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# *catena*-Poly[[[diaquacadmium(II)]-bis[$\mu$-4-*tert*-butyl-2,6-bis(1,2,4-triazol-1-ylmethyl)phenol]] dinitrate dihydrate]

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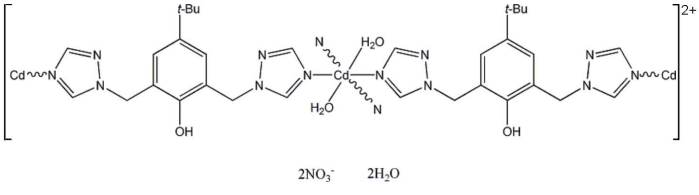
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.044; $wR$ factor = 0.107; data-to-parameter ratio = 14.3.

The title compound, $\{[Cd(C_{16}H_{20}N_6O)_2(H_2O)_2](NO_3)_2\cdot 2H_2O\}_n$, contains a $Cd^{II}$ atom, a 4-*tert*-butyl-2,6-bis(1,2,4-triazol-1-ylmethyl)phenol ligand ($L$), a nitrate anion and two water molecules in the asymmetric unit. The Cd atom resides on a crystallographic inversion centre, and the coordination about the Cd atom is distorted octahedral, formed by four equatorial N atoms from the triazole N atoms of four different $L$ ligands [Cd—N = 2.295 (3) and 2.395 (3) Å] and the O atoms from two axial water molecules [Cd—O = 2.287 (3) Å]. Two Cd atoms with two $L$ ligands form 24-membered $M_2L_2$ metallacycles along the $a$-axis direction, generating a double-stranded one-dimensional cationic chain. Inter- and intramolecular O—H···O/N hydrogen-bond interactions form a three-dimensional supramolecular network.

## Related literature

For related literature, see: Hoskins *et al.* (1997); Li *et al.* (2005); Ma *et al.* (2003); Yan *et al.* (1994); Zhu *et al.* (2004, 2007).




## Experimental

### *Crystal data*

$[Cd(C_{16}H_{20}N_6O)_2(H_2O)_2](NO_3)_2\cdot 2H_2O$
$M_r$ = 933.24
Monoclinic, $P2_1/c$
$a$ = 11.960 (4) Å
$b$ = 9.448 (3) Å
$c$ = 18.756 (6) Å
$\beta$ = 108.592 (4)°
$V$ = 2008.9 (11) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.62 mm$^{-1}$
$T$ = 293 (2) K
0.35 × 0.30 × 0.20 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.812, $T_{max}$ = 0.886
8433 measured reflections
3897 independent reflections
2974 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.107
$S$ = 1.08
3897 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.92 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.46 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cd1—O2 | 2.287 (3) | Cd1—N3 | 2.395 (3) |
| Cd1—N6$^{i}$ | 2.295 (3) | | |
| O2—Cd1—N6$^{ii}$ | 89.62 (10) | O2—Cd1—N3 | 93.35 (10) |
| O2—Cd1—N6$^{i}$ | 90.38 (10) | N6$^{ii}$—Cd1—N3 | 88.35 (10) |
| O2—Cd1—N3$^{iii}$ | 86.65 (10) | N6$^{i}$—Cd1—N3 | 91.65 (10) |

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

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 2.61 | 3.247 (4) | 135 |
| O1—H1···N2 | 0.82 | 1.99 | 2.777 (4) | 161 |
| C8—H8···O6 | 0.93 | 2.48 | 3.150 (8) | 129 |
| O2—H2$A$···O3$^{i}$ | 0.85 | 1.86 | 2.692 (4) | 164 |
| O2—H2$B$···O4$^{iv}$ | 0.85 | 2.13 | 2.951 (7) | 164 |
| O2—H2$B$···O6$^{iv}$ | 0.85 | 2.51 | 3.070 (7) | 124 |
| O3—H3$B$···N5$^{v}$ | 0.85 | 2.42 | 2.920 (5) | 118 |
| O3—H3$C$···O5$^{vi}$ | 0.85 | 2.32 | 3.163 (7) | 169 |
| C7—H7$B$···O3$^{vii}$ | 0.97 | 2.60 | 3.501 (5) | 155 |
| C8—H8···O4$^{iv}$ | 0.93 | 2.22 | 2.996 (7) | 140 |
| C12—H12···O5$^{viii}$ | 0.93 | 2.41 | 3.149 (7) | 136 |

Symmetry codes: (i) $x+1, y, z$; (iv) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $x, y+1, z$; (vi) $x-1, y+1, z$; (vii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (viii) $x-1, y, z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: GG2024).

