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catena-Poly[[bis(4-carboxycyclohexanecarboxylato-$\kappa^2O^1,O^{1'}$)cadmium(II)]-μ-1,4-bis(imidazol-1-ylmethyl)benzene-$\kappa^2N^3:N^{3'}$]

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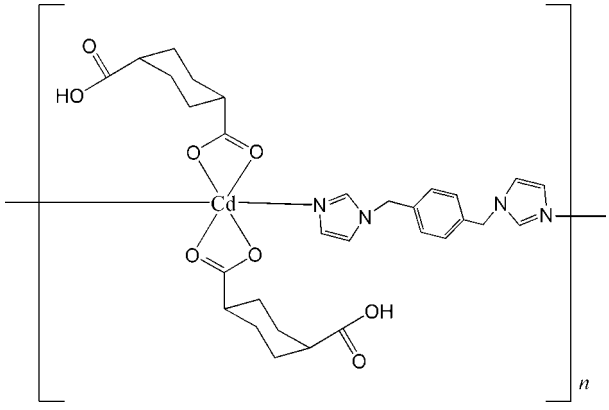
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.009 Å; R factor = 0.052; wR factor = 0.120; data-to-parameter ratio = 16.4.

In the title coordination polymer, $[Cd(C_8H_{11}O_4)_2(C_{14}H_{14}N_4)]_n$, the Cd atom (site symmetry 2) is six-coordinated by two O,O'-bidentate 4-carboxycyclohexanecarboxylate (Hchdc) ligands and two N atoms from two different 1,4-bis(imidazol-1-ylmethyl)benzene (1,4-bix) molecules in a very distorted *cis*-CdN_2O_4 octahedral environment. The 1,4-bix molecules act as bridging ligands that bind two Cd^{II} atoms, thus forming an infinite chain propagating in [100], which is decorated by the Hchdc anions. The structure is completed by O—H···O hydrogen bonds, which link the chains together.

Related literature

For related structures, see: Qi *et al.* (2003). For background to coordination polymers, see: Chen & Liu (2002); Fang *et al.* (2006); Kim & Jung (2002); Lehn (1990); Batten & Robson (1998); Yang *et al.* (2008).



Experimental

Crystal data

$[Cd(C_8H_{11}O_4)_2(C_{14}H_{14}N_4)]$
M_r = 693.03
Orthorhombic, *Pccn*
a = 12.6317 (5) Å
b = 19.9697 (12) Å
c = 12.3703 (7) Å
V = 3120.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 292 K
0.26 × 0.22 × 0.17 mm

Data collection

Oxford Diffraction Gemini R Ultra diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.816, T_{max} = 0.882
26676 measured reflections
3190 independent reflections
1658 reflections with $I > 2\sigma(I)$
R_{int} = 0.116

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.120
S = 0.95
3190 reflections
195 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.249 (4)	Cd1—O2	2.384 (4)
Cd1—O1	2.306 (4)		
O1—Cd1—O2	55.00 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O2^{i}	0.82	1.86	2.644 (6)	161

Symmetry code: (i) $x+\frac{1}{2}, -y, -z+\frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2986).

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supplementary materials

Acta Cryst. (2009). E**65**, m756-m757 [**doi:10.1107/S1600536809021618**]

catena-Poly[[bis(4-carboxycyclohexanecarboxylato-$\kappa^2O^1,O^{1'}$)cadmium(II)]-μ-1,4-bis(imidazol-1-ylmethyl)benzene-$\kappa^2N^3:N^{3'}$]

B.-B. Li and B. Xiao

Comment

The rational design and synthesis of metal-organic coordination polymers have received intense interest due to their fascinating structural topologies and potential applications as functional materials (e.g. Fang *et al.*, 2006). These coordination polymers can be specially designed by the careful selection of metal cations with preferred coordination geometries, the nature of the anions, the structure of the connecting ligands, and the reaction conditions (Kim & Jung, 2002). The selection of ligand is extremely important because changing the structures of the ligands can control and adjust the topologies of coordination frameworks. Among these mentioned above, chain structures have received much attention in coordination chemistry and life sciecnce (Lehn, 1990). So far, many chain complexes have been generated by self-assembly processes (Chen & Liu, 2002). In this regard, metal 1,4-benzenedicarboxylates (1,4-bdc) have been widely studied (Qi *et al.*, 2003). However, so far, less attention has been given to the 1,4-cyclohexanedicarboxylic acid ligand (H_2chdc). The H_2chdc as an important analogues of 1,4-bdc may be a good candidate for the construction of metal-organic architectures. On the other hand, 4,4'-byridine is a rigid rod-like spacer, well known in the construction of metal-organic polymers, and it has adopted numerous interesting supramolecular architectures (Batten & Robson, 1998). However, flexible ligands such as 1,4-bis(imidazole-1-ylmethyl)-benzene (1,4-bix) have not been so well explored to date (Yang *et al.*, 2008). In this work, the combination of 1,4-bix with H_2chdc and Cd^{II} cations resulted in the title compound [Cd(1,4-bix)(Hchdc)$_2$], (I), a new one-dimensional chain coordination polymer.

