

## Bis(2,2'-bipyridine)(5,5'-iminoditetrazolato)cadmium(II) 2,2'-bipyridine hemisolvate monohydrate

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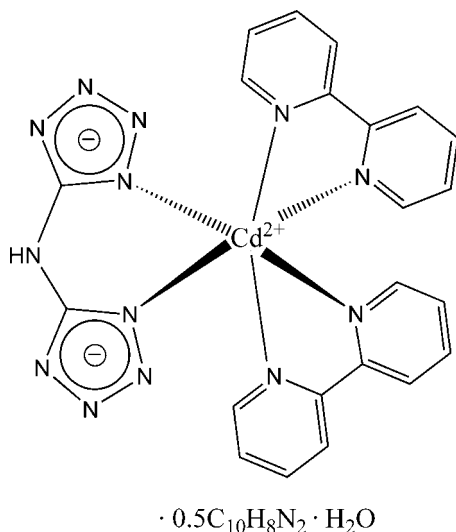
Received 19 November 2007; accepted 13 December 2007

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.024;  $wR$  factor = 0.064; data-to-parameter ratio = 13.8.

The title complex,  $[\text{Cd}(\text{C}_2\text{HN}_9)(\text{C}_{10}\text{H}_8\text{N}_2)_2] \cdot 0.5\text{C}_{10}\text{H}_8\text{N}_2 \cdot \text{H}_2\text{O}$ , was prepared under hydrothermal reaction conditions. The asymmetric unit contains the cadmium complex, half a 2,2'-bipyridine solvent molecule and a solvent water molecule. The  $\text{Cd}^{\text{II}}$  ion is coordinated by four N atoms from two 2,2'-bipyridine ligands and two N atoms from an HBTA<sup>-</sup> anion ligand [where  $\text{H}_2\text{BTA}$  is  $N,N$ -bis(1*H*-tetrazol-5-yl)amine], forming an octahedral geometry. The complex is linked into a three-dimensional network by  $\text{O}-\text{H} \cdots \text{N}$  and  $\text{N}-\text{H} \cdots \text{N}$  hydrogen bonds and by the stacking interactions of rings, with distances of 3.5–3.7 Å between the atoms of two parallel 2,2'-bipyridine rings.

### Related literature

Other complexes of the  $N,N$ -bis-[1(2)*H*-tetrazol-5-yl]imine ligand are rare; for a related copper(II) complex, see: Friedrich *et al.* (2005).



### Experimental

#### Crystal data

$[\text{Cd}(\text{C}_2\text{HN}_9)(\text{C}_{10}\text{H}_8\text{N}_2)_2] \cdot 0.5\text{C}_{10}\text{H}_8\text{N}_2 \cdot \text{H}_2\text{O}$   
 $M_r = 672.00$   
 Monoclinic,  $P2_1/n$   
 $a = 15.1919$  (12) Å  
 $b = 11.2383$  (9) Å  
 $c = 17.5759$  (14) Å

$\beta = 106.073$  (3)°  
 $V = 2883.5$  (4) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.81$  mm<sup>-1</sup>  
 $T = 296$  (2) K  
 $0.24 \times 0.23 \times 0.13$  mm

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.824$ ,  $T_{\text{max}} = 0.901$

41852 measured reflections  
 6569 independent reflections  
 5669 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.064$   
 $S = 1.07$   
 6569 reflections

477 parameters  
 All H-atom parameters refined  
 $\Delta\rho_{\text{max}} = 0.27$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.30$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N5}-\text{H1} \cdots \text{N4}^i$	0.77 (2)	2.17 (2)	2.929 (2)	174 (2)
$\text{O1}-\text{H22} \cdots \text{N9}$	0.82 (4)	2.08 (4)	2.893 (3)	172 (4)
$\text{O1}-\text{H23} \cdots \text{N3}^i$	0.92 (4)	2.02 (5)	2.901 (3)	159 (4)

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

Data collection: SMART (Bruker, 2005); cell refinement: SAINT-Plus (Bruker, 2005); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2005); software used to prepare material for publication: SHELXTL.

