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from iucrdata.iucr.org

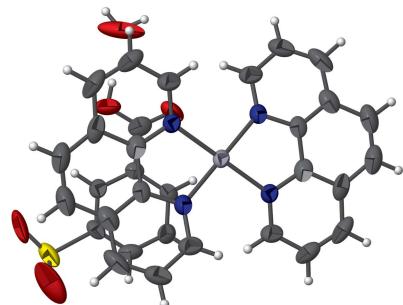
# Bis(1,10-phenanthroline- $\kappa^2 N,N'$ )platinum(II) bis(3-carboxybenzenesulfonate) dihydrate

Jing Liu and Long-Guan Zhu\*

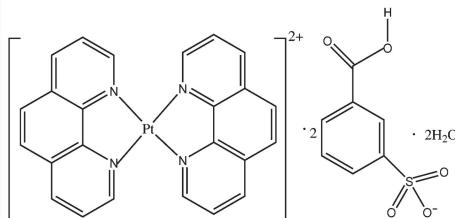
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The title complex,  $[\text{Pt}(\text{C}_{12}\text{H}_8\text{N}_2)_2](\text{C}_7\text{H}_5\text{O}_5\text{S})_2 \cdot 2\text{H}_2\text{O}$ , consists of a complex cation  $[\text{Pt}(1,10\text{-phen})_2]^{2+}$  ( $1,10\text{-phen}$  = 1,10-phenanthroline), two 3-sulfobenzoate anions and two lattice water molecules. In the crystal, anions and water molecules form hydrogen-bonded centrosymmetric dimers. In addition,  $\pi-\pi$  interactions are observed between 1,10-phenanthroline ligands and 3-sulfobenzoate anions.

## 3D view



## Chemical scheme



## Structure description

Metal complexes with sulfobenzoate ligands or anions have attracted much attention and are very interesting in material science, as they may have potential applications in fluorescence, as electric conductors or may be used as catalysts (Ma & Zhu, 2014; Zheng & Zhu, 2014). Sulfobenzoate ligands have two functional groups, sulfonate and carboxylate, and may therefore either coordinate to metal ions or form abundant hydrogen bonds. Platinum complexes are important in bio- and catalytical chemistry (Li *et al.*, 2011; Palocsay & Rund, 1969). General background to bis(1,10-phenanthroline)platinum and sulfobenzoate complexes and their applications is given by Wernberg & Hazell (1980) and Hazell *et al.* (1986).

Up to now, more than 100 platinum 1,10-phenanthroline complexes have been structurally characterized (CSD Version 5.36, 2015; Groom & Allen, 2015), but no structure analysis of a platinum complex with sulfobenzoate moieties has been reported so far. The title complex is therefore the first 3-sulfobenzoate platinum complex and consists of one centrosymmetric cation and two anions as well as two additional lattice water molecules (Fig. 1). In the cation, the platinum ion is coordinated by four nitrogen donor atoms from two 1,10-phenanthroline ligands in a square-planar geometry (Table 1). The anion is deprotonated at the sulfonate substituent. Two anions and water molecules form hydrogen-bonded centrosymmetric dimers (Table 2 and Fig. 2). There are additional

# data reports

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Pt1—N1	2.022 (7)	S1—O5	1.418 (7)
Pt1—N1 <sup>i</sup>	2.022 (7)	S1—O4	1.479 (10)
Pt1—N2 <sup>j</sup>	2.034 (6)	O2—C13	1.289 (11)
Pt1—N2	2.034 (6)	O1—C13	1.231 (12)
S1—O3	1.357 (10)		
N1—Pt1—N1 <sup>i</sup>	180.0 (4)	N2 <sup>j</sup> —Pt1—N2	180.0 (5)
N1—Pt1—N2 <sup>i</sup>	99.9 (3)	O3—S1—O5	114.6 (7)
N1 <sup>i</sup> —Pt1—N2 <sup>i</sup>	80.1 (3)	O3—S1—O4	113.4 (8)
N1—Pt1—N2	80.1 (3)	O5—S1—O4	109.7 (6)
N1 <sup>i</sup> —Pt1—N2	99.9 (3)		

