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# *cis*-(Di-2-pyridylamine- $\kappa^2N^2, N^{2'}$ )bis(thiocyanato- $\kappa S$ )platinum(II)

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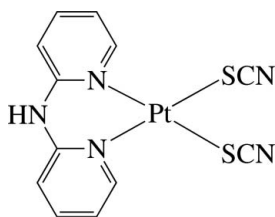
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Key indicators: single-crystal X-ray study;  $T = 200$  K; mean  $\sigma(C-C) = 0.014$  Å;  
 $R$  factor = 0.031;  $wR$  factor = 0.088; data-to-parameter ratio = 14.6.

In the title complex,  $[Pt(NCS)_2(C_{10}H_9N_3)]$ , the  $Pt^{II}$  ion is four-coordinated in a distorted square-planar environment by the two pyridine N atoms of the chelating di-2-pyridylamine (dpa) ligand and two mutually *cis* S atoms from two linear thiocyanate anions. The dpa ligand is not planar, the dihedral angle between the pyridine rings being  $30.8$  ( $4$ )°. In the crystal, the complex molecules are stacked in columns along the *a* axis and are connected by intermolecular  $N-H\cdots N$  hydrogen bonds, forming supramolecular chains along the *b* axis.

## Related literature

For the crystal structure of the related chlorido  $Pt^{II}$  complex  $[PtCl_2(dpa)]$ , see: Li & Liu (2004); Tu *et al.* (2004); Zhang *et al.* (2006).



## Experimental

## Crystal data

$[Pt(NCS)_2(C_{10}H_9N_3)]$   
 $M_r = 482.45$   
Triclinic,  $P\bar{1}$   
 $a = 7.2282$  (6) Å  
 $b = 9.8308$  (8) Å  
 $c = 10.2501$  (8) Å  
 $\alpha = 94.292$  (2)°  
 $\beta = 93.081$  (2)°

$\gamma = 106.123$  (2)°  
 $V = 695.64$  (10) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 10.38$  mm<sup>-1</sup>  
 $T = 200$  K  
 $0.19 \times 0.15 \times 0.09$  mm

## Data collection

Bruker SMART 1000 CCD  
diffractometer  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 2000)  
 $T_{min} = 0.812$ ,  $T_{max} = 1.000$

4195 measured reflections  
2636 independent reflections  
2391 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.018$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.088$   
 $S = 1.22$   
2636 reflections

181 parameters  
H-atom parameters constrained  
 $\Delta\rho_{max} = 3.96$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -1.40$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Pt1–N1	2.065 (7)	Pt1–S2	2.302 (2)
Pt1–N3	2.069 (7)	Pt1–S1	2.306 (2)
N1–Pt1–N3	88.1 (3)	S2–Pt1–S1	89.04 (9)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H2N\cdots N5^i$	0.92	1.93	2.851 (11)	176

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK5067).

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## supporting information

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***cis*-(Di-2-pyridylamine- $\kappa^2N^2,N^{2'}$ )bis(thiocyanato- $\kappa S$ )platinum(II)****Kwang Ha****S1. Comment**

Crystal structures of the related chlorido Pt<sup>II</sup> complex, [PtCl<sub>2</sub>(dpa)] (dpa = di-2-pyridylamine, C<sub>10</sub>H<sub>9</sub>N<sub>3</sub>), have been reported previously (Li & Liu, 2004; Tu *et al.*, 2004; Zhang *et al.*, 2006).

