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Aqua(benzene-1,2-dicarboxylato-κO)bis[2-(1*H*-pyrazol-3-yl-κN^2)pyridine-κN]-cadmium(II)

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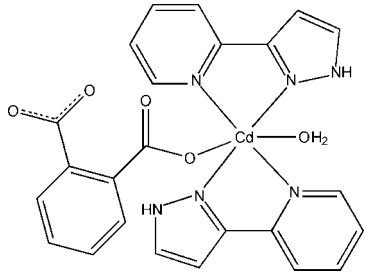
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.033; wR factor = 0.064; data-to-parameter ratio = 12.5.

In the mononuclear title complex, $[Cd(C_8H_4O_4)(C_8H_7N_3)_2(H_2O)]$, the Cd^{II} atom is six-coordinated in a distorted octahedral geometry by four N atoms from two bidentate chelating 2-(1*H*-pyrazol-3-yl)pyridine ligands, one O atom from a benzene-1,2-dicarboxylate ligand and one water molecule. The molecular structure features intramolecular O—H···O and N—H···O hydrogen bonds. In the crystal structure, the complex molecules are assembled into a two-dimensional supramolecular layer parallel to (011) *via* O—H···O and N—H···O hydrogen bonds and π–π stacking interactions between the pyridyl and pyrazole rings [centroid–centroid distances = 3.544 (2) and 3.722 (3) Å].

Related literature

For general background to the roles played by aromatic ring stacking and hydrogen bonding in biological reactions and in molecular recognition and self-organization, see: Borrows *et al.* (1995); Hunter (1994). For related structures, see: Cheng *et al.* (2006); Hu *et al.* (2008); Wan *et al.* (2003).



Experimental

Crystal data

$[Cd(C_8H_4O_4)(C_8H_7N_3)_2(H_2O)]$
M_r = 584.86
Triclinic, $P\overline{1}$
a = 10.1546 (7) Å
b = 10.7709 (7) Å
c = 12.4900 (9) Å
α = 64.986 (1)°
β = 71.209 (1)°
γ = 81.618 (1)°
V = 1171.90 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 296 K
0.28 × 0.22 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.771, T_{max} = 0.828
5869 measured reflections
4075 independent reflections
3194 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.064
S = 1.06
4075 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O3^{i}	0.85	1.84	2.672 (4)	168
O5—H5B···O3	0.85	2.07	2.892 (4)	164
N3—H3A···O4^{i}	0.86	1.79	2.646 (4)	176
N6—H6···O2	0.86	1.91	2.700 (4)	152

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: HY2347).

References

Borrows, A. D., Chan, C. M., Chowdhry, M. M., Mcgrady, J. E. & Mingos, D. M. P. (1995). *Chem. Soc. Rev.* **24**, 329–340.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cheng, J.-W., Zhang, J., Zheng, S.-T., Zhang, M.-B. & Yang, G.-Y. (2006). *Angew. Chem. Int. Ed.* **45**, 73–77.
Hu, T.-L., Zou, R.-Q., Li, J.-R. & Bu, X.-H. (2008). *Dalton Trans.* pp. 1302–1311.
Hunter, C. A. (1994). *Chem. Soc. Rev.* **23**, 101–110.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wan, Y.-H., Zhang, L.-P., Jin, L.-P., Gao, S. & Lu, S.-Z. (2003). *Inorg. Chem.* **42**, 4985–4994.

supporting information

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Aqua(benzene-1,2-dicarboxylato-κO)bis[2-(1*H*-pyrazol-3-yl-κN^2)pyridine-κN]cadmium(II)

Jian-Hua Guo

S1. Comment

The strategies for the construction of functional systems depend on the nature of the interactions responsible for creating networks. Aromatic ring stacking and hydrogen bonds are two important types of intermolecular non-covalent interactions, which play vital roles in highly efficient and specific biological reactions and are essential for molecular recognition and self-organization (Borrows *et al.*, 1995; Hunter, 1994). Benzene-1,2-dicarboxylic acid (1,2-H_2bdc) exhibits rich coordination modes to metal centers owing to its rigidity and polycarboxylate groups. Therefore, its metal complexes often show two- or three-dimensional structures (Cheng *et al.*, 2006; Wan *et al.*, 2003). 3-(2-Pyridyl)pyrazole (*L*) can act as a simple bidentate chelating ligand, similar to 2,2′-bipyridine (or 1,10-phenanthroline) (Hu *et al.*, 2008). In the present paper, we report the crystal structure of the title compound, a new Cd^{II} complex based on the mixed ligands *L* and 1,2-bdc, in which interesting hydrogen-bonding and π–π stacking interactions are observed.