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

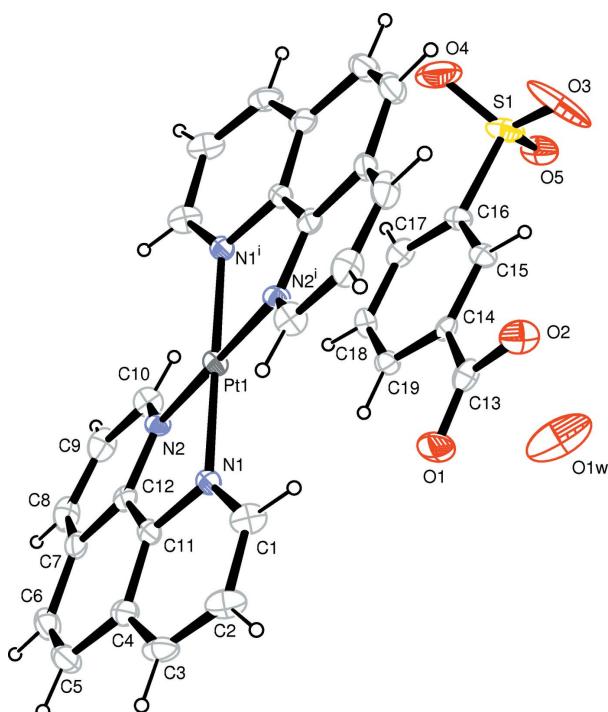
**Table 2**

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

$D\cdots H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O2—H2A $\cdots$ O1W	0.82	1.83	2.650 (10)	177
O1W—H1A $\cdots$ O3 <sup>ii</sup>	0.85 (2)	2.32 (14)	2.90 (2)	126 (14)
C6—H6 $\cdots$ O2 <sup>iii</sup>	0.93	2.57	3.468 (13)	161
C10—H1 $\cdots$ O5 <sup>iv</sup>	0.93	2.46	3.228 (12)	140

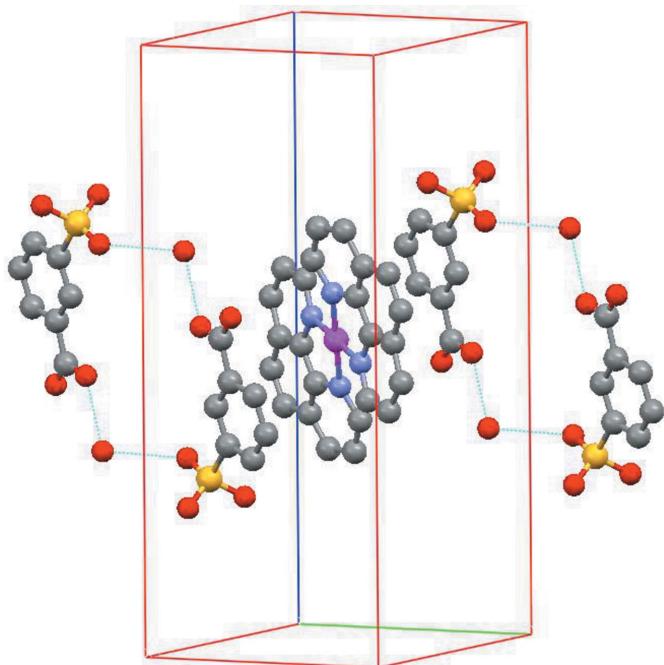
Symmetry codes: (ii)  $-x + 1, -y + 1, -z$ ; (iii)  $x, y - 1, z$ ; (iv)  $-x + \frac{1}{2}, y - \frac{1}{2}, -z - \frac{1}{2}$ .

weak C—H $\cdots$ O contacts linking the anions and cations. Furthermore,  $\pi$ — $\pi$  stacking interactions between 1,10-phenanthroline ligands and sulfobenzoate anions with centroid-to-centroid distances of 3.549 (5) and 3.733 (5)  $\text{\AA}$ , respectively, are observed.



