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Chlorido(*N*,*N*-dimethylformamide-κO)-{2-(4-methylphenyldiazenyl)-3-(methylsulfonyl)phenyl-$\kappa^2 C,N$}palladium(II)

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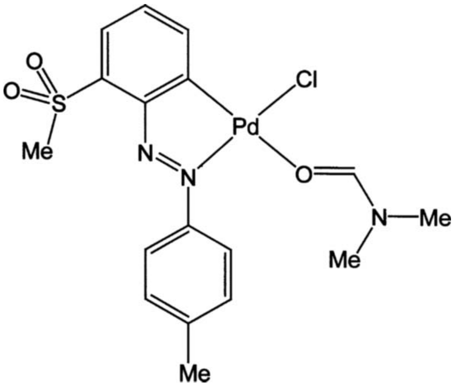
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.058; wR factor = 0.125; data-to-parameter ratio = 14.2.

In the title compound, [Pd($C_{14}H_{13}N_2O_2S$)Cl(C_3H_7NO)], the Pd atom is tetracoordinated by a phenyl C, a diazene N, a Cl and a dimethylformamide O atom in an approximate square-planar geometry. There are intramolecular C—H···O, C—H···N and C—H···Cl interactions. The crystal packing is stabilized by weak intermolecular π–π interactions; the *Cg*–*Cg* distance is 3.920 (4) Å and the perpendicular distance is 3.302 Å with a slippage of 2.113 Å.

Related literature

For related literature, see: Dupont *et al.* (2005); Ghedini *et al.* (1991); Kubo *et al.* (2005); Neogi *et al.* (2006); Suzuki & Ishiguro (2006); Yen *et al.* (2006); Şahin *et al.* (2005*a*,*b*).



Experimental

Crystal data

[Pd($C_{14}H_{13}N_2O_2S$)Cl(C_3H_7NO)]
M_r = 488.30
Monoclinic, $P2_1/n$
a = 10.199 (3) Å
b = 10.811 (3) Å
c = 18.579 (5) Å
β = 103.427 (4)°
V = 1992.5 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.19 mm^{-1}
T = 298 (2) K
0.36 × 0.28 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.676, $T_{\max}$ = 0.778
17353 measured reflections
3396 independent reflections
3235 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.125
S = 1.19
3396 reflections
239 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.65 e Å^{-3}
$\Delta\rho_{\min}$ = −0.95 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—Pd1	2.2875 (16)	Pd1—C2	1.952 (5)
O1—Pd1	2.138 (4)	Pd1—N2	2.058 (4)
C2—Pd1—N2	79.4 (2)	C2—Pd1—Cl1	93.86 (17)
N2—Pd1—O1	96.65 (16)	O1—Pd1—Cl1	89.87 (12)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Cl1	0.93	2.72	3.250 (7)	117
C5—H5···O3	0.93	2.47	2.862 (9)	106
C8—H8···O1	0.93	2.32	2.947 (7)	124
C14—H14···Cl1	0.93	2.72	3.253 (7)	118
C17—H17*B*···N1	0.96	2.48	3.140 (8)	126

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXL97* (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: BQ2012).

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supplementary materials

Acta Cryst. (2007). E**63**, m1614-m1615 [**doi:10.1107/S1600536807021526**]

Chlorido(*N,N*-dimethylformamide-*κO*){2-(4-methylphenyldiazenyl)-3-(methylsulfonyl)phenyl-κ^2*C,N*}palladium(II)

V. Bagchi and **D. Bandyopadhyay**

Comment

Cyclopalladated compounds have 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) and few *N,N*-dimethyl formamide solvated metal complexes (Suzuki & Ishiguro, 2006) have been reported in literature, report of palladium complexes with solvent molecules as donor is relatively sparse (Yen *et al.*, 2006). Against this background, we report here the crystal structure of (**I**).

The molecular structure of the title compound, (**I**), and its packing arrangement are shown in Fig. 1 and Fig. 2, respectively. The palladium atom along with donor set of four atoms lie in an almost plane.

Selected bond lengths, bond angles and torsion angles are listed in Table 1. The N=N bond length is typical of other cyclopalladated azoarenes (Neogi *et al.*, 2006), unlike those of free azoarenes (Şahin *et al.*, 2005*a*,*b*). The metal carbon bond length, 1.952 (5) Å, is slightly higher than the reported values of other *ortho*-palladated azoarenes (Ghedini *et al.*, 1991).

