

Bis(phenanthridinium) hexachlorido-platinate(IV) dimethyl sulfoxide disolvate

Selvi Karaca,^a Mehmet Akkurt,^{a*} Nasser Safari,^b Vahid Amani,^b Orhan Büyükgüngör^c and Anita Abedi^d

^aDepartment of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, ^bChemistry Department, Shahid Beheshti University, GC, Tehran, Iran, ^cDepartment of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey, and ^dDepartment of Chemistry, North Tehran Branch, Islamic Azad University, Tehran, Iran
Correspondence e-mail: akkurt@erciyes.edu.tr

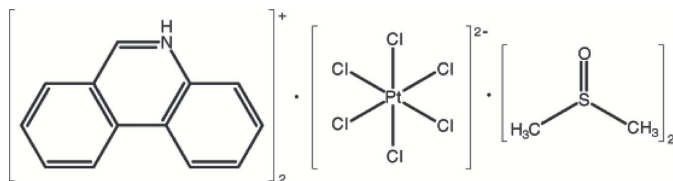
Received 21 January 2009; accepted 22 January 2009

Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.045; wR factor = 0.096; data-to-parameter ratio = 17.8.

The asymmetric unit of the title compound, $(\text{C}_{13}\text{H}_{10}\text{N})_2\text{[PtCl}_6\text{]}\cdot 2\text{C}_2\text{H}_6\text{OS}$, contains one independent protonated phenanthridinium cation, half of a centrosymmetric $[\text{PtCl}_6]^{2-}$ anion and one dimethyl sulfoxide solvent molecule. Intra-molecular $\text{N}-\text{H}\cdots\text{O}$ and intermolecular $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen-bonding interactions seem to be effective in the stabilization of the structure.

Related literature

For related literature, see: Abedi *et al.* (2008); Amani *et al.* (2008); Hasan *et al.* (2001); Hu *et al.* (2003); Juan *et al.* (1998); Kalateh *et al.* (2008); Li & Liu (2003); Terzis & Mentzafos (1983); Yousefi, Ahmadi *et al.* (2007); Yousefi, Teimouri *et al.* (2007a,b); Zafar *et al.* (2000); Zordan & Brammer (2004); Zordan *et al.* (2005).



Experimental

Crystal data

$(\text{C}_{13}\text{H}_{10}\text{N})_2[\text{PtCl}_6]\cdot 2\text{C}_2\text{H}_6\text{OS}$	$V = 3358.6$ (2) Å ³
$M_r = 924.50$	$Z = 4$
Orthorhombic, <i>Pbcn</i>	Mo $K\alpha$ radiation
$a = 24.3695$ (11) Å	$\mu = 4.81$ mm ⁻¹
$b = 7.9061$ (3) Å	$T = 295$ (2) K
$c = 17.4322$ (6) Å	$0.80 \times 0.35 \times 0.09$ mm

Data collection

Stoe IPDS-II diffractometer	33029 measured reflections
Absorption correction: integration (<i>X-RED32</i> ; Stoe & Cie, 2002)	3533 independent reflections
$T_{\min} = 0.114$, $T_{\max} = 0.671$	2992 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.106$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.096$	
$S = 1.12$	
3533 reflections	$\Delta\rho_{\text{max}} = 2.20$ e Å ⁻³
199 parameters	$\Delta\rho_{\text{min}} = -1.01$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{HN1}\cdots\text{O1}$	0.84 (9)	1.79 (9)	2.621 (8)	169 (8)
$\text{C7}-\text{H7}\cdots\text{Cl2}^i$	0.93	2.68	3.540 (7)	154

Symmetry code: (i) $-x + \frac{3}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for use of the diffractometer (purchased under grant No. F.279 of the University Research Fund). NS, VA and AA are grateful to Shahid Beheshti University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2472).

