

## Trichlorido{1-[2-(methylsulfanyl)phenyl]-diazanyl}phenyl- $\kappa^3$ C,N,S}platinum(IV)

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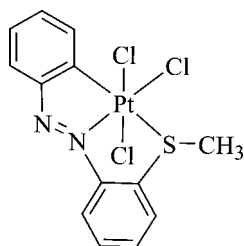
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Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.020$  Å;  $R$  factor = 0.061;  $wR$  factor = 0.116; data-to-parameter ratio = 13.8.

The Pt atom in the title compound,  $[\text{Pt}(\text{C}_{13}\text{H}_{11}\text{N}_2\text{S})\text{Cl}_3]$ , is hexacoordinated by an aromatic C, a diazene N, three Cl, and one S atoms in an approximately octahedral geometry. There are intra- and intermolecular C—H $\cdots$ Cl hydrogen-bonding interactions. The crystal packing is stabilized by a weak intermolecular  $\pi$ – $\pi$  interaction; the centroid–centroid distance is 3.924 (8) Å and the perpendicular distance is 3.656 Å, with a slippage of 1.424 Å.

### Related literature

For related literature, see: Bagchi *et al.* (2007); van Beek *et al.* (1986); Chattopadhyay *et al.* (1991); Lersch & Tilset (2005); Rendina & Puddephatt (1997); Yahav *et al.* (2005).



### Experimental

#### Crystal data

$[\text{Pt}(\text{C}_{13}\text{H}_{11}\text{N}_2\text{S})\text{Cl}_3]$   
 $M_r = 528.74$   
 Monoclinic,  $P2_1/c$   
 $a = 7.765$  (2) Å  
 $b = 16.858$  (5) Å  
 $c = 12.031$  (3) Å  
 $\beta = 105.799$  (5)°

$V = 1515.4$  (7) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 9.91$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
 $0.41 \times 0.16 \times 0.15$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.163$ ,  $T_{\max} = 0.225$

13366 measured reflections  
 2515 independent reflections

2339 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.082$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$   
 $wR(F^2) = 0.116$   
 $S = 1.25$   
 2515 reflections

182 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 1.42$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -2.85$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

N2—N1	1.274 (13)	Pt1—Cl2	2.315 (3)
Pt1—N1	1.992 (10)	Pt1—Cl3	2.317 (3)
Pt1—Cl2	2.015 (11)	Pt1—S1	2.435 (3)
Pt1—Cl1	2.306 (3)		
N1—Pt1—Cl2	80.7 (5)	Cl2—Pt1—Cl3	90.6 (4)
N1—Pt1—Cl1	88.4 (3)	Cl2—Pt1—Cl3	90.63 (13)
Cl2—Pt1—Cl1	89.0 (4)	N1—Pt1—S1	84.8 (3)
Cl2—Pt1—Cl2	96.4 (4)	Cl1—Pt1—S1	84.84 (12)
Cl1—Pt1—Cl2	91.74 (13)	Cl2—Pt1—S1	98.05 (12)
N1—Pt1—Cl3	89.2 (3)	Cl3—Pt1—S1	94.99 (11)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C13—H13B $\cdots$ Cl1 <sup>i</sup>	0.96	2.69	3.302 (13)	123
C13—H13B $\cdots$ Cl3	0.96	2.71	3.448 (14)	134

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

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); 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: BT2390).

### References

- Bagchi, V., Das, P. & Bandyopadhyay, D. (2007). *Acta Cryst.* **E63**, m1704.  
 Beek, J. A. M. van, van Koten, G., Smeets, W. J. J. & Spek, A. L. (1986). *J. Am. Chem. Soc.* **108**, 5010–5011.  
 Bruker (1997). SHELXTL. Bruker AXS Inc. Madison, Wisconsin, USA.  
 Bruker (1998). SMART (Version 5.054) and SAINT (Version 6.02a). Bruker AXS Inc., Madison, Wisconsin, USA.  
 Chattopadhyay, S., Sinha, C., Basu, P. & Chakravorty, A. (1991). *Organometallics*, **10**, 1135–1139.  
 Lersch, M. & Tilset, M. (2005). *Chem. Rev.* **105**, 2471–2526.  
 Rendina, L. M. & Puddephatt, R. J. (1997). *Chem. Rev.* **97**, 1735–1754.  
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.  
 Yahav, A., Goldberg, I. & Vignalok, A. (2005). *Organometallics*, **24**, 5654–5659.