In the title mononuclear compound, as shown in Fig. 1, the Cd^{II} atom is coordinated by four N atoms from two *L* ligands, with Cd—N bond lengths in the range of 2.241 (3)–2.525 (3) Å, one O atom from the carboxylate group of a 1,2-bdc ligand, with a Cd—O bond distance of 2.306 (3)Å and one O atom from a water molecule, with a Cd—O bond distance of 2.306 (2) Å. Thus, the coordination polyhedron around the Cd^{II} atom can be best described as distorted octahedral. The complex molecule involves intramolecular O—H···O and N—H···O hydrogen bonds (Table 1). Analysis of the crystal packing indicates that intermolecular O—H···O and N—H···O hydrogen bonds link two complex molecules, producing a dimeric unit. The dimeric units are arranged in a parallel fashion, which makes the aromatic stacking available to afford a two-dimensional supramolecular layer (Fig. 2). The centroid–centroid distances between the pyridyl and pyrazolyl rings are 3.544 (2)Å and 3.722 (3) Å and their corresponding dihedral angles are 3.40 (2) and 4.68 (1)°, respectively.

S2. Experimental

The title complex was obtained by the reaction of $Cd(CH_3CO_2)_2.2H_2O$, 3-(2-pyridyl)pyrazole and benzene-1,2-dicarboxylic acid in a molar ratio of 1:1:1, mixed with water (10 ml) under hydrothermal conditions at 413 K for 3 d. After cooled to room temperature at a rate of 5 K h^{-1}, colorless block crystals suitable for X-ray analysis were obtained in a 60% yield. Analysis, calculated for $C_{24}H_{20}CdN_6O_5$: C 49.29, H 3.45, N 14.37%; found: C 49.33, H 3.35, N 14.44%.

S3. Refinement

Although all H atoms were visible in difference Fourier maps, they were placed in geometrically calculated positions and refined as riding atoms, with C—H = 0.93, N—H = 0.86 and O—H = 0.85 Å and with U_{iso}(H) = 1.2U_{eq}(C, N) and U_{iso}(H) = 1.5U_{eq}(O).

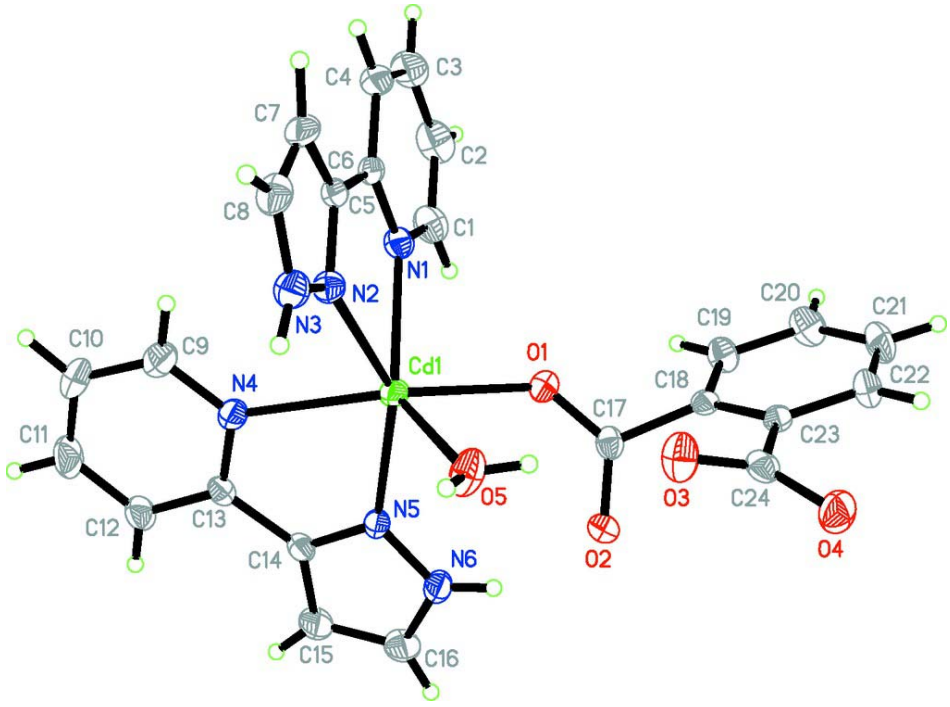

Figure 1

The molecular structure of the title complex, showing 30% probability displacement ellipsoids.

