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Poly[[(1,10-phenanthroline)cadmium(II)]-μ_3-2-(4-carboxylatophenoxy)propionato]

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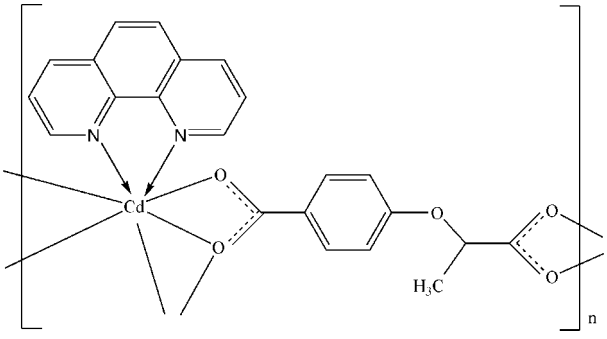
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.039; wR factor = 0.083; data-to-parameter ratio = 16.0.

In the title linear polymeric chain compound, $[Cd(C_{10}H_8O_5)(C_{12}H_8N_2)]_n$, the Cd^{II} ion exists in a monocapped triangular–prismatic geometry that is defined by two N atoms from a 1,10-phenanthroline molecule and five O atoms from three 2-(4-carboxylatophenoxy)propionate ligands. Adjacent chains are cross-linked *via* π–π stacking interactions between the 1,10-phenanthroline rings [centroid–centroid distance = 3.5894 (6) Å].

Related literature

For the cobalt(II), nickel(II) and manganese(II) complexes of 2-(4-carboxyphenoxy)propionic acid, see: Deng *et al.* (2007*a*,*b*); Xiao *et al.* (2007).



Experimental

Crystal data

$[Cd(C_{10}H_8O_5)(C_{12}H_8N_2)]$
M_r = 500.77
Monoclinic, $C2/c$
a = 21.214 (4) Å
b = 10.506 (2) Å
c = 19.775 (4) Å
β = 120.02 (3)°
V = 3816.4 (16) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 293 (2) K
0.38 × 0.25 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.662, T_{max} = 0.824
18185 measured reflections
4351 independent reflections
3474 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.083
S = 1.06
4351 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); 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: NG2338).

References

Deng, Z.-P., Gao, S. & Chen, P.-G. (2007*a*). *Acta Cryst.* E**63**, m296–m298.
Deng, Z.-P., Gao, S. & Chen, P.-G. (2007*b*). *Acta Cryst.* E**63**, m553–m554.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Rigaku Corporation (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Xiao, Y.-H., Kong, L.-L. & Gao, S. (2007). *Acta Cryst.* E**63**, m1587–m1588.

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supplementary materials

Acta Cryst. (2007). E**63**, m2759 [**doi:10.1107/S1600536807050350**]

Poly[[(1,10-phenanthroline)cadmium(II)]-μ_3-2-(4-carboxylatophenoxy)propionato]

L.-L. Kong, S. Gao and L.-H. Huo

Comment

We are interested in the solid-state coordination chemistry of carboxyphenoxypropionic combining with specific transition-metals, a ligand that is a good candidate fir fabricating versatile coordination polymers. Recently, some structures of cobalt(II), nickel(II) and manganese(II) complexes incorporating 2-(4-carboxylatophenoxy)propionate groups had been reported (Deng *et al.*, 2007*a*,b; Xiao *et al.*, 2007).

As illustrated in Fig. 1 and Fig. 2, each Cd atom displays a distorted monocapped triangular prismatic geometry, with five carboxylate oxygen donors from three 2-(4-carboxylatophenoxy)propionato ligands, two nitrogen donors from one 1,10-phenanthroline ligand. Two CdN_2O_5 one-cap triangular prisms are combined by the carboxyl O1 and $O1^i$ atoms to form a binuclear unit. Then these binuclear units are linked by the 2-(4-carboxylatophenoxy)propionato ligands into a ribbon structure along *b* axis. Furthermore, the chains are connected through π-π stacking interactions between the adjacent 1,10-phenanthroline rings, forming a two-dimensional network.