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## References


Bruker (2000). *SMART* (Version 5.622), *SAINT* (Version 6.02a), *SADABS* (Version 6.02a) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Hoskins, B. F., Robson, R. & Slizys, D. A. (1997). *J. Am. Chem. Soc.* **119**, 2952–2953.

Li, B.-L., Peng, Y.-F., Li, B.-Z. & Zhang, Y. (2005). *Chem. Commun.* pp. 2333–2335.

Ma, Y.-L., Huang, W., Yao, J.-C., Li, B., Gou, S.-H. & Fun, H.-K. (2003). *J. Mol. Struct.* **658**, 51–58.

Yan, J. M., Zhang, Z. J., Yuan, D. Q., Xie, R. G. & Zhao, H. M. (1994). *Synth. Commun.* **24**, 47–52.

Zhu, H.-B., Chu, Z.-L., Hu, D.-H., Huang, W. & Gou, S.-H. (2007). *Inorg. Chem. Commun.* **10**, 362–366.

Zhu, H.-B., Huang, C.-H., Huang, W. & Gou, S.-H. (2004). *Inorg. Chem. Commun.* **7**, 1095–1099.

# supplementary materials

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# *catena*-Poly[[[diaquacadmium(II)]-bis[$\mu$-4-*tert*-butyl-2,6-bis(1,2,4-triazol-1-ylmethyl)phenol]] dinitrate dihydrate]

**Z.-L. Chu, G. Xu, W. Huang and S.-H. Gou**

## Comment

In recent years, organic ligands with azole units have become a new class of supramolecular synthons of intense interest in creating appealing coordination polymers (Hoskins *et al.*, 1997; Li *et al.*, 2005). In our previous studies, we synthesized two kinds of flexible bidentate ligands 1,6-di(imidazole-1-yl-methyl)-4-*R*-phenol and 1,6-di(triazole-1-yl-methyl)-4-*R*-phenol (*R* = Me, *t*-Bu, or Cl), and demonstrated that they can form different structures and topologies with different metal ions (Ma *et al.*, 2003; Zhu *et al.*, 2004; Zhu *et al.*, 2007). The title compound, (I), is obtained by the reaction of 1,6-di(triazole-1-yl-methyl)-4 − *t*-Bu-phenol(dttp) with cadmium nitrate in ethanol.

The asymmetric unit of (I) contains half a Cd(II) atom, one dttp ligand, two water molecules and a nitrate ion. The metal atoms are located on the crystallographic inversion center with octahedral geometry, formed equatorially by four N atoms of triazoles from four dttp ligands and axially by two O atoms from two water molecules (Fig. 1). Each dttp adopts a *trans* conformation in which two triazole groups of a ligand with a dihedral angle of 53.9 (3) ° are on the opposite direction of the central benzene ring. In this way two metal atoms and two dttp ligands form a 24-membered $M_2L_2$ macrocycle through Cd—N coordination bonds. In each macrocycle, two phenyl rings are found strictly in a plane and the intermetallic distance between the two $Cd^{II}$ atoms is 11.96 (1) Å. Such a metallomacrocyclic unit repeats along the *a*-axis to generate a double-stranded one-dimensional cationic chain as shown in Fig. 2.

Each phenol O—H moiety is directed at the N atom of a triazole moiety with H···N distances ranging from 1.99 to 2.61 Å, indicative of strong intramolecular hydrogen-bonding interactions. It is noticed that the resulting one-dimensional chains are further linked together to a three-dimensional framework by the uncoordinated water molecules and nitrate anions through O–H···O, O–H···N and C–H···O hydrogen-bonding interactions as shown in Fig. 3.

## Experimental

All solvents and chemicals were of analytical grade and were used without further purification. Ligand dttp was prepared *via* a one-step Mannich reaction as a white powder in 57% yield (Yan *et al.*, 1994). For the synthesis of (I), an ethanol solution (10 ml) of $Cd(NO_3)_2{\cdot}6H_2O$ (34.4 mg, 0.1 mmol) was added slowly with constant stirring to a solution of dttp (31.2 mg, 0.1 mmol) in ethanol (30 ml) to give a clear solution. The reaction mixture was left to stand at room temperature for one week and colorless crystalline products were obtained (34.2 mg, 79%). Anal. Calcd. for $C_{32}H_{48}CdN_{14}O_{12}$: C, 43.84; H, 5.52; N, 22.37. Found: C, 41.18; H, 5.18; N, 21.01. Infra-red (KBr, $cm^{-1}$): 3422(*s*), 3233(*m*), 2962(*m*), 1656(*m*), 1522(*s*).