References

- Abedi, A., Bahrami Shabestari, A. & Amani, V. (2008). *Acta Cryst.* **E64**, o990.
 Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
 Amani, V., Rahimi, R. & Khavasi, H. R. (2008). *Acta Cryst.* **E64**, m1143–m1144.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Hasan, M., Kozhevnikov, I. V., Siddiqui, M. R. H., Femoni, C., Steiner, A. & Winterton, N. (2001). *Inorg. Chem.* **40**, 795–800.
 Hu, N. H., Norifusa, T. & Aoki, K. (2003). *Dalton Trans.* pp. 335–341.
 Juan, C., Mareque, R. & Lee, B. (1998). *Inorg. Chem.* **37**, 4756–4757.
 Kalateh, K., Ebadi, A., Abedi, A., Amani, V. & Khavasi, H. R. (2008). *Acta Cryst.* **E64**, m1267–m1268.
 Li, D. & Liu, D. (2003). *Anal. Sci.* **19**, 1089–1090.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Stoe & Cie (2002). *X-AREA* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.
 Terzis, A. & Mentzafos, D. (1983). *Inorg. Chem.* **22**, 1140–1143.
 Yousefi, M., Ahmadi, R., Amani, V. & Khavasi, H. R. (2007). *Acta Cryst.* **E63**, m3114–m3115.
 Yousefi, M., Teimouri, S., Amani, V. & Khavasi, H. R. (2007a). *Acta Cryst.* **E63**, m2460–m2461.
 Yousefi, M., Teimouri, S., Amani, V. & Khavasi, H. R. (2007b). *Acta Cryst.* **E63**, m2748–m2749.
 Zafar, A., Geib, S. J., Hamuro, Y., Carr, A. J. & Hamilton, A. D. (2000). *Tetrahedron*, **56**, 8419–8427.
 Zordan, F. & Brammer, L. (2004). *Acta Cryst.* **B60**, 512–519.
 Zordan, F., Purver, S. L., Adams, H. & Brammer, L. (2005). *CrystEngComm*, **7**, 350–354.

supplementary materials

Acta Cryst. (2009). E65, m235 [doi:10.1107/S1600536809002736]

Bis(phenanthridinium) hexachloridoplatinate(IV) dimethyl sulfoxide disolvate

S. Karaca, M. Akkurt, N. Safari, V. Amani, O. Büyükgüngör and A. Abedi

Comment

In recent years, there has been considerable interest in proton transfer systems and their structures (Zafar *et al.*, 2000; Abedi *et al.*, 2008). Several proton transfer systems using $\text{H}_2[\text{PtCl}_6]$ with proton acceptor molecules, such as $[\text{HpyBr-3}]_2[\text{PtCl}_6] \cdot 2\text{H}_2\text{O}$, (II), and $[\text{HpyI-3}]_2[\text{PtCl}_6] \cdot 2\text{H}_2\text{O}$, (III), (Zordan *et al.*, 2005), $[\text{BMIM}]_2[\text{PtCl}_6]$, (IV), and $[\text{EMIM}]_2[\text{PtCl}_6]$, (V), (Hasan *et al.*, 2001), $\{(\text{DABCO})\text{H}_2[\text{PtCl}_6]\}$, (VI), (Juan *et al.*, 1998), $\{p\text{-C}_6\text{H}_4(\text{CH}_2\text{ImMe})_2[\text{PtCl}_6]\}$, (VII), (Li & Liu, 2003), $[\text{het}][\text{PtCl}_6] \cdot 2\text{H}_2\text{O}$, (VIII), (Hu *et al.*, 2003), $[\text{9-MeGuaH}]_2[\text{PtCl}_6] \cdot 2\text{H}_2\text{O}$, (IX), (Terzis & Mentzafos, 1983), $[\text{HpyCl-3}]_3[\text{PtCl}_6]\text{Cl}$, (X), (Zordan *et al.*, 2004), $[\text{2,9-dmphen.H}]_2[\text{PtCl}_6]$, (XI), (Yousefi *et al.*, 2007), $[\text{H}_2\text{DA18C6}][\text{PtCl}_6] \cdot 2\text{H}_2\text{O}$, (XII), (Yousefi *et al.*, 2007a), $[\text{2,6-dmpy.H}]_2[\text{PtCl}_6]$, (XIII), (Amani *et al.*, 2008), $[\text{TBA}]_3[\text{PtCl}_6]\text{Cl}$, (XIV), (Yousefi *et al.*, 2007b) and $[\text{2,4,6-dmpy.H}]_2[\text{PtCl}_6]$, (XV), (Kalateh *et al.*, 2008) [where hpy is halo-pyridinium, BMIM^+ is 1-*n*-butyl-3-methylimidazolium, EMIM^+ is 1-ethyl-3-methylimidazolium, DABCO is 1,4-diazabicyclooctane, Im is imidazolium, het is 2-(α -hydroxyethyl) thiamine, 9-MeGuaH is 9-methylguaninium, 2,9-dmphen.H is 2,9-dimethyl-1,10-phenanthroline, $\text{H}_2\text{DA18C6}$ is 1,10-Diazonia-18-crown-6, 2,6-dmpy.H is 2,6-dimethylpyridinium, TBA is tribenzylammonium and 2,4,6-dmpy.H is 2,4,6-dimethylpyridinium] have been synthesized and characterized by single-crystal X-ray diffraction methods. We report herein the synthesis and crystal structure of the title compound, (I).