**supplementary materials**

*Acta Cryst.* (2007). E63, m1940 [ doi:10.1107/S160053680702898X ]

## Trichlorido{1-[2-(methylsulfanyl)phenyldiazenyl]phenyl- $\kappa^3$ C,N,S}platinum(IV)

V. Bagchi, P. Das and D. Bandyopadhyay

### Comment

The intramolecular C—H bond activation of aryl rings using platinum(II) is important in synthetic chemistry. There has been intense interest in C—H bond activation by platinum complexes (Lersch & Tilset, 2005; Rendina & Puddephatt, 1997). The oxidation of divalent cycloplatinates by halogens affords tetravalent cycloplatinates (Yahav *et al.*, 2005) and the structures of few tetravalent platinum complexes have appeared in literature (Chattopadhyay *et al.*, 1991; van Beek *et al.*, 1986). Herein, we report the X-ray crystallographic study of the title compound.

The molecular structure of the title compound is shown in Fig. 1, with the atom numbering scheme. The platinum atom is hexa-coordinated with a donor set of six atoms in an approximately octahedral geometry. The packing arrangement of the title compound is shown in Fig. 2. The N=N bond length is slightly greater than the typical value (Chattopadhyay *et al.*, 1991). The metal carbon and metal sulfur bond lengths are very close to the typical values; all the three Pt—Cl bond lengths are very close and are also close to the reported values (Chattopadhyay *et al.*, 1991).

There are intra and intermolecular C—H $\cdots$ Cl hydrogen bonding interactions (Table 2, Fig. 3) in the title compound. A chain structure results by the intermolecular hydrogen-bonds where C13 atom in the molecule acts as a hydrogen-bond donor, *via* H13B, to the Cl11 atom of another molecule [Symmetry code: (i)  $-1 + x, y, z$ ] (Table 2) (Fig. 3). A weak intermolecular  $\pi$ — $\pi$  interaction (Bagchi *et al.*, 2007) arranges the molecules in an anti parallel fashion (Fig. 4). The  $Cg3$ — $Cg3^{ii}$  [Symmetry code: (ii)  $-x, 1 - y, 1 - z$ .  $Cg3$  is the centroid of C1—C6 ring.] distance is 3.924 (8) Å and the perpendicular distance is 3.656 Å with a slippage of 1.424 Å.

### Experimental

The title compound was synthesized by the treatment of Chlorido{1-[2-(methylsulfanyl)phenyldiazenyl]phenyl- $\kappa^3$ C,N,S}platinum(II) with chlorinated acetonitrile following a reported procedure (Chattopadhyay *et al.*, 1991) (Yield 74%).

### Refinement

H atoms were included at calculated positions as riding atoms with C—H set to 0.93 Å for (aromatic) and 0.96 Å for (CH<sub>3</sub>) H atoms, with  $U_{iso}(H) = 1.2U_{eq}(C)$  (1.5 $U_{eq}$  for methyl group). Some low-angle reflections were excluded from the refinement, as they were probably obscured by the beam stop.

## Figures

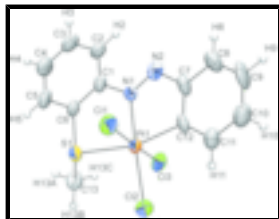


Fig. 1. The asymmetric unit of (I), with displacement ellipsoids drawn at the 50% probability level.

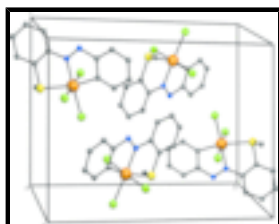


Fig. 2. The molecular arrangement of (I) in the *ac* plane.

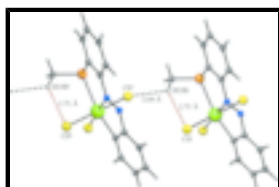


Fig. 3. Intra and intermolecular C—H...Cl interactions for (I), indicated by the dotted lines. [Symmetry code: (i)  $-1 + x, y, z$ ].