## Refinement

All non-hydrogen atoms were refined anisotropically, whereas the positions of all H atoms were fixed geometrically and treated as riding atoms in the refinement with *X*—H distances set as follows: C–H 0.93–0.97 Å and O–H 0.82–0.85 Å.

## Figures

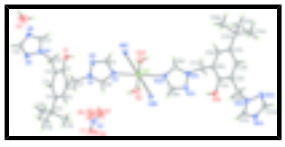

Fig. 1. Molecular structure of the title compound (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

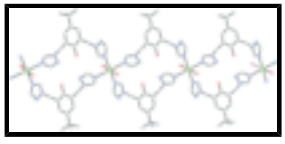

Fig. 2. A perspective view of the one-dimensional cationic chain structure of (I) along the *a*-axis.

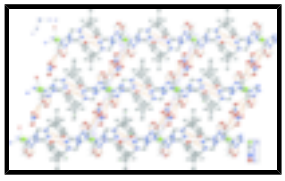

Fig. 3. A three-dimensional packing diagram of (I). For clarity, only H atoms involved in hydrogen bonds are shown. Hydrogen-bond contacts are indicated by dashed lines.

## *catena*-Poly[[[diaquacadmium(II)]-bis[μ-4-*tert*-butyl-2,6-bis(1,2,4- triazol-1-ylmethyl)phenol]] dinitrate dihydrate]

*Crystal data*

| | |
|---|---|
| $[Cd(C_{16}H_{20}N_6O)_2(H_2O)_2](NO_3)_2{\cdot}2H_2O$ | $F_{000}$ = 964 |
| $M_r$ = 933.24 | $D_x$ = 1.543 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 848 reflections |
| $a$ = 11.960 (4) Å | θ = 2.3–23.5º |
| $b$ = 9.448 (3) Å | μ = 0.62 mm$^{-1}$ |
| $c$ = 18.756 (6) Å | $T$ = 293 (2) K |
| β = 108.592 (4)º | Block, colorless |
| $V$ = 2008.9 (11) Å$^3$ | 0.35 × 0.30 × 0.20 mm |
| $Z$ = 2 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3897 independent reflections |
| Radiation source: fine-focus sealed tube | 2974 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.031 |
| $T$ = 293(2) K | $\theta_{max}$ = 26.0º |
| φ and ω scans | $\theta_{min}$ = 1.8º |
| Absorption correction: multi-scan (SADABS; Bruker, 2000) | $h$ = −12→14 |
| $T_{min}$ = 0.812, $T_{max}$ = 0.886 | $k$ = −7→11 |
| 8433 measured reflections | $l$ = −22→23 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | H-atom parameters constrained |
| $wR(F^2) = 0.107$ | $w = 1/[\sigma^2(F_o^2) + (0.047P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.08$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 3897 reflections | $\Delta\rho_{max} = 0.92$ e Å$^{-3}$ |
| 272 parameters | $\Delta\rho_{min} = -0.46$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Experimental**. The structure was solved by direct methods (Bruker, 2000) and successive difference Fourier syntheses.

**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$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cd1 | 1.0000 | 0.5000 | 0.0000 | 0.03931 (14) |
| C1 | 0.4821 (3) | 0.1571 (4) | 0.07099 (17) | 0.0367 (8) |
| C2 | 0.4142 (3) | 0.0348 (3) | 0.05930 (19) | 0.0362 (8) |
| C3 | 0.4560 (3) | −0.0813 (4) | 0.10476 (18) | 0.0389 (8) |
| H3 | 0.4097 | −0.1625 | 0.0971 | 0.047* |
| C4 | 0.5635 (3) | −0.0817 (4) | 0.16110 (18) | 0.0389 (8) |
| C5 | 0.6286 (3) | 0.0425 (4) | 0.17102 (18) | 0.0394 (8) |
| H5 | 0.7015 | 0.0455 | 0.2085 | 0.047* |
| C6 | 0.5898 (3) | 0.1625 (3) | 0.12747 (17) | 0.0359 (7) |
| C7 | 0.6600 (3) | 0.2970 (4) | 0.14719 (19) | 0.0441 (9) |
| H7A | 0.6086 | 0.3715 | 0.1542 | 0.053* |
| H7B | 0.7219 | 0.2835 | 0.1948 | 0.053* |
| C8 | 0.8256 (3) | 0.3626 (4) | 0.0972 (2) | 0.0463 (9) |
| H8 | 0.8886 | 0.3422 | 0.1401 | 0.056* |
| C9 | 0.7236 (3) | 0.4264 (4) | −0.0096 (2) | 0.0489 (9) |
| H9 | 0.7025 | 0.4610 | −0.0585 | 0.059* |
| C10 | 0.2986 (3) | 0.0280 (4) | −0.0035 (2) | 0.0433 (9) |