Experimental

Cadmium nitrate tetrahydrate (10 mmol) was added to a hot H_2O/MeOH (*v*/*v* = 1:1) solution of 2-(4-carboxylatophenoxy)propionic acid (10 mmol) and 1,10-phenanthroline (10 mmol) and the pH value was adjusted to 5 with NaOH (0.2 *M*) solution. Colorless crystals were obtained from the filtered solution at room temperature over several days. Analysis: calculated for $C_{22}H_{16}CdN_2O_5$: C 52.77, H 3.22, N 5.59%; found: C 52.75, H 3.23, N 5.60%.

Refinement

C-bound H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C), and were included in the refinement in the riding-model approximation.

Figures

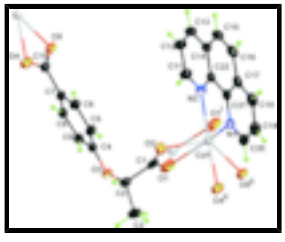

Fig. 1. **Figure 1**. A view of the title complex, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) *x*,*y* − 1,*z*; (ii) −*x*,-*y*,-*z* + 1.]

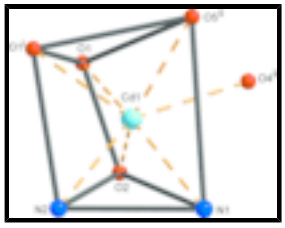

Fig. 2. **Figure 2**. Geometry of Cd.

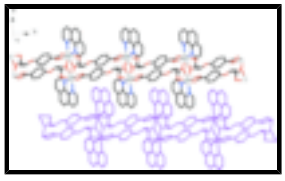

Fig. 3. **Figure 3**. The chain of (I), show the centroid···centroid distance. H atoms have been omitted for clarify.

Poly[[(1,10-phenanthroline)cadmium(II)]- μ$_3$-2-(4-carboxylatophenoxy)propionato]

Crystal data

$[Cd(C_{10}H_8O_5)(C_{12}H_8N_2)]$	F_{000} = 2000
M_r = 500.77	D_x = 1.743 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 13541 reflections
a = 21.214 (4) Å	θ = 3.1–27.5º
b = 10.506 (2) Å	μ = 1.18 mm^{-1}
c = 19.775 (4) Å	*T* = 293 (2) K
β = 120.02 (3)º	Prism, colorless
V = 3816.4 (16) Å^3	0.38 × 0.25 × 0.17 mm
Z = 8	

Data collection

Rigaku R-AXIS RAPID diffractometer	4351 independent reflections
Radiation source: fine-focus sealed tube	3474 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.5º
ω scans	*h* = −27→25
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*k* = −13→13
T_{min} = 0.662, T_{max} = 0.824	*l* = −25→25
18185 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

$R[F^2 > 2\sigma(F^2)] = 0.039$	H-atom parameters constrained
$wR(F^2) = 0.083$	$w = 1/[\sigma^2(F_o^2) + (0.0225P)^2 + 14.3767P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
4351 reflections	$\Delta\rho_{max} = 0.86$ e Å^{-3}
272 parameters	$\Delta\rho_{min} = -0.58$ 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}
Cd1	0.097015 (14)	−0.03739 (2)	0.521545 (15)	0.03668 (9)
O1	0.02629 (17)	0.0381 (3)	0.58469 (19)	0.0702 (9)
O2	0.13086 (19)	0.1237 (3)	0.6179 (2)	0.0670 (9)
O3	0.13576 (18)	0.2592 (2)	0.73727 (15)	0.0568 (8)
O4	0.15814 (16)	0.8245 (3)	0.63802 (18)	0.0588 (8)
O5	0.06814 (15)	0.7552 (3)	0.52771 (16)	0.0510 (7)
N1	0.21148 (16)	−0.0571 (3)	0.52675 (18)	0.0392 (7)
N2	0.10454 (16)	0.1131 (3)	0.43895 (18)	0.0399 (7)
C1	0.0786 (2)	0.1073 (4)	0.6289 (2)	0.0494 (10)
C2	0.0826 (3)	0.1625 (4)	0.7016 (3)	0.0531 (10)
H2	0.0348	0.1966	0.6884	0.064*
C3	0.1034 (3)	0.0580 (4)	0.7616 (3)	0.0817 (17)
H3	0.1508	0.0259	0.7757	0.123*
H4	0.0684	−0.0097	0.7402	0.123*
H7	0.1042	0.0914	0.8072	0.123*
C4	0.1260 (2)	0.3743 (3)	0.7004 (2)	0.0415 (8)
C5	0.0629 (2)	0.4110 (4)	0.6340 (2)	0.0435 (9)
H5	0.0230	0.3566	0.6108	0.052*
C6	0.0600 (2)	0.5306 (4)	0.6024 (2)	0.0414 (8)
H6	0.0175	0.5557	0.5578	0.050*
C7	0.11833 (19)	0.6129 (3)	0.6356 (2)	0.0365 (8)
C8	0.1815 (2)	0.5746 (3)	0.7026 (2)	0.0404 (8)
H8	0.2212	0.6294	0.7262	0.049*
C9	0.1856 (2)	0.4556 (4)	0.7343 (2)	0.0441 (9)

