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catena-Poly[[[aqua(1,10-phenanthroline-κ^2N,N')cadmium(II)]-μ-*o*-phenylenediacetato-$\kappa^2O,O':\kappa O''$-[bis(1,10-phenanthroline-κ^2N,N')cadmium(II)]-μ-*o*-phenylenediacetato-$\kappa O:\kappa^2O',O''$] ethanol 0.79-solvate 3.05-hydrate]

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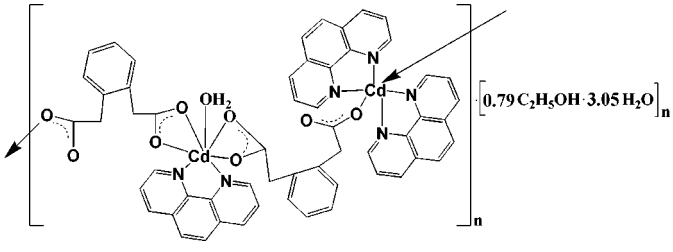
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.004 Å; H-atom completeness 97%; disorder in solvent or counterion; R factor = 0.025; wR factor = 0.093; data-to-parameter ratio = 15.7.

In the title compound, $[Cd_2(C_{10}H_8O_4)_2(C_{12}H_8N_2)_3(H_2O)]\cdot 0.79C_2H_6O\cdot 3.05H_2O$, the two independent Cd^{II} atoms in the asymmetric unit have different coordination modes. One is six-coordinate and the other is seven-coordinate, forming distorted octahedral and monocapped octahedral geometries, respectively. The Cd^{II} atoms are bridged by *o*-phenylenediacetate ligands to form a one-dimensional chain structure, which is further linked into a two-dimensional network through O—H···O hydrogen bonds.

Related literature

For related literature, see: Yam *et al.* (1999); Harvey *et al.* (2000); Ding *et al.* (2005); Shi *et al.* (2005); Tan *et al.* (2006).



Experimental

Crystal data

$[Cd_2(C_{10}H_8O_4)_2(C_{12}H_8N_2)_3(H_2O)]\cdot 0.79C_2H_6O\cdot 3.05H_2O$
M_r = 1257.16
Triclinic, $P\overline{1}$
a = 12.6568 (2) Å
b = 14.7729 (3) Å
c = 15.0674 (3) Å
α = 68.710 (1)°
β = 83.896 (1)°
γ = 78.303 (1)°
V = 2568.84 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.90 mm^{-1}
T = 153 (2) K
0.20 × 0.16 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
25428 measured reflections
11681 independent reflections
10285 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.093
S = 1.01
11681 reflections
744 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O9—H9*B*···O1^{i}	0.81 (3)	1.92 (3)	2.713 (2)	167 (4)
O9—H9*A*···O4^{i}	0.81 (3)	1.88 (3)	2.678 (2)	164 (3)
O11—H01*B*···O3^{ii}	0.82 (3)	2.07 (3)	2.860 (3)	161 (4)
O11—H01*A*···O8	0.82 (3)	1.92 (3)	2.732 (3)	170 (5)
O12—H02*A*···O10	0.80 (3)	2.22 (3)	2.844 (5)	136 (3)
O12—H02*B*···O11^{iii}	0.83 (6)	1.98 (5)	2.776 (4)	161 (6)
O10—H10···O6^{iv}	0.84	1.91	2.745 (5)	174

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: LH2456).

References

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supplementary materials

Acta Cryst. (2007). E**63**, m2392 [**doi:10.1107/S1600536807040214**]

catena-Poly[[[aqua(1,10-phenanthroline-κ^2N,N')cadmium(II)]-μ-*o*-phenylenediacetato-$\kappa^2O,O':\kappa O''$-[bis(1,10-phenanthroline-κ^2N,N')cadmium(II)]-μ-*o*-phenylenediacetato-$\kappa O:\kappa^2O',O''$] ethanol 0.79-solvate 3.05-hydrate]

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Comment

Many complexes containing phenanthroline have been reported (*e.g.* Yam,*et al.*,1999; Harvey *et al.*, 2000; Ding,*et al.*,2005) and these include dinuclear complexes containing phenanthroline bridged by carboxylate ligands (Tan, *et al.*,2006; Shi, *et al.*,2005). In this report we used phenanthroline, (2-Carboxymethyl-phenyl)-acetic acid and cadmium chloride to construct the title one-dimensional chain polymer.