The authors acknowledge financial support by the National Natural Science Foundation of China (grant No. 206710214), and the Science and Technology Program Foundation of Guang Zhou (2007 J1-co381).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2057).

### References

- Bruker (2005). SAINT-Plus (Version 6.45), SHELXTL (Version 6.14) and SMART (Version 5.054). Bruker AXS Inc., Madison, Wisconsin, USA.  
 Friedrich, M., Gólviz-Ruiz, J. C., Klapötke, T. M., Mayer, P., Weber, R. & Weigand, J. J. (2005). *Inorg. Chem.* **44**, 8044–8052.  
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.

**supplementary materials**

*Acta Cryst.* (2008). E64, m238 [ doi:10.1107/S1600536807066846 ]

## Bis(2,2'-bipyridine)(5,5'-iminoditrazolato)cadmium(II) 2,2'-bipyridine hemisolvate monohydrate

J.-M. Lin, Y.-F. Guan and W. Dong

### Comment

The H<sub>2</sub>BTA (where H<sub>2</sub>BTA is *N,N*-bis(1(2)*H*-tetrazol-5-yl)-amine) and its deprotonated anions contain nine nitrogen electron-donating atoms and show hundreds of different coordinating or bridging modes in their complexes. However, the complexes of H<sub>2</sub>BTA ligand have been not widely investigated in past decades (Friedrich *et al.*, 2005). The title complex, (I), consists of the cadmium complex of 2,2'-bipyridine and *HBTA*<sup>−</sup> anion ligands, half 2,2'-bipyridine guest molecule and a solvent water molecule (Fig. 1). The *HBTA*<sup>−</sup> ligand acts as a chelatingbidentate and the Cd<sup>II</sup> cation is coordinated to four N atoms from two 2,2'-bipyridine ligands and two N atoms from a *HBTA*<sup>−</sup> anion ligand to form an octahedral mononuclear complex. In the crystal structure, an extensive range of O—H⋯N and N—H⋯N hydrogen bonds as well as the stacking interactions of aryls between the parallel 2,2'-bipyridine molecules links the complex, 2,2'-bipyridine guest molecules and the water molecules into a three dimensional networks (Table 1 and Fig. 2).

### Experimental

A 20 mL aqueous solution of Cd(Cl)<sub>2</sub>·4H<sub>2</sub>O (0.026 g, 0.1 mmol), H<sub>2</sub>BTA (0.016 g, 0.01 mmol) and 2,2'-bipyridine (0.039 g, 0.025 mmol) was heated in a 25 ml Teflon-lined autoclave at 433 K for 3 d, followed by slow cooling to room temperature. The resulting mixture was filtered and washed with 95% methanol, and colorless crystal were collected and dried in air. Elemental analysis, calc (%) for C<sub>27</sub>H<sub>23</sub>CdN<sub>14</sub>O<sub>1</sub>: C 48.21, H 3.42, N 27.08; found (%): C 47.96, H 3.87, N 26.78.

### Refinement

All hydrogen atoms were located in difference Fourier maps and freely refined with isotropic displacement parameters.

### Figures

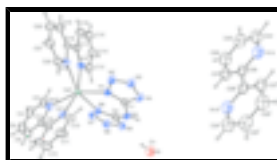


Fig. 1. The molecular structure of the complex, with atom labels and 30% probability displacement ellipsoids for non-H atoms. Symmetry code (i):  $-x, -y, -z$ .

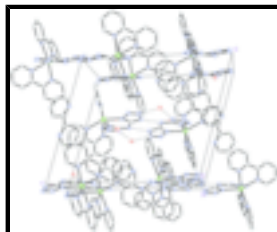


Fig. 2. The packing diagram of the complex, showing a three-dimensional network connected by O—H⋯N and N—H⋯N hydrogen bonds (dashed lines) and by the stacking interactions of aryls between the parallel 2,2'-bipyridine molecules. H atoms not involved in hydrogen bonding have been omitted.