The asymmetric unit of the title compound (I), (Fig. 1) contains one independent protonated phenanthridinium cation and one half PtCl_6^{2-} anion, and one dimethyl sulfoxide solvate. The Pt ion has an octahedral coordination (Table 1). In cation, the bond lengths and angles are normal. In PtCl_6^{2-} anion, the Pt—Cl bond lengths and Cl—Pt—Cl bond angles are also within normal ranges, as in (III) to (XV).

The intramolecular N—H \cdots O and intermolecular C—H \cdots Cl hydrogen bonding interactions (Table 1) seem to be effective in the stabilization of the structure (Fig. 2).

Experimental

For the preparation of the title compound, (I), a solution of phenanthridine (0.27 g, 1.48 mmol) in ethanol (10 ml) was added to a solution of $\text{H}_2\text{PtCl}_6 \cdot 6\text{H}_2\text{O}$, (0.38 g, 0.74 mmol) in ethanol (10 ml) at room temperature. The suitable crystals for X-ray diffraction experiment were obtained by ethanol diffusion in a solution of orange precipitated in DMSO after one week [yield; 0.51 g, 74.7%, m.p. < 573 K].

Refinement

The C-bound H-atoms were placed in calculated positions with C—H = 0.93 Å and C—H 0.96 Å, and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ (ring C) and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}$ (methyl C). The

supplementary materials

N-bound H-atom was found from a difference Fourier map and refined freely. In the final Fourier map, the highest and deepest peaks were located 1.13 and 0.47 Å from atom S1, respectively.

Figures

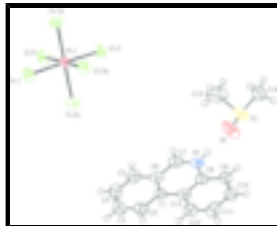


Fig. 1. ORTEP-3 view of the title molecule, with the atom-numbering scheme and 50% probability displacement ellipsoids

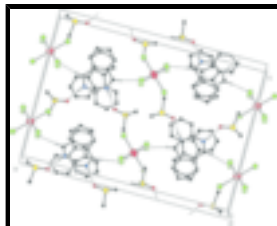


Fig. 2. View of the packing and hydrogen bonding interactions. For clarity, H atoms not involved in hydrogen bonds have been omitted.

Bis(phenanthridinium) hexachloridoplatinate(IV) dimethyl sulfoxide disolvate

Crystal data

(C₁₃H₁₀N)₂[PtCl₆]·2C₂H₆OS

M_r = 924.50

Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

a = 24.3695 (11) Å

b = 7.9061 (3) Å

c = 17.4322 (6) Å

V = 3358.6 (2) Å³

Z = 4

*F*₀₀₀ = 1816

D_x = 1.828 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 46774 reflections

θ = 1.4–27.3°

μ = 4.81 mm⁻¹

T = 295 (2) K

Prism, yellow

0.80 × 0.35 × 0.09 mm

Data collection

Stoe IPDS-2
diffractometer

Monochromator: plane graphite

Detector resolution: 6.67 pixels mm⁻¹

T = 295(3) K

ω scans

Absorption correction: integration
(X-RED32; Stoe & Cie, 2002)