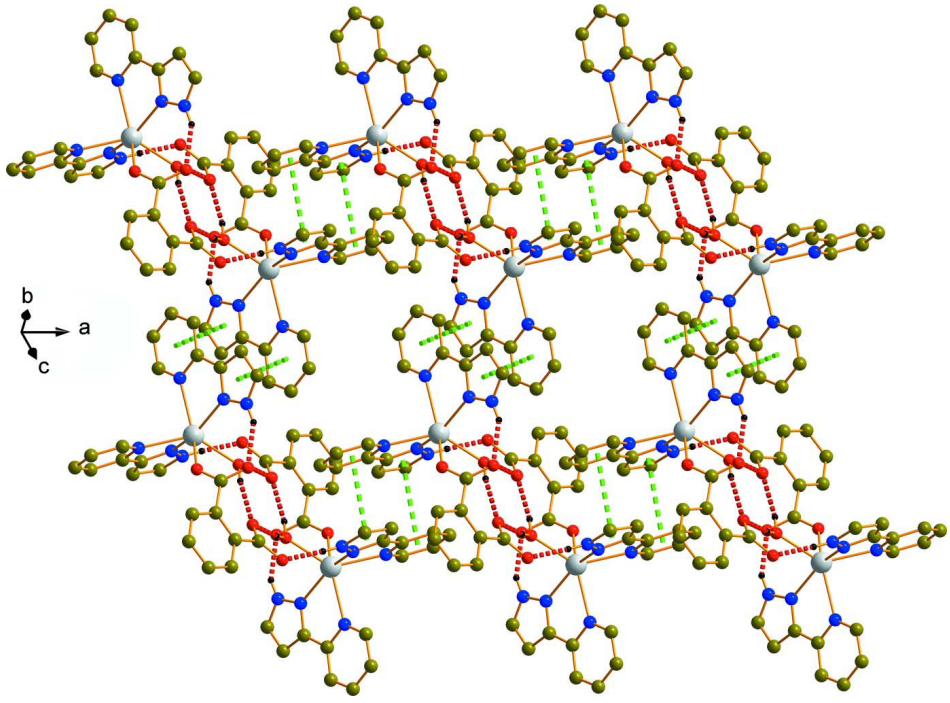

Figure 2

The two-dimensional supramolecular layer in the title complex, formed *via* O—H···O, N—H···O hydrogen bonds and π–π stacking interactions (dashed lines).

Aqua(benzene-1,2-dicarboxylato-κO)bis[2-(1*H*-pyrazol-3-yl-κN^2)pyridine-κN]cadmium(II)

Crystal data

$[Cd(C_8H_4O_4)(C_8H_7N_3)_2(H_2O)]$
$M_r = 584.86$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.1546\ (7)$ Å
$b = 10.7709\ (7)$ Å
$c = 12.4900\ (9)$ Å
$\alpha = 64.986\ (1)°$
$\beta = 71.209\ (1)°$
$\gamma = 81.618\ (1)°$
$V = 1171.90\ (14)$ Å^3
$Z = 2$
$F(000) = 588$
$D_x = 1.657$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2320 reflections
$\theta = 2.4–26.3°$
$\mu = 0.98$ mm^{-1}
$T = 296$ K
Block, colorless
0.28 × 0.22 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.771$, $T_{max} = 0.828$
5869 measured reflections
4075 independent reflections
3194 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -12\rightarrow12$
$k = -11\rightarrow12$
$l = -14\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.064$
$S = 1.06$
4075 reflections
325 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
$w = 1/[\sigma^2(F_o^2) + (0.0213P)^2 + 0.3676P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.63$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.24772 (3)	0.29292 (3)	0.32881 (3)	0.03231 (10)
O1	0.1867 (3)	0.2927 (3)	0.5234 (2)	0.0476 (7)
O2	0.3783 (3)	0.3400 (3)	0.5504 (2)	0.0436 (7)
O3	0.3964 (3)	0.0332 (3)	0.6592 (3)	0.0526 (7)
O4	0.4584 (3)	−0.0169 (3)	0.8281 (2)	0.0553 (8)
O5	0.4235 (3)	0.1523 (3)	0.3978 (2)	0.0518 (7)
H5A	0.4793	0.0992	0.3694	0.078*
H5B	0.4031	0.1299	0.4751	0.078*
N1	0.0044 (3)	0.2749 (3)	0.3848 (3)	0.0356 (7)
N2	0.1955 (3)	0.1179 (3)	0.2898 (3)	0.0335 (7)
N3	0.2667 (3)	0.0223 (3)	0.2516 (3)	0.0414 (8)
H3A	0.3558	0.0203	0.2226	0.050*