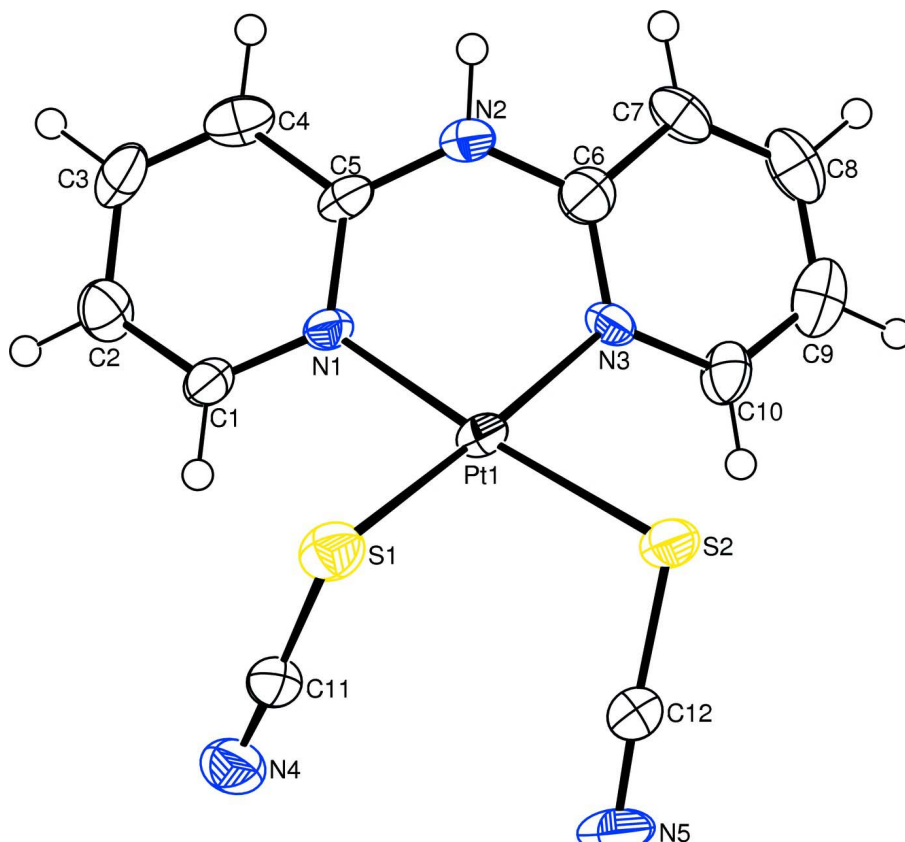
In the title complex, [Pt(NCS)<sub>2</sub>(dpa)], the Pt<sup>II</sup> ion is four-coordinated in a distorted square-planar environment by the two pyridyl N atoms of the chelating dpa ligand and two S atoms from two thiocyanate anions (Fig. 1). The dpa ligand is not planar with the dihedral angle between the least-squares planes of the pyridyl rings being 30.8 (4)°. The thiocyanato ligands are located on the same sides of the PtS<sub>2</sub>N<sub>2</sub> plane and are almost linear with the bond angles <S1—C11—N4 = 177.4 (9)° and <S2—C12—N5 = 177.3 (9)°. The pairs of Pt—N and Pt—S bond lengths are nearly equivalent (Table 1). The complex molecules are stacked in columns along the *a* axis and are connected by intermolecular N—H⋯N hydrogen bonds, forming chains along the *b* axis (Fig. 2 and Table 2). In the columns, intermolecular  $\pi$ - $\pi$  interactions between the pyridine rings are present, the ring centroid-centroid distance being 4.155 (5) Å.

**S2. Experimental**

To a solution of K<sub>2</sub>PtCl<sub>4</sub> (0.2066 g, 0.498 mmol) in H<sub>2</sub>O (20 ml) and MeOH (10 ml) were added KSCN (0.5232 g, 5.384 mmol) and di-2-pyridylamine (0.0883 g, 0.516 mmol) and stirred for 7 h at room temperature. The formed precipitate was separated by filtration and washed with H<sub>2</sub>O and MeOH, and dried at 50 °C, to give a yellow powder (0.2182 g). Crystals suitable for X-ray analysis were obtained by slow evaporation from a CH<sub>3</sub>CN solution.