*T*_{min} = 0.114, *T*_{max} = 0.671

33029 measured reflections

3533 independent reflections

2992 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.106

θ_{max} = 26.8°

θ_{min} = 1.7°

h = -30→30

k = -9→10

l = -22→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.096$	$w = 1/[\sigma^2(F_o^2) + (0.0192P)^2 + 15.6678P]$
$S = 1.12$	where $P = (F_o^2 + 2F_c^2)/3$
3533 reflections	$(\Delta/\sigma)_{\max} = 0.001$
199 parameters	$\Delta\rho_{\max} = 2.20 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -1.01 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.3026 (2)	0.7872 (7)	0.9147 (3)	0.0450 (17)
C1	0.2284 (2)	0.9236 (7)	0.8111 (3)	0.0380 (17)
C2	0.1935 (3)	0.9962 (8)	0.7558 (4)	0.051 (2)
C3	0.2148 (3)	1.0700 (9)	0.6916 (4)	0.057 (3)
C4	0.2715 (3)	1.0779 (9)	0.6797 (4)	0.059 (3)
C5	0.3067 (3)	1.0107 (9)	0.7327 (4)	0.052 (2)
C6	0.2855 (2)	0.9333 (8)	0.7987 (3)	0.0417 (17)
C7	0.3209 (3)	0.8621 (8)	0.8539 (4)	0.048 (2)
C8	0.2463 (3)	0.7702 (8)	0.9301 (3)	0.0403 (17)
C9	0.2309 (3)	0.6859 (9)	0.9972 (4)	0.049 (2)
C10	0.1764 (3)	0.6683 (9)	1.0126 (4)	0.056 (2)
C11	0.1378 (3)	0.7337 (9)	0.9637 (5)	0.060 (3)
C12	0.1527 (3)	0.8186 (8)	0.8981 (4)	0.051 (2)
C13	0.2085 (2)	0.8394 (7)	0.8797 (3)	0.0383 (17)
S1	0.42059 (10)	0.6422 (3)	1.04509 (15)	0.0776 (8)
O1	0.3643 (2)	0.7031 (10)	1.0318 (4)	0.099 (3)
C14	0.4292 (4)	0.6686 (12)	1.1452 (5)	0.080 (3)

