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Diaquabis(2,2′-biimidazole)cadmium(II) benzene-1,4-dicarboxylate

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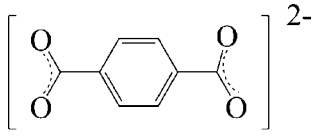
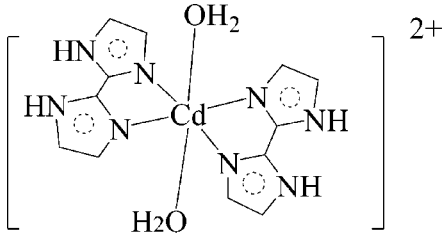
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.018; wR factor = 0.049; data-to-parameter ratio = 14.2.

In the title compound, $[Cd(C_6H_6N_4)_2(H_2O)_2](C_8H_4O_4)$, the Cd^{II} atom (site symmetry $\overline{1}$) is chelated by two 2,2′-biimidazole (H_2biim) ligands in the equatorial plane and two axial water molecules to result in a *trans*-CdN_4O_2 octahedral geometry. The complex dication and centrosymmetric benzene-1,4-dicarboxylate (bdc) dianion interact *via* O—H···O and N—H···O hydrogen bonds. Centrosymmetric aromatic π–π stacking involving one of the C_3N_2 rings of the H_2biim species also occurs with a short centroid–centroid separation of 3.4164 (14) Å.

Related literature

For a related structure, see: Ding *et al.* (2005). For the ligand synthesis, see: Fieselmann *et al.* (1978). For reference geometrical data, see: Allen *et al.* (1987).





Experimental

Crystal data

$[Cd(C_6H_6N_4)_2(H_2O)_2](C_8H_4O_4)$
M_r = 580.84
Monoclinic, $P2_1/n$
a = 8.336 (2) Å
b = 11.009 (3) Å
c = 12.688 (4) Å
β = 93.674 (3)°
V = 1161.9 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.99 mm^{-1}
T = 293 (2) K
0.58 × 0.53 × 0.25 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.596, T_{max} = 0.786
9682 measured reflections
2294 independent reflections
2139 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.049
S = 1.04
2294 reflections
162 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N4	2.2759 (14)	Cd1—O*W*1	2.4007 (14)
Cd1—N1	2.3178 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O*W*1—H*W*1*A*···O1^{i}	0.84	1.88	2.718 (2)	171
O*W*1—H*W*1*B*···O2^{ii}	0.89	1.97	2.822 (2)	161
N2—H2*A*···O1^{iii}	0.86	1.89	2.7471 (18)	171
N3—H3*A*···O2^{iii}	0.86	1.86	2.6972 (19)	165

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2453).

References

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supplementary materials

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Diaquabis(2,2'-biimidazole)cadmium(II) benzene-1,4-dicarboxylate

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Comment

As part of the ongoing study of complexes containing 2,2'-biimidazole (H_2biim) as a ligand (Ding *et al.*,2005), we now report the title compound, (I), which contains Cd^{2+}-containing complex ions, charge balanced by benzene-1,4-dicarboxylate dianions.

The Cd atom (site symmetry $\bar{1}$) in (I) is coordinated by four N atoms of two H_2biim ligands and two O atoms from two water molecules, in a octahedral geometry (Table 1, Fig. 1). The cation and anion interact by way of N—H···O and O—H···O hydrogen bonds (Table 2).

The plane-to-plane distance of 3.26 Å between the C1 imidazol ring and its symmetry equivalent partner at (3 − *x*, −*y*, 2 − *z*), in an offset fashion (slippage = 1.10 Å) indicates a strong π–π interaction (Fig. 2).

Experimental

2,2'-Biimidazole was synthesized according to the literature method (Fieselmann *et al.*, 1978). Benzene-1,4-dicarboxylic acid, 2,2'-biimidazole and cadmium acetate dihydrate were reacted in a molar ratio of 1:2:1. The mixture was stirred for 30 min, then the pH was adjusted to 6.5 with an aqueous solution of NaOH (0.1 *M*). The mixture with a total volume of 21 ml was heated at 433 K for 5 d in a sealed 25 ml Teflon-lined stainless steel vessel under autogenous pressure. After the reaction mixture was slowly cooled to room temperature at a rate of 5 K h^{-1}, colourless blocks of (I) were obtained.