## Bis(2,2'-bipyridine)(5,5'-iminoditrazolato)cadmium(II) 2,2'-bipyridine hemisolvate monohydrate

### Crystal data

[Cd(C<sub>2</sub>HN<sub>9</sub>)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>] $\cdot$ 0.5C<sub>10</sub>H<sub>8</sub>N<sub>2</sub> $\cdot$ H<sub>2</sub>O

$M_r = 672.00$

Monoclinic,  $P2_1/n$

Hall symbol: - $P2_1n$

$a = 15.1919$  (12) Å

$b = 11.2383$  (9) Å

$c = 17.5759$  (14) Å

$\beta = 106.073$  (3)°

$V = 2883.5$  (4) Å<sup>3</sup>

$Z = 4$

$F_{000} = 1356$

$D_x = 1.548$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 6569 reflections

$\theta = 27.5$ – $1.0$ °

$\mu = 0.81$  mm<sup>-1</sup>

$T = 296$  (2) K

Block, colourless

$0.24 \times 0.23 \times 0.13$  mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296$ (2) K

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.824$ ,  $T_{\max} = 0.901$

41852 measured reflections

6569 independent reflections

5669 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\text{max}} = 27.5$ °

$\theta_{\text{min}} = 1.6$ °

$h = -19$ → $19$

$k = -14$ → $14$

$l = -21$ → $22$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.064$

$S = 1.07$

6569 reflections

477 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.9028P]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.003$

$\Delta\rho_{\text{max}} = 0.27$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.30$  e Å<sup>-3</sup>

Extinction correction: SHELXL97 (Sheldrick, 1997),

$$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Extinction coefficient: 0.00357 (18)

*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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.532267 (9)	0.270422 (13)	0.774688 (8)	0.04977 (6)
N1	0.53723 (11)	0.28970 (14)	0.64584 (10)	0.0532 (4)
N2	0.56948 (13)	0.20365 (15)	0.60598 (11)	0.0626 (4)
N6	0.49834 (12)	0.46846 (15)	0.74874 (10)	0.0562 (4)
N3	0.56653 (15)	0.24290 (15)	0.53653 (11)	0.0669 (5)
N5	0.48085 (12)	0.48791 (16)	0.60938 (11)	0.0576 (4)
N9	0.47554 (13)	0.64671 (15)	0.69592 (11)	0.0663 (5)
N8	0.48433 (14)	0.65384 (17)	0.77468 (12)	0.0714 (5)
N4	0.53314 (12)	0.35578 (15)	0.52681 (9)	0.0592 (4)
N7	0.49775 (13)	0.54972 (17)	0.80637 (11)	0.0652 (4)
C1	0.51621 (12)	0.38009 (16)	0.59524 (10)	0.0479 (4)
C2	0.48555 (12)	0.53204 (16)	0.68325 (11)	0.0495 (4)
N10	0.45883 (14)	0.27233 (15)	0.87647 (11)	0.0621 (4)
N12	0.68118 (11)	0.31927 (17)	0.85200 (11)	0.0624 (4)
N11	0.39018 (11)	0.17392 (15)	0.73247 (11)	0.0594 (4)
N13	0.62379 (11)	0.09995 (15)	0.79609 (10)	0.0553 (4)
C7	0.37105 (17)	0.23839 (18)	0.85718 (15)	0.0639 (6)
C17	0.74399 (14)	0.2331 (2)	0.86491 (13)	0.0602 (5)
C12	0.36175 (15)	0.1183 (2)	0.66307 (16)	0.0735 (6)
C8	0.33420 (13)	0.18067 (18)	0.77886 (14)	0.0606 (5)
C18	0.71146 (13)	0.1114 (2)	0.83875 (12)	0.0579 (5)
C16	0.83514 (18)	0.2601 (3)	0.9003 (2)	0.0903 (9)
C6	0.3187 (3)	0.2561 (3)	0.9092 (2)	0.0921 (9)
C3	0.4959 (2)	0.3204 (3)	0.94745 (15)	0.0824 (7)
C11	0.27651 (18)	0.0677 (3)	0.6357 (2)	0.0915 (9)
C22	0.59252 (17)	-0.0076 (2)	0.77108 (16)	0.0703 (6)
C14	0.79708 (19)	0.4612 (3)	0.90888 (19)	0.0904 (8)
C15	0.8608 (2)	0.3740 (3)	0.9222 (2)	0.1035 (10)
C9	0.24676 (18)	0.1321 (3)	0.7531 (2)	0.0864 (8)
C13	0.70807 (17)	0.4305 (2)	0.87371 (17)	0.0808 (7)
C19	0.76731 (19)	0.0129 (3)	0.8578 (2)	0.0885 (8)
C10	0.21877 (19)	0.0756 (3)	0.6815 (2)	0.0998 (10)
C4	0.4464 (4)	0.3369 (3)	1.00196 (19)	0.1007 (11)