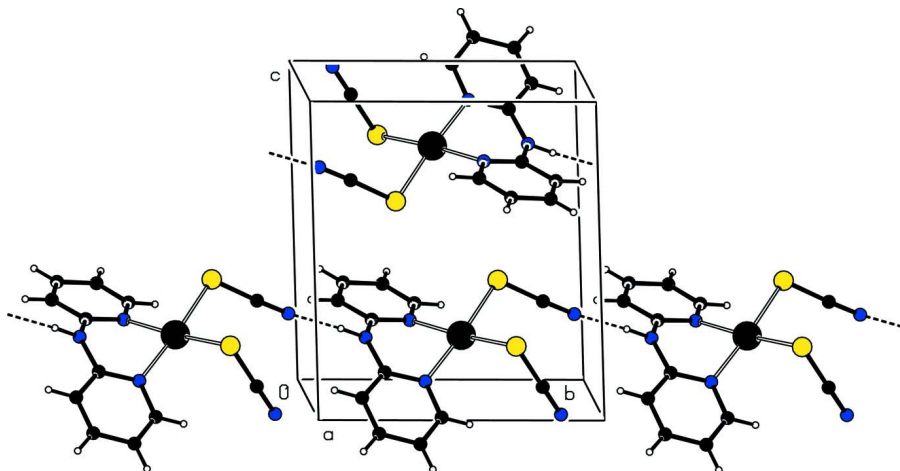
**S3. Refinement**

Carbon-bound H atoms were positioned geometrically and allowed to ride on their respective parent atoms [C—H = 0.95 Å and  $U_{iso}(H) = 1.2U_{eq}(C)$ ]. Nitrogen-bound H atom was located from Fourier difference maps then allowed to ride on its parent atom in the final cycles of refinement with N—H = 0.92 Å and  $U_{iso}(H) = 1.5U_{eq}(N)$ . The highest peak (3.96 e Å<sup>-3</sup>) and the deepest hole (-1.40 e Å<sup>-3</sup>) in the difference Fourier map are located 0.98 Å and 0.99 Å from the Pt1 atom, respectively. Owing to poor agreement, the following reflections were omitted from the final refinement: ( $\bar{8}$  7 2), (0  $\bar{1}$  1 4), ( $\bar{7}$  8 4), (2  $\bar{9}$  9), ( $\bar{7}$  0 8), ( $\bar{7}$  5 7), (8  $\bar{7}$  3), ( $\bar{8}$  8 0), (0  $\bar{9}$  8), (7  $\bar{4}$  7), ( $\bar{6}$  8 6), (8  $\bar{6}$  3), ( $\bar{5}$  7 8), ( $\bar{4}$  7 9), (3 1 11), ( $\bar{6}$   $\bar{6}$  2), (8  $\bar{8}$  1), (8  $\bar{7}$  1), (1  $\bar{9}$  9), (0 10 5), (7  $\bar{7}$  5), ( $\bar{2}$  4 11), ( $\bar{8}$   $\bar{1}$  4), ( $\bar{4}$  8 8), (8  $\bar{7}$  2), ( $\bar{2}$  5 11), (3  $\bar{2}$  11), (1 10 4), and ( $\bar{2}$  11 4).



**Figure 1**

The molecular structure of the title complex, with displacement ellipsoids drawn at the 50% probability level for non-H atoms.



**Figure 2**

A view of the unit-cell contents of the title complex. Intermolecular N—H...N hydrogen-bond interactions are drawn with dashed lines.