**Figure 1**

View of the molecular structure of (I), showing displacement ellipsoids at the 30% probability level. [Symmetry code: (i)  $-x, -y, -z$ .]



**Figure 2**

Perspective view of the centrosymmetric hydrogen-bonded dimers consisting of anions and water molecules in (I).

**Table 3**

Experimental details.

Crystal data	[Pt(C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> ) <sub>2</sub> ](C <sub>7</sub> H <sub>5</sub> O <sub>5</sub> S) <sub>2</sub> ·2H <sub>2</sub> O
Chemical formula	993.87
$M_r$	Monoclinic, $P2_1/n$
Crystal system, space group	295
Temperature (K)	6.9957 (7), 12.0819 (10), 20.904 (2)
$a, b, c$ ( $\text{\AA}$ )	97.296 (10)
$\beta$ ( $^\circ$ )	1752.5 (3)
$V$ ( $\text{\AA}^3$ )	2
Z	Mo $K\alpha$
Radiation type	4.20
$\mu$ ( $\text{mm}^{-1}$ )	0.40 $\times$ 0.15 $\times$ 0.13
Crystal size (mm)	
Data collection	Oxford Diffraction Xcalibur Atlas
Diffractometer	Gemini ultra
Absorption correction	Multi-scan ( <i>CrysAlis PRO</i> ; Oxford Diffraction, 2009)
$T_{\min}, T_{\max}$	0.285, 0.611
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	7677, 3087, 2202
$R_{\text{int}}$	0.047
( $\sin \theta/\lambda$ ) <sub>max</sub> ( $\text{\AA}^{-1}$ )	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.050, 0.122, 1.16
No. of reflections	3087
No. of parameters	265
No. of restraints	5
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ( $e \text{\AA}^{-3}$ )	1.35, -0.76

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2009), *ORTEP-3 for Windows* (Farrugia, 2012), *WinGX* (Farrugia, 2012).

## Synthesis and crystallization

A mixture of  $\text{K}_2\text{PtCl}_4$  (52 mg, 0.125 mmol), 3-sulfobenzoic acid monosodium salt (48 mg, 0.25 mmol), and 1,10-phenanthroline (50 mg 0.25 mmol) was dissolved in  $\text{H}_2\text{O}$  (15 ml). The resulting mixture was sealed in a 30 ml Teflon-lined autoclave in a stainless-steel reactor and heated to 150°C for 24 h. The resulting clear solution was set aside for about two weeks at room temperature. Brownish needle-shaped crystals were obtained by filtration (Yield: 85 mg, 69%).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Although the sulfonate group seems to be disordered due to the elongated displacement parameters of oxygen atoms, disorder has not been resolved because the refinement then did not converge.

## Acknowledgements

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## References

- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.  
Groom, C. R. & Allen, F. H. (2014). *Angew. Chem. Int. Ed.* **53**, 662–671.  
Hazell, A., Simonsen, O. & Wernberg, O. (1986). *Acta Cryst. C* **42**, 1707–1711.  
Li, Q. P., Zhang, Q., Xian, P. & Song, Y. M. (2011). *Chemistry*, **74**, 164–169.  
Ma, A. Q. & Zhu, L. G. (2014). *RSC Adv.* **4**, 14691–14699.  
Oxford Diffraction (2009). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, UK.  
Palocsay, F. A. & Rund, J. V. (1969). *Inorg. Chem.* **8**, 524–528.  
Wernberg, O. & Hazell, A. (1980). *J. Chem. Soc. Dalton Trans.* pp. 973.  
Zheng, X. F. & Zhu, L. G. (2014). *J. Mol. Struct.* **1065**, 113–119.