## supplementary materials

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C21	0.6447 (2)	-0.1090 (2)	0.7879 (2)	0.0860 (8)
C5	0.3577 (3)	0.3043 (3)	0.9816 (2)	0.1103 (12)
C20	0.7331 (2)	-0.0975 (3)	0.8319 (2)	0.1006 (10)
O1	0.40434 (19)	0.8585 (2)	0.60636 (19)	0.1105 (8)
C28	0.54281 (19)	0.0235 (2)	0.02531 (14)	0.0757 (6)
C27	0.5463 (2)	0.0710 (2)	0.09726 (16)	0.0844 (7)
H21	0.4938	0.0743	0.1147	0.101*
C26	0.6255 (3)	0.1129 (3)	0.1425 (2)	0.1115 (11)
C25	0.7028 (3)	0.1084 (3)	0.1179 (2)	0.1102 (11)
N14	0.6182 (2)	0.0168 (2)	-0.00166 (16)	0.1035 (8)
H1	0.4760 (15)	0.533 (2)	0.5756 (13)	0.062 (7)*
H9	0.4053 (16)	0.116 (2)	0.6320 (13)	0.072 (7)*
H6	0.2165 (19)	0.139 (2)	0.7846 (16)	0.087 (9)*
H7	0.158 (2)	0.044 (3)	0.6619 (17)	0.106 (9)*
H8	0.260 (2)	0.026 (3)	0.5852 (19)	0.121 (11)*
H2	0.5629 (19)	0.338 (3)	0.9605 (16)	0.096 (9)*
H4	0.323 (2)	0.316 (3)	1.021 (2)	0.131 (11)*
H5	0.259 (2)	0.233 (3)	0.894 (2)	0.105 (11)*
H3	0.475 (2)	0.365 (3)	1.0450 (19)	0.098 (10)*
H17	0.5337 (17)	-0.013 (2)	0.7381 (14)	0.074 (7)*
H13	0.874 (2)	0.201 (3)	0.9080 (16)	0.088 (9)*
H11	0.8101 (19)	0.542 (3)	0.9196 (16)	0.100 (9)*
H10	0.6577 (19)	0.491 (2)	0.8614 (16)	0.095 (9)*
H16	0.6172 (18)	-0.179 (3)	0.7664 (16)	0.089 (8)*
H15	0.769 (2)	-0.165 (3)	0.8439 (19)	0.121 (11)*
H12	0.923 (2)	0.395 (3)	0.9494 (19)	0.126 (11)*
H14	0.828 (2)	0.027 (3)	0.8895 (18)	0.108 (10)*
H20	0.632 (2)	0.143 (3)	0.194 (2)	0.130 (13)*
H19	0.764 (2)	0.129 (3)	0.150 (2)	0.125 (12)*
C24	0.6980 (3)	0.0596 (4)	0.0460 (2)	0.1138 (11)
H22	0.421 (3)	0.801 (4)	0.635 (2)	0.123 (14)*
H23	0.398 (3)	0.830 (4)	0.556 (3)	0.163 (17)*
H18	0.747 (2)	0.040 (3)	0.0236 (19)	0.113 (11)*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cd1	0.04460 (8)	0.04959 (9)	0.05279 (9)	0.00138 (5)	0.00960 (6)	-0.00035 (6)
N1	0.0591 (9)	0.0464 (9)	0.0542 (9)	0.0083 (7)	0.0155 (7)	-0.0006 (7)
N2	0.0781 (12)	0.0494 (9)	0.0594 (10)	0.0113 (8)	0.0176 (9)	-0.0033 (7)
N6	0.0640 (10)	0.0518 (9)	0.0536 (9)	0.0071 (8)	0.0176 (7)	-0.0036 (7)
N3	0.0874 (14)	0.0537 (10)	0.0578 (11)	0.0134 (9)	0.0172 (9)	-0.0073 (8)
N5	0.0724 (11)	0.0490 (9)	0.0507 (10)	0.0141 (8)	0.0161 (8)	0.0047 (8)
N9	0.0865 (12)	0.0474 (9)	0.0725 (11)	0.0051 (8)	0.0345 (10)	-0.0034 (8)
N8	0.0873 (13)	0.0584 (11)	0.0757 (13)	0.0026 (9)	0.0346 (10)	-0.0135 (9)
N4	0.0760 (11)	0.0510 (9)	0.0475 (9)	0.0117 (8)	0.0117 (8)	-0.0035 (7)
N7	0.0777 (12)	0.0613 (11)	0.0613 (10)	0.0061 (9)	0.0270 (9)	-0.0092 (8)
C1	0.0464 (9)	0.0465 (10)	0.0471 (10)	0.0024 (7)	0.0070 (7)	-0.0037 (7)