H9	0.2284	0.4299	0.7783	0.053*
C10	0.1149 (2)	0.7393 (3)	0.5986 (2)	0.0387 (8)
C11	0.0535 (2)	0.1983 (4)	0.3986 (2)	0.0506 (10)
H11	0.0109	0.1962	0.4012	0.061*
C12	0.0604 (2)	0.2910 (4)	0.3524 (2)	0.0532 (10)
H12	0.0231	0.3492	0.3248	0.064*
C13	0.1224 (2)	0.2952 (4)	0.3481 (2)	0.0519 (10)
H13	0.1277	0.3561	0.3171	0.062*
C14	0.1783 (2)	0.2079 (4)	0.3904 (2)	0.0423 (9)
C15	0.2456 (2)	0.2076 (4)	0.3900 (3)	0.0516 (10)
H15	0.2531	0.2669	0.3598	0.062*
C16	0.2979 (2)	0.1233 (4)	0.4325 (2)	0.0524 (11)
H16	0.3411	0.1256	0.4313	0.063*
C17	0.2891 (2)	0.0296 (4)	0.4796 (2)	0.0447 (9)
C18	0.3425 (2)	−0.0587 (4)	0.5262 (3)	0.0555 (11)
H18	0.3862	−0.0611	0.5260	0.067*
C19	0.3310 (2)	−0.1409 (4)	0.5718 (3)	0.0571 (11)
H19	0.3669	−0.1986	0.6036	0.069*
C20	0.2645 (2)	−0.1377 (4)	0.5704 (2)	0.0477 (9)
H20	0.2571	−0.1949	0.6016	0.057*
C21	0.22354 (18)	0.0268 (3)	0.4822 (2)	0.0370 (8)
C22	0.16690 (19)	0.1176 (3)	0.4360 (2)	0.0362 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03487 (14)	0.03534 (14)	0.04202 (15)	−0.00154 (12)	0.02086 (12)	0.00385 (12)
O1	0.0508 (18)	0.0507 (18)	0.070 (2)	−0.0104 (15)	0.0014 (16)	0.0131 (16)
O2	0.090 (2)	0.0516 (18)	0.083 (2)	−0.0095 (17)	0.061 (2)	−0.0080 (17)
O3	0.084 (2)	0.0342 (14)	0.0413 (15)	−0.0031 (14)	0.0229 (16)	0.0033 (12)
O4	0.0590 (19)	0.0427 (16)	0.0630 (19)	−0.0142 (14)	0.0218 (16)	0.0026 (14)
O5	0.0501 (17)	0.0388 (15)	0.0534 (17)	0.0005 (12)	0.0180 (15)	0.0075 (13)
N1	0.0387 (16)	0.0376 (17)	0.0435 (17)	−0.0003 (13)	0.0222 (15)	−0.0026 (14)
N2	0.0359 (16)	0.0396 (17)	0.0482 (18)	0.0004 (13)	0.0241 (15)	0.0036 (14)
C1	0.055 (3)	0.0289 (19)	0.050 (2)	0.0017 (18)	0.016 (2)	0.0108 (17)
C2	0.067 (3)	0.038 (2)	0.063 (3)	−0.0015 (19)	0.040 (2)	0.0083 (19)
C3	0.131 (5)	0.050 (3)	0.067 (3)	−0.010 (3)	0.052 (4)	0.011 (2)
C4	0.056 (2)	0.0328 (18)	0.039 (2)	0.0022 (17)	0.0260 (19)	0.0010 (16)
C5	0.039 (2)	0.0355 (19)	0.053 (2)	−0.0056 (16)	0.0211 (19)	−0.0018 (17)
C6	0.0352 (19)	0.0395 (19)	0.045 (2)	0.0029 (16)	0.0167 (17)	0.0043 (17)
C7	0.0371 (19)	0.0323 (18)	0.042 (2)	0.0021 (15)	0.0209 (17)	0.0004 (15)
C8	0.040 (2)	0.0387 (19)	0.039 (2)	−0.0020 (15)	0.0172 (18)	−0.0063 (15)
C9	0.045 (2)	0.044 (2)	0.0324 (18)	0.0059 (18)	0.0110 (17)	0.0005 (17)
C10	0.037 (2)	0.0325 (18)	0.050 (2)	0.0015 (15)	0.0248 (19)	0.0002 (16)
C11	0.044 (2)	0.050 (2)	0.061 (3)	0.0047 (19)	0.029 (2)	0.010 (2)
C12	0.056 (3)	0.052 (2)	0.053 (2)	0.008 (2)	0.028 (2)	0.015 (2)
C13	0.066 (3)	0.047 (2)	0.048 (2)	−0.007 (2)	0.032 (2)	0.0052 (19)
C14	0.053 (2)	0.0376 (19)	0.042 (2)	−0.0096 (17)	0.029 (2)	−0.0046 (17)