*cis*-(Di-2-pyridylamine- $\kappa^2N^2,N^2$ )bis(thiocyanato- $\kappa S$ )platinum(II)*Crystal data*[Pt(NCS)<sub>2</sub>(C<sub>10</sub>H<sub>6</sub>N<sub>3</sub>)] $M_r = 482.45$ Triclinic,  $P\bar{1}$ 

Hall symbol: -P 1

 $a = 7.2282$  (6) Å $b = 9.8308$  (8) Å $c = 10.2501$  (8) Å $\alpha = 94.292$  (2)° $\beta = 93.081$  (2)° $\gamma = 106.123$  (2)° $V = 695.64$  (10) Å<sup>3</sup> $Z = 2$  $F(000) = 452$  $D_x = 2.303$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3201 reflections

 $\theta = 2.8$ – $25.9$ ° $\mu = 10.38$  mm<sup>-1</sup> $T = 200$  K

Block, yellow

 $0.19 \times 0.15 \times 0.09$  mm*Data collection*

Bruker SMART 1000 CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 2000)

 $T_{\min} = 0.812$ ,  $T_{\max} = 1.000$ 

4195 measured reflections

2636 independent reflections

2391 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.018$  $\theta_{\text{max}} = 26.0$ °,  $\theta_{\text{min}} = 2.0$ ° $h = -8 \rightarrow 8$  $k = -12 \rightarrow 11$  $l = -12 \rightarrow 12$ *Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.031$  $wR(F^2) = 0.088$  $S = 1.22$ 

2636 reflections

181 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0179P)^2 + 8.2228P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} = 0.001$  $\Delta\rho_{\text{max}} = 3.96$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -1.40$  e Å<sup>-3</sup>*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<sup>2</sup>)*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Pt1	1.01671 (5)	0.50573 (3)	0.26893 (3)	0.02699 (12)
S1	1.3097 (3)	0.6767 (2)	0.2720 (2)	0.0351 (5)
S2	0.9284 (4)	0.6445 (2)	0.4314 (2)	0.0367 (5)

N1	1.0971 (10)	0.3699 (7)	0.1344 (7)	0.0256 (15)
N2	0.9426 (11)	0.1761 (8)	0.2524 (7)	0.0307 (16)
H2N	0.9464	0.0901	0.2805	0.046*
N3	0.7667 (10)	0.3445 (7)	0.2845 (7)	0.0254 (15)
N4	1.2719 (12)	0.8295 (9)	0.0535 (9)	0.043 (2)
N5	0.9605 (17)	0.9069 (9)	0.3291 (10)	0.060 (3)
C1	1.2059 (12)	0.4162 (9)	0.0350 (9)	0.0293 (19)
H1	1.2247	0.5119	0.0157	0.035*