The asymmetric unit contains two independent Cd^{II} atoms, two L^{2-} ligands, three phenanthroline ligands, 3.05 H_2O molecules and one partial occupancy C_2H_5OH molecule. The two Cd^{II} atoms have different coordination modes. Atom Cd1 is coordinated by four O atoms from two different L^{2-} ligands, two N atoms from one phenanthroline ligand and by atom O9 from a water molecule, forming a distorted monocapped octahedral geometry. Atom Cd2 is coordinated by four N atoms from two different phenanthroline ligands and two O atoms from a two bridging L^{2-}, ligands, forming a distorted octahedral geometry. The two independent Cd^{II} atoms are bridged by a L^{2-} ligand forming a one-dimensional chain structure. Part of the one dimensional chain structure is shown in Fig. 1. A l l bond distances and angles are as expected. In the crystal structure, intermolecular O—H···O hydrogen bonds connect molecules to form a two-dimensional network (Fig. 2).

Experimental

A solution of (2-Carboxymethyl-phenyl)-acetic acid(2 mmol,0.388 g), phenanthroline(3 mmol,0.594 g),cadmium chloride(3 mmol,0.37 g) in the mixture solution of ethanol-water. The mixture solution was stirred for 30 min at room temperature,then filtered. The filtrate were added to 30 ml sealed teflon-lined stainless steel vessels, and the teflon-lined stainless steel vessels was placed at 413 K vacuum case for 4 d under autogenous pressure. After cooled to room temperature, colorless crystals were produced(yield: 48.8%, based on Cd).

Refinement

The crystal contains various partial occupancy solvent molecules, namely a 0.79 occupancy ethanol molecule and in addition to the two full occupancy water solvent molecules there are two more sites for water atoms adding to a further occupancy of 1.05. The H atoms of the partial occupancy water atoms were not located and were not included in the refinement. The contribution of these H atoms is included in the molecular formula.

H atoms boned to C and N atoms were positioned geometrically and refined in a riding-model approximation, with C—H distances of 0.95–0.99 Å, N—H distances of 0.92 Å, and with U_{iso}(H) = 1.2U_{eq}(C & N). The H atom of the partially occupied ethanol solvent was included in a calculated position with O—H = 0.84Å and U_{iso}(H) = 1.1U_{eq}(O). The H atoms

of the water molecules were located in difference Fourier maps and were refined with a distance restraint of 0.84 (2)Å and their isotropic displacement parameters were refined.

Figures

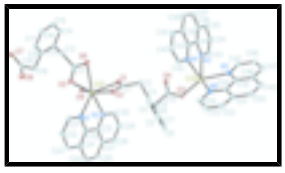


Fig. 1. A section of a one-dimensional chain of the title compound showing 30% probability displacement ellipsoids. All solvent molecules have been omitted.

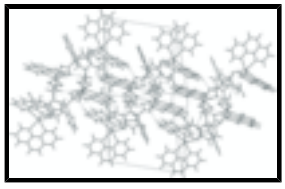


Fig. 2. The packing of title structure, showing hydrogen bonds as dashed lines.

catena-Poly[[[aqua(1,10-phenanthroline-κ^2_N_,_N_')cadmium(II)]-μ-_o_-phenylenediacetato-κ^2_O_,_O_':κ_O_''-[bis(1,10-phenanthroline-κ^2_N_,_N_')cadmium(II)]-μ-_o_-phenylenediacetato-κ_O_:κ^2_O_',_O_''] ethanol 0.79-solvate 3.05-hydrate]

Crystal data

$[Cd_2(C_{10}H_8O_4)_2(C_{12}H_8N_2)_3(H_2O)]\cdot 0.79C_2H_6O\cdot 3.05H_2O$	$Z = 2$
$M_r = 1257.16$	$F_{000} = 1274$
Triclinic, $P\overline{1}$	$D_x = 1.625$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 12.6568$ (2) Å	Cell parameters from 21913 reflections
$b = 14.7729$ (3) Å	$\theta = 3.0$–27.5º
$c = 15.0674$ (3) Å	$\mu = 0.90$ mm^{-1}
$\alpha = 68.710$ (1)º	$T = 153$ (2) K
$\beta = 83.896$ (1)º	Block, colorless
$\gamma = 78.303$ (1)º	0.20 × 0.16 × 0.11 mm
$V = 2568.84$ (9) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	10285 reflections with $I > 2\sigma(I)$
Radiation source: Rotating Anode	$R_{int} = 0.016$
Monochromator: graphite	$\theta_{max} = 27.5$º
$T = 153(2)$ K	$\theta_{min} = 3.0$º
ω scans	$h = -16\rightarrow16$
Absorption correction: none	$k = -19\rightarrow19$
25428 measured reflections	$l = -19\rightarrow19$
11681 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.025$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.093$	$w = 1/[\sigma^2(F_o^2) + (0.0676P)^2 + 0.93P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
11681 reflections	$\Delta\rho_{max} = 0.82$ e Å^{-3}
744 parameters	$\Delta\rho_{min} = -0.85$ e Å^{-3}
9 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997a), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0017 (3)