supplementary materials

C15	0.4641 (5)	0.7984 (15)	1.0151 (6)	0.111 (5)
Pt1	1.00000	0.67772 (4)	0.25000	0.0358 (1)
C11	0.95124 (7)	0.8825 (2)	0.18305 (10)	0.0533 (5)
C12	1.04739 (6)	0.4687 (2)	0.31590 (9)	0.0509 (5)
C13	1.06735 (7)	0.6805 (2)	0.15568 (9)	0.0525 (5)
HN1	0.325 (4)	0.753 (11)	0.948 (5)	0.09 (3)*
H2	0.15570	0.99380	0.76300	0.0610*
H3	0.19120	1.11580	0.65520	0.0690*
H4	0.28520	1.12890	0.63560	0.0710*
H5	0.34440	1.01640	0.72490	0.0620*
H7	0.35860	0.86920	0.84640	0.0580*
H9	0.25720	0.64290	1.03050	0.0590*
H10	0.16530	0.61150	1.05660	0.0670*
H11	0.10070	0.72030	0.97510	0.0710*
H12	0.12590	0.86250	0.86580	0.0610*
H14A	0.40670	0.58810	1.17200	0.1200*
H14B	0.41840	0.78110	1.15950	0.1200*
H14C	0.46700	0.65100	1.15850	0.1200*
H15A	0.46470	0.80150	0.96010	0.1660*
H15B	0.50040	0.77600	1.03400	0.1660*
H15C	0.45170	0.90540	1.03450	0.1660*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.030 (3)	0.053 (3)	0.052 (3)	-0.001 (2)	-0.008 (2)	-0.008 (3)
C1	0.036 (3)	0.037 (3)	0.041 (3)	0.002 (2)	-0.004 (2)	-0.009 (2)
C2	0.043 (3)	0.056 (4)	0.054 (4)	0.007 (3)	-0.005 (3)	-0.007 (3)
C3	0.062 (5)	0.059 (4)	0.051 (4)	0.011 (4)	-0.007 (4)	-0.001 (3)
C4	0.074 (5)	0.057 (4)	0.046 (4)	0.004 (4)	0.013 (4)	0.000 (3)
C5	0.051 (4)	0.061 (4)	0.044 (4)	-0.005 (3)	0.008 (3)	-0.009 (3)
C6	0.034 (3)	0.047 (3)	0.044 (3)	0.005 (3)	0.001 (3)	-0.013 (3)
C7	0.026 (3)	0.057 (4)	0.061 (4)	0.002 (3)	-0.002 (3)	-0.012 (3)
C8	0.036 (3)	0.043 (3)	0.042 (3)	0.002 (3)	-0.001 (3)	-0.013 (3)
C9	0.053 (4)	0.053 (4)	0.042 (3)	-0.002 (3)	-0.006 (3)	-0.004 (3)
C10	0.059 (4)	0.055 (4)	0.053 (4)	-0.005 (4)	0.006 (4)	0.000 (3)
C11	0.040 (4)	0.061 (4)	0.078 (5)	0.000 (3)	0.018 (4)	0.003 (4)
C12	0.035 (3)	0.054 (4)	0.064 (4)	0.005 (3)	0.002 (3)	0.000 (3)
C13	0.032 (3)	0.041 (3)	0.042 (3)	0.004 (2)	-0.001 (2)	-0.013 (3)
S1	0.0602 (13)	0.0891 (16)	0.0836 (15)	-0.0018 (11)	-0.0189 (11)	-0.0056 (12)
O1	0.049 (3)	0.170 (7)	0.077 (4)	0.013 (4)	-0.021 (3)	0.027 (4)
C14	0.072 (6)	0.106 (7)	0.062 (5)	-0.016 (5)	-0.017 (4)	0.030 (5)
C15	0.095 (8)	0.166 (11)	0.071 (6)	-0.051 (8)	0.009 (6)	-0.023 (7)
Pt1	0.0247 (2)	0.0484 (2)	0.0342 (2)	0.0000	0.0005 (1)	0.0000
C11	0.0434 (9)	0.0616 (9)	0.0548 (9)	0.0150 (8)	-0.0025 (7)	0.0076 (8)
C12	0.0390 (8)	0.0611 (9)	0.0527 (9)	0.0007 (7)	-0.0073 (7)	0.0160 (8)
C13	0.0396 (8)	0.0715 (10)	0.0463 (8)	0.0082 (8)	0.0145 (7)	0.0067 (8)

Geometric parameters (Å, °)

Pt1—C11 ⁱ	2.3228 (17)	C8—C13	1.386 (8)
Pt1—C12 ⁱ	2.3204 (16)	C9—C10	1.362 (10)
Pt1—C13 ⁱ	2.3233 (16)	C10—C11	1.371 (11)
Pt1—C13	2.3233 (16)	C11—C12	1.375 (11)
Pt1—C11	2.3228 (17)	C12—C13	1.407 (9)
Pt1—C12	2.3204 (16)	C2—H2	0.9300
S1—C14	1.770 (9)	C3—H3	0.9300
S1—C15	1.710 (12)	C4—H4	0.9300
S1—O1	1.472 (6)	C5—H5	0.9300
N1—C7	1.293 (9)	C7—H7	0.9300
N1—C8	1.405 (9)	C9—H9	0.9300
N1—HN1	0.84 (9)	C10—H10	0.9300
C1—C6	1.410 (7)	C11—H11	0.9300
C1—C2	1.408 (9)	C12—H12	0.9300
C1—C13	1.452 (7)	C14—H14B	0.9600
C2—C3	1.365 (10)	C14—H14A	0.9600
C3—C4	1.399 (10)	C14—H14C	0.9600
C4—C5	1.368 (10)	C15—H15C	0.9600
C5—C6	1.402 (9)	C15—H15A	0.9600
C6—C7	1.410 (9)	C15—H15B	0.9600
C8—C9	1.398 (9)		
C11...C11 ⁱ	3.331 (2)	C8...O1	3.420 (9)
C11...C12 ⁱ	3.272 (2)	C8...C6 ^{ix}	3.598 (8)
C11...C13 ⁱ	3.265 (2)	C8...C9 ^{viii}	3.533 (9)
C11...C13	3.284 (2)	C8...C1 ^{ix}	3.492 (8)
C12...C11 ⁱ	3.272 (2)	C9...O1	3.309 (9)
C12...C13 ⁱ	3.297 (2)	C9...C8 ^{ix}	3.533 (9)
C12...C13	3.293 (2)	C10...C13 ^{xi}	3.646 (7)
C12...C7 ⁱⁱ	3.540 (7)	C13...C6 ^{ix}	3.511 (8)
C12...C12 ⁱ	3.258 (2)	C2...H12	2.7400
C13...C12	3.293 (2)	C2...H14A ^{xii}	2.9200
C13...C11	3.284 (2)	C4...H10 ^{xii}	3.0400
C13...C11 ⁱ	3.265 (2)	C10...H3 ^{xiii}	3.0400
C13...C10 ⁱⁱⁱ	3.646 (7)	C12...H2	2.7300
C13...C12 ⁱ	3.297 (2)	HN1...H9	2.3600
C11...H15A ^{iv}	2.9100	HN1...S1	3.01 (9)
C11...H14C ^v	2.9400	HN1...O1	1.79 (9)
C11...H2 ^{vi}	2.9400	H2...H12	2.1900
C11...H7 ^{iv}	3.0500	H2...H14A ^{xii}	2.2900
C11...H12 ^{vi}	2.8900	H2...C12	2.7300
C12...H7 ⁱⁱ	2.6800	H2...C11 ^{vi}	2.9400