C15	0.059 (3)	0.057 (3)	0.056 (3)	−0.015 (2)	0.041 (2)	−0.006 (2)
C16	0.048 (2)	0.067 (3)	0.059 (3)	−0.014 (2)	0.039 (2)	−0.014 (2)
C17	0.040 (2)	0.052 (2)	0.048 (2)	−0.0061 (18)	0.0261 (18)	−0.0157 (19)
C18	0.039 (2)	0.065 (3)	0.065 (3)	0.000 (2)	0.028 (2)	−0.014 (2)
C19	0.042 (2)	0.060 (3)	0.060 (3)	0.010 (2)	0.019 (2)	−0.006 (2)
C20	0.047 (2)	0.043 (2)	0.050 (2)	0.0031 (18)	0.022 (2)	−0.0030 (18)
C21	0.0340 (18)	0.0376 (19)	0.0416 (19)	−0.0043 (15)	0.0205 (16)	−0.0103 (16)
C22	0.0379 (19)	0.0364 (18)	0.0376 (19)	−0.0060 (15)	0.0214 (17)	−0.0089 (15)

Geometric parameters (Å, °)

Cd1—O5^{i}	2.283 (3)	C5—H5	0.9300
Cd1—N2	2.335 (3)	C6—C7	1.378 (5)
Cd1—O2	2.375 (3)	C6—H6	0.9300
Cd1—N1	2.388 (3)	C7—C8	1.392 (5)
Cd1—O1^{ii}	2.400 (3)	C7—C10	1.500 (5)
Cd1—O4^{i}	2.471 (3)	C8—C9	1.381 (5)
Cd1—O1	2.513 (4)	C8—H8	0.9300
O1—C1	1.247 (5)	C9—H9	0.9300
O1—Cd1^{ii}	2.400 (3)	C10—Cd1^{iii}	2.719 (4)
O2—C1	1.243 (5)	C11—C12	1.392 (6)
O3—C4	1.374 (4)	C11—H11	0.9300
O3—C2	1.416 (5)	C12—C13	1.362 (6)
O4—C10	1.239 (4)	C12—H12	0.9300
O4—Cd1^{iii}	2.471 (3)	C13—C14	1.397 (6)
O5—C10	1.259 (4)	C13—H13	0.9300
O5—Cd1^{iii}	2.283 (3)	C14—C22	1.410 (5)
N1—C20	1.325 (5)	C14—C15	1.433 (5)
N1—C21	1.358 (5)	C15—C16	1.337 (6)
N2—C11	1.321 (5)	C15—H15	0.9300
N2—C22	1.354 (4)	C16—C17	1.430 (6)
C1—C2	1.512 (6)	C16—H16	0.9300
C2—C3	1.513 (6)	C17—C18	1.395 (6)
C2—H2	0.9800	C17—C21	1.418 (5)
C3—H3	0.9600	C18—C19	1.356 (6)
C3—H4	0.9600	C18—H18	0.9300
C3—H7	0.9600	C19—C20	1.397 (6)
C4—C5	1.381 (5)	C19—H19	0.9300
C4—C9	1.389 (5)	C20—H20	0.9300
C5—C6	1.390 (5)	C21—C22	1.446 (5)
O5^{i}—Cd1—N2	142.89 (11)	C7—C6—C5	121.7 (3)
O5^{i}—Cd1—O2	128.22 (11)	C7—C6—H6	119.1
N2—Cd1—O2	88.83 (11)	C5—C6—H6	119.1
O5^{i}—Cd1—N1	102.07 (10)	C6—C7—C8	118.6 (3)
N2—Cd1—N1	70.43 (10)	C6—C7—C10	120.7 (3)
O2—Cd1—N1	97.73 (11)	C8—C7—C10	120.6 (3)
O5^{i}—Cd1—O1^{ii}	80.78 (10)	C9—C8—C7	120.4 (3)