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}	Occ. (<1)
Cd1	0.689294 (11)	0.421799 (11)	0.608438 (11)	0.02153 (6)	
Cd2	0.053959 (11)	0.793489 (11)	0.773349 (10)	0.02087 (6)	
O1	0.49865 (13)	0.49043 (12)	0.63061 (12)	0.0290 (3)	
O2	0.61249 (13)	0.45434 (12)	0.74444 (12)	0.0296 (3)	
O3	0.22400 (12)	0.79301 (12)	0.71617 (11)	0.0253 (3)	
O4	0.20909 (13)	0.70938 (13)	0.62286 (13)	0.0324 (4)	
O5	0.78141 (15)	0.26364 (13)	0.67143 (16)	0.0418 (5)	
O6	0.60941 (16)	0.26266 (14)	0.66945 (18)	0.0471 (5)	
O7	0.98151 (13)	−0.07694 (12)	0.65385 (12)	0.0287 (3)	
O8	1.02815 (15)	0.03295 (15)	0.70485 (15)	0.0399 (4)	
O9	0.68968 (15)	0.41970 (15)	0.45880 (14)	0.0365 (4)	
N1	0.85996 (15)	0.45969 (14)	0.61669 (13)	0.0243 (4)	
N2	0.69086 (15)	0.59301 (14)	0.51893 (14)	0.0253 (4)	
N3	−0.08039 (15)	0.72071 (13)	0.74069 (13)	0.0233 (4)	
N4	0.09081 (15)	0.61537 (14)	0.85106 (14)	0.0249 (4)	

N5	−0.08516 (17)	0.84413 (15)	0.88096 (15)	0.0304 (4)
N6	0.13219 (18)	0.80485 (15)	0.90742 (14)	0.0301 (4)
C1	0.51985 (18)	0.48876 (16)	0.71056 (17)	0.0249 (4)
C2	0.43193 (19)	0.52965 (17)	0.77025 (17)	0.0293 (5)
H2A	0.3641	0.5545	0.7351	0.035*
H2B	0.4186	0.4758	0.8304	0.035*
C3	0.46247 (17)	0.61267 (18)	0.79344 (17)	0.0274 (5)
C4	0.5117 (2)	0.5908 (2)	0.8791 (2)	0.0435 (7)
H4	0.5267	0.5242	0.9213	0.052*
C5	0.5390 (2)	0.6647 (3)	0.9037 (3)	0.0588 (11)
H5	0.5712	0.6488	0.9629	0.071*
C6	0.5195 (2)	0.7610 (3)	0.8422 (3)	0.0551 (10)
H6	0.5383	0.8118	0.8587	0.066*
C7	0.47280 (19)	0.7833 (2)	0.7570 (2)	0.0399 (6)
H7	0.4602	0.8499	0.7146	0.048*
C8	0.44330 (16)	0.71033 (17)	0.73112 (17)	0.0264 (5)
C9	0.38516 (17)	0.73898 (17)	0.64020 (16)	0.0258 (4)
H9A	0.4114	0.6891	0.6097	0.031*
H9B	0.4012	0.8033	0.5957	0.031*
C10	0.26244 (17)	0.74676 (16)	0.65953 (15)	0.0232 (4)
C11	0.7039 (2)	0.21884 (17)	0.68541 (18)	0.0291 (5)
C12	0.7269 (2)	0.10595 (17)	0.72501 (18)	0.0295 (5)
H12A	0.8017	0.0827	0.7475	0.035*
H12B	0.6771	0.0819	0.7802	0.035*
C13	0.71312 (17)	0.06376 (15)	0.64981 (16)	0.0237 (4)
C14	0.61860 (18)	0.02941 (17)	0.65013 (17)	0.0283 (5)
H14	0.5647	0.0302	0.6989	0.034*
C15	0.60195 (19)	−0.00598 (17)	0.58005 (18)	0.0299 (5)
H15	0.5368	−0.0288	0.5809	0.036*
C16	0.6798 (2)	−0.00801 (17)	0.50930 (18)	0.0306 (5)
H16	0.6682	−0.0315	0.4608	0.037*
C17	0.77596 (19)	0.02477 (17)	0.50944 (16)	0.0280 (5)
H17	0.8300	0.0227	0.4610	0.034*
C18	0.79385 (17)	0.06027 (15)	0.57926 (16)	0.0244 (4)
C19	0.90071 (18)	0.09020 (16)	0.58026 (18)	0.0282 (5)
H19A	0.8879	0.1513	0.5956	0.034*
H19B	0.9360	0.1047	0.5160	0.034*
C20	0.97616 (17)	0.00966 (17)	0.65299 (17)	0.0260 (4)
C21	0.94063 (19)	0.39586 (18)	0.66638 (17)	0.0296 (5)
H21	0.9310	0.3296	0.6995	0.035*
C22	1.03977 (19)	0.4216 (2)	0.67239 (18)	0.0340 (5)
H22	1.0952	0.3738	0.7097	0.041*
C23	1.05560 (19)	0.5164 (2)	0.62381 (18)	0.0344 (5)
H23	1.1221	0.5352	0.6271	0.041*
C24	0.97165 (19)	0.58586 (19)	0.56868 (17)	0.0295 (5)
C25	0.9833 (2)	0.6857 (2)	0.5142 (2)	0.0354 (5)
H25	1.0487	0.7071	0.5157	0.042*
C26	0.9022 (2)	0.74954 (19)	0.4609 (2)	0.0358 (5)
H26	0.9125	0.8146	0.4230	0.043*