| | | | | |
|---|---|---|---|---|
| H10A | 0.3098 | 0.0617 | −0.0496 | 0.052* |
| H10B | 0.2725 | −0.0696 | −0.0113 | 0.052* |
| C11 | 0.1637 (3) | 0.2360 (4) | −0.01451 (19) | 0.0452 (9) |
| H11 | 0.1845 | 0.2853 | −0.0513 | 0.054* |
| C12 | 0.0861 (3) | 0.1758 (4) | 0.0643 (2) | 0.0594 (11) |
| H12 | 0.0388 | 0.1771 | 0.0952 | 0.071* |
| C13 | 0.6105 (3) | −0.2113 (4) | 0.21066 (18) | 0.0456 (9) |
| C14 | 0.5190 (4) | −0.3283 (4) | 0.1967 (2) | 0.0707 (13) |
| H14A | 0.5023 | −0.3633 | 0.1464 | 0.106* |
| H14B | 0.4480 | −0.2915 | 0.2032 | 0.106* |
| H14C | 0.5489 | −0.4039 | 0.2318 | 0.106* |
| C15 | 0.6439 (4) | −0.1696 (5) | 0.2937 (2) | 0.0679 (12) |
| H15A | 0.5759 | −0.1321 | 0.3038 | 0.102* |
| H15B | 0.7048 | −0.0990 | 0.3048 | 0.102* |
| H15C | 0.6720 | −0.2514 | 0.3246 | 0.102* |
| C16 | 0.7174 (4) | −0.2704 (5) | 0.1931 (3) | 0.0804 (14) |
| H16A | 0.7468 | −0.3518 | 0.2240 | 0.121* |
| H16B | 0.7779 | −0.1994 | 0.2031 | 0.121* |
| H16C | 0.6948 | −0.2971 | 0.1410 | 0.121* |
| N1 | 0.7139 (2) | 0.3441 (3) | 0.09105 (15) | 0.0391 (7) |
| N2 | 0.6458 (2) | 0.3859 (3) | 0.02182 (16) | 0.0488 (8) |
| N3 | 0.8359 (2) | 0.4139 (3) | 0.03429 (16) | 0.0452 (7) |
| N4 | 0.2073 (2) | 0.1133 (3) | 0.01273 (14) | 0.0390 (7) |
| N5 | 0.1576 (3) | 0.0706 (4) | 0.06402 (18) | 0.0564 (8) |
| N6 | 0.0867 (2) | 0.2805 (3) | 0.01688 (16) | 0.0439 (7) |
| N7 | 0.9577 (4) | 0.0212 (6) | 0.2125 (3) | 0.0825 (13) |
| O1 | 0.43423 (19) | 0.2713 (2) | 0.02633 (14) | 0.0460 (6) |
| H1 | 0.4874 | 0.3215 | 0.0216 | 0.069* |
| O2 | 1.1054 (2) | 0.5603 (3) | 0.12084 (14) | 0.0670 (8) |
| H2A | 1.1197 | 0.6486 | 0.1253 | 0.080* |
| H2B | 1.0652 | 0.5326 | 0.1483 | 0.080* |
| O3 | 0.1714 (3) | 0.8280 (3) | 0.16290 (17) | 0.0990 (11) |
| H3B | 0.2153 | 0.8576 | 0.1383 | 0.149* |
| H3C | 0.1105 | 0.8802 | 0.1535 | 0.149* |
| O4 | 0.9864 (7) | −0.0496 (6) | 0.2614 (3) | 0.239 (4) |
| O5 | 0.9399 (5) | 0.0037 (5) | 0.1480 (3) | 0.164 (3) |
| O6 | 0.9167 (5) | 0.1339 (7) | 0.2248 (4) | 0.178 (2) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd1 | 0.0348 (2) | 0.0368 (2) | 0.0502 (2) | 0.00473 (15) | 0.01896 (15) | 0.00747 (17) |
| C1 | 0.0419 (18) | 0.032 (2) | 0.0437 (18) | 0.0064 (15) | 0.0250 (15) | 0.0041 (15) |
| C2 | 0.0361 (17) | 0.032 (2) | 0.0462 (19) | 0.0023 (13) | 0.0206 (15) | −0.0034 (14) |
| C3 | 0.0436 (19) | 0.031 (2) | 0.050 (2) | 0.0004 (15) | 0.0257 (16) | −0.0005 (16) |
| C4 | 0.046 (2) | 0.033 (2) | 0.0445 (19) | 0.0035 (16) | 0.0247 (16) | 0.0019 (16) |
| C5 | 0.0402 (18) | 0.042 (2) | 0.0401 (18) | 0.0016 (15) | 0.0187 (15) | 0.0037 (15) |
| C6 | 0.0406 (18) | 0.034 (2) | 0.0409 (17) | −0.0034 (14) | 0.0241 (15) | −0.0016 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C7 | 0.050 (2) | 0.041 (2) | 0.049 (2) | −0.0056 (16) | 0.0279 (17) | −0.0027 (17) |
| C8 | 0.0394 (19) | 0.049 (2) | 0.050 (2) | −0.0010 (16) | 0.0137 (16) | 0.0048 (18) |
| C9 | 0.044 (2) | 0.052 (3) | 0.050 (2) | −0.0069 (17) | 0.0143 (17) | 0.0138 (19) |
| C10 | 0.046 (2) | 0.036 (2) | 0.051 (2) | 0.0047 (15) | 0.0189 (16) | −0.0055 (15) |
| C11 | 0.049 (2) | 0.038 (2) | 0.052 (2) | 0.0077 (16) | 0.0210 (17) | 0.0092 (17) |
| C12 | 0.059 (2) | 0.056 (3) | 0.080 (3) | 0.012 (2) | 0.046 (2) | 0.018 (2) |
| C13 | 0.055 (2) | 0.039 (2) | 0.048 (2) | 0.0038 (16) | 0.0224 (17) | 0.0107 (17) |
| C14 | 0.087 (3) | 0.046 (3) | 0.073 (3) | −0.006 (2) | 0.016 (2) | 0.019 (2) |
| C15 | 0.087 (3) | 0.060 (3) | 0.053 (2) | 0.002 (2) | 0.018 (2) | 0.014 (2) |
| C16 | 0.080 (3) | 0.066 (3) | 0.110 (4) | 0.032 (2) | 0.051 (3) | 0.037 (3) |
| N1 | 0.0404 (15) | 0.0347 (17) | 0.0460 (16) | −0.0040 (12) | 0.0190 (13) | 0.0022 (13) |
| N2 | 0.0390 (16) | 0.051 (2) | 0.0560 (18) | −0.0041 (14) | 0.0148 (14) | 0.0149 (15) |
| N3 | 0.0421 (17) | 0.044 (2) | 0.0533 (17) | −0.0008 (13) | 0.0206 (14) | 0.0075 (14) |
| N4 | 0.0381 (15) | 0.0352 (18) | 0.0442 (15) | −0.0003 (12) | 0.0138 (12) | −0.0010 (13) |
| N5 | 0.0540 (19) | 0.048 (2) | 0.079 (2) | 0.0102 (16) | 0.0372 (17) | 0.0191 (18) |
| N6 | 0.0391 (16) | 0.0387 (18) | 0.0575 (18) | 0.0058 (13) | 0.0205 (14) | 0.0071 (14) |
| N7 | 0.088 (3) | 0.090 (4) | 0.071 (3) | 0.004 (2) | 0.028 (2) | 0.010 (3) |
| O1 | 0.0433 (13) | 0.0332 (15) | 0.0646 (15) | 0.0034 (11) | 0.0215 (12) | 0.0128 (12) |
| O2 | 0.086 (2) | 0.0573 (18) | 0.0549 (16) | 0.0001 (16) | 0.0189 (15) | 0.0034 (14) |
| O3 | 0.118 (3) | 0.070 (2) | 0.100 (2) | −0.0065 (19) | 0.022 (2) | 0.0237 (19) |
| O4 | 0.374 (10) | 0.121 (4) | 0.116 (4) | 0.077 (5) | −0.069 (5) | 0.028 (3) |
| O5 | 0.171 (5) | 0.258 (7) | 0.079 (3) | −0.079 (4) | 0.063 (3) | −0.017 (3) |
| O6 | 0.169 (5) | 0.143 (5) | 0.242 (7) | 0.026 (4) | 0.093 (5) | 0.025 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cd1—O2$^{i}$ | 2.287 (3) | C11—N4 | 1.307 (4) |
| Cd1—O2 | 2.287 (3) | C11—N6 | 1.311 (4) |
| Cd1—N6$^{ii}$ | 2.295 (3) | C11—H11 | 0.9300 |
| Cd1—N6$^{iii}$ | 2.295 (3) | C12—N5 | 1.312 (5) |
| Cd1—N3$^{i}$ | 2.395 (3) | C12—N6 | 1.332 (4) |
| Cd1—N3 | 2.395 (3) | C12—H12 | 0.9300 |
| C1—O1 | 1.374 (4) | C13—C14 | 1.518 (5) |
| C1—C6 | 1.383 (4) | C13—C16 | 1.524 (5) |
| C1—C2 | 1.389 (4) | C13—C15 | 1.531 (5) |
| C2—C3 | 1.382 (5) | C14—H14A | 0.9600 |
| C2—C10 | 1.505 (5) | C14—H14B | 0.9600 |
| C3—C4 | 1.380 (4) | C14—H14C | 0.9600 |
| C3—H3 | 0.9300 | C15—H15A | 0.9600 |
| C4—C5 | 1.387 (5) | C15—H15B | 0.9600 |
| C4—C13 | 1.532 (5) | C15—H15C | 0.9600 |
| C5—C6 | 1.388 (4) | C16—H16A | 0.9600 |
| C5—H5 | 0.9300 | C16—H16B | 0.9600 |
| C6—C7 | 1.502 (4) | C16—H16C | 0.9600 |
| C7—N1 | 1.469 (4) | N1—N2 | 1.353 (4) |
| C7—H7A | 0.9700 | N4—N5 | 1.343 (4) |
| C7—H7B | 0.9700 | N6—Cd1$^{iv}$ | 2.295 (3) |
| C8—N1 | 1.315 (4) | N7—O4 | 1.099 (6) |

