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

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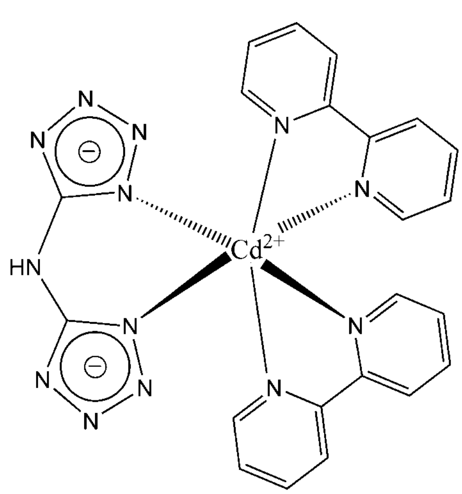
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.024; wR factor = 0.064; data-to-parameter ratio = 13.8.

The title complex, $[Cd(C_2HN_9)(C_{10}H_8N_2)_2]\cdot0.5C_{10}H_8N_2\cdot H_2O$, 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 Cd^{II} ion is coordinated by four N atoms from two 2,2′-bipyridine ligands and two N atoms from an $HBTA^-$ anion ligand [where H_2BTA is *N*,*N*-bis(1*H*-tetrazol-5-yl)amine], forming an octahedral geometry. The complex is linked into a three-dimensional network by O—H···N and N—H···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).



$\cdot 0.5C_{10}H_8N_2\cdot H_2O$

Experimental

Crystal data

$[Cd(C_2HN_9)(C_{10}H_8N_2)_2]\cdot0.5C_{10}H_8N_2\cdot H_2O$
M_r = 672.00
Monoclinic, $P2_1/n$
a = 15.1919 (12) Å
b = 11.2383 (9) Å
c = 17.5759 (14) Å
β = 106.073 (3)°
V = 2883.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.81 mm^{-1}
T = 296 (2) K
0.24 × 0.23 × 0.13 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
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_{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
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H1···N4^i	0.77 (2)	2.17 (2)	2.929 (2)	174 (2)
O1—H22···N9	0.82 (4)	2.08 (4)	2.893 (3)	172 (4)
O1—H23···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*.

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

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  doi:10.1107/S1600536807066846

supplementary materials

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

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

Comment

The H_2BTA (where H_2BTA 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_2BTA 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 $HBTA^{-}$ anion ligands, half 2,2'-bipyridine guest molecule and a solvent water molecule (Fig. 1). The $HBTA^{-}$ ligand acts as a chelatingbidentate and the Cd^{II} cation is coordinated to four N atoms from two 2,2'-bipyridine ligands and two N atoms from a $HBTA^{-}$ 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 $Cd(Cl)_2·4H_2O$ (0.026 g, 0.1 mmol), H_2BTA (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 $C_{27}H_{23}Cd_1N_{14}O_1$: 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

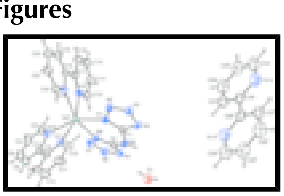


Fig. 1. The molecular structure of the complex, with atom labels and 30% probability displacement ellipsoids for non-H atoms. Symmetry code (i): $-x$, $-y$, $-z$.

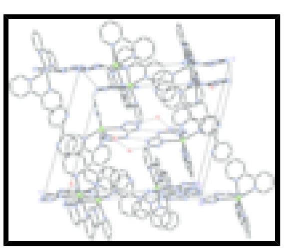


Fig. 2. The packing diagram of the complex, showing a three-dimensional network connected by O—H···N and N—H···N hydrogen bonds (dashed lines) and by the stacking interactions of aryls between the parallel 2,2'-bipyridine molecules. H atoms not involved in hydrogen bonding have been omitted.

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

Crystal data

$[Cd(C_2HN_9)(C_{10}H_8N_2)_2]\cdot0.5C_{10}H_8N_2\cdot H_2O$	$F_{000} = 1356$
$M_r = 672.00$	$D_x = 1.548$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P2yn	Cell parameters from 6569 reflections
$a = 15.1919$ (12) Å	$\theta = 27.5–1.0°$
$b = 11.2383$ (9) Å	$\mu = 0.81$ mm^{-1}
$c = 17.5759$ (14) Å	$T = 296$ (2) K
$\beta = 106.073$ (3)°	Block, colourless
$V = 2883.5$ (4) Å^3	0.24 × 0.23 × 0.13 mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	6569 independent reflections
Radiation source: fine-focus sealed tube	5669 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 296(2)$ K	$\theta_{max} = 27.5°$
φ and ω scans	$\theta_{min} = 1.6°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -19\rightarrow19$
$T_{min} = 0.824$, $T_{max} = 0.901$	$k = -14\rightarrow14$
41852 measured reflections	$l = -21\rightarrow22$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.025$	$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.9028P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.064$	$(\Delta/\sigma)_{max} = 0.003$
$S = 1.07$	$\Delta\rho_{max} = 0.27$ e Å^{-3}
6569 reflections	$\Delta\rho_{min} = -0.30$ e Å^{-3}
477 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00357 (18)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{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)

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 (Å^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)

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^{i}	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^{i}	117.6 (3)
N10—C7—C6	120.5 (3)	C27—C28—C28^{i}	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)		

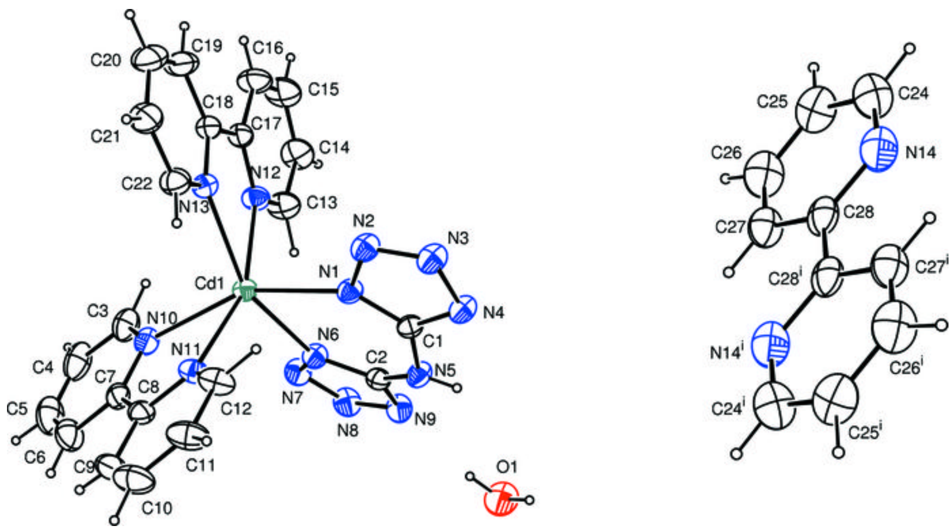
Symmetry codes: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H1···N4^{ii}	0.77 (2)	2.17 (2)	2.929 (2)	174 (2)
O1—H22···N9	0.82 (4)	2.08 (4)	2.893 (3)	172 (4)
O1—H23···N3^{ii}	0.92 (4)	2.02 (5)	2.901 (3)	159 (4)

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*+1.

Fig. 1


C20
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N8
C6
C9
C11
C10
O1
C25
C24
C26
N14
C28
C27
C28i
C27i
N14i
C26i
C24i
C25i

Fig. 2