C27	0.8011 (2)	0.72061 (17)	0.46086 (17)	0.0290 (5)
C28	0.7118 (2)	0.78729 (18)	0.41059 (19)	0.0359 (5)
H28	0.7185	0.8533	0.3726	0.043*
C29	0.6160 (2)	0.7556 (2)	0.4174 (2)	0.0391 (6)
H29	0.5549	0.7998	0.3856	0.047*
C30	0.6090 (2)	0.65751 (19)	0.47168 (19)	0.0320 (5)
H30	0.5424	0.6361	0.4748	0.038*
C31	0.78632 (18)	0.62377 (16)	0.51401 (16)	0.0237 (4)
C32	0.87444 (17)	0.55413 (17)	0.56788 (16)	0.0237 (4)
C33	−0.16356 (18)	0.77187 (17)	0.68545 (16)	0.0263 (4)
H33	−0.1626	0.8391	0.6479	0.032*
C34	−0.25225 (19)	0.73094 (19)	0.68023 (18)	0.0297 (5)
H34	−0.3102	0.7702	0.6405	0.036*
C35	−0.25462 (19)	0.63431 (19)	0.73267 (17)	0.0292 (5)
H35	−0.3149	0.6058	0.7308	0.035*
C36	−0.16710 (19)	0.57734 (17)	0.78951 (16)	0.0262 (4)
C37	−0.1615 (2)	0.47415 (19)	0.84237 (18)	0.0329 (5)
H37	−0.2200	0.4428	0.8422	0.040*
C38	−0.0735 (2)	0.42123 (18)	0.89247 (18)	0.0349 (5)
H38	−0.0706	0.3526	0.9262	0.042*
C39	0.0153 (2)	0.46562 (17)	0.89621 (17)	0.0294 (5)
C40	0.1087 (2)	0.41219 (18)	0.9472 (2)	0.0383 (6)
H40	0.1154	0.3431	0.9805	0.046*
C41	0.1895 (2)	0.4603 (2)	0.9484 (2)	0.0391 (6)
H41	0.2532	0.4250	0.9820	0.047*
C42	0.17758 (19)	0.56245 (19)	0.89955 (18)	0.0320 (5)
H42	0.2342	0.5952	0.9013	0.038*
C43	0.01141 (18)	0.56768 (16)	0.84802 (15)	0.0232 (4)
C44	−0.08122 (17)	0.62421 (16)	0.79162 (15)	0.0221 (4)
C45	−0.1902 (2)	0.8629 (2)	0.8677 (2)	0.0384 (6)
H45	−0.2145	0.8535	0.8146	0.046*
C46	−0.2673 (3)	0.8960 (2)	0.9283 (2)	0.0487 (7)
H46	−0.3421	0.9087	0.9166	0.058*
C47	−0.2321 (3)	0.9095 (3)	1.0047 (2)	0.0544 (8)
H47	−0.2829	0.9325	1.0463	0.065*
C48	−0.1213 (3)	0.8896 (2)	1.0217 (2)	0.0448 (7)
C49	−0.0793 (3)	0.8993 (3)	1.1015 (2)	0.0560 (9)
H49	−0.1279	0.9225	1.1443	0.067*
C50	0.0272 (3)	0.8765 (3)	1.1178 (2)	0.0528 (8)
H50	0.0526	0.8825	1.1722	0.063*
C51	0.1025 (3)	0.8431 (2)	1.0527 (2)	0.0421 (6)
C52	0.2130 (3)	0.8170 (3)	1.0670 (2)	0.0517 (8)
H52	0.2413	0.8204	1.1214	0.062*
C53	0.2808 (3)	0.7866 (3)	1.0024 (2)	0.0490 (7)
H53	0.3564	0.7687	1.0113	0.059*
C54	0.2367 (2)	0.7823 (2)	0.92304 (19)	0.0370 (6)
H54	0.2844	0.7621	0.8780	0.044*
C55	0.0641 (2)	0.83559 (17)	0.97167 (17)	0.0307 (5)
C56	−0.0501 (2)	0.85692 (17)	0.95655 (18)	0.0325 (5)