The sulfur atom in methyl-sulfonyl group is nearly in tetrahedral geometry. Three nearly planar fragment in the molecular structure of (**I**) may be identified: the palladium atom, diazene unit and the *ortho*-palladated phenyl unit (*A*), the *para*-methyl phenyl group (*B*) and the *N,N*-dimethyl formamide molecule (*C*). The dihedral angles between the planes *A/B*, *A/C* & *B/C* are 26.60 (20)°, 20.61 (38)° & 24.78 (37)°, respectively. Actual geometry of the compound can be understood by the four torsion angles listed in Table 1. An weak inter molecular π—π interaction (Kubo *et al.*, 2005) arranges the molecules in anti parallel fashion (Fig. 3). The *Cg3*—*Cg3*$^{\rm i}$ [Symmetry code: (i) $1-x$, $1-y$, $-z$. *Cg3* is the centroid of C7—C12 ring.] distance is 3.920 (4)Å and the perpendicular distance is 3.302Å with a slippage of 2.113 Å. There are intra molecular C—H···O, C—H···N and C—H···Cl interactions (Table 2, Fig. 1) in compound (**I**).

Experimental

2-(Methyl sulfonyl)azo-*p*-toluene was synthesized by the over oxidation of corresponding thio-ether ligand using hydrogen peroxide. An ethanolic solution (15 ml) of the 2-(methyl sulfonyl)azo-*p*-toluene (0.21 mmol) was added drop wise to an ethanolic solution (15 ml) of Na_2PdCl_4 (0.27 mmol) under stirring condition. The orange-red colored solution was evaporated in air, the solid thus left was washed with water followed by washing with 50% aqueous ethanol (5x3 ml). The compound was then chromatographed over silica-gel column (1x50 cm) which was pre-equilibrated in dicholoromethane. The title compound (**I**) was eluted with methanol-dichloromethane (1:9 *v/v*) mixture. The solvent was evaporated in vacuum to obtain the pure product (yield: 0.065 g, 74.9%). Suitable crystals of (**I**) were grown from an *N,N*-dimethyl formamide solution by slow evaporation.

Refinement

H atoms were included at calculated positions as riding atoms with C–H set to 0.93Å for (aromatic) and 0.96Å for (CH_3) H atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$ ($1.5U_{eq}$ for methyl group). Some low-angle reflections were excluded from the refinement, as they were probably obscured by the beam stop.

Figures

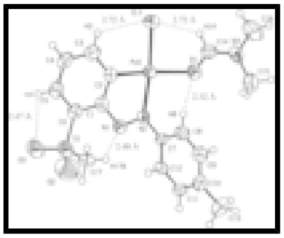


Figure 1
The asymmetric unit of (**I**), with displacement ellipsoids drawn at the 50% probability level. The intra molecular C—H···O, C—H···N and C—H···Cl interactions are shown by dotted lines.

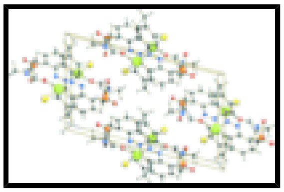


Figure 2
The molecular arrangement of (**I**) in the *ac* plane.

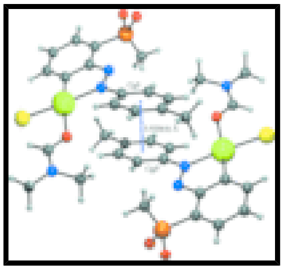


Figure 3
The inter molecular π—π interaction for (**I**), indicated by the dotted line. [Symmetry code: (i) $1 - x$, $1 - y$, $-z$.]. *Cg3* is the centroid of C7—C12 ring.