The selected bond lengthes and angles are listed in Table 1. In compound (I), the Cd^{II} atom is is six-coordinated by four carboxylate O atoms from two different Hchdc ligands, and two N atoms from two different 1,4-bix molecules in a distorted octahedral environment (Fig. 1). The O1, O2, O2^i and N1^i atoms comprise the basal plane, whereas the N1 and O1^i occupy the axial positions of the octahedron. As shown in Fig. 2, each 1,4-bix acts as a bridging ligand that binds two Cd^{II} atoms, thus forming a unique chain. The chain is decorated with Hchdc molecules alternately at two sides. Furthermore, the O—H···O hydrogen bonds link the chains together, stablizing the structure of (I).

Experimental

A mixture of $CdCl_2{\cdot}2H_2O$ (0.5 mmol), H_2chdc acid (0.5 mmol), 1,4-bix (0.5 mmol), and H_2O (500 mmol) was adjusted to pH = 5.8 by addition of aqueous NaOH solution, and heated at 453 K for 5 days. After the mixture was slowly cooled to room temperature, colorless blocks of (I) were recovered in a 28% yield.

Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.97 Å, O—H = 0.82Å) and refined as riding, with U_{iso}(H)=1.2U_{eq}(carrier).

Figures

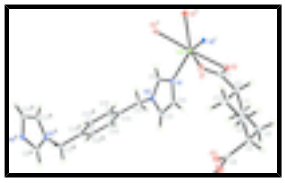

Fig. 1. The structure of (I), showing displacement ellipsoids drawn at the 20% probability level. Symmetry code: (i) 3/2 - *x*, 1/2 - *y*, *z*; (ii) 5/2 - *x*, -1/2 - *y*, *z*.

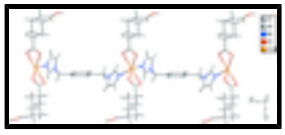

Fig. 2. View of the chain structure of (I).

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Crystal data

$[Cd(C_8H_{11}O_4)_2(C_{14}H_{14}N_4)]$	F_{000} = 1424
M_r = 693.03	D_x = 1.475 Mg m^{-3}
Orthorhombic, *Pccn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ab 2ac	Cell parameters from 3190 reflections
a = 12.6317 (5) Å	θ = 3.0–26.5º
b = 19.9697 (12) Å	μ = 0.75 mm^{-1}
c = 12.3703 (7) Å	*T* = 292 K
V = 3120.4 (3) Å^3	Block, colorless
Z = 4	0.26 × 0.22 × 0.17 mm

