

## (Acetato- $\kappa^2O,O'$ )(aqua- $\kappa O$ )[1-(2-pyridylmethylidene- $\kappa N$ )semicarbazide- $\kappa^2N^1,O$ ](thiocyanato- $\kappa S$ )cadmium(II) monohydrate

Ling-Feng Deng,<sup>a\*</sup> Gui-Quan Guo,<sup>b</sup> Di-Chang Zhong,<sup>c</sup> Ji-Hua Deng<sup>c\*</sup> and Meng-Ping Guo<sup>c</sup>

<sup>a</sup>College of Materials Science and Engineering, Central South University of Forestry and Technology, Changsha, Hunan 410004, People's Republic of China, <sup>b</sup>College of Chemistry and Chemical Engineering, Anyang Normal University, Anyang, Henan 455000, People's Republic of China, and <sup>c</sup>College of Chemistry and Bio-engineering, Yichun University, Yichun, Jiangxi 336000, People's Republic of China  
Correspondence e-mail: zhong\_dichang@yahoo.com.cn

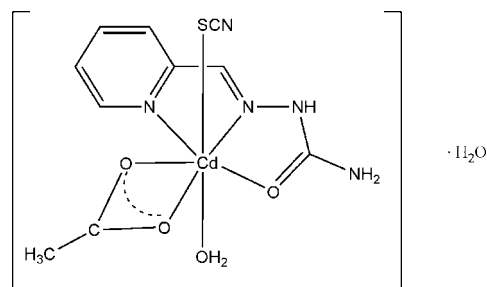
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Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(C-C) = 0.004$  Å;  $R$  factor = 0.028;  $wR$  factor = 0.056; data-to-parameter ratio = 19.7.

The Cd atom in the title complex,  $[Cd(C_2H_3O_2)(NCS)(C_7H_8N_4O)(H_2O)] \cdot H_2O$ , is coordinated by one neutral Schiff base ligand, one acetate anion, one thiocyanate anion and one water molecule, forming a distorted pentagonal-bipyramidal geometry. The thiocyanate S atom and the coordinated water ligand occupy the apical positions of the coordination polyhedron. The acetate acts as a bidentate ligand through the carboxylate O atoms. The Schiff base, derived from the condensation of pyridine-2-carbaldehyde and semicarbazone, acts as a tridentate ligand, coordinating the metal through the amide, imine and pyridyl N atoms in a meridional fashion. The crystal packing is stabilized by  $\pi-\pi$  stacking interactions between the neighboring pyridine rings and hydrogen bonds involving the Schiff base, thiocyanate, water molecules and uncoordinated solvent water molecules.

### Related literature

For related literature, see: Carcelli *et al.* (1999); Chen, Zhou, Liang *et al.* (2004); Chen, Zhou, Li *et al.* (2004); Kaur *et al.* (2002); Zhong *et al.* (2007); Zhou *et al.* (2004).



### Experimental

#### Crystal data

$[Cd(C_2H_3O_2)(NCS)(C_7H_8N_4O)(H_2O)] \cdot H_2O$   
 $M_r = 429.73$   
 Monoclinic,  $P2_1/c$   
 $a = 14.767$  (1) Å  
 $b = 7.7345$  (7) Å  
 $c = 13.964$  (1) Å

$\beta = 99.340$  (1)°  
 $V = 1573.7$  (3) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.55$  mm<sup>-1</sup>  
 $T = 173$  (2) K  
 $0.35 \times 0.28 \times 0.22$  mm

#### Data collection

Bruker SMART APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{min} = 0.601$ ,  $T_{max} = 0.718$

14208 measured reflections  
 3919 independent reflections  
 2921 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.072$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$   
 $wR(F^2) = 0.056$   
 $S = 0.93$   
 3919 reflections

199 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 0.48$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.63$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1W-H1A \cdots S1^i$	0.89	2.46	3.348 (2)	170
$O1W-H1B \cdots O3^{iii}$	0.90	1.79	2.689 (2)	177
$O2W-H2A \cdots N5^{iii}$	0.89	2.21	3.038 (4)	154
$O2W-H2B \cdots O2^i$	0.89	1.91	2.791 (3)	169
$N3-H3A \cdots O2W$	0.86	2.05	2.773 (3)	141
$N4-H4A \cdots O1^{iv}$	0.86	2.07	2.916 (3)	169
$N4-H4B \cdots O1W^v$	0.86	2.24	2.959 (3)	141

Symmetry codes: (i)  $x, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (ii)  $-x + 1, -y, -z + 1$ ; (iii)  $x, -y + \frac{3}{2}, z + \frac{1}{2}$ ; (iv)  $-x + 1, -y + 1, -z + 1$ ; (v)  $x, y + 1, z$ .