N4	0.2559 (3)	0.4476 (3)	0.1084 (3)	0.0391 (8)
N5	0.3742 (3)	0.4808 (3)	0.2559 (3)	0.0337 (7)
N6	0.4404 (3)	0.5217 (3)	0.3126 (3)	0.0428 (8)
H6	0.4467	0.4744	0.3861	0.051*
C1	−0.0887 (4)	0.3532 (4)	0.4319 (4)	0.0483 (11)
H1	−0.0561	0.4242	0.4401	0.058*
C2	−0.2294 (5)	0.3350 (5)	0.4689 (4)	0.0587 (12)
H2	−0.2909	0.3935	0.4993	0.070*
C3	−0.2772 (4)	0.2280 (5)	0.4598 (4)	0.0601 (13)
H3	−0.3722	0.2125	0.4851	0.072*
C4	−0.1854 (4)	0.1449 (4)	0.4138 (3)	0.0453 (11)
H4	−0.2169	0.0719	0.4077	0.054*
C5	−0.0440 (4)	0.1701 (4)	0.3760 (3)	0.0330 (9)
C6	0.0611 (4)	0.0854 (4)	0.3267 (3)	0.0324 (9)
C7	0.0489 (4)	−0.0336 (4)	0.3124 (3)	0.0452 (11)
H7	−0.0324	−0.0786	0.3316	0.054*
C8	0.1816 (5)	−0.0697 (4)	0.2642 (4)	0.0462 (11)
H8	0.2082	−0.1450	0.2437	0.055*
C9	0.1999 (5)	0.4256 (5)	0.0353 (4)	0.0578 (12)
H9	0.1482	0.3466	0.0681	0.069*
C10	0.2141 (5)	0.5130 (5)	−0.0862 (4)	0.0635 (13)
H10	0.1728	0.4939	−0.1340	0.076*
C11	0.2908 (4)	0.6286 (5)	−0.1340 (4)	0.0579 (12)
H11	0.3027	0.6895	−0.2158	0.069*
C12	0.3501 (4)	0.6549 (4)	−0.0614 (3)	0.0431 (10)
H12	0.4024	0.7333	−0.0931	0.052*
C13	0.3305 (3)	0.5622 (3)	0.0601 (3)	0.0312 (9)
C14	0.3906 (4)	0.5814 (3)	0.1437 (3)	0.0313 (8)
C15	0.4666 (4)	0.6870 (4)	0.1304 (4)	0.0485 (11)
H15	0.4923	0.7688	0.0615	0.058*
C16	0.4951 (4)	0.6451 (4)	0.2400 (4)	0.0529 (12)
H16	0.5442	0.6941	0.2604	0.064*
C17	0.2603 (4)	0.2903 (3)	0.5888 (3)	0.0330 (9)
C18	0.1943 (3)	0.2270 (3)	0.7271 (3)	0.0284 (8)
C19	0.0726 (4)	0.2855 (4)	0.7768 (3)	0.0423 (10)
H19	0.0285	0.3548	0.7243	0.051*
C20	0.0159 (4)	0.2427 (4)	0.9027 (4)	0.0514 (11)
H20	−0.0655	0.2833	0.9347	0.062*
C21	0.0796 (4)	0.1403 (4)	0.9804 (4)	0.0523 (11)
H21	0.0423	0.1121	1.0655	0.063*
C22	0.1987 (4)	0.0793 (4)	0.9329 (3)	0.0434 (10)
H22	0.2414	0.0099	0.9866	0.052*
C23	0.2569 (3)	0.1189 (3)	0.8060 (3)	0.0288 (8)
C24	0.3806 (4)	0.0414 (4)	0.7593 (4)	0.0365 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03555 (16)	0.02947 (15)	0.03196 (15)	−0.00863 (11)	−0.01207 (12)	−0.00811 (11)
O1	0.0392 (16)	0.0718 (19)	0.0339 (15)	−0.0109 (14)	−0.0121 (13)	−0.0188 (14)
O2	0.0391 (15)	0.0525 (17)	0.0334 (14)	−0.0165 (13)	−0.0063 (12)	−0.0098 (13)
O3	0.0638 (19)	0.0536 (18)	0.0454 (17)	0.0198 (14)	−0.0187 (15)	−0.0289 (15)