Data collection

Oxford Diffraction Gemini R Ultra diffractometer	3190 independent reflections
Radiation source: fine-focus sealed tube	1658 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.116
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 26.5º
T = 292 K	θ_{min} = 4.7º
ω scans	*h* = −15→15
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006)	*k* = −24→24
T_{min} = 0.816, T_{max} = 0.882	*l* = −15→15
26676 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.120$	$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(\Delta/\sigma)_{max} < 0.001$
3190 reflections	$\Delta\rho_{max} = 0.62$ e Å^{-3}
195 parameters	$\Delta\rho_{min} = -0.30$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > \sigma(F^2)$ 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}
C1	0.7200 (5)	0.1255 (3)	0.1946 (5)	0.0556 (16)
C2	0.7134 (5)	0.0551 (3)	0.1562 (5)	0.0703 (18)
H2	0.6472	0.0495	0.1158	0.084*
C3	0.8075 (6)	0.0347 (3)	0.0813 (6)	0.089 (2)
H3A	0.8072	0.0627	0.0172	0.107*
H3B	0.8738	0.0420	0.1190	0.107*
C4	0.7998 (7)	−0.0363 (4)	0.0488 (6)	0.106 (3)
H4A	0.8606	−0.0478	0.0045	0.127*
H4B	0.7367	−0.0427	0.0054	0.127*
C5	0.7956 (5)	−0.0833 (3)	0.1467 (6)	0.082 (2)
H5	0.7788	−0.1281	0.1192	0.099*
C6	0.7065 (7)	−0.0639 (4)	0.2243 (7)	0.098 (2)
H6A	0.6387	−0.0729	0.1905	0.118*
H6B	0.7113	−0.0910	0.2891	0.118*
C7	0.7123 (6)	0.0065 (3)	0.2537 (6)	0.089 (2)
H7A	0.7758	0.0137	0.2961	0.107*
H7B	0.6521	0.0172	0.2992	0.107*
C8	0.9032 (6)	−0.0881 (3)	0.2022 (7)	0.078 (2)
C9	0.9060 (3)	0.2554 (3)	0.4765 (4)	0.0524 (13)
H9	0.8851	0.2997	0.4856	0.063*
C10	0.9221 (4)	0.1567 (3)	0.4138 (5)	0.0657 (16)
H10	0.9152	0.1192	0.3699	0.079*
C11	0.9818 (5)	0.1601 (3)	0.5038 (5)	0.0665 (18)
H11	1.0218	0.1258	0.5339	0.080*

C12	1.0206 (3)	0.2510 (3)	0.6389 (4)	0.0612 (14)
H12A	0.9962	0.2257	0.7010	0.073*
H12B	0.9972	0.2969	0.6481	0.073*
C13	1.1951 (4)	0.2506 (5)	0.5441 (5)	0.125 (4)
H13	1.1592	0.2521	0.4785	0.150*
C14	1.1390 (3)	0.2497 (3)	0.6368 (4)	0.0479 (11)
C15	1.1954 (4)	0.2499 (4)	0.7277 (5)	0.0693 (15)
H15	1.1599	0.2498	0.7936	0.083*
N1	0.8735 (3)	0.2166 (2)	0.3967 (4)	0.0527 (11)
N2	0.9721 (3)	0.2237 (2)	0.5420 (4)	0.0515 (12)
O1	0.7903 (3)	0.1640 (2)	0.1601 (3)	0.0683 (11)
O2	0.6563 (3)	0.1466 (2)	0.2657 (4)	0.0700 (12)
O3	0.9194 (5)	−0.0730 (3)	0.2950 (5)	0.120 (2)
O4	0.9764 (4)	−0.1119 (2)	0.1406 (4)	0.0951 (15)
H4	1.0323	−0.1134	0.1741	0.143*
Cd1	0.7500	0.2500	0.27740 (4)	0.04487 (19)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.062 (4)	0.045 (3)	0.059 (4)	0.007 (3)	−0.007 (3)	0.005 (3)
C2	0.096 (5)	0.045 (3)	0.069 (4)	0.000 (3)	0.000 (4)	0.002 (3)
C3	0.149 (6)	0.058 (4)	0.061 (4)	−0.006 (4)	0.036 (5)	0.000 (4)
C4	0.118 (6)	0.103 (6)	0.096 (6)	0.048 (5)	−0.013 (5)	−0.008 (5)
C5	0.085 (4)	0.068 (4)	0.093 (6)	0.022 (4)	−0.020 (4)	0.014 (4)
C6	0.095 (5)	0.078 (5)	0.123 (7)	0.020 (4)	0.014 (5)	0.016 (5)
C7	0.111 (6)	0.065 (4)	0.092 (6)	−0.013 (4)	0.027 (4)	0.005 (4)
C8	0.089 (5)	0.058 (4)	0.087 (6)	0.029 (4)	−0.001 (4)	0.002 (4)
C9	0.036 (2)	0.060 (3)	0.062 (3)	0.015 (3)	−0.002 (3)	0.001 (4)
C10	0.067 (4)	0.055 (4)	0.075 (5)	0.009 (3)	−0.018 (3)	0.002 (3)
C11	0.060 (4)	0.062 (4)	0.077 (5)	0.014 (3)	−0.018 (3)	0.006 (3)
C12	0.037 (2)	0.094 (4)	0.052 (3)	0.009 (4)	−0.006 (2)	0.000 (4)
C13	0.042 (3)	0.291 (12)	0.042 (4)	−0.020 (7)	−0.008 (3)	−0.003 (6)
C14	0.040 (2)	0.062 (3)	0.042 (3)	−0.002 (3)	0.001 (2)	−0.009 (4)
C15	0.048 (3)	0.119 (5)	0.041 (3)	−0.006 (5)	0.004 (2)	−0.004 (5)
N1	0.039 (2)	0.056 (3)	0.064 (3)	0.000 (2)	−0.007 (2)	0.006 (3)
N2	0.030 (2)	0.069 (3)	0.056 (3)	−0.0009 (19)	−0.002 (2)	0.006 (2)
O1	0.083 (3)	0.058 (2)	0.064 (3)	0.001 (2)	0.021 (2)	−0.004 (2)
O2	0.051 (2)	0.059 (2)	0.100 (3)	−0.0010 (18)	0.015 (2)	−0.025 (2)
O3	0.143 (5)	0.130 (5)	0.088 (4)	0.059 (4)	−0.019 (4)	−0.005 (4)
O4	0.077 (3)	0.099 (4)	0.110 (4)	0.027 (3)	−0.007 (3)	−0.027 (3)
Cd1	0.0318 (2)	0.0523 (3)	0.0505 (3)	0.0036 (3)	0.000	0.000