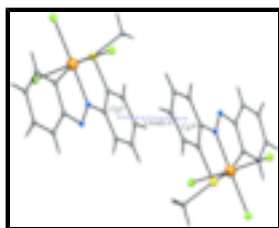


Fig. 4. The intermolecular  $\pi$ — $\pi$  interaction for (I), indicated by dotted line [Symmetry code: (i)  $-x, 1 - y, 1 - z$ .  $Cg3$  is the centroid of C1—C6 ring.].

## Trichlorido{1-[2-(methylsulfanyl)phenyldiazenyl]phenyl- $\lambda$ - $\kappa^3C,N,S$ }platinum(IV)

### Crystal data

[Pt(C<sub>13</sub>H<sub>11</sub>N<sub>2</sub>S)Cl<sub>3</sub>]

$M_r = 528.74$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 7.765$  (2) Å

$b = 16.858$  (5) Å

$c = 12.031$  (3) Å

$\beta = 105.799$  (5)°

$V = 1515.4$  (7) Å<sup>3</sup>

$Z = 4$

$F_{000} = 992$

$D_x = 2.317$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 2515 reflections

$\theta = 2.1$ – $25.0$ °

$\mu = 9.91$  mm<sup>-1</sup>

$T = 295$  (2) K

Block, yellow

$0.41 \times 0.16 \times 0.15$  mm

### Data collection

Bruker SMART CCD area-detector

2515 independent reflections

diffractometer	
Radiation source: fine-focus sealed tube	2339 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.082$
$T = 298(2)$ K	$\theta_{\text{max}} = 25.0^\circ$
$\varphi$ and $\omega$ scans	$\theta_{\text{min}} = 2.1^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.163$ , $T_{\text{max}} = 0.225$	$k = -20 \rightarrow 20$
13366 measured reflections	$l = -14 \rightarrow 14$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.061$	H-atom parameters constrained
$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2 + 10.465P]$
$S = 1.25$	where $P = (F_o^2 + 2F_c^2)/3$
2515 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
182 parameters	$\Delta\rho_{\text{max}} = 1.42 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -2.84 \text{ e } \text{\AA}^{-3}$
	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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
N2	0.3697 (12)	0.3572 (6)	0.4335 (9)	0.038 (3)
C13	-0.1878 (15)	0.4983 (8)	0.1296 (13)	0.049 (4)
H13A	-0.2277	0.5445	0.1622	0.074*
H13B	-0.2244	0.4515	0.1624	0.074*
H13C	-0.2393	0.4981	0.0474	0.074*
C3	0.2107 (19)	0.5732 (8)	0.5385 (13)	0.052 (4)
H3	0.2400	0.5884	0.6157	0.062*
C9	0.580 (2)	0.1686 (10)	0.4006 (17)	0.073 (5)
H9	0.6655	0.1338	0.4439	0.088*