O4	0.0462 (17)	0.068 (2)	0.0481 (17)	0.0108 (15)	−0.0218 (15)	−0.0174 (15)
O5	0.0597 (18)	0.0574 (18)	0.0525 (17)	0.0234 (14)	−0.0305 (15)	−0.0327 (15)
N1	0.0378 (18)	0.0329 (18)	0.0318 (17)	−0.0021 (15)	−0.0107 (15)	−0.0080 (15)
N2	0.0373 (18)	0.0305 (17)	0.0340 (18)	−0.0020 (15)	−0.0107 (15)	−0.0134 (15)
N3	0.043 (2)	0.042 (2)	0.041 (2)	0.0027 (16)	−0.0156 (17)	−0.0165 (17)
N4	0.0442 (19)	0.0408 (19)	0.0325 (18)	−0.0096 (16)	−0.0151 (16)	−0.0092 (15)
N5	0.0397 (18)	0.0361 (17)	0.0258 (16)	−0.0100 (14)	−0.0106 (14)	−0.0089 (15)
N6	0.053 (2)	0.045 (2)	0.0325 (18)	−0.0139 (17)	−0.0164 (16)	−0.0110 (16)
C1	0.057 (3)	0.036 (2)	0.043 (2)	0.001 (2)	−0.012 (2)	−0.010 (2)
C2	0.050 (3)	0.058 (3)	0.054 (3)	0.016 (2)	−0.008 (2)	−0.020 (2)
C3	0.032 (2)	0.083 (4)	0.052 (3)	0.001 (3)	−0.013 (2)	−0.014 (3)
C4	0.037 (2)	0.055 (3)	0.040 (2)	−0.010 (2)	−0.016 (2)	−0.010 (2)
C5	0.038 (2)	0.032 (2)	0.0241 (19)	−0.0078 (18)	−0.0155 (17)	0.0004 (17)
C6	0.037 (2)	0.033 (2)	0.0236 (19)	−0.0105 (18)	−0.0107 (17)	−0.0037 (17)
C7	0.059 (3)	0.040 (2)	0.041 (2)	−0.020 (2)	−0.019 (2)	−0.011 (2)
C8	0.068 (3)	0.033 (2)	0.042 (2)	−0.005 (2)	−0.022 (2)	−0.014 (2)
C9	0.067 (3)	0.064 (3)	0.048 (3)	−0.022 (2)	−0.021 (2)	−0.017 (2)
C10	0.072 (3)	0.087 (4)	0.045 (3)	−0.011 (3)	−0.030 (3)	−0.026 (3)
C11	0.063 (3)	0.068 (3)	0.030 (2)	0.004 (3)	−0.020 (2)	−0.006 (2)
C12	0.046 (2)	0.042 (2)	0.032 (2)	−0.0029 (19)	−0.0107 (19)	−0.0053 (19)
C13	0.0270 (19)	0.032 (2)	0.0267 (19)	0.0024 (16)	−0.0052 (16)	−0.0075 (17)
C14	0.033 (2)	0.030 (2)	0.027 (2)	−0.0046 (17)	−0.0037 (17)	−0.0100 (17)
C15	0.058 (3)	0.039 (2)	0.042 (2)	−0.022 (2)	−0.009 (2)	−0.007 (2)
C16	0.063 (3)	0.047 (3)	0.051 (3)	−0.028 (2)	−0.008 (2)	−0.019 (2)
C17	0.042 (2)	0.029 (2)	0.028 (2)	−0.0002 (18)	−0.0095 (19)	−0.0121 (17)
C18	0.030 (2)	0.030 (2)	0.0287 (19)	−0.0084 (16)	−0.0068 (17)	−0.0146 (17)
C19	0.046 (2)	0.037 (2)	0.037 (2)	0.0019 (19)	−0.010 (2)	−0.0114 (19)
C20	0.048 (3)	0.056 (3)	0.045 (3)	0.006 (2)	0.000 (2)	−0.028 (2)
C21	0.062 (3)	0.059 (3)	0.027 (2)	−0.005 (2)	0.001 (2)	−0.017 (2)
C22	0.051 (3)	0.043 (2)	0.028 (2)	0.000 (2)	−0.010 (2)	−0.0078 (19)
C23	0.031 (2)	0.0283 (19)	0.030 (2)	−0.0057 (16)	−0.0089 (17)	−0.0122 (17)
C24	0.041 (2)	0.028 (2)	0.035 (2)	−0.0080 (18)	−0.006 (2)	−0.0080 (18)