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); 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: IM2029).

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**supplementary materials**

*Acta Cryst.* (2007). E63, m2434-m2435 [ doi:10.1107/S1600536807041487 ]

**(Acetato- $\kappa^2 O, O'$ )(aqua- $\kappa O$ )[1-(2-pyridylmethylidene- $\kappa N$ )semicarbazide- $\kappa^2 N^1, O$ ](thiocyanato- $\kappa S$ )cadmium(II) monohydrate**

**L.-F. Deng, G.-Q. Guo, D.-C. Zhong, J.-H. Deng and M.-P. Guo**

**Comment**

Crystal structures and properties of metal complexes based on pyridine-2-carbaldehyde semicarbazone (H-Pysc), owing to their antimicrobial, cytotoxic and antioxidant activities, have been reported in numerous papers (Zhou *et al.*, 2004; Kaur *et al.*, 2002; Carcelli *et al.*, 1999; Zhong *et al.*, 2007) in last several years. Herein, we report the synthesis and crystal structure of the title compound, (**I**).

Compound (**I**) is composed of one [Cd(HPysc)(SCN)(Ac)(H<sub>2</sub>O)] unit and one lattice water. The Cd atom in compound (**I**) is seven-coordinated (Fig. 1) by one S atom (from thiocyanate), two N atoms (from H-Pysc ligand) and four O atoms (one from the coordinated water molecule, one from H-Pysc ligand, and two from the acetate anion), forming a slightly distorted pentagonal bipyramidal geometry (Table 1). S1 and O1W occupy the apical positions of the coordination polyhedron. Similar to the corresponding nickel(II) complex (Zhou *et al.*, 2004), the H-Pysc ligand is planar and utilizes its pyridyl N atom, amide O atom and imine N atom for metal coordination. This is in contrast to the highly related ligand pyridine-3-carbaldehyde-semicarbazone in its cobalt(II) (Chen, Zhou, Liang *et al.*, 2004) and nickel(II) (Chen, Zhou, Li *et al.*, 2004) complexes, in which only the pyridyl N atoms bind to the metal ions. The acetate anion acts as a bidentate chelating ligand leading to two short C—O distances (O(2)—C(8) 1.261 (3) Å, O(3)—C(8) 1.260 (3) Å).

The molecules are connected by intermolecular hydrogen bonding interactions and  $\pi$  -  $\pi$  stacking interactions to form a three-dimensional supramolecular network. The coordinated water molecules (O1W) act as hydrogen bond donor sites towards the thiocyanate S1 atoms and acetate O3 atoms to form O—H $\cdots$ S<sup>i</sup> and O—H $\cdots$ O<sup>ii</sup> hydrogen bonds, respectively [symmetry codes  $i=x, 1/2 - y, 1/2 + z$ ;  $ii = 1 - x, -y, 1 - z$ ]. The uncoordinated water molecules (O2W) also act as a H atom donors, the accepters being the thiocyanate N5 atoms and acetate O2 atoms, respectively, forming O—H $\cdots$ N<sup>iii</sup> and O—H $\cdots$ O<sup>i</sup> hydrogen bonds [symmetry codes  $iii=x, 3/2 - y, 1/2 + z$ ]. In addition, the O1W atoms and semicarbazone O1 atoms accept H atoms from N4 to form N—H $\cdots$ O<sup>v</sup> and N—H $\cdots$ O<sup>iv</sup> hydrogen bonds [symmetry codes  $iv = 1 - x, 1 - y, 1 - z$ ;  $v = x, 1 + y, z$ ] (Table 2, Fig. 2).

**Experimental**

H-Pysc (1.0 mmol) and Cd(Ac)<sub>2</sub> × 4H<sub>2</sub>O (0.5 mmol) were dissolved in a water-ethanol mixture (1:1 v/v; 16 ml) at 353 K. After stirring for *ca* 2 hrs, 10 ml of a solution containing 1.0 mmol (NH<sub>4</sub>)SCN was added, then the mixture was further stirred for another 2 hrs. The resulting solution was filtered and the filtrate allowed to standing at room temperature. Well shaped colorless crystals suitable for X-rays diffraction were obtained in 58% yield after two weeks.