## supplementary materials

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Pt1	0.18423 (6)	0.36801 (3)	0.19692 (4)	0.03112 (19)
S1	0.0533 (4)	0.49996 (18)	0.1610 (3)	0.0383 (7)
Cl3	-0.0645 (4)	0.31058 (19)	0.2355 (3)	0.0462 (8)
Cl1	0.4357 (4)	0.4267 (2)	0.1665 (3)	0.0467 (8)
Cl2	0.0959 (5)	0.3211 (2)	0.0091 (3)	0.0502 (9)
N1	0.2666 (13)	0.4032 (6)	0.3610 (8)	0.036 (2)
C12	0.3348 (16)	0.2734 (7)	0.2651 (12)	0.039 (3)
C6	0.1158 (16)	0.5285 (7)	0.3087 (11)	0.038 (3)
C1	0.2150 (15)	0.4783 (7)	0.3953 (11)	0.036 (3)
C7	0.4102 (17)	0.2864 (7)	0.3837 (12)	0.044 (3)
C8	0.5301 (18)	0.2333 (8)	0.4501 (13)	0.050 (4)
H8	0.5763	0.2420	0.5289	0.060*
C4	0.113 (2)	0.6234 (8)	0.4548 (14)	0.058 (4)
H4	0.0757	0.6720	0.4763	0.070*
C10	0.501 (2)	0.1546 (9)	0.2809 (15)	0.061 (4)
H10	0.5317	0.1095	0.2460	0.073*
C2	0.2650 (18)	0.5011 (8)	0.5083 (12)	0.045 (3)
H2	0.3353	0.4679	0.5644	0.054*
C11	0.3794 (19)	0.2074 (8)	0.2171 (13)	0.050 (4)
H11	0.3269	0.1973	0.1392	0.060*
C5	0.0690 (17)	0.6028 (7)	0.3395 (14)	0.046 (3)
H5	0.0087	0.6384	0.2832	0.056*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N2	0.023 (5)	0.041 (6)	0.055 (7)	-0.014 (5)	0.020 (5)	0.006 (5)
Cl3	0.023 (6)	0.044 (8)	0.076 (11)	0.008 (6)	0.004 (6)	-0.001 (7)
C3	0.054 (9)	0.041 (8)	0.059 (10)	-0.009 (7)	0.014 (7)	-0.017 (7)
C9	0.053 (10)	0.050 (10)	0.112 (16)	0.038 (8)	0.014 (10)	0.020 (10)
Pt1	0.0311 (3)	0.0261 (3)	0.0346 (3)	-0.0006 (2)	0.00616 (19)	0.0012 (2)
S1	0.0403 (17)	0.0294 (16)	0.0424 (19)	0.0008 (13)	0.0062 (14)	0.0065 (14)
Cl3	0.0432 (18)	0.0395 (18)	0.060 (2)	-0.0096 (14)	0.0199 (16)	-0.0019 (16)
Cl1	0.0351 (17)	0.049 (2)	0.057 (2)	-0.0091 (14)	0.0135 (15)	0.0054 (16)
Cl2	0.060 (2)	0.045 (2)	0.0408 (19)	-0.0004 (16)	0.0067 (16)	-0.0042 (15)
N1	0.045 (6)	0.029 (5)	0.030 (6)	-0.005 (5)	0.004 (5)	0.006 (5)
C12	0.031 (7)	0.028 (7)	0.054 (9)	0.007 (5)	0.004 (6)	0.014 (6)
C6	0.038 (7)	0.023 (6)	0.050 (8)	0.000 (5)	0.006 (6)	0.000 (6)
C1	0.030 (6)	0.027 (6)	0.053 (8)	0.001 (5)	0.011 (6)	-0.003 (6)
C7	0.044 (8)	0.034 (7)	0.053 (9)	0.019 (6)	0.013 (7)	0.014 (6)
C8	0.046 (8)	0.053 (9)	0.048 (9)	0.013 (7)	0.008 (7)	0.014 (7)
C4	0.062 (10)	0.040 (8)	0.068 (11)	0.015 (7)	0.010 (8)	-0.009 (8)
C10	0.063 (10)	0.044 (9)	0.077 (12)	0.011 (7)	0.022 (9)	-0.010 (8)
C2	0.050 (8)	0.041 (8)	0.041 (8)	-0.008 (6)	0.006 (6)	-0.008 (6)
C11	0.055 (9)	0.036 (8)	0.060 (10)	0.011 (7)	0.018 (7)	-0.001 (7)
C5	0.041 (7)	0.024 (6)	0.072 (10)	0.005 (6)	0.010 (7)	-0.005 (7)