# full crystallographic data

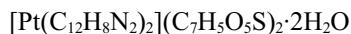
*IUCrData* (2016). **1**, x160211 [https://doi.org/10.1107/S241431461600211X]

## Bis(1,10-phenanthroline- $\kappa^2N,N'$ )platinum(II) bis(3-carboxybenzenesulfonate) dihydrate

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### Bis(1,10-phenanthroline- $\kappa^2N,N'$ )platinum(II) bis(3-carboxybenzenesulfonate) dihydrate

#### Crystal data



$M_r = 993.87$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 6.9957 (7)$  Å

$b = 12.0819 (10)$  Å

$c = 20.904 (2)$  Å

$\beta = 97.296 (10)^\circ$

$V = 1752.5 (3)$  Å<sup>3</sup>

$Z = 2$

$F(000) = 984$

$D_x = 1.883$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2156 reflections

$\theta = 2.9\text{--}29.2^\circ$

$\mu = 4.20$  mm<sup>-1</sup>

$T = 295$  K

Needle, brown

0.40 × 0.15 × 0.13 mm

#### Data collection

Oxford Diffraction Xcalibur Atlas Gemini ultra diffractometer

7677 measured reflections

Radiation source: fine-focus sealed tube

3087 independent reflections

Graphite monochromator

2202 reflections with  $I > 2\sigma(I)$

$\omega$  scans

$R_{\text{int}} = 0.047$

Absorption correction: multi-scan

$\theta_{\text{max}} = 25.1^\circ$ ,  $\theta_{\text{min}} = 3.4^\circ$

(CrysAlis PRO; Oxford Diffraction, 2009)

$h = -8 \rightarrow 7$

$T_{\text{min}} = 0.285$ ,  $T_{\text{max}} = 0.611$

$k = -14 \rightarrow 11$

$l = -24 \rightarrow 22$

#### Refinement

Refinement on  $F^2$

Secondary atom site location: difference Fourier map

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.050$

H atoms treated by a mixture of independent and constrained refinement

$wR(F^2) = 0.122$

$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 1.9422P]$   
where  $P = (F_o^2 + 2F_c^2)/3$