| | | | |
|---|---|---|---|
| C8—N3 | 1.318 (4) | N7—O5 | 1.170 (6) |
| C8—H8 | 0.9300 | N7—O6 | 1.225 (6) |
| C9—N2 | 1.307 (4) | O1—H1 | 0.8200 |
| C9—N3 | 1.338 (4) | O2—H2A | 0.8500 |
| C9—H9 | 0.9300 | O2—H2B | 0.8500 |
| C10—N4 | 1.465 (4) | O3—H3B | 0.8500 |
| C10—H10A | 0.9700 | O3—H3C | 0.8499 |
| C10—H10B | 0.9700 | | |
| $O2^{i}$—Cd1—O2 | 180.00 (8) | N4—C11—H11 | 124.5 |
| $O2^{i}$—Cd1—$N6^{ii}$ | 90.38 (10) | N6—C11—H11 | 124.5 |
| O2—Cd1—$N6^{ii}$ | 89.62 (10) | N5—C12—N6 | 114.7 (3) |
| $O2^{i}$—Cd1—$N6^{iii}$ | 89.62 (10) | N5—C12—H12 | 122.7 |
| O2—Cd1—$N6^{iii}$ | 90.38 (10) | N6—C12—H12 | 122.7 |
| $N6^{ii}$—Cd1—$N6^{iii}$ | 180.0 | C14—C13—C16 | 107.7 (3) |
| $O2^{i}$—Cd1—$N3^{i}$ | 93.35 (10) | C14—C13—C15 | 107.6 (3) |
| O2—Cd1—$N3^{i}$ | 86.65 (10) | C16—C13—C15 | 110.5 (3) |
| $N6^{ii}$—Cd1—$N3^{i}$ | 91.65 (10) | C14—C13—C4 | 111.9 (3) |
| $N6^{iii}$—Cd1—$N3^{i}$ | 88.35 (10) | C16—C13—C4 | 109.4 (3) |
| $O2^{i}$—Cd1—N3 | 86.65 (10) | C15—C13—C4 | 109.7 (3) |
| O2—Cd1—N3 | 93.35 (10) | C13—C14—H14A | 109.5 |
| $N6^{ii}$—Cd1—N3 | 88.35 (10) | C13—C14—H14B | 109.5 |
| $N6^{iii}$—Cd1—N3 | 91.65 (10) | H14A—C14—H14B | 109.5 |
| $N3^{i}$—Cd1—N3 | 180.00 (12) | C13—C14—H14C | 109.5 |
| O1—C1—C6 | 122.9 (3) | H14A—C14—H14C | 109.5 |
| O1—C1—C2 | 116.6 (3) | H14B—C14—H14C | 109.5 |
| C6—C1—C2 | 120.4 (3) | C13—C15—H15A | 109.5 |
| C3—C2—C1 | 119.0 (3) | C13—C15—H15B | 109.5 |
| C3—C2—C10 | 120.7 (3) | H15A—C15—H15B | 109.5 |
| C1—C2—C10 | 120.3 (3) | C13—C15—H15C | 109.5 |
| C4—C3—C2 | 122.7 (3) | H15A—C15—H15C | 109.5 |
| C4—C3—H3 | 118.7 | H15B—C15—H15C | 109.5 |
| C2—C3—H3 | 118.7 | C13—C16—H16A | 109.5 |
| C3—C4—C5 | 116.5 (3) | C13—C16—H16B | 109.5 |
| C3—C4—C13 | 122.6 (3) | H16A—C16—H16B | 109.5 |
| C5—C4—C13 | 120.9 (3) | C13—C16—H16C | 109.5 |
| C4—C5—C6 | 123.0 (3) | H16A—C16—H16C | 109.5 |
| C4—C5—H5 | 118.5 | H16B—C16—H16C | 109.5 |
| C6—C5—H5 | 118.5 | C8—N1—N2 | 109.3 (3) |
| C1—C6—C5 | 118.4 (3) | C8—N1—C7 | 130.0 (3) |
| C1—C6—C7 | 122.0 (3) | N2—N1—C7 | 120.6 (3) |
| C5—C6—C7 | 119.4 (3) | C9—N2—N1 | 102.7 (3) |
| N1—C7—C6 | 114.7 (3) | C8—N3—C9 | 102.8 (3) |
| N1—C7—H7A | 108.6 | C8—N3—Cd1 | 133.2 (2) |
| C6—C7—H7A | 108.6 | C9—N3—Cd1 | 123.6 (2) |
| N1—C7—H7B | 108.6 | C11—N4—N5 | 109.5 (3) |
| C6—C7—H7B | 108.6 | C11—N4—C10 | 129.6 (3) |