## Refinement

Hydrogen atoms bound to carbon atoms and nitrogen atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, N—H = 0.86 Å, and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C or N})$ . Water Hydrogen atoms were located in difference maps and constrained to ride at the as-found O—H distances (0.89 Å), with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .

## Figures

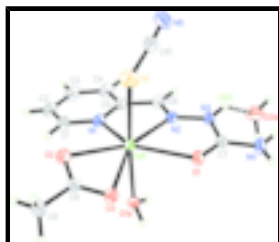


Fig. 1. The structure of **(I)**, showing 30% probability displacement ellipsoids and the atom-labeling scheme.

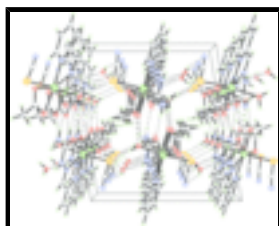


Fig. 2. Three-dimensional supramolecular network constructed by hydrogen bonding interactions (dashed lines) and p-p stacking interaction.

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### Crystal data

$[\text{Cd}(\text{C}_2\text{H}_3\text{O}_2)(\text{NCS})(\text{C}_7\text{H}_8\text{N}_4\text{O})(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}$	$Z = 4$
$M_r = 429.73$	$F_{000} = 856$
Monoclinic, $P2_1/c$	$D_x = 1.814 \text{ Mg m}^{-3}$
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation
$a = 14.767 (1) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 7.7345 (7) \text{ \AA}$	$\theta = 2.8\text{--}28.4^\circ$
$c = 13.964 (1) \text{ \AA}$	$\mu = 1.55 \text{ mm}^{-1}$
$\beta = 99.340 (1)^\circ$	$T = 173 (2) \text{ K}$
$V = 1573.7 (3) \text{ \AA}^3$	Block, colourless
	$0.35 \times 0.28 \times 0.22 \text{ mm}$

### Data collection

Bruker SMART APEXII CCD diffractometer	3919 independent reflections
Radiation source: fine-focus sealed tube	2921 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.072$
$T = 173(2) \text{ K}$	$\theta_{\text{max}} = 28.4^\circ$

$\omega$ scans	$\theta_{\min} = 2.8^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -19 \rightarrow 19$
$T_{\min} = 0.601$ , $T_{\max} = 0.718$	$k = -9 \rightarrow 10$
14208 measured reflections	$l = -18 \rightarrow 18$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.028$	H-atom parameters constrained
$wR(F^2) = 0.056$	$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2]$
$S = 0.93$	where $P = (F_o^2 + 2F_c^2)/3$
3919 reflections	$(\Delta/\sigma)_{\max} = 0.001$
199 parameters	$\Delta\rho_{\max} = 0.48 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.63 \text{ e } \text{\AA}^{-3}$
	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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.688818 (11)	0.12412 (2)	0.472629 (12)	0.02909 (6)
S1	0.72697 (6)	0.26945 (11)	0.30933 (5)	0.0539 (2)
O1	0.59934 (11)	0.3712 (2)	0.50308 (13)	0.0371 (4)
N1	0.83695 (13)	0.0190 (3)	0.54372 (14)	0.0336 (5)
O3	0.54727 (11)	-0.0111 (2)	0.39860 (11)	0.0369 (4)
O1W	0.63610 (11)	0.0075 (2)	0.61140 (11)	0.0330 (4)
O2	0.67697 (12)	-0.1351 (2)	0.38194 (14)	0.0451 (5)
C8	0.59050 (17)	-0.1326 (3)	0.36624 (17)	0.0331 (5)
N3	0.73204 (13)	0.4873 (3)	0.58458 (14)	0.0341 (5)
H3A	0.7617	0.5745	0.6121	0.041*
N2	0.77331 (13)	0.3339 (3)	0.57216 (14)	0.0303 (5)
N4	0.59726 (15)	0.6374 (3)	0.56943 (16)	0.0416 (5)
H4A	0.5394	0.6496	0.5494	0.050*