O11	1.24607 (16)	−0.02220 (14)	0.72639 (15)	0.0380 (4)	
O12	−0.3976 (3)	0.9918 (3)	1.1718 (3)	0.0813 (9)	
O13	−0.4695 (4)	1.0800 (4)	0.9987 (4)	0.112 (2)	0.846 (12)
O10	−0.4680 (3)	0.8163 (3)	1.1848 (3)	0.0728 (10)	0.792 (4)
H10	−0.5096	0.7944	1.2318	0.080*	0.792 (4)
C58	−0.4086 (5)	0.7355 (4)	1.1573 (5)	0.115 (3)	0.792 (4)
H58A	−0.3846	0.7615	1.0895	0.137*	0.792 (4)
H58B	−0.4571	0.6885	1.1636	0.137*	0.792 (4)
C57	−0.3117 (5)	0.6815 (5)	1.2168 (6)	0.121 (3)	0.792 (4)
H57A	−0.2627	0.7274	1.2099	0.133*	0.792 (4)
H57B	−0.2741	0.6278	1.1953	0.133*	0.792 (4)
H57C	−0.3351	0.6541	1.2838	0.133*	0.792 (4)
O10W	−0.4956 (12)	0.7129 (10)	1.1176 (10)	0.0728 (10)	0.208 (4)
H9AO	0.720 (2)	0.3728 (16)	0.444 (2)	0.035 (8)*	
H9BO	0.6380 (19)	0.454 (2)	0.428 (2)	0.046 (9)*	
H01A	1.1821 (14)	0.001 (3)	0.716 (3)	0.090 (16)*	
H01B	1.255 (3)	−0.0762 (14)	0.720 (3)	0.055 (10)*	
H02A	−0.388 (3)	0.9327 (8)	1.194 (2)	0.035 (9)*	
H02B	−0.363 (4)	1.013 (4)	1.201 (4)	0.12 (2)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02012 (9)	0.01939 (9)	0.02826 (10)	−0.00338 (6)	−0.00033 (6)	−0.01231 (7)
Cd2	0.02013 (9)	0.01867 (9)	0.02286 (9)	−0.00310 (6)	0.00037 (6)	−0.00666 (6)
O1	0.0257 (7)	0.0303 (8)	0.0330 (9)	−0.0016 (7)	−0.0018 (6)	−0.0150 (7)
O2	0.0261 (8)	0.0292 (8)	0.0339 (9)	0.0007 (7)	−0.0021 (6)	−0.0142 (7)
O3	0.0217 (7)	0.0269 (8)	0.0292 (8)	−0.0026 (6)	0.0023 (6)	−0.0137 (7)
O4	0.0250 (8)	0.0390 (9)	0.0403 (10)	−0.0025 (7)	−0.0031 (7)	−0.0234 (8)
O5	0.0389 (10)	0.0234 (8)	0.0653 (13)	−0.0052 (8)	−0.0126 (9)	−0.0155 (9)
O6	0.0359 (10)	0.0292 (9)	0.0783 (15)	0.0020 (8)	−0.0095 (10)	−0.0233 (10)
O7	0.0275 (8)	0.0199 (7)	0.0335 (9)	−0.0013 (6)	−0.0038 (7)	−0.0042 (7)
O8	0.0361 (9)	0.0392 (10)	0.0492 (11)	−0.0002 (8)	−0.0122 (8)	−0.0218 (9)
O9	0.0324 (9)	0.0444 (10)	0.0418 (10)	0.0077 (8)	−0.0110 (8)	−0.0307 (9)
N1	0.0229 (8)	0.0278 (9)	0.0242 (9)	−0.0046 (7)	−0.0009 (7)	−0.0112 (8)
N2	0.0256 (9)	0.0238 (9)	0.0289 (10)	−0.0055 (7)	−0.0011 (7)	−0.0112 (8)
N3	0.0236 (8)	0.0215 (8)	0.0251 (9)	−0.0042 (7)	−0.0017 (7)	−0.0080 (7)
N4	0.0245 (9)	0.0233 (9)	0.0244 (9)	−0.0007 (7)	0.0000 (7)	−0.0075 (8)
N5	0.0377 (11)	0.0227 (9)	0.0291 (10)	−0.0059 (8)	0.0061 (8)	−0.0089 (8)
N6	0.0409 (11)	0.0250 (9)	0.0253 (10)	−0.0108 (8)	0.0032 (8)	−0.0082 (8)
C1	0.0258 (10)	0.0164 (9)	0.0318 (11)	−0.0054 (8)	0.0040 (9)	−0.0081 (9)
C2	0.0290 (11)	0.0248 (11)	0.0314 (12)	−0.0053 (9)	0.0081 (9)	−0.0089 (9)
C3	0.0214 (10)	0.0338 (12)	0.0288 (11)	−0.0002 (9)	0.0024 (8)	−0.0167 (10)
C4	0.0361 (13)	0.0577 (18)	0.0336 (13)	0.0140 (13)	−0.0068 (11)	−0.0226 (13)
C5	0.0310 (13)	0.105 (3)	0.059 (2)	0.0126 (17)	−0.0159 (13)	−0.060 (2)
C6	0.0233 (12)	0.083 (2)	0.089 (3)	−0.0018 (14)	−0.0059 (14)	−0.069 (2)
C7	0.0214 (10)	0.0419 (14)	0.0691 (19)	−0.0071 (10)	0.0031 (11)	−0.0348 (14)
C8	0.0162 (9)	0.0288 (11)	0.0392 (13)	−0.0021 (8)	0.0024 (8)	−0.0195 (10)