| | | | |
|---|---|---|---|
| H7A—C7—H7B | 107.6 | N5—N4—C10 | 120.8 (3) |
| N1—C8—N3 | 110.6 (3) | C12—N5—N4 | 102.3 (3) |
| N1—C8—H8 | 124.7 | C11—N6—C12 | 102.4 (3) |
| N3—C8—H8 | 124.7 | C11—N6—Cd1$^{iv}$ | 125.4 (2) |
| N2—C9—N3 | 114.6 (3) | C12—N6—Cd1$^{iv}$ | 131.7 (2) |
| N2—C9—H9 | 122.7 | O4—N7—O5 | 133.1 (7) |
| N3—C9—H9 | 122.7 | O4—N7—O6 | 114.0 (7) |
| N4—C10—C2 | 111.9 (3) | O5—N7—O6 | 111.5 (6) |
| N4—C10—H10A | 109.2 | C1—O1—H1 | 109.5 |
| C2—C10—H10A | 109.2 | Cd1—O2—H2A | 111.9 |
| N4—C10—H10B | 109.2 | Cd1—O2—H2B | 106.5 |
| C2—C10—H10B | 109.2 | H2A—O2—H2B | 112.2 |
| H10A—C10—H10B | 107.9 | H3B—O3—H3C | 109.5 |
| N4—C11—N6 | 111.0 (3) | | |