Refinement

The water H atoms were located in a difference map and refined as riding in their as-found relative positions with free refinement for their U_{iso} values. The other H atoms were positioned geometrically (C—H = 0.93 Å, N—H = 0.86 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

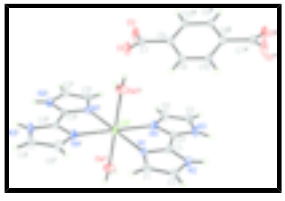

Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms). Symmetry codes: (i) 2 − *x*, −*y*, 2 − *z*; (ii) 2 − *x*, −*y*, 3 − *z*.

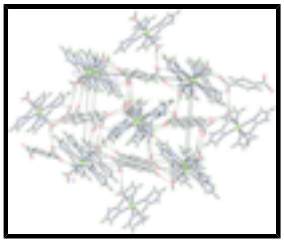

Fig. 2. The packing diagrame for (I). The dotted lines indicate the hydrogen bonds.

Diaquabis(2,2'-biimidazole)cadmium(II) benzene-1,4-dicarboxylate

Crystal data

$[Cd(C_6H_6N_4)_2(H_2O)_2](C_8H_4O_4)$	F_{000} = 584
M_r = 580.84	D_x = 1.660 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 903 reflections
a = 8.336 (2) Å	θ = 2.6–25.8º
b = 11.009 (3) Å	μ = 0.99 mm^{-1}
c = 12.688 (4) Å	T = 293 (2) K
β = 93.674 (3)º	Block, colourless
V = 1161.9 (6) Å^3	0.58 × 0.53 × 0.25 mm
Z = 2	

Data collection

Bruker SMART CCD diffractometer	2294 independent reflections
Radiation source: fine-focus sealed tube	2139 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.014
T = 293(2) K	θ_{max} = 26.1º
ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996) or Bruker (1997)?	h = −10→10
T_{min} = 0.596, T_{max} = 0.786	k = −13→13
9682 measured reflections	l = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.018	H-atom parameters constrained
$wR(F^2)$ = 0.049	$w = 1/[\sigma^2(F_o^2) + (0.0258P)^2 + 0.5043P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.003
2294 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}

