—N2—C11—C12 | 169.0 (3) | C12—C13—C14—C15 | 0.4 (5) |
| Pd1—N2—C11—C12 | −16.0 (4) | C16—C15—C14—C13 | −2.4 (5) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C3—H3···Cl1 | 0.93 | 2.77 | 3.297 (4) | 117 |
| C13—H13···O3 | 0.93 | 2.41 | 2.841 (5) | 108 |
| C18—H18A···O3$^{i}$ | 0.97 | 2.52 | 3.443 (4) | 158 |

Symmetry codes: (i) −*x*+1/2, −*y*+5/2, −*z*+2.

**Fig. 1**

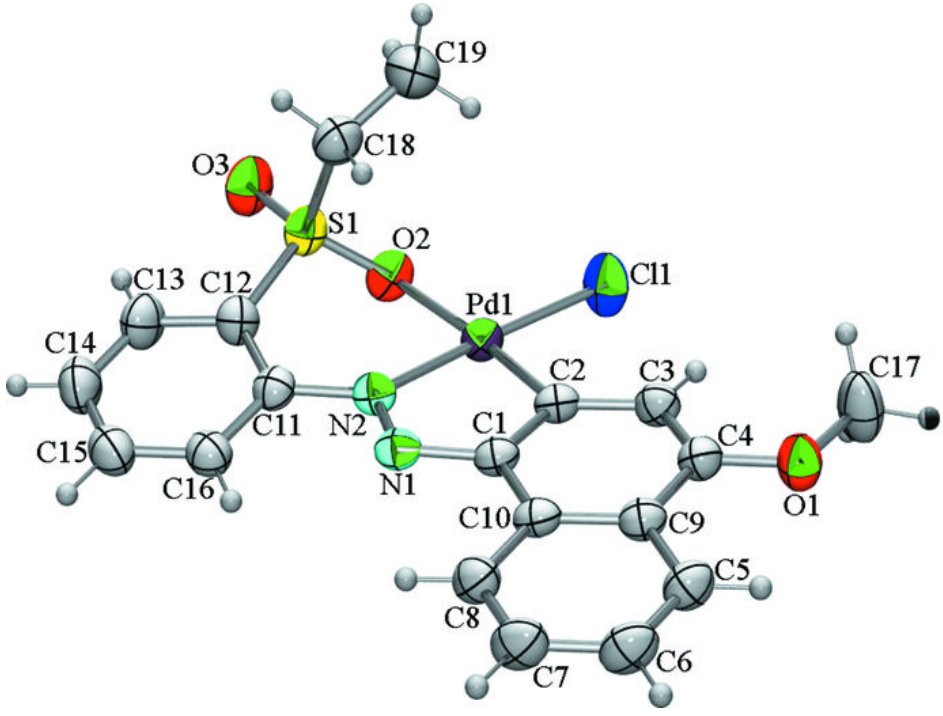

C19
C18
O3
S1
O2
C13
C12
Cl1
Pd1