C2	0.0452 (9)	0.0479 (10)	0.0574 (11)	0.0037 (7)	0.0173 (8)	-0.0024 (8)
N10	0.0755 (12)	0.0562 (10)	0.0570 (10)	0.0062 (8)	0.0224 (9)	0.0046 (8)
N12	0.0481 (9)	0.0621 (10)	0.0714 (11)	-0.0040 (8)	0.0073 (8)	-0.0030 (9)
N11	0.0478 (8)	0.0524 (9)	0.0789 (12)	0.0007 (7)	0.0189 (8)	-0.0104 (8)
N13	0.0517 (9)	0.0550 (9)	0.0579 (9)	0.0049 (7)	0.0129 (7)	0.0045 (7)
C7	0.0736 (14)	0.0490 (11)	0.0790 (15)	0.0158 (10)	0.0377 (12)	0.0169 (10)
C17	0.0468 (10)	0.0762 (14)	0.0556 (11)	0.0014 (9)	0.0107 (8)	0.0070 (10)
C12	0.0545 (12)	0.0710 (15)	0.0938 (17)	-0.0029 (10)	0.0184 (12)	-0.0273 (13)
C8	0.0520 (10)	0.0483 (10)	0.0850 (15)	0.0097 (9)	0.0247 (10)	0.0091 (10)
C18	0.0489 (10)	0.0693 (13)	0.0558 (11)	0.0089 (9)	0.0152 (8)	0.0094 (9)
C16	0.0484 (13)	0.103 (2)	0.108 (2)	0.0046 (13)	0.0014 (13)	0.0003 (17)
C6	0.105 (2)	0.0825 (19)	0.109 (3)	0.0165 (16)	0.064 (2)	0.0100 (16)
C3	0.110 (2)	0.0793 (17)	0.0581 (14)	0.0035 (16)	0.0240 (14)	0.0028 (12)
C11	0.0566 (13)	0.0860 (19)	0.123 (2)	-0.0047 (12)	0.0092 (15)	-0.0384 (17)
C22	0.0635 (13)	0.0597 (13)	0.0857 (16)	0.0034 (10)	0.0174 (12)	0.0001 (11)
C14	0.0697 (16)	0.088 (2)	0.102 (2)	-0.0256 (15)	0.0054 (14)	-0.0134 (16)
C15	0.0550 (14)	0.122 (3)	0.118 (2)	-0.0214 (17)	-0.0017 (15)	-0.013 (2)
C9	0.0552 (13)	0.0894 (19)	0.122 (2)	0.0056 (12)	0.0370 (15)	0.0111 (17)
C13	0.0613 (14)	0.0732 (16)	0.0964 (19)	-0.0095 (12)	0.0028 (13)	-0.0129 (13)
C19	0.0597 (14)	0.0825 (19)	0.117 (2)	0.0207 (13)	0.0145 (15)	0.0136 (16)
C10	0.0529 (14)	0.091 (2)	0.148 (3)	-0.0109 (13)	0.0150 (17)	-0.0166 (19)
C4	0.169 (4)	0.0783 (19)	0.0608 (17)	0.014 (2)	0.041 (2)	0.0034 (14)
C21	0.0878 (19)	0.0567 (15)	0.120 (2)	0.0085 (13)	0.0395 (17)	0.0005 (14)
C5	0.162 (4)	0.095 (2)	0.103 (3)	0.022 (2)	0.085 (3)	0.0110 (19)
C20	0.0833 (19)	0.0758 (19)	0.143 (3)	0.0311 (16)	0.0323 (19)	0.0184 (18)
O1	0.146 (2)	0.0835 (14)	0.1159 (19)	0.0489 (14)	0.0601 (16)	-0.0008 (14)
C28	0.110 (2)	0.0503 (12)	0.0725 (16)	0.0102 (12)	0.0343 (13)	0.0153 (10)
C27	0.113 (2)	0.0722 (16)	0.0732 (16)	0.0032 (15)	0.0348 (16)	-0.0052 (13)
C26	0.155 (4)	0.087 (2)	0.098 (3)	-0.002 (2)	0.043 (3)	-0.0129 (19)
C25	0.130 (3)	0.093 (2)	0.101 (3)	-0.022 (2)	0.020 (2)	-0.0030 (19)
N14	0.130 (2)	0.0973 (18)	0.0890 (17)	0.0021 (17)	0.0396 (17)	0.0085 (14)
C24	0.123 (3)	0.115 (3)	0.112 (3)	-0.008 (2)	0.046 (2)	0.006 (2)