Chlorido(*N*,*N*-dimethylformamide-κ*O*){2-(4-methylphenyldiazenyl)-\ 3-(methylsulfonyl)phenyl-κ^2*C*,*N*}palladium(II)

Crystal data

$[Pd(C_{14}H_{13}N_2O_2S)Cl(C_3H_7NO)]$

$M_r = 488.30$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 10.199\ (3)$ Å

$b = 10.811\ (3)$ Å

$c = 18.579\ (5)$ Å

$\beta = 103.427\ (4)^\circ$

$V = 1992.5\ (9)$ Å^3

$Z = 4$

$F_{000} = 980$

$D_x = 1.624$ Mg m^{-3}

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 3396 reflections

θ = 2.1–25.0°

$\mu = 1.19$ mm^{-1}

$T = 298\ (2)$ K

Rod, pink

0.36 × 0.28 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3396 independent reflections
Radiation source: fine-focus sealed tube	3235 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.040$
$T = 298(2)$ K	$\theta_{\text{max}} = 25.0°$
φ and ω scans	$\theta_{\text{min}} = 2.1°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12\rightarrow12$
$T_{\text{min}} = 0.676$, $T_{\text{max}} = 0.778$	$k = -12\rightarrow12$
17353 measured reflections	$l = -22\rightarrow22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.058$	H-atom parameters constrained
$wR(F^2) = 0.125$	$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 6.1689P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.19$	$(\Delta/\sigma)_{\text{max}} = 0.001$
3396 reflections	$\Delta\rho_{\text{max}} = 0.65$ e Å^{-3}
239 parameters	$\Delta\rho_{\text{min}} = -0.95$ 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}
Cl1	0.73827 (17)	−0.00332 (16)	0.12741 (9)	0.0585 (4)
C7	0.4027 (5)	0.3422 (4)	−0.0256 (3)	0.0337 (11)
N3	0.5275 (5)	0.2477 (5)	0.2563 (3)	0.0501 (12)
C15	0.4787 (8)	0.3729 (7)	0.2414 (4)	0.072 (2)
H15A	0.5216	0.4102	0.2059	0.107*

H15B	0.4992	0.4200	0.2864	0.107*
H15C	0.3829	0.3716	0.2218	0.107*
C16	0.5317 (11)	0.1970 (10)	0.3296 (5)	0.094 (3)
H16A	0.4437	0.2025	0.3397	0.141*
H16B	0.5948	0.2433	0.3661	0.141*
H16C	0.5593	0.1120	0.3312	0.141*
O1	0.5559 (4)	0.2239 (4)	0.1413 (2)	0.0505 (10)
Pd1	0.60269 (4)	0.13137 (4)	0.04867 (2)	0.03753 (17)
S1	0.57175 (17)	0.21103 (17)	−0.24762 (9)	0.0535 (4)
C12	0.3833 (6)	0.4436 (5)	−0.0730 (3)	0.0387 (12)
H12	0.4294	0.4486	−0.1106	0.046*
N2	0.4923 (4)	0.2455 (4)	−0.0316 (2)	0.0352 (10)
C2	0.6572 (5)	0.0695 (5)	−0.0387 (3)	0.0389 (12)
C8	0.3343 (6)	0.3391 (6)	0.0315 (3)	0.0445 (14)
H8	0.3485	0.2739	0.0650	0.053*
N1	0.5120 (5)	0.2341 (4)	−0.0962 (2)	0.0397 (10)
C1	0.6010 (5)	0.1385 (5)	−0.1014 (3)	0.0376 (12)
C6	0.6283 (6)	0.1130 (5)	−0.1701 (3)	0.0433 (13)
C11	0.2968 (6)	0.5358 (5)	−0.0644 (3)	0.0438 (13)
H11	0.2844	0.6027	−0.0967	0.053*
C10	0.2264 (6)	0.5323 (5)	−0.0081 (3)	0.0439 (13)
C5	0.7106 (6)	0.0153 (6)	−0.1767 (4)	0.0496 (15)
H5	0.7264	−0.0053	−0.2225	0.060*
O3	0.6033 (7)	0.1501 (6)	−0.3099 (3)	0.0905 (19)
C14	0.5605 (6)	0.1832 (6)	0.2041 (3)	0.0489 (14)
H14	0.5892	0.1021	0.2145	0.059*
C4	0.7698 (7)	−0.0520 (6)	−0.1146 (4)	0.0554 (16)
H4	0.8275	−0.1168	−0.1188	0.066*
C9	0.2460 (6)	0.4323 (6)	0.0382 (3)	0.0473 (14)
H9	0.1984	0.4271	0.0751	0.057*
C3	0.7452 (6)	−0.0253 (6)	−0.0461 (4)	0.0531 (15)
H3	0.7877	−0.0710	−0.0048	0.064*
C13	0.1332 (7)	0.6366 (6)	0.0003 (5)	0.0669 (19)
H13A	0.0802	0.6128	0.0345	0.100*
H13B	0.0745	0.6548	−0.0469	0.100*
H13C	0.1853	0.7087	0.0186	0.100*
C17	0.6273 (6)	0.3294 (5)	−0.2288 (3)	0.0406 (13)
H17A	0.7239	0.3239	−0.2166	0.061*
H17B	0.5973	0.3605	−0.1870	0.061*
H17C	0.5986	0.3844	−0.2700	0.061*
O2	0.3937 (7)	0.2197 (8)	−0.2636 (4)	0.113 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0639 (10)	0.0573 (9)	0.0491 (9)	0.0143 (8)	0.0025 (7)	0.0075 (7)
C7	0.040 (3)	0.026 (2)	0.036 (3)	0.000 (2)	0.012 (2)	0.006 (2)
N3	0.051 (3)	0.066 (3)	0.036 (3)	−0.003 (3)	0.015 (2)	−0.003 (2)