N2—Cd1—O1^{ii}	79.38 (11)	C9—C8—H8	119.8
O2—Cd1—O1^{ii}	117.66 (12)	C7—C8—H8	119.8
N1—Cd1—O1^{ii}	132.63 (12)	C8—C9—C4	120.1 (3)
O5^{i}—Cd1—O4^{i}	54.50 (10)	C8—C9—H9	119.9
N2—Cd1—O4^{i}	149.55 (10)	C4—C9—H9	119.9
O2—Cd1—O4^{i}	82.17 (11)	O4—C10—O5	121.8 (3)
N1—Cd1—O4^{i}	81.99 (11)	O4—C10—C7	119.5 (3)
O1^{ii}—Cd1—O4^{i}	130.40 (10)	O5—C10—C7	118.7 (3)
O5^{i}—Cd1—O1	91.82 (10)	O4—C10—Cd1^{iii}	65.2 (2)
N2—Cd1—O1	113.62 (10)	O5—C10—Cd1^{iii}	56.63 (19)
O2—Cd1—O1	52.59 (10)	C7—C10—Cd1^{iii}	175.1 (3)
N1—Cd1—O1	148.57 (10)	N2—C11—C12	123.2 (4)
O1^{ii}—Cd1—O1	77.04 (13)	N2—C11—H11	118.4
O4^{i}—Cd1—O1	83.54 (10)	C12—C11—H11	118.4
C1—O1—Cd1^{ii}	144.5 (3)	C13—C12—C11	119.0 (4)
C1—O1—Cd1	89.3 (3)	C13—C12—H12	120.5
Cd1^{ii}—O1—Cd1	102.96 (13)	C11—C12—H12	120.5
C1—O2—Cd1	96.0 (3)	C12—C13—C14	119.8 (4)
C4—O3—C2	119.8 (3)	C12—C13—H13	120.1
C10—O4—Cd1^{iii}	87.7 (2)	C14—C13—H13	120.1
C10—O5—Cd1^{iii}	95.9 (2)	C13—C14—C22	117.4 (4)
C20—N1—C21	117.6 (3)	C13—C14—C15	123.2 (4)
C20—N1—Cd1	126.7 (3)	C22—C14—C15	119.5 (4)
C21—N1—Cd1	115.7 (2)	C16—C15—C14	120.9 (4)
C11—N2—C22	118.2 (3)	C16—C15—H15	119.5
C11—N2—Cd1	124.0 (2)	C14—C15—H15	119.5
C22—N2—Cd1	117.6 (2)	C15—C16—C17	121.9 (4)
O2—C1—O1	121.2 (4)	C15—C16—H16	119.1
O2—C1—C2	118.8 (4)	C17—C16—H16	119.1
O1—C1—C2	119.7 (4)	C18—C17—C21	116.7 (4)
O3—C2—C1	113.7 (3)	C18—C17—C16	124.1 (4)
O3—C2—C3	106.4 (4)	C21—C17—C16	119.2 (4)
C1—C2—C3	108.9 (4)	C19—C18—C17	120.4 (4)
O3—C2—H2	109.2	C19—C18—H18	119.8
C1—C2—H2	109.2	C17—C18—H18	119.8
C3—C2—H2	109.2	C18—C19—C20	119.1 (4)
C2—C3—H3	109.5	C18—C19—H19	120.4
C2—C3—H4	109.5	C20—C19—H19	120.4
H3—C3—H4	109.5	N1—C20—C19	123.3 (4)
C2—C3—H7	109.5	N1—C20—H20	118.4
H3—C3—H7	109.5	C19—C20—H20	118.4
H4—C3—H7	109.5	N1—C21—C17	122.9 (3)
O3—C4—C5	124.6 (4)	N1—C21—C22	118.1 (3)
O3—C4—C9	115.3 (3)	C17—C21—C22	118.9 (3)
C5—C4—C9	120.2 (3)	N2—C22—C14	122.3 (3)