*Geometric parameters (Å, °)*

Cd1—N1	2.2970 (17)	C6—C5	1.358 (5)
Cd1—N6	2.3015 (17)	C6—H5	0.91 (3)
Cd1—N13	2.3357 (16)	C3—C4	1.384 (4)
Cd1—N11	2.3451 (16)	C3—H2	1.00 (3)
Cd1—N10	2.3559 (18)	C11—C10	1.348 (5)
Cd1—N12	2.3587 (16)	C11—H8	0.97 (3)
N1—C1	1.329 (2)	C22—C21	1.373 (3)
N1—N2	1.362 (2)	C22—H17	0.92 (2)
N2—N3	1.287 (3)	C14—C15	1.352 (5)
N6—C2	1.322 (2)	C14—C13	1.366 (3)
N6—N7	1.366 (2)	C14—H11	0.93 (3)
N3—N4	1.359 (2)	C15—H12	0.96 (3)
N5—C2	1.373 (2)	C9—C10	1.367 (5)
N5—C1	1.376 (2)	C9—H6	0.82 (3)

## supplementary materials

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N5—H1	0.77 (2)	C13—H10	1.00 (3)
N9—C2	1.324 (3)	C19—C20	1.373 (4)
N9—N8	1.356 (3)	C19—H14	0.95 (3)
N8—N7	1.288 (3)	C10—H7	0.96 (3)
N4—C1	1.326 (2)	C4—C5	1.346 (5)
N10—C3	1.333 (3)	C4—H3	0.82 (3)
N10—C7	1.337 (3)	C21—C20	1.357 (4)
N12—C17	1.334 (3)	C21—H16	0.92 (3)
N12—C13	1.338 (3)	C5—H4	0.98 (4)
N11—C12	1.332 (3)	C20—H15	0.92 (3)
N11—C8	1.333 (3)	O1—H22	0.82 (4)
N13—C22	1.328 (3)	O1—H23	0.92 (4)
N13—C18	1.341 (2)	C28—N14	1.357 (4)
C7—C6	1.382 (4)	C28—C27	1.361 (3)
C7—C8	1.484 (3)	C28—C28 <sup>i</sup>	1.456 (5)
C17—C16	1.386 (3)	C27—C26	1.332 (5)
C17—C18	1.483 (3)	C27—H21	0.9300
C12—C11	1.373 (3)	C26—C25	1.360 (5)
C12—H9	0.97 (2)	C26—H20	0.94 (4)
C8—C9	1.391 (3)	C25—C24	1.361 (5)
C18—C19	1.378 (3)	C25—H19	0.97 (3)
C16—C15	1.362 (5)	N14—C24	1.357 (5)
C16—H13	0.88 (3)	C24—H18	0.96 (3)
N1—Cd1—N6	77.29 (6)	C15—C16—C17	120.4 (3)
N1—Cd1—N13	93.18 (6)	C15—C16—H13	123.0 (19)
N6—Cd1—N13	156.31 (6)	C17—C16—H13	117 (2)
N1—Cd1—N11	90.59 (6)	C5—C6—C7	119.7 (4)
N6—Cd1—N11	104.39 (6)	C5—C6—H5	122 (2)
N13—Cd1—N11	97.26 (6)	C7—C6—H5	119 (2)
N1—Cd1—N10	154.10 (7)	N10—C3—C4	122.2 (3)
N6—Cd1—N10	90.83 (6)	N10—C3—H2	115.7 (16)
N13—Cd1—N10	105.73 (6)	C4—C3—H2	122.0 (16)
N11—Cd1—N10	69.92 (7)	C10—C11—C12	118.0 (3)
N1—Cd1—N12	104.95 (6)	C10—C11—H8	122 (2)
N6—Cd1—N12	90.89 (6)	C12—C11—H8	120 (2)
N13—Cd1—N12	70.42 (6)	N13—C22—C21	123.5 (2)
N11—Cd1—N12	160.38 (7)	N13—C22—H17	117.5 (15)
N10—Cd1—N12	98.09 (7)	C21—C22—H17	118.9 (16)
C1—N1—N2	104.62 (16)	C15—C14—C13	117.9 (3)
C1—N1—Cd1	131.62 (12)	C15—C14—H11	124.4 (18)
N2—N1—Cd1	123.69 (12)	C13—C14—H11	117.6 (18)
N3—N2—N1	108.74 (16)	C14—C15—C16	119.8 (3)
C2—N6—N7	104.75 (16)	C14—C15—H12	118 (2)
C2—N6—Cd1	131.75 (13)	C16—C15—H12	122 (2)
N7—N6—Cd1	123.14 (13)	C10—C9—C8	120.5 (3)
N2—N3—N4	110.66 (16)	C10—C9—H6	125 (2)
C2—N5—C1	124.64 (17)	C8—C9—H6	114 (2)
C2—N5—H1	117.6 (18)	N12—C13—C14	123.4 (3)