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*; (ii) −*x*+1, −*y*+1, −*z*; (iii) *x*+1, *y*, *z*; (iv) *x*−1, *y*, *z*.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 2.61 | 3.247 (4) | 135 |
| O1—H1···N2 | 0.82 | 1.99 | 2.777 (4) | 161 |
| C8—H8···O6 | 0.93 | 2.48 | 3.150 (8) | 129 |
| O2—H2A···O3$^{iii}$ | 0.85 | 1.86 | 2.692 (4) | 164 |
| O2—H2B···O4$^{v}$ | 0.85 | 2.13 | 2.951 (7) | 164 |
| O2—H2B···O6$^{v}$ | 0.85 | 2.51 | 3.070 (7) | 124 |
| O3—H3B···N5$^{vi}$ | 0.85 | 2.42 | 2.920 (5) | 118 |
| O3—H3C···O5$^{vii}$ | 0.85 | 2.32 | 3.163 (7) | 169 |
| C7—H7B···O3$^{viii}$ | 0.97 | 2.60 | 3.501 (5) | 155 |
| C8—H8···O4$^{v}$ | 0.93 | 2.22 | 2.996 (7) | 140 |
| C12—H12···O5$^{iv}$ | 0.93 | 2.41 | 3.149 (7) | 136 |