Geometric parameters (Å, º)

Cd1—N5	2.241 (3)	C4—H4	0.9300
Cd1—N2	2.304 (3)	C5—C6	1.456 (5)
Cd1—O1	2.306 (3)	C6—C7	1.394 (5)
Cd1—O5	2.306 (2)	C7—C8	1.360 (5)
Cd1—N1	2.355 (3)	C7—H7	0.9300
Cd1—N4	2.525 (3)	C8—H8	0.9300

O1—C17	1.263 (4)	C9—C10	1.378 (6)
O2—C17	1.246 (4)	C9—H9	0.9300
O3—C24	1.248 (4)	C10—C11	1.367 (6)
O4—C24	1.262 (4)	C10—H10	0.9300
O5—H5A	0.8500	C11—C12	1.372 (5)
O5—H5B	0.8500	C11—H11	0.9300
N1—C1	1.334 (5)	C12—C13	1.387 (5)
N1—C5	1.352 (4)	C12—H12	0.9300
N2—N3	1.336 (4)	C13—C14	1.461 (5)
N2—C6	1.340 (4)	C14—C15	1.389 (5)
N3—C8	1.336 (4)	C15—C16	1.363 (5)
N3—H3A	0.8600	C15—H15	0.9300
N4—C9	1.331 (5)	C16—H16	0.9300
N4—C13	1.345 (4)	C17—C18	1.513 (5)
N5—C14	1.336 (4)	C18—C19	1.385 (5)
N5—N6	1.343 (4)	C18—C23	1.395 (5)
N6—C16	1.329 (4)	C19—C20	1.377 (5)
N6—H6	0.8600	C19—H19	0.9300
C1—C2	1.369 (5)	C20—C21	1.367 (5)
C1—H1	0.9300	C20—H20	0.9300
C2—C3	1.373 (6)	C21—C22	1.372 (5)
C2—H2	0.9300	C21—H21	0.9300
C3—C4	1.360 (6)	C22—C23	1.394 (5)
C3—H3	0.9300	C22—H22	0.9300
C4—C5	1.389 (5)	C23—C24	1.500 (5)

N5—Cd1—N2	146.39 (10)	C8—C7—C6	105.2 (3)
N5—Cd1—O1	89.21 (9)	C8—C7—H7	127.4
N2—Cd1—O1	123.55 (9)	C6—C7—H7	127.4
N5—Cd1—O5	91.79 (10)	N3—C8—C7	107.9 (4)
N2—Cd1—O5	86.61 (10)	N3—C8—H8	126.1
O1—Cd1—O5	81.39 (9)	C7—C8—H8	126.1
N5—Cd1—N1	128.46 (10)	N4—C9—C10	123.9 (4)
N2—Cd1—N1	70.85 (11)	N4—C9—H9	118.1
O1—Cd1—N1	79.65 (10)	C10—C9—H9	118.1
O5—Cd1—N1	134.70 (10)	C11—C10—C9	117.8 (4)
N5—Cd1—N4	67.54 (10)	C11—C10—H10	121.1
N2—Cd1—N4	86.92 (10)	C9—C10—H10	121.1
O1—Cd1—N4	141.67 (10)	C10—C11—C12	120.0 (4)
O5—Cd1—N4	127.21 (10)	C10—C11—H11	120.0
N1—Cd1—N4	91.24 (10)	C12—C11—H11	120.0
C17—O1—Cd1	131.2 (2)	C11—C12—C13	118.7 (4)
Cd1—O5—H5A	130.4	C11—C12—H12	120.7
Cd1—O5—H5B	107.9	C13—C12—H12	120.7
H5A—O5—H5B	116.4	N4—C13—C12	122.0 (3)
C1—N1—C5	117.7 (3)	N4—C13—C14	115.6 (3)
C1—N1—Cd1	125.5 (3)	C12—C13—C14	122.4 (3)
C5—N1—Cd1	116.6 (2)	N5—C14—C15	110.1 (3)