C1—N5—H1	113.5 (18)	N12—C13—H10	114.6 (16)
C2—N9—N8	104.23 (17)	C14—C13—H10	122.0 (16)
N7—N8—N9	110.31 (16)	C20—C19—C18	119.6 (3)
C1—N4—N3	103.75 (16)	C20—C19—H14	124.2 (19)
N8—N7—N6	108.63 (17)	C18—C19—H14	116 (2)
N4—C1—N1	112.23 (16)	C11—C10—C9	119.5 (3)
N4—C1—N5	121.93 (17)	C11—C10—H7	118.7 (18)
N1—C1—N5	125.85 (17)	C9—C10—H7	121.8 (18)
N6—C2—N9	112.07 (17)	C5—C4—C3	118.3 (3)
N6—C2—N5	125.76 (17)	C5—C4—H3	125 (2)
N9—C2—N5	122.17 (18)	C3—C4—H3	116 (2)
C3—N10—C7	119.1 (2)	C20—C21—C22	117.7 (3)
C3—N10—Cd1	123.25 (19)	C20—C21—H16	125.4 (17)
C7—N10—Cd1	116.97 (15)	C22—C21—H16	116.9 (18)
C17—N12—C13	118.86 (19)	C4—C5—C6	120.2 (3)
C17—N12—Cd1	117.10 (14)	C4—C5—H4	118 (2)
C13—N12—Cd1	123.39 (16)	C6—C5—H4	122 (2)
C12—N11—C8	119.13 (19)	C21—C20—C19	119.9 (3)
C12—N11—Cd1	122.94 (15)	C21—C20—H15	119 (2)
C8—N11—Cd1	117.85 (14)	C19—C20—H15	121 (2)
C22—N13—C18	118.75 (19)	H22—O1—H23	104 (4)
C22—N13—Cd1	123.41 (14)	N14—C28—C27	121.8 (3)
C18—N13—Cd1	117.78 (14)	N14—C28—C28 <sup>i</sup>	117.6 (3)