C15	0.077 (5)	0.080 (5)	0.057 (4)	0.015 (4)	0.014 (4)	−0.015 (4)
C16	0.120 (8)	0.113 (7)	0.057 (5)	0.010 (6)	0.036 (5)	0.017 (5)
O1	0.061 (3)	0.055 (3)	0.038 (2)	0.008 (2)	0.0163 (19)	0.0042 (19)
Pd1	0.0418 (3)	0.0362 (3)	0.0351 (3)	0.00051 (18)	0.00993 (17)	0.00318 (18)
S1	0.0621 (10)	0.0628 (10)	0.0408 (8)	0.0054 (8)	0.0222 (7)	0.0065 (7)
C12	0.052 (3)	0.036 (3)	0.030 (3)	−0.001 (2)	0.014 (2)	0.013 (2)
N2	0.041 (2)	0.033 (2)	0.034 (2)	−0.0030 (19)	0.0128 (19)	0.0004 (18)
C2	0.039 (3)	0.040 (3)	0.039 (3)	−0.004 (2)	0.012 (2)	−0.005 (2)
C8	0.047 (3)	0.045 (3)	0.044 (3)	0.003 (3)	0.014 (3)	0.008 (3)
N1	0.043 (3)	0.040 (3)	0.037 (3)	0.002 (2)	0.011 (2)	0.002 (2)
C1	0.041 (3)	0.036 (3)	0.038 (3)	−0.008 (2)	0.014 (2)	−0.002 (2)
C6	0.047 (3)	0.036 (3)	0.050 (3)	−0.006 (2)	0.018 (3)	0.001 (3)
C11	0.051 (3)	0.032 (3)	0.045 (3)	0.002 (2)	0.004 (3)	0.008 (2)
C10	0.037 (3)	0.044 (3)	0.050 (3)	−0.002 (2)	0.010 (2)	−0.008 (3)
C5	0.052 (3)	0.051 (4)	0.052 (4)	0.000 (3)	0.024 (3)	−0.007 (3)
O3	0.124 (5)	0.113 (5)	0.044 (3)	0.044 (4)	0.040 (3)	0.011 (3)
C14	0.052 (4)	0.046 (3)	0.050 (4)	0.003 (3)	0.014 (3)	0.006 (3)
C4	0.060 (4)	0.043 (3)	0.070 (4)	0.014 (3)	0.027 (3)	−0.001 (3)
C9	0.042 (3)	0.057 (4)	0.047 (3)	0.002 (3)	0.018 (3)	0.005 (3)
C3	0.054 (4)	0.047 (4)	0.059 (4)	0.007 (3)	0.016 (3)	0.006 (3)
C13	0.060 (4)	0.051 (4)	0.092 (6)	0.007 (3)	0.021 (4)	−0.005 (4)
C17	0.045 (3)	0.035 (3)	0.044 (3)	−0.008 (2)	0.015 (2)	0.020 (2)
O2	0.094 (5)	0.135 (6)	0.107 (5)	0.011 (4)	0.020 (4)	0.011 (5)