N3—N2—C6	105.9 (3)	N5—C14—C13	117.4 (3)
N3—N2—Cd1	136.5 (2)	C15—C14—C13	132.5 (3)
C6—N2—Cd1	117.0 (2)	C16—C15—C14	105.1 (3)
C8—N3—N2	111.2 (3)	C16—C15—H15	127.4
C8—N3—H3A	124.4	C14—C15—H15	127.4
N2—N3—H3A	124.4	N6—C16—C15	108.0 (3)
C9—N4—C13	117.6 (3)	N6—C16—H16	126.0
C9—N4—Cd1	127.5 (3)	C15—C16—H16	126.0
C13—N4—Cd1	114.9 (2)	O2—C17—O1	126.4 (3)
C14—N5—N6	105.8 (3)	O2—C17—C18	117.4 (3)
C14—N5—Cd1	124.4 (2)	O1—C17—C18	116.1 (3)
N6—N5—Cd1	129.7 (2)	C19—C18—C23	119.4 (3)
C16—N6—N5	111.1 (3)	C19—C18—C17	118.2 (3)
C16—N6—H6	124.5	C23—C18—C17	122.3 (3)
N5—N6—H6	124.5	C20—C19—C18	121.0 (4)
N1—C1—C2	123.7 (4)	C20—C19—H19	119.5
N1—C1—H1	118.2	C18—C19—H19	119.5
C2—C1—H1	118.2	C21—C20—C19	119.9 (4)
C1—C2—C3	118.1 (4)	C21—C20—H20	120.1
C1—C2—H2	121.0	C19—C20—H20	120.1
C3—C2—H2	121.0	C20—C21—C22	119.9 (4)
C4—C3—C2	119.9 (4)	C20—C21—H21	120.0
C4—C3—H3	120.1	C22—C21—H21	120.0
C2—C3—H3	120.1	C21—C22—C23	121.4 (4)
C3—C4—C5	119.2 (4)	C21—C22—H22	119.3
C3—C4—H4	120.4	C23—C22—H22	119.3
C5—C4—H4	120.4	C22—C23—C18	118.3 (3)
N1—C5—C4	121.4 (4)	C22—C23—C24	119.2 (3)
N1—C5—C6	115.9 (3)	C18—C23—C24	122.5 (3)
C4—C5—C6	122.6 (3)	O3—C24—O4	124.5 (4)
N2—C6—C7	109.8 (3)	O3—C24—C23	118.6 (3)
N2—C6—C5	119.2 (3)	O4—C24—C23	116.8 (3)
C7—C6—C5	131.0 (3)		

N5—Cd1—O1—C17	−56.3 (3)	C3—C4—C5—N1	0.5 (5)
N2—Cd1—O1—C17	115.7 (3)	C3—C4—C5—C6	179.5 (3)
O5—Cd1—O1—C17	35.6 (3)	N3—N2—C6—C7	0.7 (4)
N1—Cd1—O1—C17	174.3 (3)	Cd1—N2—C6—C7	−171.7 (2)
N4—Cd1—O1—C17	−107.0 (3)	N3—N2—C6—C5	178.9 (3)
N5—Cd1—N1—C1	−31.9 (3)	Cd1—N2—C6—C5	6.6 (4)
N2—Cd1—N1—C1	179.9 (3)	N1—C5—C6—N2	−2.3 (5)
O1—Cd1—N1—C1	48.7 (3)	C4—C5—C6—N2	178.6 (3)
O5—Cd1—N1—C1	115.5 (3)	N1—C5—C6—C7	175.5 (4)
N4—Cd1—N1—C1	−93.8 (3)	C4—C5—C6—C7	−3.6 (6)
N5—Cd1—N1—C5	152.8 (2)	N2—C6—C7—C8	−0.6 (4)
N2—Cd1—N1—C5	4.6 (2)	C5—C6—C7—C8	−178.6 (4)
O1—Cd1—N1—C5	−126.5 (2)	N2—N3—C8—C7	0.1 (4)
O5—Cd1—N1—C5	−59.8 (3)	C6—C7—C8—N3	0.3 (4)