## supplementary materials

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H4B	0.6278	0.7186	0.6021	0.050*
C7	0.63933 (17)	0.4936 (3)	0.54996 (17)	0.0313 (5)
C6	0.85542 (17)	0.3042 (3)	0.61182 (18)	0.0359 (6)
H6	0.8905	0.3889	0.6477	0.043*
C1	0.86846 (18)	-0.1400 (4)	0.5326 (2)	0.0422 (7)
H1	0.8304	-0.2183	0.4948	0.051*
C5	0.89292 (16)	0.1320 (3)	0.59916 (17)	0.0347 (6)
N5	0.8725 (2)	0.5003 (4)	0.3657 (2)	0.0673 (8)
C9	0.5393 (2)	-0.2757 (4)	0.3088 (2)	0.0486 (7)
C2	0.95532 (19)	-0.1941 (4)	0.5746 (2)	0.0495 (8)
H2	0.9748	-0.3064	0.5657	0.059*
C4	0.98095 (18)	0.0857 (4)	0.6424 (2)	0.0468 (7)
H4	1.0185	0.1654	0.6797	0.056*
C10	0.8116 (2)	0.4066 (4)	0.3455 (2)	0.0478 (7)
C3	1.0120 (2)	-0.0781 (4)	0.6296 (2)	0.0521 (8)
H3	1.0709	-0.1105	0.6580	0.062*
O2W	0.79164 (14)	0.6935 (3)	0.74484 (15)	0.0604 (6)
H9C	0.4875	-0.3189	0.3348	0.091*
H9B	0.5195	-0.2523	0.2396	0.091*
H9A	0.5857	-0.3653	0.3135	0.091*
H2B	0.7535	0.6609	0.7848	0.091*
H1B	0.5745	0.0123	0.6070	0.091*
H1A	0.6617	0.0540	0.6679	0.091*
H2A	0.8207	0.7926	0.7617	0.091*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cd1	0.02724 (9)	0.02820 (10)	0.03121 (10)	0.00117 (8)	0.00290 (6)	-0.00288 (8)
S1	0.0649 (5)	0.0621 (5)	0.0335 (4)	-0.0032 (4)	0.0041 (3)	0.0104 (4)
O1	0.0324 (9)	0.0285 (9)	0.0484 (11)	0.0034 (8)	0.0007 (8)	-0.0104 (9)
N1	0.0293 (11)	0.0400 (13)	0.0316 (12)	0.0045 (10)	0.0054 (9)	0.0037 (10)
O3	0.0344 (10)	0.0398 (11)	0.0361 (10)	-0.0003 (8)	0.0043 (8)	-0.0082 (8)
O1W	0.0320 (9)	0.0350 (10)	0.0318 (9)	-0.0012 (8)	0.0047 (7)	-0.0025 (8)
O2	0.0356 (10)	0.0459 (12)	0.0537 (12)	-0.0028 (9)	0.0068 (8)	-0.0107 (10)
C8	0.0378 (13)	0.0347 (14)	0.0269 (12)	-0.0052 (12)	0.0058 (10)	0.0005 (12)
N3	0.0334 (11)	0.0265 (12)	0.0410 (13)	-0.0023 (9)	0.0020 (9)	-0.0086 (9)
N2	0.0315 (11)	0.0307 (12)	0.0292 (11)	0.0011 (9)	0.0065 (9)	-0.0010 (9)
N4	0.0398 (12)	0.0303 (12)	0.0532 (14)	0.0053 (10)	0.0030 (10)	-0.0113 (11)
C7	0.0357 (13)	0.0293 (14)	0.0291 (13)	0.0011 (11)	0.0056 (10)	0.0021 (11)
C6	0.0330 (13)	0.0428 (16)	0.0304 (14)	-0.0021 (12)	0.0007 (11)	-0.0068 (12)
C1	0.0393 (14)	0.0395 (17)	0.0490 (17)	0.0081 (13)	0.0108 (12)	0.0035 (13)
C5	0.0289 (12)	0.0450 (16)	0.0304 (13)	0.0022 (12)	0.0054 (10)	0.0037 (12)
N5	0.0597 (17)	0.0463 (17)	0.096 (2)	0.0005 (15)	0.0134 (16)	0.0116 (16)
C9	0.0502 (17)	0.0477 (18)	0.0483 (18)	-0.0103 (15)	0.0092 (14)	-0.0194 (14)
C2	0.0474 (17)	0.0512 (18)	0.0519 (18)	0.0213 (15)	0.0141 (15)	0.0142 (15)
C4	0.0337 (14)	0.067 (2)	0.0368 (16)	0.0091 (14)	-0.0014 (12)	0.0015 (14)
C10	0.0564 (19)	0.0404 (18)	0.0489 (18)	0.0171 (15)	0.0150 (15)	0.0139 (14)