supplementary materials

C12...H15A ⁱⁱ	3.1200	H3...C10 ^{xiv}	3.0400
C12...H5 ⁱⁱ	3.0800	H5...H7	2.4400
C13...H15C ^{vii}	3.0700	H5...C12 ^x	3.0800
C13...H10 ⁱⁱⁱ	3.0000	H5...C13 ^x	2.9200
C13...H5 ⁱⁱ	2.9200	H7...C11 ^{xv}	3.0500
S1...HN1	3.01 (9)	H7...H5	2.4400
O1...N1	2.621 (8)	H7...C12 ^x	2.6800
O1...C9	3.309 (9)	H9...O1	2.6500
O1...C8	3.420 (9)	H9...HN1	2.3600
O1...HN1	1.79 (9)	H10...C4 ^{xvi}	3.0400
O1...H9	2.6500	H10...C13 ^{xi}	3.0000
N1...O1	2.621 (8)	H11...H15B ^{xvii}	2.4500
C1...C8 ^{viii}	3.492 (8)	H12...C2	2.7400
C1...C4 ^{ix}	3.566 (9)	H12...H2	2.1900
C2...C7 ^{viii}	3.379 (9)	H12...C11 ^{vi}	2.8900
C2...C6 ^{viii}	3.573 (9)	H14A...C2 ^{xvi}	2.9200
C3...C6 ^{viii}	3.426 (9)	H14A...H2 ^{xvi}	2.2900
C3...C5 ^{viii}	3.596 (10)	H14B...H15C	2.5200
C4...C1 ^{viii}	3.566 (9)	H14C...H15B	2.5200
C5...C3 ^{ix}	3.596 (10)	H14C...C11 ^{xviii}	2.9400
C6...C3 ^{ix}	3.426 (9)	H15A...C12 ^x	3.1200
C6...C13 ^{viii}	3.511 (8)	H15A...C11 ^{xv}	2.9100
C6...C2 ^{ix}	3.573 (9)	H15B...H14C	2.5200
C6...C8 ^{viii}	3.598 (8)	H15B...H11 ^{xix}	2.4500
C7...C2 ^{ix}	3.379 (9)	H15C...H14B	2.5200
C7...C12 ^x	3.540 (7)	H15C...C13 ^{xx}	3.0700
C11 ⁱ —Pt1—C12	89.60 (6)	C9—C10—C11	120.5 (7)
C12—Pt1—C12 ⁱ	89.18 (6)	C10—C11—C12	121.4 (7)
C12—Pt1—C13 ⁱ	90.46 (5)	C11—C12—C13	120.1 (6)
C11 ⁱ —Pt1—C13	89.29 (6)	C1—C13—C8	118.8 (5)
C12 ⁱ —Pt1—C13	90.46 (5)	C1—C13—C12	124.4 (5)
C13—Pt1—C13 ⁱ	178.92 (6)	C8—C13—C12	116.9 (5)
C11 ⁱ —Pt1—C12 ⁱ	178.75 (6)	C1—C2—H2	120.00
C11 ⁱ —Pt1—C13 ⁱ	89.96 (6)	C3—C2—H2	120.00
C12 ⁱ —Pt1—C13 ⁱ	90.32 (5)	C2—C3—H3	119.00
C12—Pt1—C13	90.32 (5)	C4—C3—H3	120.00
C11—Pt1—C11 ⁱ	91.62 (6)	C3—C4—H4	120.00
C11—Pt1—C12	178.75 (6)	C5—C4—H4	120.00
C11—Pt1—C13	89.96 (6)	C6—C5—H5	120.00
C11—Pt1—C12 ⁱ	89.60 (6)	C4—C5—H5	120.00
C11—Pt1—C13 ⁱ	89.29 (6)	N1—C7—H7	119.00
O1—S1—C14	103.1 (4)	C6—C7—H7	119.00