Geometric parameters (Å, °)

C1—O1	1.250 (6)	C9—N2	1.325 (7)
C1—O2	1.265 (6)	C9—H9	0.9300
C1—C2	1.487 (8)	C10—C11	1.347 (8)
C1—Cd1	2.716 (6)	C10—N1	1.361 (6)

C2—C7	1.548 (8)	C10—H10	0.9300
C2—C3	1.561 (8)	C11—N2	1.360 (7)
C2—H2	0.9800	C11—H11	0.9300
C3—C4	1.478 (9)	C12—N2	1.453 (7)
C3—H3A	0.9700	C12—C14	1.496 (6)
C3—H3B	0.9700	C12—H12A	0.9700
C4—C5	1.533 (10)	C12—H12B	0.9700
C4—H4A	0.9700	C13—C14	1.347 (7)
C4—H4B	0.9700	C13—C13^{i}	1.388 (11)
C5—C8	1.526 (9)	C13—H13	0.9300
C5—C6	1.529 (9)	C14—C15	1.331 (7)
C5—H5	0.9800	C15—C15^{i}	1.379 (10)
C6—C7	1.453 (9)	C15—H15	0.9300
C6—H6A	0.9700	O4—H4	0.8200
C6—H6B	0.9700	Cd1—N1	2.249 (4)
C7—H7A	0.9700	Cd1—O1	2.306 (4)
C7—H7B	0.9700	Cd1—O2	2.384 (4)
C8—O3	1.205 (8)	Cd1—N1^{ii}	2.249 (4)
C8—O4	1.288 (8)	Cd1—O1^{ii}	2.306 (4)
C9—N1	1.320 (7)	Cd1—O2^{ii}	2.384 (4)
O1—C1—O2	119.0 (5)	C11—C10—N1	109.7 (5)
O1—C1—C2	120.8 (5)	C11—C10—H10	125.2
O2—C1—C2	120.2 (6)	N1—C10—H10	125.2
C1—C2—C7	110.2 (5)	C10—C11—N2	106.5 (5)
C1—C2—C3	113.2 (5)	C10—C11—H11	126.8
C7—C2—C3	107.8 (5)	N2—C11—H11	126.8
C1—C2—H2	108.5	N2—C12—C14	113.6 (4)
C7—C2—H2	108.5	N2—C12—H12A	108.8
C3—C2—H2	108.5	C14—C12—H12A	108.8
C4—C3—C2	111.2 (6)	N2—C12—H12B	108.8
C4—C3—H3A	109.4	C14—C12—H12B	108.8
C2—C3—H3A	109.4	H12A—C12—H12B	107.7
C4—C3—H3B	109.4	C14—C13—C13^{i}	121.7 (3)
C2—C3—H3B	109.4	C14—C13—H13	119.2
H3A—C3—H3B	108.0	C13^{i}—C13—H13	119.2
C3—C4—C5	112.0 (6)	C15—C14—C13	115.9 (4)
C3—C4—H4A	109.2	C15—C14—C12	121.3 (4)
C5—C4—H4A	109.2	C13—C14—C12	122.7 (5)
C3—C4—H4B	109.2	C14—C15—C15^{i}	122.4 (3)
C5—C4—H4B	109.2	C14—C15—H15	118.8
H4A—C4—H4B	107.9	C15^{i}—C15—H15	118.8
C8—C5—C6	112.9 (6)	C9—N1—C10	105.1 (5)
C8—C5—C4	111.2 (6)	C9—N1—Cd1	122.2 (4)
C6—C5—C4	111.5 (6)	C10—N1—Cd1	132.5 (4)
C8—C5—H5	106.9	C9—N2—C11	106.9 (5)
C6—C5—H5	106.9	C9—N2—C12	126.2 (5)
C4—C5—H5	106.9	C11—N2—C12	126.8 (5)