C2	1.2890 (14)	0.3335 (10)	-0.0382 (9)	0.036 (2)
H2	1.3633	0.3698	-0.1081	0.044*
C3	1.2635 (14)	0.1923 (11)	-0.0089 (10)	0.041 (2)
H3	1.3234	0.1322	-0.0570	0.050*
C4	1.1520 (13)	0.1437 (9)	0.0890 (9)	0.034 (2)
H4	1.1351	0.0490	0.1107	0.041*
C5	1.0619 (12)	0.2315 (9)	0.1582 (9)	0.0272 (18)
C6	0.7784 (14)	0.2105 (10)	0.2872 (9)	0.034 (2)
C7	0.6286 (13)	0.1040 (10)	0.3285 (10)	0.038 (2)
H7	0.6401	0.0104	0.3319	0.045*
C8	0.4652 (15)	0.1353 (12)	0.3638 (10)	0.048 (3)
H8	0.3619	0.0636	0.3925	0.058*
C9	0.4500 (14)	0.2743 (12)	0.3578 (9)	0.042 (2)
H9	0.3369	0.2980	0.3818	0.051*
C10	0.6011 (12)	0.3736 (11)	0.3166 (9)	0.035 (2)
H10	0.5906	0.4670	0.3101	0.042*
C11	1.2825 (13)	0.7673 (10)	0.1414 (10)	0.035 (2)
C12	0.9486 (13)	0.7994 (10)	0.3678 (9)	0.033 (2)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pt1	0.0312 (2)	0.02336 (19)	0.0312 (2)	0.01455 (14)	0.00534 (13)	0.00443 (13)
S1	0.0337 (12)	0.0298 (12)	0.0411 (13)	0.0094 (10)	-0.0007 (10)	-0.0008 (10)
S2	0.0573 (15)	0.0285 (12)	0.0319 (12)	0.0220 (11)	0.0132 (11)	0.0064 (9)
N1	0.025 (4)	0.017 (3)	0.036 (4)	0.007 (3)	0.005 (3)	0.003 (3)
N2	0.039 (4)	0.023 (4)	0.034 (4)	0.014 (3)	0.006 (3)	0.006 (3)
N3	0.025 (4)	0.021 (3)	0.029 (4)	0.003 (3)	0.004 (3)	0.009 (3)
N4	0.031 (4)	0.033 (5)	0.064 (6)	0.006 (4)	0.005 (4)	0.014 (4)
N5	0.100 (8)	0.028 (5)	0.066 (7)	0.033 (5)	0.030 (6)	0.018 (4)
C1	0.027 (4)	0.025 (4)	0.038 (5)	0.012 (4)	0.005 (4)	0.002 (4)
C2	0.041 (5)	0.037 (5)	0.028 (5)	0.007 (4)	0.007 (4)	-0.002 (4)
C3	0.030 (5)	0.046 (6)	0.053 (6)	0.020 (5)	0.007 (5)	-0.002 (5)
C4	0.039 (5)	0.021 (4)	0.039 (5)	0.007 (4)	-0.012 (4)	-0.007 (4)
C5	0.025 (4)	0.021 (4)	0.037 (5)	0.010 (3)	-0.003 (4)	-0.003 (3)
C6	0.039 (5)	0.039 (5)	0.028 (5)	0.015 (4)	0.001 (4)	0.003 (4)
C7	0.033 (5)	0.028 (5)	0.044 (6)	-0.008 (4)	0.004 (4)	0.010 (4)
C8	0.035 (6)	0.056 (7)	0.042 (6)	-0.007 (5)	0.007 (5)	0.010 (5)
C9	0.032 (5)	0.068 (7)	0.025 (5)	0.018 (5)	-0.006 (4)	-0.011 (5)
C10	0.022 (4)	0.047 (6)	0.040 (5)	0.014 (4)	0.004 (4)	0.005 (4)