*Geometric parameters (Å, °)*

N2—N1	1.274 (13)	Pt1—S1	2.435 (3)
N2—C7	1.409 (16)	S1—C6	1.776 (13)
C13—S1	1.807 (11)	N1—C1	1.422 (15)
C13—H13A	0.9600	C12—C11	1.343 (18)
C13—H13B	0.9600	C12—C7	1.404 (19)
C13—H13C	0.9600	C6—C5	1.382 (17)
C3—C2	1.369 (19)	C6—C1	1.400 (17)
C3—C4	1.37 (2)	C1—C2	1.365 (17)
C3—H3	0.9300	C7—C8	1.378 (17)
C9—C8	1.35 (2)	C8—H8	0.9300
C9—C10	1.42 (2)	C4—C5	1.38 (2)
C9—H9	0.9300	C4—H4	0.9300
Pt1—N1	1.992 (10)	C10—C11	1.37 (2)
Pt1—C12	2.015 (11)	C10—H10	0.9300
Pt1—C11	2.306 (3)	C2—H2	0.9300
Pt1—C12	2.315 (3)	C11—H11	0.9300
Pt1—C13	2.317 (3)	C5—H5	0.9300
N1—N2—C7	113.3 (11)	N2—N1—Pt1	118.1 (8)
S1—C13—H13A	109.5	C1—N1—Pt1	120.8 (8)
S1—C13—H13B	109.5	C11—C12—C7	118.8 (12)
H13A—C13—H13B	109.5	C11—C12—Pt1	132.1 (11)
S1—C13—H13C	109.5	C7—C12—Pt1	109.0 (9)
H13A—C13—H13C	109.5	C5—C6—C1	118.7 (13)
H13B—C13—H13C	109.5	C5—C6—S1	119.6 (10)
C2—C3—C4	120.1 (14)	C1—C6—S1	121.7 (9)
C2—C3—H3	120.0	C2—C1—C6	121.4 (12)
C4—C3—H3	120.0	C2—C1—N1	120.9 (11)
C8—C9—C10	118.9 (13)	C6—C1—N1	117.6 (11)
C8—C9—H9	120.6	C8—C7—C12	121.1 (12)
C10—C9—H9	120.6	C8—C7—N2	119.9 (13)
N1—Pt1—C12	80.7 (5)	C12—C7—N2	118.9 (11)
N1—Pt1—C11	88.4 (3)	C9—C8—C7	120.0 (15)
C12—Pt1—C11	89.0 (4)	C9—C8—H8	120.0
N1—Pt1—C12	177.1 (3)	C7—C8—H8	120.0
C12—Pt1—C12	96.4 (4)	C3—C4—C5	121.2 (13)
C11—Pt1—C12	91.74 (13)	C3—C4—H4	119.4
N1—Pt1—C13	89.2 (3)	C5—C4—H4	119.4
C12—Pt1—C13	90.6 (4)	C11—C10—C9	120.1 (14)
C11—Pt1—C13	177.63 (12)	C11—C10—H10	119.9
C12—Pt1—C13	90.63 (13)	C9—C10—H10	119.9
N1—Pt1—S1	84.8 (3)	C1—C2—C3	119.4 (13)
C12—Pt1—S1	164.4 (4)	C1—C2—H2	120.3
C11—Pt1—S1	84.84 (12)	C3—C2—H2	120.3
C12—Pt1—S1	98.05 (12)	C12—C11—C10	121.1 (14)
C13—Pt1—S1	94.99 (11)	C12—C11—H11	119.5
C6—S1—C13	101.5 (6)	C10—C11—H11	119.5

## supplementary materials

C6—S1—Pt1	94.7 (4)	C4—C5—C6	119.1 (13)
C13—S1—Pt1	112.4 (5)	C4—C5—H5	120.5
N2—N1—C1	121.1 (10)	C6—C5—H5	120.5
N1—Pt1—S1—C6	-3.3 (5)	C13—S1—C6—C1	116.4 (11)
C12—Pt1—S1—C6	-25.2 (15)	Pt1—S1—C6—C1	2.3 (10)
C11—Pt1—S1—C6	-92.2 (4)	C5—C6—C1—C2	0.2 (19)
C12—Pt1—S1—C6	176.8 (4)	S1—C6—C1—C2	178.9 (10)
C13—Pt1—S1—C6	85.5 (4)	C5—C6—C1—N1	-178.0 (11)
N1—Pt1—S1—C13	-107.8 (6)	S1—C6—C1—N1	0.7 (16)
C12—Pt1—S1—C13	-129.6 (15)	N2—N1—C1—C2	-4.3 (17)
C11—Pt1—S1—C13	163.4 (5)	Pt1—N1—C1—C2	177.2 (9)
C12—Pt1—S1—C13	72.3 (5)	N2—N1—C1—C6	173.9 (10)
C13—Pt1—S1—C13	-19.0 (5)	Pt1—N1—C1—C6	-4.6 (14)
C7—N2—N1—C1	-178.5 (10)	C11—C12—C7—C8	1(2)
C7—N2—N1—Pt1	0.1 (12)	Pt1—C12—C7—C8	-175.2 (11)
C11—Pt1—N1—N2	-88.8 (8)	C11—C12—C7—N2	177.3 (12)
C13—Pt1—N1—N2	91.2 (8)	Pt1—C12—C7—N2	1.1 (14)
S1—Pt1—N1—N2	-173.8 (8)	N1—N2—C7—C8	175.5 (11)
C11—Pt1—N1—C1	89.7 (8)	N1—N2—C7—C12	-0.8 (16)
C13—Pt1—N1—C1	-90.3 (8)	C10—C9—C8—C7	-3(2)
S1—Pt1—N1—C1	4.8 (8)	C12—C7—C8—C9	2(2)
N1—Pt1—C12—C11	-176.3 (14)	N2—C7—C8—C9	-174.5 (13)
C11—Pt1—C12—C11	-87.8 (13)	C2—C3—C4—C5	-1(2)
C12—Pt1—C12—C11	3.9 (13)	C8—C9—C10—C11	2(2)
C13—Pt1—C12—C11	94.6 (13)	C6—C1—C2—C3	2.8 (19)
S1—Pt1—C12—C11	-154.2 (11)	N1—C1—C2—C3	-179.0 (11)
N1—Pt1—C12—C7	-0.8 (9)	C4—C3—C2—C1	-3(2)
C11—Pt1—C12—C7	87.8 (9)	C7—C12—C11—C10	-2(2)
C12—Pt1—C12—C7	179.4 (8)	Pt1—C12—C11—C10	172.9 (11)
C13—Pt1—C12—C7	-89.9 (9)	C9—C10—C11—C12	1(2)
S1—Pt1—C12—C7	21 (2)	C3—C4—C5—C6	4(2)
C13—S1—C6—C5	-64.9 (11)	C1—C6—C5—C4	-3.4 (19)
Pt1—S1—C6—C5	-179.0 (10)	S1—C6—C5—C4	177.8 (11)