C7—C6—C5	111.5 (6)	C1—O1—Cd1	94.9 (3)
C7—C6—H6A	109.3	C1—O2—Cd1	90.9 (3)
C5—C6—H6A	109.3	C8—O4—H4	109.5
C7—C6—H6B	109.3	N1—Cd1—N1^{ii}	97.9 (2)
C5—C6—H6B	109.3	N1—Cd1—O1	92.24 (16)
H6A—C6—H6B	108.0	N1^{ii}—Cd1—O1	141.92 (15)
C6—C7—C2	114.3 (6)	N1—Cd1—O1^{ii}	141.92 (15)
C6—C7—H7A	108.7	N1^{ii}—Cd1—O1^{ii}	92.24 (16)
C2—C7—H7A	108.7	O1—Cd1—O1^{ii}	102.0 (2)
C6—C7—H7B	108.7	N1—Cd1—O2	97.33 (15)
C2—C7—H7B	108.7	N1^{ii}—Cd1—O2	87.24 (15)
H7A—C7—H7B	107.6	O1—Cd1—O2	55.00 (14)
O3—C8—O4	122.2 (7)	O1^{ii}—Cd1—O2	119.83 (15)
O3—C8—C5	124.4 (7)	N1—Cd1—O2^{ii}	87.24 (15)
O4—C8—C5	113.3 (7)	N1^{ii}—Cd1—O2^{ii}	97.33 (15)
N1—C9—N2	111.8 (6)	O1—Cd1—O2^{ii}	119.83 (15)
N1—C9—H9	124.1	O1^{ii}—Cd1—O2^{ii}	55.00 (14)
N2—C9—H9	124.1	O2—Cd1—O2^{ii}	173.1 (2)

Symmetry codes: (i) −*x*+5/2, −*y*+1/2, *z*; (ii) −*x*+3/2, −*y*+1/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O2^{iii}	0.82	1.86	2.644 (6)	161

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

Fig. 1

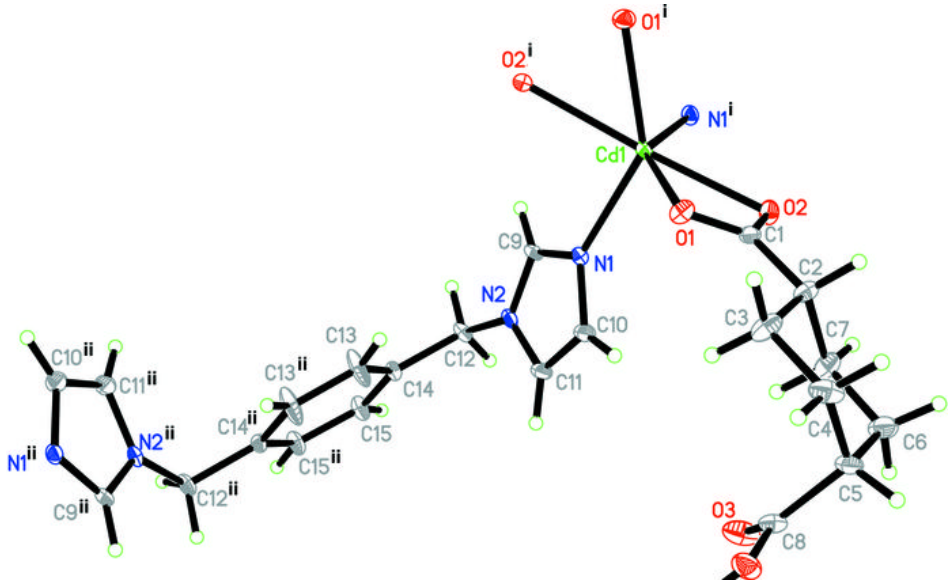
O1i
O2i
N1i
Cd1
O2
O1
C1
C9
N1
C2
N2
C10
C3
C7
C13
C10ii
C13ii
C12
C14
C11
C11ii
C14ii
C15
C4
C6
N2ii
N1ii
C15ii
C5
C12ii
O3
C9ii
C8

Fig. 2