C4—C5—C6	118.9 (3)	N2—C22—C21	118.1 (3)
C4—C5—H5	120.5	C14—C22—C21	119.6 (3)
C6—C5—H5	120.5		
O5^{i}—Cd1—O1—C1	133.5 (2)	O2—C1—C2—C3	−100.2 (5)
N2—Cd1—O1—C1	−74.2 (2)	O1—C1—C2—C3	74.0 (5)
O2—Cd1—O1—C1	−5.5 (2)	C2—O3—C4—C5	8.6 (6)
N1—Cd1—O1—C1	16.6 (3)	C2—O3—C4—C9	−170.9 (3)
O1^{ii}—Cd1—O1—C1	−146.4 (3)	O3—C4—C5—C6	179.8 (3)
O4^{i}—Cd1—O1—C1	79.6 (2)	C9—C4—C5—C6	−0.7 (6)
C10^{i}—Cd1—O1—C1	106.6 (2)	C4—C5—C6—C7	0.1 (6)
O5^{i}—Cd1—O1—Cd1^{ii}	−80.10 (11)	C5—C6—C7—C8	−0.3 (5)
N2—Cd1—O1—Cd1^{ii}	72.12 (13)	C5—C6—C7—C10	177.5 (3)
O2—Cd1—O1—Cd1^{ii}	140.88 (17)	C6—C7—C8—C9	1.0 (5)
N1—Cd1—O1—Cd1^{ii}	162.94 (15)	C10—C7—C8—C9	−176.8 (3)
O1^{ii}—Cd1—O1—Cd1^{ii}	0.0	C7—C8—C9—C4	−1.5 (6)
O4^{i}—Cd1—O1—Cd1^{ii}	−134.06 (12)	O3—C4—C9—C8	−179.1 (3)
C10^{i}—Cd1—O1—Cd1^{ii}	−107.07 (12)	C5—C4—C9—C8	1.3 (6)
O5^{i}—Cd1—O2—C1	−51.0 (3)	Cd1^{iii}—O4—C10—O5	2.2 (4)
N2—Cd1—O2—C1	126.9 (3)	Cd1^{iii}—O4—C10—C7	−178.5 (3)
N1—Cd1—O2—C1	−163.1 (2)	Cd1^{iii}—O5—C10—O4	−2.4 (4)
O1^{ii}—Cd1—O2—C1	49.5 (3)	Cd1^{iii}—O5—C10—C7	178.3 (3)
O4^{i}—Cd1—O2—C1	−82.3 (3)	C8—C7—C10—O4	−21.2 (5)
O1—Cd1—O2—C1	5.5 (2)	C6—C7—C10—O5	−19.6 (5)
C10^{i}—Cd1—O2—C1	−68.1 (3)	C8—C7—C10—O5	158.2 (3)
O5^{i}—Cd1—N1—C20	−39.4 (3)	C22—N2—C11—C12	1.0 (6)
N2—Cd1—N1—C20	178.5 (3)	Cd1—N2—C11—C12	177.0 (3)
O2—Cd1—N1—C20	92.5 (3)	N2—C11—C12—C13	−0.1 (7)
O1^{ii}—Cd1—N1—C20	−127.9 (3)	C11—C12—C13—C14	−0.6 (6)
O4^{i}—Cd1—N1—C20	11.6 (3)	C12—C13—C14—C22	0.3 (6)
O1—Cd1—N1—C20	75.0 (4)	C12—C13—C14—C15	−178.9 (4)
C10^{i}—Cd1—N1—C20	−13.3 (3)	C13—C14—C15—C16	178.9 (4)
O5^{i}—Cd1—N1—C21	143.2 (2)	C22—C14—C15—C16	−0.2 (6)
N2—Cd1—N1—C21	1.1 (2)	C14—C15—C16—C17	0.4 (6)
O2—Cd1—N1—C21	−84.9 (3)	C15—C16—C17—C18	−178.6 (4)
O1^{ii}—Cd1—N1—C21	54.7 (3)	C15—C16—C17—C21	−0.8 (6)
O4^{i}—Cd1—N1—C21	−165.8 (3)	C21—C17—C18—C19	−0.7 (6)
O1—Cd1—N1—C21	−102.4 (3)	C16—C17—C18—C19	177.1 (4)
C10^{i}—Cd1—N1—C21	169.3 (2)	C17—C18—C19—C20	1.2 (6)
O5^{i}—Cd1—N2—C11	98.3 (3)	C21—N1—C20—C19	−0.7 (6)
O2—Cd1—N2—C11	−78.9 (3)	Cd1—N1—C20—C19	−178.1 (3)
N1—Cd1—N2—C11	−177.6 (3)	C18—C19—C20—N1	−0.5 (6)
O1^{ii}—Cd1—N2—C11	39.5 (3)	C20—N1—C21—C17	1.2 (5)
O4^{i}—Cd1—N2—C11	−151.3 (3)	Cd1—N1—C21—C17	178.9 (3)