C9	0.0218 (10)	0.0245 (10)	0.0293 (11)	−0.0029 (8)	0.0049 (8)	−0.0097 (9)
C10	0.0230 (9)	0.0197 (9)	0.0239 (10)	−0.0006 (8)	0.0010 (8)	−0.0065 (8)
C11	0.0337 (12)	0.0251 (11)	0.0328 (12)	−0.0030 (9)	−0.0051 (9)	−0.0153 (10)
C12	0.0342 (12)	0.0249 (11)	0.0312 (12)	−0.0048 (9)	−0.0037 (9)	−0.0116 (10)
C13	0.0255 (10)	0.0166 (9)	0.0277 (11)	−0.0021 (8)	−0.0037 (8)	−0.0066 (8)
C14	0.0244 (10)	0.0231 (10)	0.0342 (12)	−0.0033 (9)	0.0002 (9)	−0.0072 (9)
C15	0.0281 (11)	0.0254 (11)	0.0358 (12)	−0.0077 (9)	−0.0075 (9)	−0.0069 (10)
C16	0.0371 (12)	0.0237 (11)	0.0319 (12)	−0.0020 (9)	−0.0119 (10)	−0.0098 (10)
C17	0.0301 (11)	0.0227 (10)	0.0264 (11)	0.0004 (9)	0.0002 (9)	−0.0062 (9)
C18	0.0222 (9)	0.0153 (9)	0.0315 (11)	−0.0014 (8)	−0.0034 (8)	−0.0034 (8)
C19	0.0251 (10)	0.0185 (10)	0.0360 (12)	−0.0054 (8)	−0.0017 (9)	−0.0028 (9)
C20	0.0200 (9)	0.0251 (10)	0.0293 (11)	−0.0044 (8)	0.0027 (8)	−0.0062 (9)
C21	0.0275 (11)	0.0306 (11)	0.0306 (12)	−0.0050 (9)	−0.0018 (9)	−0.0106 (10)
C22	0.0247 (11)	0.0445 (14)	0.0332 (12)	−0.0025 (10)	−0.0035 (9)	−0.0152 (11)
C23	0.0231 (10)	0.0506 (15)	0.0350 (13)	−0.0109 (10)	0.0033 (9)	−0.0203 (12)
C24	0.0271 (11)	0.0372 (13)	0.0289 (11)	−0.0108 (10)	0.0054 (9)	−0.0160 (10)
C25	0.0323 (12)	0.0377 (13)	0.0430 (14)	−0.0183 (11)	0.0055 (10)	−0.0178 (12)
C26	0.0435 (14)	0.0293 (12)	0.0394 (14)	−0.0183 (11)	0.0058 (11)	−0.0134 (11)
C27	0.0342 (12)	0.0254 (11)	0.0313 (12)	−0.0094 (9)	0.0040 (9)	−0.0137 (10)
C28	0.0466 (14)	0.0212 (11)	0.0379 (13)	−0.0061 (10)	−0.0002 (11)	−0.0083 (10)
C29	0.0366 (13)	0.0293 (12)	0.0463 (15)	0.0000 (11)	−0.0068 (11)	−0.0091 (12)
C30	0.0278 (11)	0.0283 (12)	0.0382 (13)	−0.0026 (10)	−0.0049 (10)	−0.0099 (10)
C31	0.0271 (10)	0.0242 (10)	0.0241 (10)	−0.0062 (8)	0.0013 (8)	−0.0134 (9)
C32	0.0242 (10)	0.0279 (11)	0.0242 (10)	−0.0094 (9)	0.0022 (8)	−0.0136 (9)
C33	0.0272 (10)	0.0224 (10)	0.0279 (11)	−0.0010 (9)	−0.0036 (8)	−0.0083 (9)