162 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	1.0000	0.0000	1.0000	0.02922 (7)
OW1	1.08556 (16)	0.14916 (12)	0.87749 (10)	0.0465 (3)
HW1A	1.1376	0.1233	0.8272	0.058 (7)*
HW1B	1.1015	0.2283	0.8870	0.061 (7)*
O2	0.62681 (16)	0.09753 (13)	1.35814 (11)	0.0526 (4)
O1	0.72382 (15)	−0.05438 (15)	1.26778 (11)	0.0510 (4)
N1	1.25379 (15)	−0.08664 (12)	1.01642 (10)	0.0272 (3)
N2	1.48489 (15)	−0.08867 (12)	1.11125 (10)	0.0289 (3)
H2A	1.5591	−0.0698	1.1587	0.035*
N3	1.34980 (16)	0.12255 (13)	1.23815 (11)	0.0352 (3)
H3A	1.4448	0.1088	1.2661	0.042*
N4	1.13014 (16)	0.10607 (13)	1.13365 (10)	0.0321 (3)
C8	0.8710 (2)	0.00788 (13)	1.42460 (14)	0.0297 (4)
C7	0.7303 (2)	0.01824 (15)	1.34368 (14)	0.0340 (4)
C9	1.0192 (2)	−0.03370 (17)	1.39653 (14)	0.0342 (4)
H9	1.0326	−0.0567	1.3271	0.041*
C3	1.33955 (18)	−0.03673 (14)	1.09696 (12)	0.0249 (3)
C1	1.3500 (2)	−0.17504 (15)	0.97813 (13)	0.0322 (3)
H1	1.3222	−0.2257	0.9212	0.039*
C10	1.1479 (2)	−0.04125 (17)	1.47141 (13)	0.0340 (4)
H10	1.2471	−0.0688	1.4518	0.041*
C4	1.27572 (18)	0.06208 (14)	1.15733 (12)	0.0264 (3)
C2	1.4928 (2)	−0.17705 (15)	1.03637 (14)	0.0336 (4)
H2	1.5791	−0.2286	1.0270	0.040*
C6	1.1112 (2)	0.19951 (17)	1.20294 (15)	0.0414 (4)
H6	1.0202	0.2481	1.2052	0.050*
C5	1.2461 (2)	0.20980 (19)	1.26767 (15)	0.0436 (4)
H5	1.2644	0.2658	1.3220	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02300 (10)	0.03417 (11)	0.02907 (10)	0.00073 (6)	−0.00917 (7)	−0.00343 (6)
OW1	0.0536 (8)	0.0415 (8)	0.0455 (8)	0.0030 (6)	0.0117 (6)	0.0052 (6)
O2	0.0464 (8)	0.0513 (8)	0.0563 (8)	0.0186 (7)	−0.0271 (7)	−0.0148 (7)
O1	0.0353 (7)	0.0740 (10)	0.0412 (8)	0.0118 (7)	−0.0167 (6)	−0.0207 (7)
N1	0.0257 (6)	0.0282 (7)	0.0270 (6)	−0.0006 (5)	−0.0036 (5)	−0.0018 (5)
N2	0.0227 (6)	0.0315 (7)	0.0316 (7)	0.0014 (5)	−0.0058 (5)	0.0000 (5)
N3	0.0281 (7)	0.0417 (8)	0.0340 (7)	0.0040 (6)	−0.0115 (6)	−0.0114 (6)
N4	0.0261 (7)	0.0364 (8)	0.0326 (7)	0.0045 (6)	−0.0061 (5)	−0.0080 (6)
C8	0.0278 (8)	0.0277 (8)	0.0321 (9)	−0.0017 (6)	−0.0102 (7)	0.0019 (6)
C7	0.0297 (9)	0.0391 (9)	0.0317 (9)	−0.0003 (7)	−0.0104 (7)	0.0007 (7)
C9	0.0327 (9)	0.0412 (9)	0.0277 (8)	0.0006 (7)	−0.0057 (7)	−0.0021 (7)
C3	0.0231 (7)	0.0254 (7)	0.0258 (7)	−0.0006 (6)	−0.0023 (6)	0.0019 (6)
C1	0.0343 (8)	0.0297 (8)	0.0322 (8)	0.0014 (7)	−0.0002 (7)	−0.0057 (6)
C10	0.0265 (8)	0.0398 (9)	0.0346 (9)	0.0031 (7)	−0.0052 (7)	−0.0013 (7)
C4	0.0244 (7)	0.0290 (8)	0.0251 (7)	0.0000 (6)	−0.0043 (6)	−0.0017 (6)
C2	0.0315 (8)	0.0297 (8)	0.0397 (9)	0.0055 (6)	0.0023 (7)	−0.0025 (7)
C6	0.0348 (9)	0.0444 (10)	0.0440 (10)	0.0117 (8)	−0.0062 (8)	−0.0160 (8)
C5	0.0415 (10)	0.0463 (10)	0.0412 (10)	0.0083 (8)	−0.0100 (8)	−0.0216 (8)

Geometric parameters (Å, °)

Cd1—N4	2.2759 (14)	N3—H3A	0.8600
Cd1—N4^{i}	2.2759 (14)	N4—C4	1.323 (2)
Cd1—N1^{i}	2.3178 (14)	N4—C6	1.369 (2)
Cd1—N1	2.3178 (14)	C8—C9	1.385 (3)
Cd1—OW1	2.4007 (14)	C8—C10^{ii}	1.388 (3)
Cd1—OW1^{i}	2.4007 (14)	C8—C7	1.513 (2)
OW1—HW1A	0.8438	C9—C10	1.389 (2)
OW1—HW1B	0.8879	C9—H9	0.9300
O2—C7	1.249 (2)	C3—C4	1.451 (2)
O1—C7	1.250 (2)	C1—C2	1.360 (2)
N1—C3	1.328 (2)	C1—H1	0.9300
N1—C1	1.370 (2)	C10—C8^{ii}	1.388 (3)
N2—C3	1.341 (2)	C10—H10	0.9300
N2—C2	1.364 (2)	C2—H2	0.9300
N2—H2A	0.8600	C6—C5	1.354 (2)
N3—C4	1.340 (2)	C6—H6	0.9300
N3—C5	1.361 (2)	C5—H5	0.9300
N4—Cd1—N4^{i}	180.0	C9—C8—C10^{ii}	119.26 (16)
N4—Cd1—N1^{i}	104.16 (5)	C9—C8—C7	121.05 (16)
N4^{i}—Cd1—N1^{i}	75.84 (5)	C10^{ii}—C8—C7	119.68 (16)
N4—Cd1—N1	75.84 (5)	O2—C7—O1	124.34 (16)
N4^{i}—Cd1—N1	104.16 (5)	O2—C7—C8	117.75 (16)