$S = 1.16$

$(\Delta/\sigma)_{\text{max}} < 0.001$

3087 reflections

$\Delta\rho_{\text{max}} = 1.35$  e Å<sup>-3</sup>

265 parameters

$\Delta\rho_{\text{min}} = -0.76$  e Å<sup>-3</sup>

5 restraints

Primary atom site location: structure-invariant direct methods

*Special details*

**Experimental.** Absorption correction: CrysAlisPro, Oxford Diffraction Ltd., Version 1.171.33.53 (release 17-11-2009 CrysAlis171 .NET) (compiled Nov 17 2009, 16:58:22) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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  $F^2 > 2\text{sigma}(F^2)$  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	$U_{\text{iso}}^*/U_{\text{eq}}$
O1W	0.4465 (17)	0.3570 (11)	0.1629 (4)	0.135 (5)
H1A	0.48 (3)	0.413 (4)	0.186 (3)	0.160*
H1B	0.44 (3)	0.302 (5)	0.189 (2)	0.160*
Pt1	0.0000	0.0000	0.0000	0.03467 (18)
S1	0.2546 (4)	0.3824 (3)	-0.22026 (14)	0.0649 (8)
N1	0.1230 (9)	-0.0662 (5)	0.0841 (3)	0.0354 (16)
C12	0.1129 (11)	-0.2246 (7)	0.0181 (5)	0.040 (2)
C11	0.1365 (11)	-0.1803 (7)	0.0815 (4)	0.037 (2)
C14	0.3660 (11)	0.2165 (7)	-0.0524 (4)	0.0346 (19)
C19	0.3717 (12)	0.1080 (7)	-0.0727 (4)	0.042 (2)
H19	0.4000	0.0515	-0.0427	0.050*
N2	0.0730 (9)	-0.1517 (5)	-0.0315 (3)	0.0356 (16)
C15	0.3292 (11)	0.3015 (7)	-0.0961 (4)	0.040 (2)
H15	0.3283	0.3746	-0.0822	0.047*
C16	0.2934 (12)	0.2762 (8)	-0.1612 (4)	0.042 (2)
C8	0.1435 (14)	-0.3731 (8)	-0.0563 (6)	0.062 (3)
H8	0.1646	-0.4472	-0.0652	0.074*
O2	0.3736 (11)	0.3364 (6)	0.0359 (3)	0.070 (2)
H2A	0.3916	0.3416	0.0753	0.106*
C18	0.3351 (13)	0.0836 (8)	-0.1375 (5)	0.047 (2)
H18	0.3365	0.0106	-0.1515	0.057*
C4	0.1922 (12)	-0.2446 (8)	0.1343 (5)	0.048 (2)
O1	0.4453 (11)	0.1592 (6)	0.0573 (3)	0.072 (2)
O5	0.4059 (10)	0.3743 (6)	-0.2592 (3)	0.071 (2)
C7	0.1426 (12)	-0.3370 (7)	0.0087 (5)	0.051 (3)
C5	0.2090 (15)	-0.3632 (9)	0.1251 (6)	0.065 (3)
H5	0.2319	-0.4104	0.1604	0.078*
C17	0.2968 (13)	0.1676 (9)	-0.1812 (5)	0.051 (2)
H17	0.2728	0.1512	-0.2250	0.061*
C6	0.1908 (14)	-0.4040 (9)	0.0645 (6)	0.063 (3)
H6	0.2107	-0.4793	0.0589	0.075*
C2	0.2373 (14)	-0.0813 (10)	0.1967 (5)	0.060 (3)
H2	0.2756	-0.0454	0.2356	0.071*