Geometric parameters (Å, °)

Cl1—Pd1	2.2875 (16)	C2—C1	1.389 (8)
C7—C12	1.391 (7)	C2—C3	1.391 (8)
C7—C8	1.400 (8)	C8—C9	1.376 (8)
C7—N2	1.409 (7)	C8—H8	0.9300
N3—C14	1.302 (8)	N1—C1	1.394 (7)
N3—C15	1.446 (9)	C1—C6	1.396 (8)
N3—C16	1.459 (9)	C6—C5	1.373 (8)
C15—H15A	0.9600	C11—C10	1.399 (8)
C15—H15B	0.9600	C11—H11	0.9300
C15—H15C	0.9600	C10—C9	1.367 (8)
C16—H16A	0.9600	C10—C13	1.507 (8)
C16—H16B	0.9600	C5—C4	1.379 (9)
C16—H16C	0.9600	C5—H5	0.9300
O1—C14	1.238 (7)	C14—H14	0.9300
O1—Pd1	2.138 (4)	C4—C3	1.383 (9)
Pd1—C2	1.952 (5)	C4—H4	0.9300
Pd1—N2	2.058 (4)	C9—H9	0.9300
S1—C17	1.410 (6)	C3—H3	0.9300
S1—O3	1.432 (5)	C13—H13A	0.9600
S1—C6	1.773 (6)	C13—H13B	0.9600
S1—O2	1.774 (7)	C13—H13C	0.9600
C12—C11	1.365 (8)	C17—H17A	0.9600
C12—H12	0.9300	C17—H17B	0.9600

N2—N1	1.270 (6)	C17—H17C	0.9600

C12—C7—C8	118.4 (5)	C7—C8—H8	119.9
C12—C7—N2	122.3 (5)	N2—N1—C1	112.7 (4)
C8—C7—N2	119.2 (5)	C2—C1—N1	119.3 (5)
C14—N3—C15	119.7 (6)	C2—C1—C6	122.0 (5)
C14—N3—C16	122.5 (6)	N1—C1—C6	118.7 (5)
C15—N3—C16	117.7 (6)	C5—C6—C1	119.3 (6)
N3—C15—H15A	109.5	C5—C6—S1	118.5 (5)
N3—C15—H15B	109.5	C1—C6—S1	122.0 (4)
H15A—C15—H15B	109.5	C12—C11—C10	121.7 (5)
N3—C15—H15C	109.5	C12—C11—H11	119.1
H15A—C15—H15C	109.5	C10—C11—H11	119.1
H15B—C15—H15C	109.5	C9—C10—C11	117.8 (5)
N3—C16—H16A	109.5	C9—C10—C13	122.0 (6)
N3—C16—H16B	109.5	C11—C10—C13	120.2 (6)
H16A—C16—H16B	109.5	C6—C5—C4	119.3 (6)
N3—C16—H16C	109.5	C6—C5—H5	120.4
H16A—C16—H16C	109.5	C4—C5—H5	120.4
H16B—C16—H16C	109.5	O1—C14—N3	123.5 (6)
C14—O1—Pd1	128.7 (4)	O1—C14—H14	118.2
C2—Pd1—N2	79.4 (2)	N3—C14—H14	118.2
C2—Pd1—O1	171.7 (2)	C5—C4—C3	121.5 (6)
N2—Pd1—O1	96.65 (16)	C5—C4—H4	119.2
C2—Pd1—Cl1	93.86 (17)	C3—C4—H4	119.2
N2—Pd1—Cl1	173.19 (13)	C10—C9—C8	121.7 (6)
O1—Pd1—Cl1	89.87 (12)	C10—C9—H9	119.2
C17—S1—O3	117.7 (4)	C8—C9—H9	119.2
C17—S1—C6	107.7 (3)	C4—C3—C2	120.2 (6)
O3—S1—C6	106.9 (3)	C4—C3—H3	119.9
C17—S1—O2	109.3 (4)	C2—C3—H3	119.9
O3—S1—O2	107.6 (4)	C10—C13—H13A	109.5
C6—S1—O2	107.1 (3)	C10—C13—H13B	109.5
C11—C12—C7	120.1 (5)	H13A—C13—H13B	109.5
C11—C12—H12	119.9	C10—C13—H13C	109.5
C7—C12—H12	119.9	H13A—C13—H13C	109.5
N1—N2—C7	113.2 (4)	H13B—C13—H13C	109.5
N1—N2—Pd1	116.5 (3)	S1—C17—H17A	109.5
C7—N2—Pd1	130.1 (3)	S1—C17—H17B	109.5
C1—C2—C3	117.6 (5)	H17A—C17—H17B	109.5
C1—C2—Pd1	111.8 (4)	S1—C17—H17C	109.5
C3—C2—Pd1	130.5 (5)	H17A—C17—H17C	109.5
C9—C8—C7	120.2 (5)	H17B—C17—H17C	109.5
C9—C8—H8	119.9		