C14
C2
C3
C17
C11
N2
C1
C4
C15
N1
C16
O1
C10
C9
C5
C8
C6
C7

**Fig. 2**

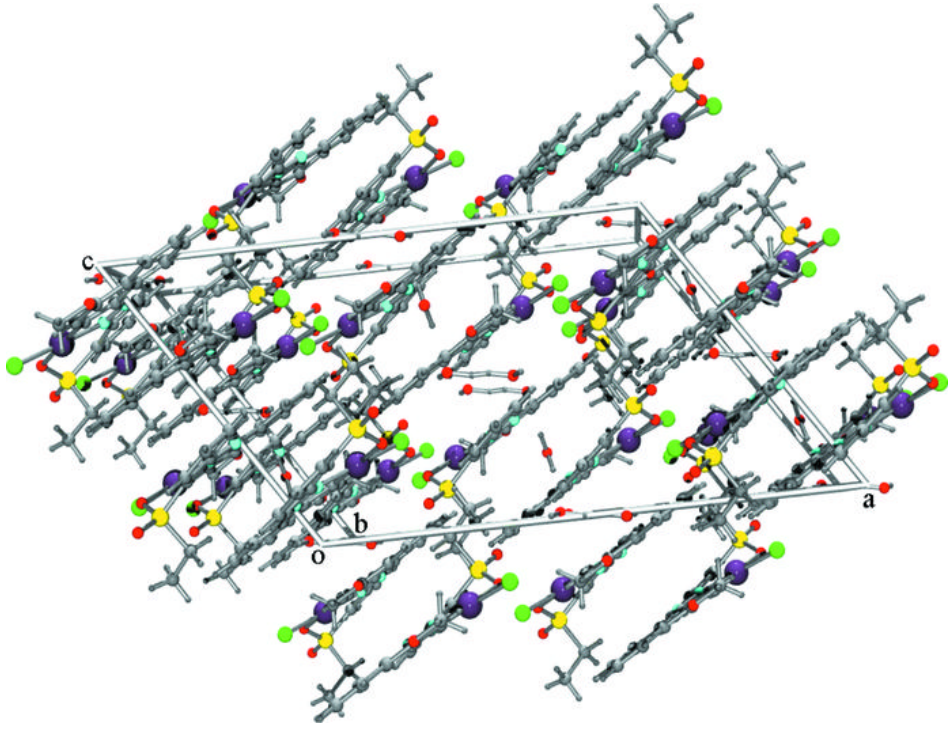


**Fig. 3**

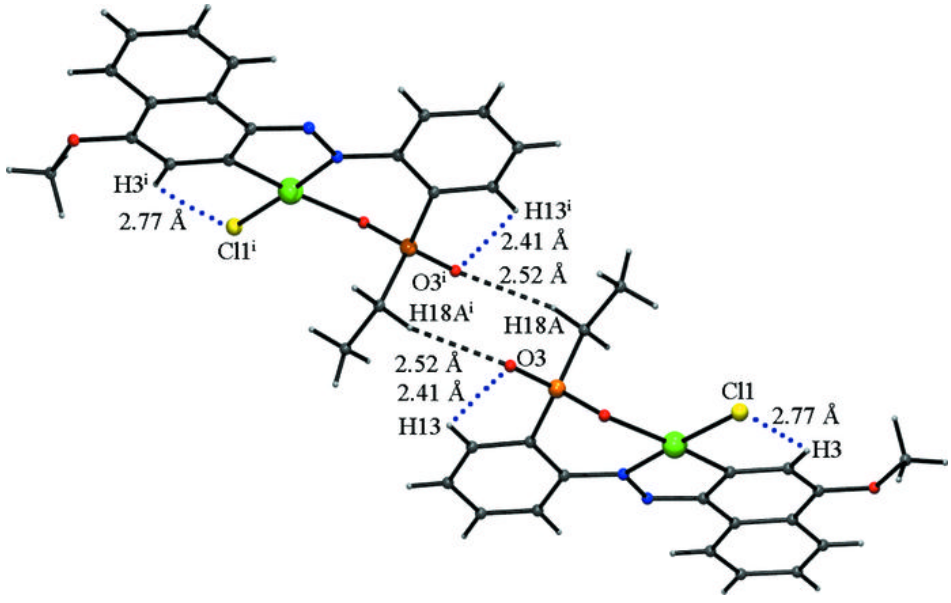
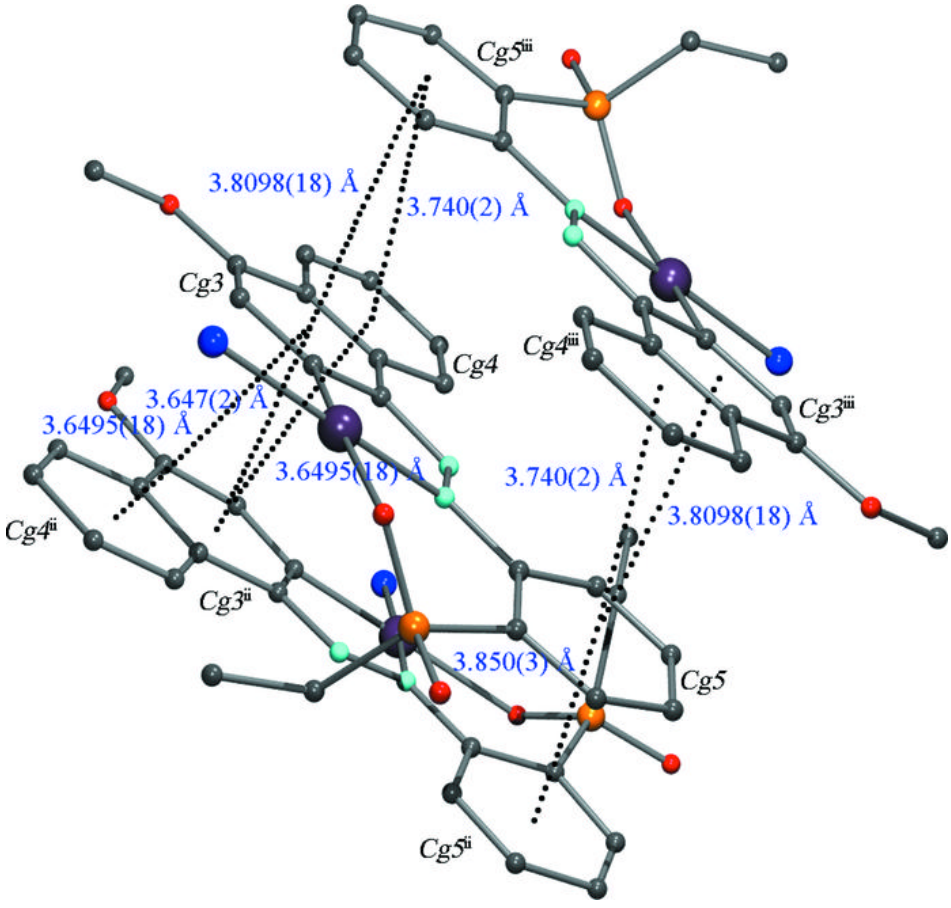

H3i
2.77 Å
Cl1i
H13i
2.41 Å
2.52 Å
O3i
H18Ai
H18A
2.52 Å
O3
2.41 Å
H13
Cl1
2.77 Å
H3

**Fig. 4**


Cg5iii
3.8098(18) Å
3.740(2) Å
Cg3
Cg4
Cg4iii
3.647(2) Å
3.6495(18) Å
3.6495(18) Å
3.740(2) Å
Cg3iii
3.8098(18) Å
Cg4ii
Cg3ii
3.850(3) Å
Cg5
Cg5ii