C13	0.3961 (13)	0.2350 (9)	0.0194 (5)	0.051 (2)
C9	0.1130 (14)	-0.2979 (9)	-0.1053 (5)	0.058 (3)
H9	0.1125	-0.3205	-0.1479	0.070*
C10	0.0829 (13)	-0.1876 (8)	-0.0911 (5)	0.050 (2)
H10	0.0690	-0.1366	-0.1247	0.060*
C1	0.1804 (14)	-0.0196 (8)	0.1412 (5)	0.052 (3)
H1	0.1826	0.0572	0.1440	0.062*
C3	0.2370 (13)	-0.1932 (10)	0.1941 (5)	0.060 (3)
H3	0.2659	-0.2350	0.2314	0.071*
O3	0.249 (2)	0.4796 (7)	-0.1881 (5)	0.158 (6)
O4	0.0693 (13)	0.3532 (9)	-0.2588 (5)	0.132 (4)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1W	0.098 (7)	0.268 (15)	0.039 (5)	0.036 (10)	0.005 (5)	-0.033 (6)
Pt1	0.0381 (3)	0.0305 (3)	0.0373 (3)	0.0038 (3)	0.01218 (19)	0.0002 (2)
S1	0.0707 (18)	0.0720 (19)	0.0559 (17)	0.0306 (16)	0.0230 (14)	0.0305 (15)
N1	0.031 (4)	0.035 (4)	0.043 (4)	0.004 (3)	0.013 (3)	0.003 (3)
C12	0.021 (4)	0.040 (5)	0.063 (6)	0.006 (4)	0.014 (4)	0.001 (4)
C11	0.025 (4)	0.038 (5)	0.051 (6)	0.004 (4)	0.017 (4)	0.008 (4)
C14	0.023 (4)	0.045 (5)	0.036 (5)	-0.004 (4)	0.005 (4)	-0.001 (4)
C19	0.040 (5)	0.046 (5)	0.040 (5)	0.000 (4)	0.006 (4)	0.008 (4)
N2	0.033 (4)	0.034 (4)	0.041 (4)	0.008 (3)	0.007 (3)	0.000 (3)
C15	0.038 (5)	0.037 (5)	0.046 (6)	0.011 (4)	0.014 (4)	0.000 (4)
C16	0.041 (5)	0.051 (6)	0.038 (5)	0.006 (4)	0.014 (4)	0.013 (4)
C8	0.047 (6)	0.037 (6)	0.105 (10)	0.001 (5)	0.020 (6)	-0.027 (6)
O2	0.089 (5)	0.082 (6)	0.037 (4)	0.015 (5)	0.001 (4)	-0.015 (4)
C18	0.052 (6)	0.040 (5)	0.051 (6)	-0.012 (5)	0.013 (5)	-0.001 (4)
C4	0.029 (5)	0.062 (6)	0.057 (7)	0.004 (5)	0.013 (4)	0.019 (5)
O1	0.094 (6)	0.078 (5)	0.042 (4)	0.001 (5)	-0.006 (4)	0.020 (4)
O5	0.071 (5)	0.090 (5)	0.057 (5)	0.016 (4)	0.029 (4)	0.028 (4)
C7	0.033 (5)	0.031 (5)	0.089 (8)	-0.002 (4)	0.004 (5)	0.001 (5)
C5	0.059 (7)	0.053 (7)	0.084 (9)	0.007 (6)	0.016 (6)	0.029 (6)
C17	0.046 (5)	0.070 (7)	0.035 (5)	-0.002 (5)	0.004 (4)	-0.014 (5)
C6	0.052 (6)	0.037 (6)	0.102 (10)	0.003 (5)	0.020 (6)	0.009 (6)
C2	0.058 (6)	0.085 (8)	0.036 (6)	0.021 (6)	0.008 (5)	0.001 (5)
C13	0.034 (5)	0.063 (7)	0.056 (7)	-0.009 (5)	0.011 (5)	-0.014 (6)
C9	0.052 (6)	0.054 (7)	0.071 (8)	0.000 (5)	0.014 (5)	-0.029 (6)
C10	0.056 (6)	0.056 (6)	0.041 (6)	0.003 (5)	0.018 (5)	-0.007 (5)
C1	0.054 (6)	0.061 (7)	0.041 (6)	0.014 (5)	0.011 (5)	-0.010 (5)
C3	0.043 (5)	0.091 (9)	0.046 (7)	0.011 (6)	0.008 (5)	0.031 (6)
O3	0.328 (19)	0.060 (6)	0.110 (8)	0.082 (8)	0.120 (10)	0.058 (6)
O4	0.078 (6)	0.169 (11)	0.142 (9)	0.017 (7)	-0.013 (6)	0.098 (8)

Geometric parameters ( $\text{\AA}$ ,  $\text{^{\circ}}$ )