O1—S1—C15	107.1 (5)	C8—C9—H9	121.00
C14—S1—C15	98.2 (5)	C10—C9—H9	121.00
C7—N1—C8	122.5 (5)	C11—C10—H10	120.00
C8—N1—HN1	118 (6)	C9—C10—H10	120.00
C7—N1—HN1	119 (6)	C12—C11—H11	119.00
C2—C1—C13	123.3 (5)	C10—C11—H11	119.00
C2—C1—C6	118.0 (5)	C13—C12—H12	120.00
C6—C1—C13	118.7 (5)	C11—C12—H12	120.00
C1—C2—C3	120.4 (6)	S1—C14—H14A	109.00
C2—C3—C4	121.1 (7)	S1—C14—H14B	109.00
C3—C4—C5	120.1 (7)	S1—C14—H14C	110.00
C4—C5—C6	119.5 (6)	H14A—C14—H14B	109.00
C1—C6—C5	120.9 (5)	H14A—C14—H14C	110.00
C5—C6—C7	120.6 (5)	H14B—C14—H14C	110.00
C1—C6—C7	118.5 (5)	S1—C15—H15A	109.00
N1—C7—C6	122.1 (6)	S1—C15—H15B	109.00
C9—C8—C13	122.7 (6)	S1—C15—H15C	109.00
N1—C8—C9	117.9 (6)	H15A—C15—H15B	109.00
N1—C8—C13	119.4 (5)	H15A—C15—H15C	110.00
C8—C9—C10	118.4 (7)	H15B—C15—H15C	109.00
C7—N1—C8—C9	179.5 (6)	C4—C5—C6—C1	0.1 (10)
C7—N1—C8—C13	-1.7 (9)	C4—C5—C6—C7	179.6 (6)
C8—N1—C7—C6	0.4 (10)	C1—C6—C7—N1	0.7 (9)
C6—C1—C2—C3	1.4 (9)	C5—C6—C7—N1	-178.8 (6)
C13—C1—C2—C3	-178.4 (6)	N1—C8—C9—C10	-179.8 (6)
C13—C1—C6—C7	-0.6 (8)	C13—C8—C9—C10	1.4 (10)
C2—C1—C13—C8	179.2 (6)	N1—C8—C13—C1	1.7 (8)
C2—C1—C13—C12	1.0 (9)	N1—C8—C13—C12	-179.9 (5)
C6—C1—C13—C8	-0.6 (8)	C9—C8—C13—C1	-179.5 (6)
C6—C1—C13—C12	-178.8 (6)	C9—C8—C13—C12	-1.2 (9)
C2—C1—C6—C5	-0.9 (9)	C8—C9—C10—C11	-0.8 (11)
C2—C1—C6—C7	179.6 (6)	C9—C10—C11—C12	-0.1 (11)
C13—C1—C6—C5	178.9 (6)	C10—C11—C12—C13	0.3 (11)
C1—C2—C3—C4	-1.1 (10)	C11—C12—C13—C1	178.6 (6)
C2—C3—C4—C5	0.2 (11)	C11—C12—C13—C8	0.4 (9)
C3—C4—C5—C6	0.3 (10)		