C3	0.0358 (15)	0.074 (2)	0.0447 (17)	0.0203 (15)	0.0013 (13)	0.0126 (16)
O2W	0.0694 (14)	0.0664 (15)	0.0482 (12)	-0.0270 (12)	0.0179 (11)	-0.0203 (11)

*Geometric parameters (Å, °)*

Cd1—N2	2.357 (2)	N2—C6	1.269 (3)
Cd1—O2	2.3629 (18)	N4—C7	1.323 (3)
Cd1—O1W	2.3800 (15)	N4—H4A	0.8600
Cd1—N1	2.393 (2)	N4—H4B	0.8600
Cd1—O1	2.4000 (16)	C6—C5	1.464 (4)
Cd1—O3	2.4146 (16)	C6—H6	0.9300
Cd1—S1	2.6829 (8)	C1—C2	1.386 (4)
Cd1—C8	2.749 (3)	C1—H1	0.9300
S1—C10	1.655 (4)	C5—C4	1.388 (4)
O1—C7	1.244 (3)	N5—C10	1.154 (4)
N1—C1	1.332 (3)	C9—H9C	0.9582
N1—C5	1.356 (3)	C9—H9B	0.9803
O3—C8	1.260 (3)	C9—H9A	0.9695
O1W—H1B	0.9021	C2—C3	1.374 (4)
O1W—H1A	0.8926	C2—H2	0.9300
O2—C8	1.260 (3)	C4—C3	1.369 (4)
C8—C9	1.497 (4)	C4—H4	0.9300
N3—N2	1.358 (3)	C3—H3	0.9300
N3—C7	1.377 (3)	O2W—H2B	0.8910
N3—H3A	0.8600	O2W—H2A	0.8910
N2—Cd1—O2	152.38 (7)	O2—C8—Cd1	59.06 (13)
N2—Cd1—O1W	89.57 (6)	O3—C8—Cd1	61.41 (12)
O2—Cd1—O1W	96.27 (6)	C9—C8—Cd1	178.4 (2)
N2—Cd1—N1	68.20 (7)	N2—N3—C7	115.3 (2)
O2—Cd1—N1	85.24 (7)	N2—N3—H3A	122.4
O1W—Cd1—N1	86.06 (6)	C7—N3—H3A	122.4
N2—Cd1—O1	66.52 (6)	C6—N2—N3	121.3 (2)
O2—Cd1—O1	140.86 (6)	C6—N2—Cd1	120.63 (17)
O1W—Cd1—O1	83.98 (6)	N3—N2—Cd1	118.12 (14)
N1—Cd1—O1	133.60 (7)	C7—N4—H4A	120.0
N2—Cd1—O3	152.75 (6)	C7—N4—H4B	120.0
O2—Cd1—O3	54.50 (6)	H4A—N4—H4B	120.0
O1W—Cd1—O3	79.02 (5)	O1—C7—N4	123.3 (2)
N1—Cd1—O3	134.41 (7)	O1—C7—N3	121.2 (2)
O1—Cd1—O3	87.56 (6)	N4—C7—N3	115.5 (2)
N2—Cd1—S1	92.79 (5)	N2—C6—C5	117.7 (2)
O2—Cd1—S1	84.69 (5)	N2—C6—H6	121.1
O1W—Cd1—S1	172.92 (4)	C5—C6—H6	121.1
N1—Cd1—S1	101.01 (5)	N1—C1—C2	123.1 (3)
O1—Cd1—S1	90.84 (5)	N1—C1—H1	118.5
O3—Cd1—S1	95.98 (4)	C2—C1—H1	118.5
N2—Cd1—C8	176.58 (7)	N1—C5—C4	121.5 (3)
O2—Cd1—C8	27.22 (7)	N1—C5—C6	116.6 (2)
O1W—Cd1—C8	87.27 (6)	C4—C5—C6	121.9 (3)