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C13—H13B $\cdots$ C11 <sup>i</sup>	0.96	2.69	3.302 (13)	123
C13—H13B $\cdots$ C13	0.96	2.71	3.448 (14)	134

Symmetry codes: (i)  $x-1, y, z$ .



Fig. 1

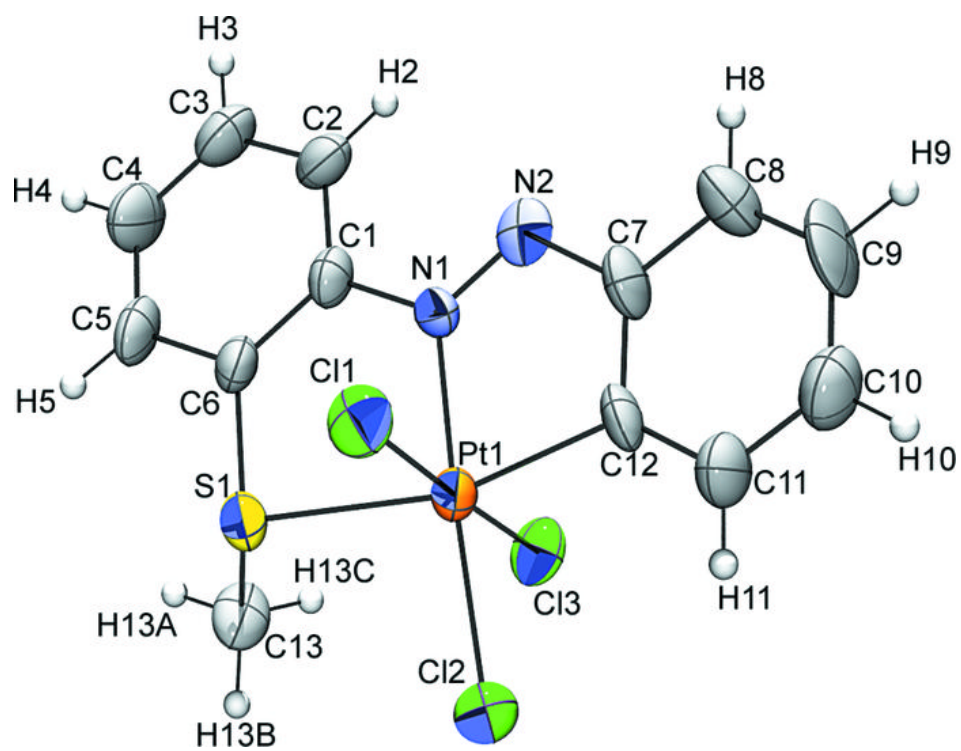


Fig. 2

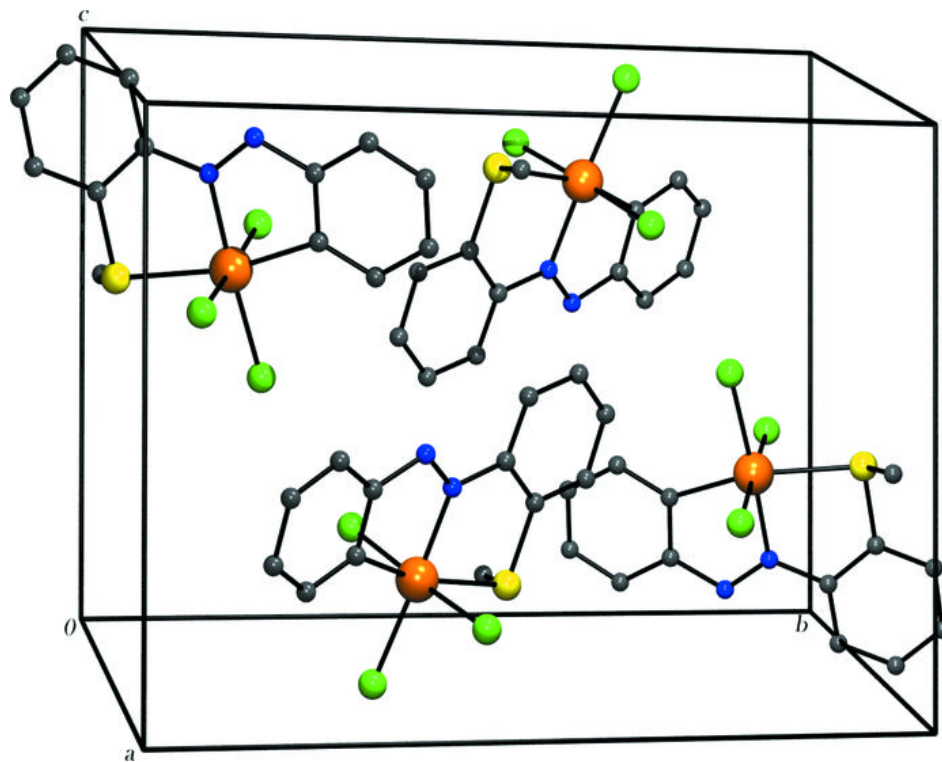


Fig. 3

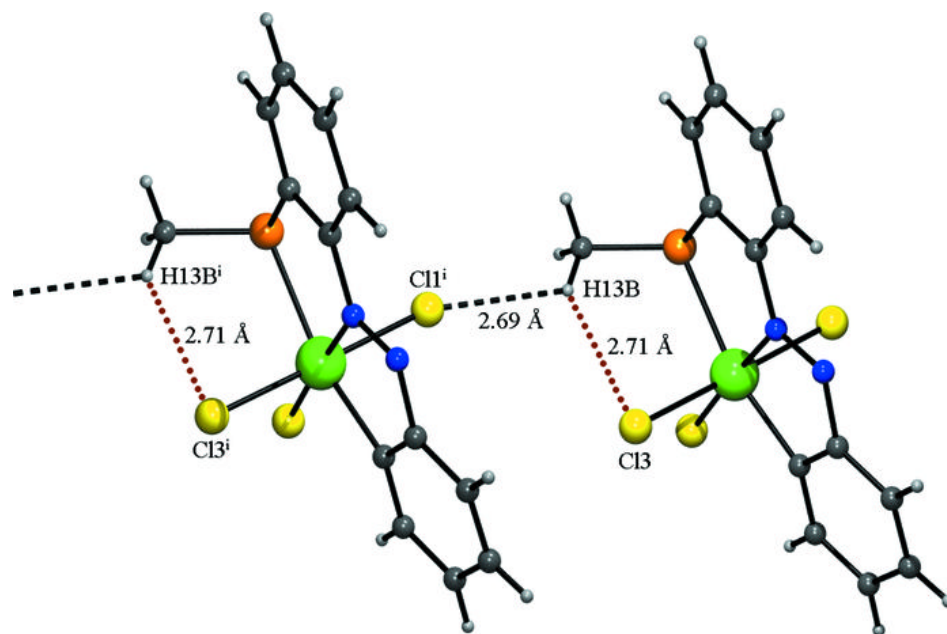


Fig. 4