N4—Cd1—N1—C5	90.9 (2)	C13—N4—C9—C10	0.0 (7)
N5—Cd1—N2—N3	53.0 (4)	Cd1—N4—C9—C10	−177.2 (3)
O1—Cd1—N2—N3	−112.4 (3)	N4—C9—C10—C11	0.3 (7)
O5—Cd1—N2—N3	−35.1 (3)	C9—C10—C11—C12	−0.3 (7)
N1—Cd1—N2—N3	−175.1 (3)	C10—C11—C12—C13	0.0 (6)
N4—Cd1—N2—N3	92.5 (3)	C9—N4—C13—C12	−0.3 (5)
N5—Cd1—N2—C6	−137.6 (2)	Cd1—N4—C13—C12	177.2 (3)
O1—Cd1—N2—C6	56.9 (3)	C9—N4—C13—C14	−179.6 (3)
O5—Cd1—N2—C6	134.2 (2)	Cd1—N4—C13—C14	−2.1 (4)
N1—Cd1—N2—C6	−5.8 (2)	C11—C12—C13—N4	0.3 (6)
N4—Cd1—N2—C6	−98.2 (2)	C11—C12—C13—C14	179.5 (4)
C6—N2—N3—C8	−0.5 (4)	N6—N5—C14—C15	−0.7 (4)
Cd1—N2—N3—C8	169.6 (3)	Cd1—N5—C14—C15	175.8 (2)
N5—Cd1—N4—C9	177.2 (4)	N6—N5—C14—C13	178.7 (3)
N2—Cd1—N4—C9	19.5 (3)	Cd1—N5—C14—C13	−4.8 (4)
O1—Cd1—N4—C9	−126.0 (3)	N4—C13—C14—N5	4.3 (5)
O5—Cd1—N4—C9	102.9 (3)	C12—C13—C14—N5	−175.0 (3)
N1—Cd1—N4—C9	−51.2 (4)	N4—C13—C14—C15	−176.5 (4)
N5—Cd1—N4—C13	−0.1 (2)	C12—C13—C14—C15	4.3 (6)
N2—Cd1—N4—C13	−157.7 (3)	N5—C14—C15—C16	0.0 (5)
O1—Cd1—N4—C13	56.8 (3)	C13—C14—C15—C16	−179.2 (4)
O5—Cd1—N4—C13	−74.3 (3)	N5—N6—C16—C15	−1.1 (5)
N1—Cd1—N4—C13	131.5 (2)	C14—C15—C16—N6	0.6 (5)
N2—Cd1—N5—C14	46.0 (4)	Cd1—O1—C17—O2	30.6 (6)
O1—Cd1—N5—C14	−146.1 (3)	Cd1—O1—C17—C18	−152.7 (2)
O5—Cd1—N5—C14	132.5 (3)	O2—C17—C18—C19	116.8 (4)
N1—Cd1—N5—C14	−70.0 (3)	O1—C17—C18—C19	−60.2 (4)
N4—Cd1—N5—C14	2.6 (3)	O2—C17—C18—C23	−58.5 (5)
N2—Cd1—N5—N6	−138.4 (3)	O1—C17—C18—C23	124.5 (4)
O1—Cd1—N5—N6	29.5 (3)	C23—C18—C19—C20	2.8 (5)
O5—Cd1—N5—N6	−51.8 (3)	C17—C18—C19—C20	−172.6 (4)
N1—Cd1—N5—N6	105.6 (3)	C18—C19—C20—C21	−0.4 (6)
N4—Cd1—N5—N6	178.2 (3)	C19—C20—C21—C22	−0.9 (7)
C14—N5—N6—C16	1.1 (4)	C20—C21—C22—C23	−0.2 (6)
Cd1—N5—N6—C16	−175.2 (3)	C21—C22—C23—C18	2.6 (5)
C5—N1—C1—C2	−1.5 (6)	C21—C22—C23—C24	−175.2 (3)
Cd1—N1—C1—C2	−176.7 (3)	C19—C18—C23—C22	−3.8 (5)
N1—C1—C2—C3	1.7 (6)	C17—C18—C23—C22	171.4 (3)
C1—C2—C3—C4	−0.7 (7)	C19—C18—C23—C24	173.9 (3)
C2—C3—C4—C5	−0.3 (6)	C17—C18—C23—C24	−10.8 (5)
C1—N1—C5—C4	0.4 (5)	C22—C23—C24—O3	149.6 (3)
Cd1—N1—C5—C4	176.0 (3)	C18—C23—C24—O3	−28.2 (5)
C1—N1—C5—C6	−178.7 (3)	C22—C23—C24—O4	−27.2 (5)
Cd1—N1—C5—C6	−3.1 (4)	C18—C23—C24—O4	155.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O3^{i}	0.85	1.84	2.672 (4)	168
O5—H5*B*···O3	0.85	2.07	2.892 (4)	164
N3—H3*A*···O4^{i}	0.86	1.79	2.646 (4)	176
N6—H6···O2	0.86	1.91	2.700 (4)	152

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