C11	0.031 (5)	0.024 (5)	0.050 (6)	0.008 (4)	0.011 (4)	0.006 (4)
C12	0.036 (5)	0.027 (5)	0.038 (5)	0.012 (4)	0.009 (4)	0.003 (4)

*Geometric parameters (Å, °)*

Pt1—N1	2.065 (7)	C1—H1	0.9500
Pt1—N3	2.069 (7)	C2—C3	1.406 (14)
Pt1—S2	2.302 (2)	C2—H2	0.9500
Pt1—S1	2.306 (2)	C3—C4	1.352 (14)
S1—C11	1.694 (10)	C3—H3	0.9500
S2—C12	1.674 (9)	C4—C5	1.394 (12)
N1—C1	1.349 (11)	C4—H4	0.9500
N1—C5	1.356 (10)	C6—C7	1.390 (13)
N2—C5	1.371 (11)	C7—C8	1.361 (15)
N2—C6	1.379 (12)	C7—H7	0.9500
N2—H2N	0.9200	C8—C9	1.407 (16)
N3—C6	1.346 (11)	C8—H8	0.9500
N3—C10	1.356 (11)	C9—C10	1.358 (14)
N4—C11	1.137 (12)	C9—H9	0.9500
N5—C12	1.139 (12)	C10—H10	0.9500
C1—C2	1.347 (12)		
N1—Pt1—N3	88.1 (3)	C2—C3—H3	120.6
N1—Pt1—S2	175.3 (2)	C3—C4—C5	120.5 (9)
N3—Pt1—S2	89.9 (2)	C3—C4—H4	119.7
N1—Pt1—S1	92.6 (2)	C5—C4—H4	119.7
N3—Pt1—S1	173.6 (2)	N1—C5—N2	121.2 (7)
S2—Pt1—S1	89.04 (9)	N1—C5—C4	120.0 (8)
C11—S1—Pt1	103.7 (3)	N2—C5—C4	118.7 (8)
C12—S2—Pt1	104.4 (3)	N3—C6—N2	120.6 (8)
C1—N1—C5	118.6 (7)	N3—C6—C7	121.3 (9)
C1—N1—Pt1	122.7 (5)	N2—C6—C7	118.1 (9)
C5—N1—Pt1	118.0 (6)	C8—C7—C6	119.3 (10)
C5—N2—C6	127.6 (7)	C8—C7—H7	120.3
C5—N2—H2N	118.5	C6—C7—H7	120.3
C6—N2—H2N	111.5	C7—C8—C9	119.7 (9)
C6—N3—C10	118.9 (8)	C7—C8—H8	120.2
C6—N3—Pt1	118.7 (6)	C9—C8—H8	120.2
C10—N3—Pt1	121.3 (6)	C10—C9—C8	118.2 (9)
C2—C1—N1	123.3 (8)	C10—C9—H9	120.9
C2—C1—H1	118.4	C8—C9—H9	120.9
N1—C1—H1	118.4	N3—C10—C9	122.6 (9)
C1—C2—C3	118.5 (9)	N3—C10—H10	118.7
C1—C2—H2	120.7	C9—C10—H10	118.7
C3—C2—H2	120.7	N4—C11—S1	177.4 (9)
C4—C3—C2	118.8 (9)	N5—C12—S2	177.3 (9)
C4—C3—H3	120.6		

N1—Pt1—S1—C11	84.1 (4)	C1—N1—C5—C4	6.0 (12)
S2—Pt1—S1—C11	-100.3 (3)	Pt1—N1—C5—C4	-164.9 (6)
N3—Pt1—S2—C12	-129.1 (4)	C6—N2—C5—N1	35.0 (13)
S1—Pt1—S2—C12	57.3 (4)	C6—N2—C5—C4	-146.8 (9)
N3—Pt1—N1—C1	149.1 (7)	C3—C4—C5—N1	-4.9 (13)
S1—Pt1—N1—C1	-37.3 (7)	C3—C4—C5—N2	176.8 (8)
N3—Pt1—N1—C5	-40.4 (6)	C10—N3—C6—N2	178.5 (8)
S1—Pt1—N1—C5	133.2 (6)	Pt1—N3—C6—N2	-13.8 (11)
N1—Pt1—N3—C6	40.9 (7)	C10—N3—C6—C7	-3.3 (13)
S2—Pt1—N3—C6	-134.9 (6)	Pt1—N3—C6—C7	164.4 (7)
N1—Pt1—N3—C10	-151.7 (7)	C5—N2—C6—N3	-34.6 (14)
S2—Pt1—N3—C10	32.5 (7)	C5—N2—C6—C7	147.1 (9)
C5—N1—C1—C2	-3.2 (13)	N3—C6—C7—C8	1.5 (15)
Pt1—N1—C1—C2	167.3 (7)	N2—C6—C7—C8	179.8 (9)
N1—C1—C2—C3	-0.8 (14)	C6—C7—C8—C9	0.2 (15)
C1—C2—C3—C4	1.9 (14)	C7—C8—C9—C10	-0.2 (15)
C2—C3—C4—C5	0.9 (14)	C6—N3—C10—C9	3.4 (13)
C1—N1—C5—N2	-175.9 (8)	Pt1—N3—C10—C9	-164.0 (7)
Pt1—N1—C5—N2	13.2 (10)	C8—C9—C10—N3	-1.6 (14)

*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>
N2—H2N...N5 <sup>i</sup>	0.92	1.93	2.851 (11)	176

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