C34	0.0245 (10)	0.0342 (12)	0.0324 (12)	−0.0010 (9)	−0.0042 (9)	−0.0155 (10)
C35	0.0261 (10)	0.0359 (12)	0.0323 (12)	−0.0092 (10)	0.0015 (9)	−0.0185 (10)
C36	0.0328 (11)	0.0267 (11)	0.0229 (10)	−0.0110 (9)	0.0040 (8)	−0.0113 (9)
C37	0.0427 (13)	0.0299 (12)	0.0309 (12)	−0.0175 (10)	0.0025 (10)	−0.0112 (10)
C38	0.0518 (15)	0.0201 (10)	0.0315 (12)	−0.0128 (10)	0.0007 (11)	−0.0048 (9)
C39	0.0396 (12)	0.0207 (10)	0.0265 (11)	−0.0043 (9)	0.0000 (9)	−0.0075 (9)
C40	0.0480 (15)	0.0199 (11)	0.0378 (14)	0.0028 (10)	−0.0048 (11)	−0.0029 (10)
C41	0.0354 (13)	0.0343 (13)	0.0387 (14)	0.0091 (11)	−0.0084 (11)	−0.0085 (11)
C42	0.0253 (11)	0.0318 (12)	0.0360 (13)	0.0007 (10)	−0.0035 (9)	−0.0107 (10)
C43	0.0277 (10)	0.0206 (10)	0.0200 (10)	−0.0025 (8)	0.0021 (8)	−0.0075 (8)
C44	0.0265 (10)	0.0209 (9)	0.0203 (10)	−0.0054 (8)	0.0016 (8)	−0.0089 (8)
C45	0.0406 (14)	0.0369 (13)	0.0382 (14)	−0.0075 (11)	0.0071 (11)	−0.0159 (12)
C46	0.0420 (15)	0.0547 (18)	0.0521 (18)	−0.0080 (14)	0.0146 (13)	−0.0268 (15)
C47	0.0562 (18)	0.060 (2)	0.0553 (19)	−0.0157 (16)	0.0265 (15)	−0.0350 (17)
C48	0.0592 (18)	0.0409 (15)	0.0430 (15)	−0.0206 (14)	0.0193 (13)	−0.0246 (13)
C49	0.076 (2)	0.065 (2)	0.0465 (17)	−0.0284 (18)	0.0256 (16)	−0.0413 (17)
C50	0.077 (2)	0.061 (2)	0.0393 (16)	−0.0317 (18)	0.0136 (15)	−0.0335 (15)
C51	0.0629 (18)	0.0391 (14)	0.0341 (14)	−0.0238 (13)	0.0078 (12)	−0.0191 (12)
C52	0.066 (2)	0.065 (2)	0.0375 (15)	−0.0264 (17)	−0.0035 (14)	−0.0253 (15)
C53	0.0491 (16)	0.065 (2)	0.0400 (16)	−0.0140 (15)	−0.0048 (13)	−0.0233 (15)
C54	0.0410 (13)	0.0420 (14)	0.0295 (12)	−0.0111 (12)	0.0003 (10)	−0.0128 (11)
C55	0.0483 (14)	0.0223 (10)	0.0256 (11)	−0.0158 (10)	0.0070 (10)	−0.0104 (9)
C56	0.0494 (14)	0.0226 (11)	0.0285 (12)	−0.0154 (10)	0.0106 (10)	−0.0111 (9)
O11	0.0382 (10)	0.0286 (9)	0.0483 (11)	−0.0083 (8)	0.0015 (8)	−0.0143 (8)