O1W—H1A	0.845 (19)	C16—C17	1.378 (13)
O1W—H1B	0.87 (2)	C8—C9	1.365 (15)
Pt1—N1	2.022 (7)	C8—C7	1.428 (14)
Pt1—N1 <sup>i</sup>	2.022 (7)	C8—H8	0.9300
Pt1—N2 <sup>i</sup>	2.034 (6)	O2—C13	1.289 (11)
Pt1—N2	2.034 (6)	O2—H2A	0.8200
S1—O3	1.357 (10)	C18—C17	1.368 (13)
S1—O5	1.418 (7)	C18—H18	0.9300
S1—O4	1.479 (10)	C4—C3	1.396 (14)
S1—C16	1.777 (9)	C4—C5	1.452 (14)
N1—C1	1.333 (11)	O1—C13	1.231 (12)
N1—C11	1.384 (10)	C7—C6	1.424 (14)
C12—N2	1.362 (11)	C5—C6	1.349 (15)
C12—C7	1.392 (12)	C5—H5	0.9300
C12—C11	1.419 (12)	C17—H17	0.9300
C11—C4	1.365 (12)	C6—H6	0.9300
C14—C15	1.377 (11)	C2—C3	1.353 (15)
C14—C19	1.381 (12)	C2—C1	1.394 (13)
C14—C13	1.505 (12)	C2—H2	0.9300
C19—C18	1.380 (12)	C9—C10	1.388 (13)
C19—H19	0.9300	C9—H9	0.9300
N2—C10	1.331 (11)	C10—H10	0.9300
C15—C16	1.386 (12)	C1—H1	0.9300
C15—H15	0.9300	C3—H3	0.9300
H1A—O1W—H1B	107 (3)	C7—C8—H8	120.2
N1—Pt1—N1 <sup>i</sup>	180.0 (4)	C13—O2—H2A	109.5
N1—Pt1—N2 <sup>i</sup>	99.9 (3)	C17—C18—C19	119.6 (9)
N1 <sup>i</sup> —Pt1—N2 <sup>i</sup>	80.1 (3)	C17—C18—H18	120.2
N1—Pt1—N2	80.1 (3)	C19—C18—H18	120.2
N1 <sup>i</sup> —Pt1—N2	99.9 (3)	C11—C4—C3	118.6 (10)
N2 <sup>i</sup> —Pt1—N2	180.0 (5)	C11—C4—C5	118.3 (10)
O3—S1—O5	114.6 (7)	C3—C4—C5	123.1 (9)
O3—S1—O4	113.4 (8)	C12—C7—C6	117.6 (10)
O5—S1—O4	109.7 (6)	C12—C7—C8	116.7 (9)
O3—S1—C16	107.0 (5)	C6—C7—C8	125.2 (10)
O5—S1—C16	106.8 (4)	C6—C5—C4	119.0 (10)
O4—S1—C16	104.6 (5)	C6—C5—H5	120.5
C1—N1—C11	116.2 (8)	C4—C5—H5	120.5
C1—N1—Pt1	131.1 (6)	C18—C17—C16	120.8 (9)
C11—N1—Pt1	112.5 (6)	C18—C17—H17	119.6
N2—C12—C7	123.0 (9)	C16—C17—H17	119.6
N2—C12—C11	117.1 (8)	C5—C6—C7	123.0 (10)
C7—C12—C11	119.8 (9)	C5—C6—H6	118.5
C4—C11—N1	123.3 (9)	C7—C6—H6	118.5
C4—C11—C12	121.8 (9)	C3—C2—C1	120.1 (10)