O1—Cd1—N2—C11	−31.2 (3)	C20—N1—C21—C22	−178.3 (3)
C10^{i}—Cd1—N2—C11	146.5 (4)	Cd1—N1—C21—C22	−0.6 (4)
O5^{i}—Cd1—N2—C22	−85.7 (3)	C18—C17—C21—N1	−0.5 (5)
O2—Cd1—N2—C22	97.1 (3)	C16—C17—C21—N1	−178.5 (3)
N1—Cd1—N2—C22	−1.5 (2)	C18—C17—C21—C22	179.0 (3)
O1^{ii}—Cd1—N2—C22	−144.5 (3)	C16—C17—C21—C22	1.0 (5)
O4^{i}—Cd1—N2—C22	24.8 (4)	C11—N2—C22—C14	−1.3 (5)
O1—Cd1—N2—C22	144.9 (2)	Cd1—N2—C22—C14	−177.5 (3)
C10^{i}—Cd1—N2—C22	−37.4 (5)	C11—N2—C22—C21	178.1 (3)
Cd1—O2—C1—O1	−10.4 (4)	Cd1—N2—C22—C21	1.8 (4)
Cd1—O2—C1—C2	163.7 (3)	C13—C14—C22—N2	0.6 (5)
Cd1^{ii}—O1—C1—O2	−101.9 (6)	C15—C14—C22—N2	179.9 (3)
Cd1—O1—C1—O2	9.8 (4)	C13—C14—C22—C21	−178.7 (3)
Cd1^{ii}—O1—C1—C2	84.1 (6)	C15—C14—C22—C21	0.5 (5)
Cd1—O1—C1—C2	−164.2 (3)	N1—C21—C22—N2	−0.8 (5)
C4—O3—C2—C1	68.7 (5)	C17—C21—C22—N2	179.7 (3)
C4—O3—C2—C3	−171.4 (4)	N1—C21—C22—C14	178.6 (3)
O2—C1—C2—O3	18.3 (5)	C17—C21—C22—C14	−0.9 (5)
O1—C1—C2—O3	−167.6 (3)		