Symmetry codes: (i) $-x+2, y, -z+1/2$; (ii) $-x+3/2, -y+3/2, z-1/2$; (iii) $x+1, y, z-1$; (iv) $x+1/2, -y+3/2, -z+1$; (v) $-x+3/2, y+1/2, z-1$; (vi) $-x+1, -y+2, -z+1$; (vii) $-x+3/2, y-1/2, z-1$; (viii) $-x+1/2, y+1/2, z$; (ix) $-x+1/2, y-1/2, z$; (x) $-x+3/2, -y+3/2, z+1/2$; (xi) $x-1, y, z+1$; (xii) $-x+1/2, -y+3/2, z-1/2$; (xiii) $x, -y+2, z+1/2$; (xiv) $x, -y+2, z-1/2$; (xv) $x-1/2, -y+3/2, -z+1$; (xvi) $-x+1/2, -y+3/2, z+1/2$; (xvii) $x-1/2, -y+3/2, -z+2$; (xviii) $-x+3/2, y-1/2, z+1$; (xix) $x+1/2, -y+3/2, -z+2$; (xx) $-x+3/2, y+1/2, z+1$.

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>
N1—HN1...O1	0.84 (9)	1.79 (9)	2.621 (8)	169 (8)
C7—H7...Cl2 ^x	0.93	2.68	3.540 (7)	154

Symmetry codes: (x) $-x+3/2, -y+3/2, z+1/2$.

Fig. 1

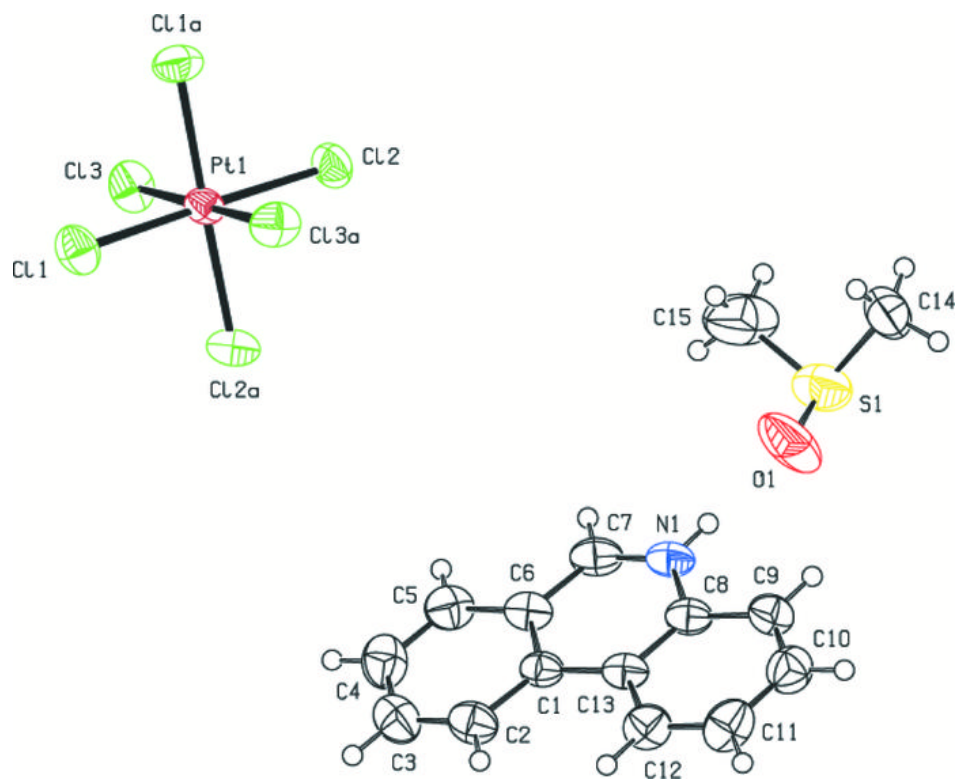


Fig. 2