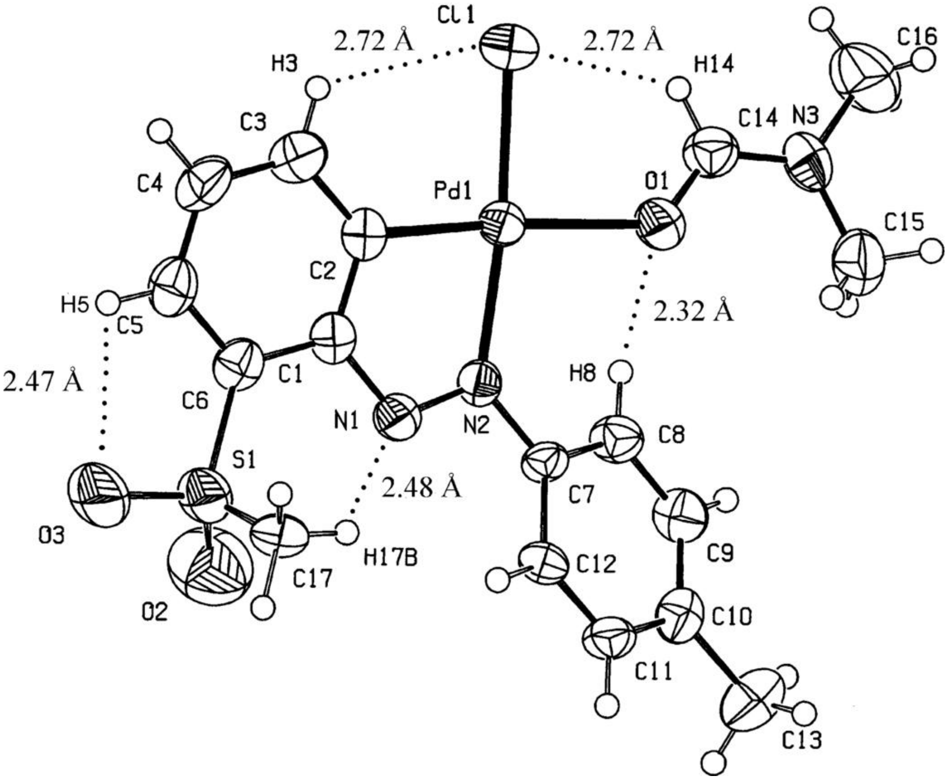
C14—O1—Pd1—N2	158.0 (5)	C2—C1—C6—C5	1.5 (8)
C14—O1—Pd1—Cl1	−24.0 (5)	N1—C1—C6—C5	−176.9 (5)
C8—C7—C12—C11	−1.5 (8)	C2—C1—C6—S1	−172.9 (4)
N2—C7—C12—C11	−179.1 (5)	N1—C1—C6—S1	8.7 (7)
C12—C7—N2—N1	−25.2 (7)	C17—S1—C6—C5	−115.2 (5)