N1^{i}—Cd1—N1	180.0	O1—C7—C8	117.90 (16)
N4—Cd1—OW1	89.10 (5)	C8—C9—C10	120.43 (17)
N4^{i}—Cd1—OW1	90.90 (5)	C8—C9—H9	119.8
N1^{i}—Cd1—OW1	88.15 (5)	C10—C9—H9	119.8
N1—Cd1—OW1	91.85 (5)	N1—C3—N2	111.39 (14)
N4—Cd1—OW1^{i}	90.90 (5)	N1—C3—C4	121.26 (13)
N4^{i}—Cd1—OW1^{i}	89.10 (5)	N2—C3—C4	127.35 (14)
N1^{i}—Cd1—OW1^{i}	91.85 (5)	C2—C1—N1	109.33 (14)
N1—Cd1—OW1^{i}	88.15 (5)	C2—C1—H1	125.3
OW1—Cd1—OW1^{i}	180.0	N1—C1—H1	125.3
Cd1—OW1—HW1A	116.5	C8^{ii}—C10—C9	120.31 (17)
Cd1—OW1—HW1B	129.1	C8^{ii}—C10—H10	119.8
HW1A—OW1—HW1B	110.8	C9—C10—H10	119.8
C3—N1—C1	105.55 (13)	N4—C4—N3	111.29 (14)
C3—N1—Cd1	110.01 (10)	N4—C4—C3	121.10 (13)
C1—N1—Cd1	144.33 (11)	N3—C4—C3	127.58 (14)
C3—N2—C2	107.07 (13)	C1—C2—N2	106.66 (14)
C3—N2—H2A	126.5	C1—C2—H2	126.7
C2—N2—H2A	126.5	N2—C2—H2	126.7
C4—N3—C5	106.95 (14)	C5—C6—N4	109.06 (15)
C4—N3—H3A	126.5	C5—C6—H6	125.5
C5—N3—H3A	126.5	N4—C6—H6	125.5
C4—N4—C6	105.74 (13)	C6—C5—N3	106.96 (15)
C4—N4—Cd1	111.59 (10)	C6—C5—H5	126.5
C6—N4—Cd1	142.64 (11)	N3—C5—H5	126.5
N4—Cd1—N1—C3	3.63 (10)	C1—N1—C3—C4	179.68 (14)
N4^{i}—Cd1—N1—C3	−176.37 (10)	Cd1—N1—C3—C4	−3.15 (18)
OW1—Cd1—N1—C3	92.23 (11)	C2—N2—C3—N1	−0.33 (18)
OW1^{i}—Cd1—N1—C3	−87.77 (11)	C2—N2—C3—C4	−179.77 (16)
N4—Cd1—N1—C1	178.95 (19)	C3—N1—C1—C2	0.00 (19)
N4^{i}—Cd1—N1—C1	−1.05 (19)	Cd1—N1—C1—C2	−175.44 (13)
OW1—Cd1—N1—C1	−92.45 (19)	C8—C9—C10—C8^{ii}	0.4 (3)
OW1^{i}—Cd1—N1—C1	87.55 (19)	C6—N4—C4—N3	0.15 (19)
N1^{i}—Cd1—N4—C4	176.15 (11)	Cd1—N4—C4—N3	−178.11 (11)
N1—Cd1—N4—C4	−3.85 (11)	C6—N4—C4—C3	−177.99 (15)
OW1—Cd1—N4—C4	−95.99 (11)	Cd1—N4—C4—C3	3.75 (19)
OW1^{i}—Cd1—N4—C4	84.01 (11)	C5—N3—C4—N4	0.0 (2)
N1^{i}—Cd1—N4—C6	−1.1 (2)	C5—N3—C4—C3	177.98 (17)
N1—Cd1—N4—C6	178.9 (2)	N1—C3—C4—N4	−0.4 (2)
OW1—Cd1—N4—C6	86.8 (2)	N2—C3—C4—N4	179.02 (15)
OW1^{i}—Cd1—N4—C6	−93.2 (2)	N1—C3—C4—N3	−178.18 (15)
C9—C8—C7—O2	−151.17 (18)	N2—C3—C4—N3	1.2 (3)
C10^{ii}—C8—C7—O2	28.4 (2)	N1—C1—C2—N2	−0.2 (2)
C9—C8—C7—O1	30.0 (3)	C3—N2—C2—C1	0.31 (18)