N1—C11—C12	114.3 (8)	C3—C2—H2	119.9
C15—C14—C19	121.0 (8)	C1—C2—H2	119.9
C15—C14—C13	122.8 (8)	O1—C13—O2	124.7 (10)
C19—C14—C13	116.2 (8)	O1—C13—C14	121.6 (9)
C18—C19—C14	119.7 (8)	O2—C13—C14	113.7 (9)
C18—C19—H19	120.2	C8—C9—C10	119.5 (10)
C14—C19—H19	120.2	C8—C9—H9	120.3
C10—N2—C12	118.2 (8)	C10—C9—H9	120.3
C10—N2—Pt1	129.9 (6)	N2—C10—C9	122.7 (9)
C12—N2—Pt1	111.9 (6)	N2—C10—H10	118.6
C14—C15—C16	118.8 (8)	C9—C10—H10	118.6
C14—C15—H15	120.6	N1—C1—C2	122.7 (10)
C16—C15—H15	120.6	N1—C1—H1	118.6
C17—C16—C15	120.0 (8)	C2—C1—H1	118.6
C17—C16—S1	118.9 (7)	C2—C3—C4	118.7 (9)
C15—C16—S1	121.0 (7)	C2—C3—H3	120.6
C9—C8—C7	119.5 (9)	C4—C3—H3	120.6
C9—C8—H8	120.2		
N2 <sup>i</sup> —Pt1—N1—C1	-13.2 (8)	N1—C11—C4—C3	0.4 (13)
N2—Pt1—N1—C1	166.8 (8)	C12—C11—C4—C3	171.7 (8)
N2 <sup>i</sup> —Pt1—N1—C11	162.1 (5)	N1—C11—C4—C5	-177.4 (8)
N2—Pt1—N1—C11	-17.9 (5)	C12—C11—C4—C5	-6.1 (13)
C1—N1—C11—C4	4.4 (12)	N2—C12—C7—C6	177.6 (8)
Pt1—N1—C11—C4	-171.7 (6)	C11—C12—C7—C6	1.8 (12)
C1—N1—C11—C12	-167.5 (7)	N2—C12—C7—C8	4.4 (13)
Pt1—N1—C11—C12	16.4 (8)	C11—C12—C7—C8	-171.3 (8)
N2—C12—C11—C4	-174.5 (7)	C9—C8—C7—C12	-0.9 (14)
C7—C12—C11—C4	1.5 (12)	C9—C8—C7—C6	-173.5 (9)
N2—C12—C11—N1	-2.5 (11)	C11—C4—C5—C6	7.5 (14)
C7—C12—C11—N1	173.5 (7)	C3—C4—C5—C6	-170.2 (9)
C15—C14—C19—C18	-1.7 (12)	C19—C18—C17—C16	-0.3 (14)
C13—C14—C19—C18	176.6 (8)	C15—C16—C17—C18	0.1 (14)
C7—C12—N2—C10	-7.2 (12)	S1—C16—C17—C18	176.9 (7)
C11—C12—N2—C10	168.7 (7)	C4—C5—C6—C7	-4.4 (16)
C7—C12—N2—Pt1	171.6 (6)	C12—C7—C6—C5	-0.2 (15)
C11—C12—N2—Pt1	-12.5 (9)	C8—C7—C6—C5	172.3 (10)
N1—Pt1—N2—C10	-165.0 (8)	C15—C14—C13—O1	-173.6 (9)
N1 <sup>i</sup> —Pt1—N2—C10	15.0 (8)	C19—C14—C13—O1	8.2 (12)
N1—Pt1—N2—C12	16.4 (5)	C15—C14—C13—O2	3.7 (12)
N1 <sup>i</sup> —Pt1—N2—C12	-163.6 (5)	C19—C14—C13—O2	-174.5 (8)
C19—C14—C15—C16	1.4 (12)	C7—C8—C9—C10	0.4 (15)
C13—C14—C15—C16	-176.7 (7)	C12—N2—C10—C9	6.6 (13)
C14—C15—C16—C17	-0.6 (13)	Pt1—N2—C10—C9	-172.0 (7)
C14—C15—C16—S1	-177.4 (6)	C8—C9—C10—N2	-3.3 (15)
O3—S1—C16—C17	177.2 (10)	C11—N1—C1—C2	-4.8 (13)
O5—S1—C16—C17	-59.7 (8)	Pt1—N1—C1—C2	170.4 (7)
O4—S1—C16—C17	56.6 (9)	C3—C2—C1—N1	0.4 (15)

O3—S1—C16—C15	−6.0 (11)	C1—C2—C3—C4	4.6 (15)
O5—S1—C16—C15	117.2 (8)	C11—C4—C3—C2	−4.9 (14)
O4—S1—C16—C15	−126.6 (8)	C5—C4—C3—C2	172.8 (9)
C14—C19—C18—C17	1.1 (13)		

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

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

$D\text{—H}\cdots A$	$D\text{—H}$	$H\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
O2—H2A $\cdots$ O1W	0.82	1.83	2.650 (10)	177
O1W—H1A $\cdots$ O3 <sup>ii</sup>	0.85 (2)	2.32 (14)	2.90 (2)	126 (14)
C6—H6 $\cdots$ O2 <sup>iii</sup>	0.93	2.57	3.468 (13)	161
C10—H1 $\cdots$ O5 <sup>iv</sup>	0.93	2.46	3.228 (12)	140

Symmetry codes: (ii)  $-x+1, -y+1, -z$ ; (iii)  $x, y-1, z$ ; (iv)  $-x+1/2, y-1/2, -z-1/2$ .