## supplementary materials

N1—Cd1—C8	110.22 (8)	C8—C9—H9C	114.8
O1—Cd1—C8	114.40 (7)	C8—C9—H9B	115.8
O3—Cd1—C8	27.28 (6)	H9C—C9—H9B	108.0
S1—Cd1—C8	90.50 (5)	C8—C9—H9A	101.7
C10—S1—Cd1	105.18 (10)	H9C—C9—H9A	108.9
C7—O1—Cd1	118.10 (15)	H9B—C9—H9A	107.1
C1—N1—C5	118.0 (2)	C3—C2—C1	118.5 (3)
C1—N1—Cd1	125.32 (18)	C3—C2—H2	120.7
C5—N1—Cd1	116.69 (16)	C1—C2—H2	120.7
C8—O3—Cd1	91.31 (14)	C3—C4—C5	119.5 (3)
Cd1—O1W—H1B	112.9	C3—C4—H4	120.3
Cd1—O1W—H1A	114.8	C5—C4—H4	120.3
H1B—O1W—H1A	108.8	N5—C10—S1	176.0 (3)
C8—O2—Cd1	93.72 (15)	C4—C3—C2	119.4 (3)
O2—C8—O3	120.5 (2)	C4—C3—H3	120.3
O2—C8—C9	119.4 (2)	C2—C3—H3	120.3
O3—C8—C9	120.1 (2)	H2B—O2W—H2A	113.8

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

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1W—H1A $\cdots$ S1 <sup>i</sup>	0.89	2.46	3.348 (2)	170
O1W—H1B $\cdots$ O3 <sup>ii</sup>	0.90	1.79	2.689 (2)	177
O2W—H2A $\cdots$ N5 <sup>iii</sup>	0.89	2.21	3.038 (4)	154
O2W—H2B $\cdots$ O2 <sup>i</sup>	0.89	1.91	2.791 (3)	169
N3—H3A $\cdots$ O2W	0.86	2.05	2.773 (3)	141
N4—H4A $\cdots$ O1 <sup>iv</sup>	0.86	2.07	2.916 (3)	169
N4—H4B $\cdots$ O1W <sup>v</sup>	0.86	2.24	2.959 (3)	141

Symmetry codes: (i)  $x, -y+1/2, z+1/2$ ; (ii)  $-x+1, -y, -z+1$ ; (iii)  $x, -y+3/2, z+1/2$ ; (iv)  $-x+1, -y+1, -z+1$ ; (v)  $x, y+1, z$ .

Fig. 1

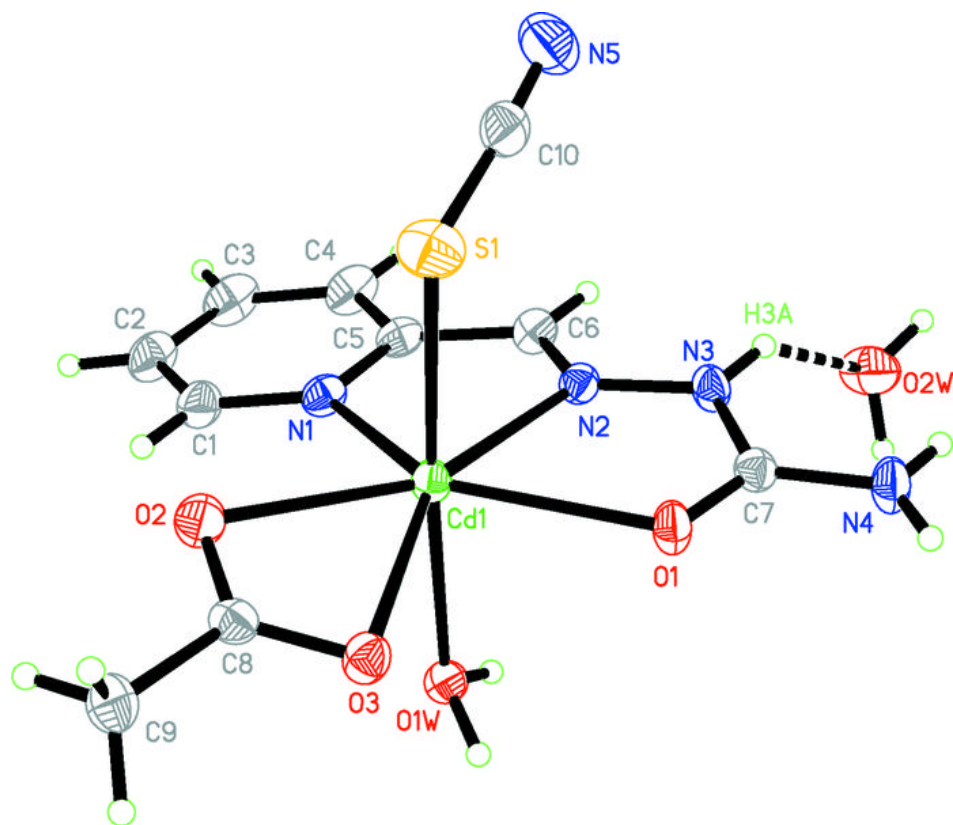


Fig. 2