C10^{ii}—C8—C7—O1	−150.43 (18)	C4—N4—C6—C5	−0.2 (2)
C10^{ii}—C8—C9—C10	−0.4 (3)	Cd1—N4—C6—C5	177.10 (16)
C7—C8—C9—C10	179.16 (16)	N4—C6—C5—N3	0.2 (2)
C1—N1—C3—N2	0.21 (18)	C4—N3—C5—C6	−0.1 (2)
Cd1—N1—C3—N2	177.38 (10)		

Symmetry codes: (i) −*x*+2, −*y*, −*z*+2; (ii) −*x*+2, −*y*, −*z*+3.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
OW1—HW1A···O1^{i}	0.84	1.88	2.718 (2)	171
OW1—HW1B···O2^{iii}	0.89	1.97	2.822 (2)	161
N2—H2A···O1^{iv}	0.86	1.89	2.7471 (18)	171
N3—H3A···O2^{iv}	0.86	1.86	2.6972 (19)	165

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

Fig. 1

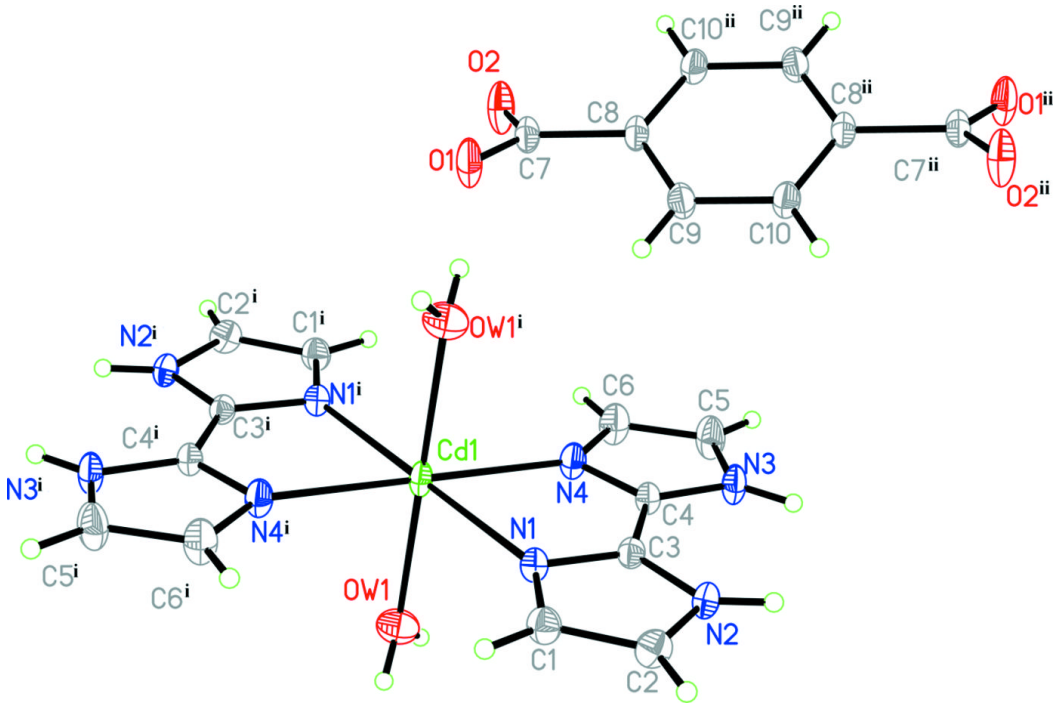
C10ii
C9ii
O2
C8ii
O1ii
C8
O1
C7
C7ii
O2ii
C9
C10
C2i
OW1i
N2i
C1i
N1i
C6
C5
C3i
C4i
Cd1
N3
N3i
N4
C4
N4i
N1
C3
C5i
OW1
N2
C6i
C1
C2

Fig. 2