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

Fig. 1

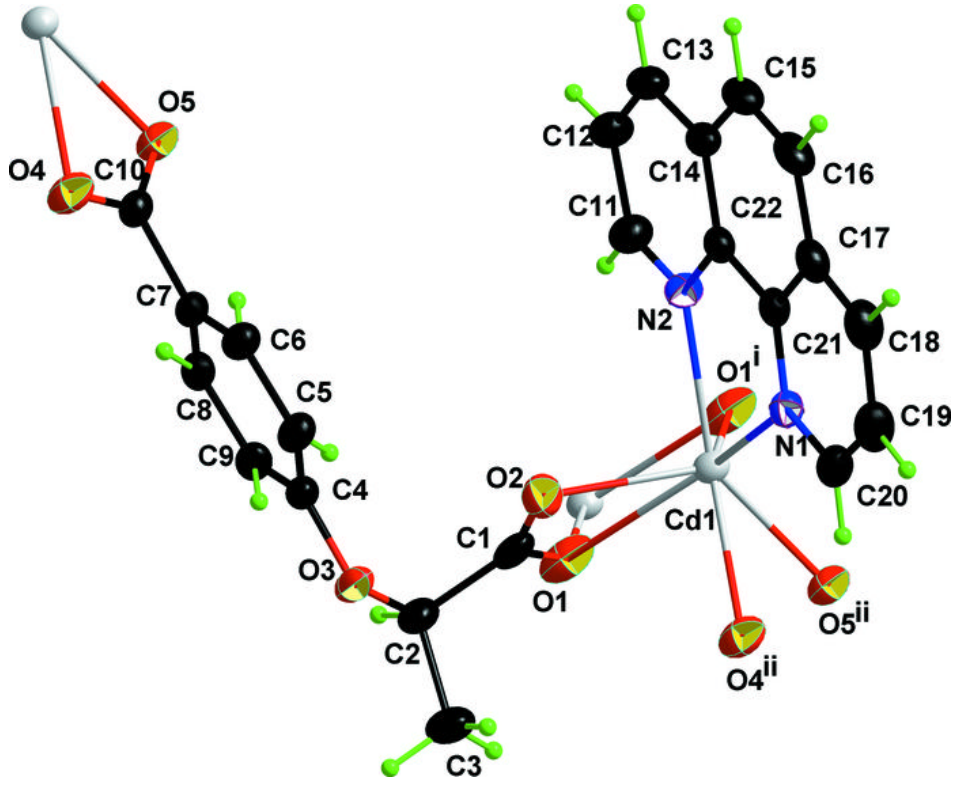
O5
O4
C10
C7
C6
C5
C8
C9
C4
O3
C2
C3
C1
O2
O1
Cd1
O1i
N2
C13
C15
C12
C14
C16
C11
C22
C17
C21
C18
C19
N1
C20
O5ii
O4ii

Fig. 2

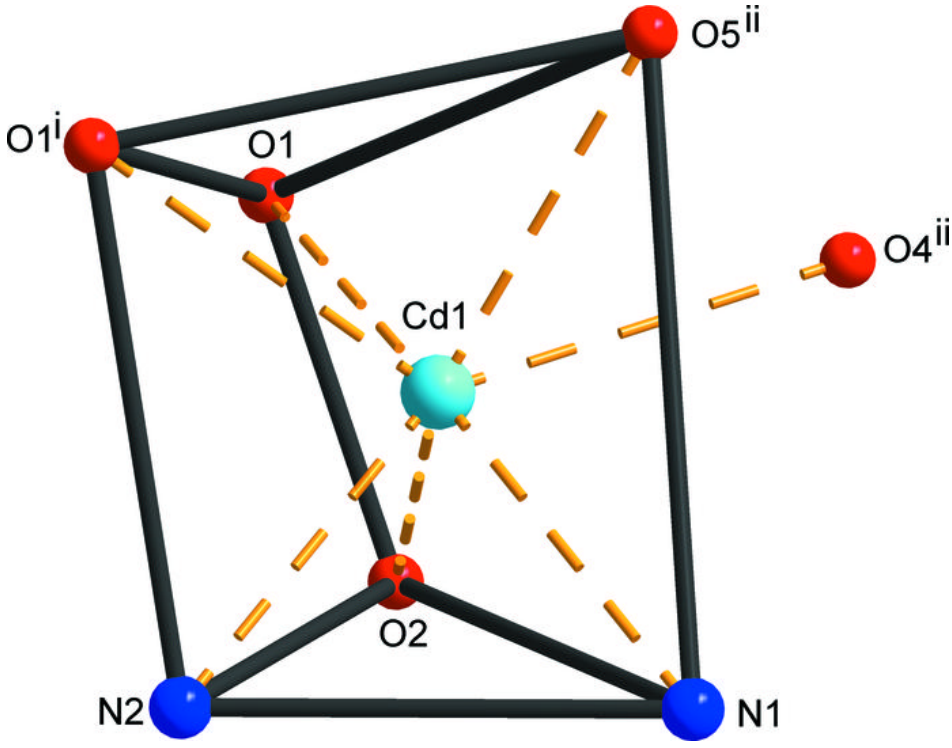

Fig. 3