Symmetry codes: (iii) *x*+1, *y*, *z*; (v) −*x*+2, *y*+1/2, −*z*+1/2; (vi) *x*, *y*+1, *z*; (vii) *x*−1, *y*+1, *z*; (viii) −*x*+1, *y*−1/2, −*z*+1/2; (iv) *x*−1, *y*, *z*.

**Fig. 1**

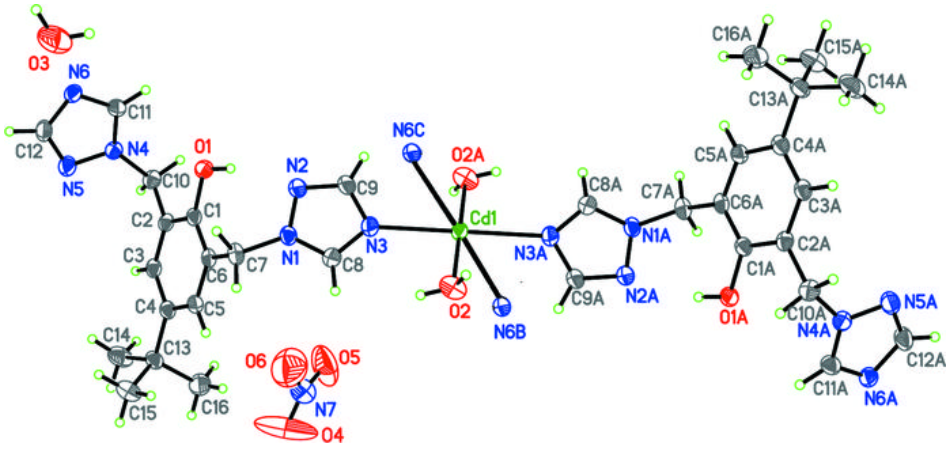
O3
N6
C11
C12
N4
N5
C10
O1
C2
C1
C3
C6
C7
C4
C5
C14
C13
C15
C16
N2
C9
N1
C8
N3
N6C
O2A
Cd1
O2
N6B
N3A
C8A
C9A
N2A
C7A
N1A
C6A
C5A
C4A
C3A
C2A
C1A
O1A
C16A
C15A
C14A
C13A
C10A
N4A
N5A
C12A
C11A
N6A
O6
O5
N7
O4

**Fig. 2**

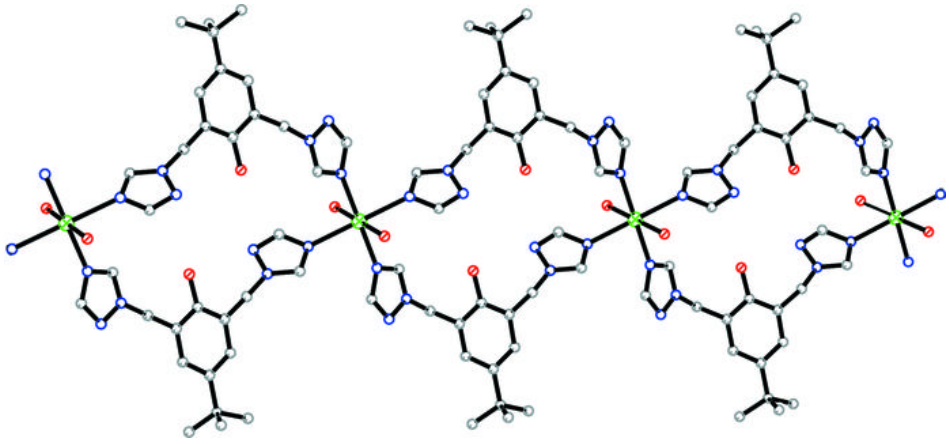

**Fig. 3**