C8—C7—N2—N1	157.2 (5)	O3—S1—C6—C5	12.2 (6)
C12—C7—N2—Pd1	150.1 (4)	O2—S1—C6—C5	127.3 (5)
C8—C7—N2—Pd1	−27.5 (7)	C17—S1—C6—C1	59.3 (6)
C2—Pd1—N2—N1	−4.4 (4)	O3—S1—C6—C1	−173.3 (5)
O1—Pd1—N2—N1	168.2 (4)	O2—S1—C6—C1	−58.2 (6)
C2—Pd1—N2—C7	−179.6 (5)	C7—C12—C11—C10	0.5 (9)
O1—Pd1—N2—C7	−7.0 (4)	C12—C11—C10—C9	−0.5 (9)
N2—Pd1—C2—C1	3.7 (4)	C12—C11—C10—C13	179.2 (6)
Cl1—Pd1—C2—C1	−175.1 (4)	C1—C6—C5—C4	−3.0 (9)
N2—Pd1—C2—C3	−179.7 (6)	S1—C6—C5—C4	171.5 (5)
Cl1—Pd1—C2—C3	1.4 (6)	Pd1—O1—C14—N3	−178.8 (4)
C12—C7—C8—C9	2.6 (9)	C15—N3—C14—O1	1.8 (10)
N2—C7—C8—C9	−179.8 (5)	C16—N3—C14—O1	179.0 (7)
C7—N2—N1—C1	179.8 (4)	C6—C5—C4—C3	1.7 (10)
Pd1—N2—N1—C1	3.8 (6)	C11—C10—C9—C8	1.6 (9)
C3—C2—C1—N1	179.8 (5)	C13—C10—C9—C8	−178.1 (6)
Pd1—C2—C1—N1	−3.2 (6)	C7—C8—C9—C10	−2.7 (9)
C3—C2—C1—C6	1.5 (8)	C5—C4—C3—C2	1.3 (10)
Pd1—C2—C1—C6	178.5 (4)	C1—C2—C3—C4	−2.8 (9)
N2—N1—C1—C2	−0.5 (7)	Pd1—C2—C3—C4	−179.2 (5)
N2—N1—C1—C6	177.9 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Cl1	0.93	2.72	3.250 (7)	117
C5—H5···O3	0.93	2.47	2.862 (9)	106
C8—H8···O1	0.93	2.32	2.947 (7)	124
C14—H14···Cl1	0.93	2.72	3.253 (7)	118
C17—H17B···N1	0.96	2.48	3.140 (8)	126

Fig. 1



Cl1
2.72 Å
2.72 Å
H3
H14
C16
C3
C14
N3
C4
Pd1
O1
C15
C2
H5
C5
2.32 Å
2.47 Å
C6
C1
H8
N1
N2
C8
S1
C7
2.48 Å
O3
H17B
C9
C12
C17
O2
C10
C11
C13

Fig. 2

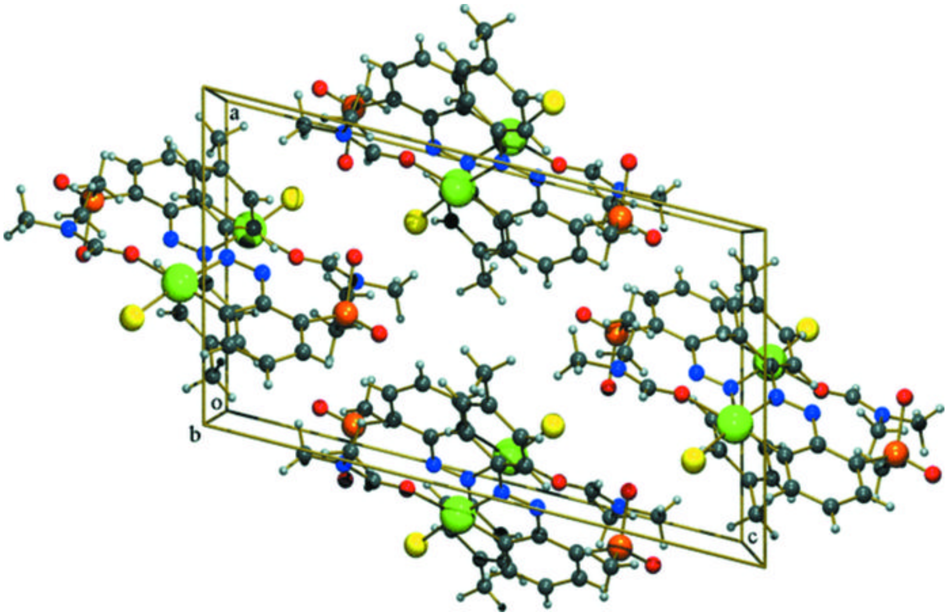


Fig. 3