N10—C7—C6	120.5 (3)	C27—C28—C28 <sup>i</sup>	120.5 (3)
N10—C7—C8	116.96 (19)	C26—C27—C28	119.3 (3)
C6—C7—C8	122.6 (3)	C26—C27—H21	120.3
N12—C17—C16	119.7 (2)	C28—C27—H21	120.3
N12—C17—C18	117.10 (18)	C27—C26—C25	121.0 (4)
C16—C17—C18	123.2 (2)	C27—C26—H20	123 (2)
N11—C12—C11	123.4 (3)	C25—C26—H20	116 (2)
N11—C12—H9	115.5 (14)	C26—C25—C24	118.7 (4)
C11—C12—H9	121.1 (14)	C26—C25—H19	126 (2)
N11—C8—C9	119.5 (2)	C24—C25—H19	115 (2)
N11—C8—C7	116.84 (19)	C28—N14—C24	117.4 (3)
C9—C8—C7	123.7 (2)	N14—C24—C25	121.7 (4)
N13—C18—C19	120.5 (2)	N14—C24—H18	109 (2)
N13—C18—C17	117.10 (18)	C25—C24—H18	129 (2)
C19—C18—C17	122.3 (2)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N5—H1 $\cdots$ N4 <sup>ii</sup>	0.77 (2)	2.17 (2)	2.929 (2)	174 (2)
O1—H22 $\cdots$ N9	0.82 (4)	2.08 (4)	2.893 (3)	172 (4)
O1—H23 $\cdots$ N3 <sup>ii</sup>	0.92 (4)	2.02 (5)	2.901 (3)	159 (4)

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

Fig. 1

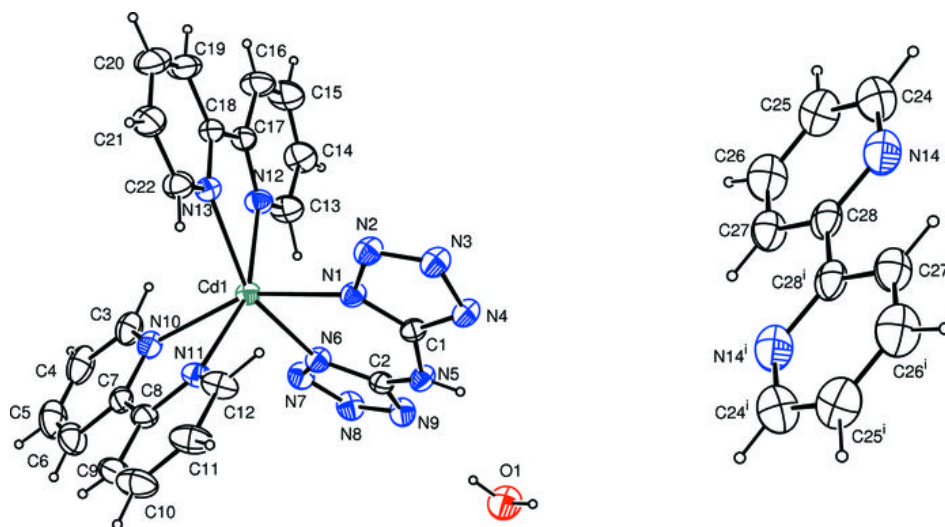


Fig. 2