O12	0.088 (2)	0.087 (2)	0.100 (2)	−0.0421 (19)	0.0266 (18)	−0.065 (2)
O13	0.098 (3)	0.112 (4)	0.133 (4)	−0.023 (3)	−0.035 (3)	−0.039 (3)
O10	0.083 (2)	0.067 (2)	0.073 (2)	−0.0356 (18)	0.0166 (18)	−0.0234 (18)
C58	0.165 (8)	0.113 (6)	0.091 (5)	−0.092 (6)	0.021 (5)	−0.036 (5)
C57	0.088 (5)	0.176 (9)	0.155 (8)	−0.045 (5)	0.036 (5)	−0.122 (7)
O10W	0.083 (2)	0.067 (2)	0.073 (2)	−0.0356 (18)	0.0166 (18)	−0.0234 (18)

Geometric parameters (Å, °)

Cd1—O9	2.2656 (18)	C21—C22	1.404 (3)
Cd1—O5	2.2891 (18)	C21—H21	0.9500
Cd1—O2	2.3404 (16)	C22—C23	1.369 (4)
Cd1—N1	2.3649 (19)	C22—H22	0.9500
Cd1—N2	2.399 (2)	C23—C24	1.414 (3)
Cd1—O1	2.4586 (15)	C23—H23	0.9500
Cd1—O6	2.567 (2)	C24—C32	1.405 (3)
Cd1—C1	2.737 (2)	C24—C25	1.433 (4)
Cd2—O7^{i}	2.2098 (16)	C25—C26	1.349 (4)
Cd2—O3	2.2312 (15)	C25—H25	0.9500
Cd2—N3	2.3650 (19)	C26—C27	1.430 (4)
Cd2—N6	2.414 (2)	C26—H26	0.9500
Cd2—N4	2.4277 (19)	C27—C31	1.403 (3)
Cd2—N5	2.455 (2)	C27—C28	1.417 (4)
O1—C1	1.252 (3)	C28—C29	1.367 (4)
O2—C1	1.261 (3)	C28—H28	0.9500
O3—C10	1.278 (3)	C29—C30	1.397 (4)
O4—C10	1.232 (3)	C29—H29	0.9500
O5—C11	1.251 (3)	C30—H30	0.9500
O6—C11	1.241 (3)	C31—C32	1.443 (3)
O7—C20	1.263 (3)	C33—C34	1.400 (3)
O7—Cd2^{ii}	2.2099 (16)	C33—H33	0.9500
O8—C20	1.248 (3)	C34—C35	1.362 (4)
O9—H9AO	0.81 (3)	C34—H34	0.9500
O9—H9BO	0.81 (3)	C35—C36	1.403 (3)
N1—C21	1.324 (3)	C35—H35	0.9500
N1—C32	1.360 (3)	C36—C44	1.411 (3)
N2—C30	1.324 (3)	C36—C37	1.432 (3)
N2—C31	1.360 (3)	C37—C38	1.349 (4)
N3—C33	1.334 (3)	C37—H37	0.9500
N3—C44	1.353 (3)	C38—C39	1.427 (4)
N4—C42	1.326 (3)	C38—H38	0.9500
N4—C43	1.352 (3)	C39—C43	1.409 (3)
N5—C45	1.324 (4)	C39—C40	1.409 (4)
N5—C56	1.352 (3)	C40—C41	1.364 (4)
N6—C54	1.322 (3)	C40—H40	0.9500
N6—C55	1.367 (3)	C41—C42	1.402 (4)
C1—C2	1.524 (3)	C41—H41	0.9500
C2—C3	1.519 (3)	C42—H42	0.9500
C2—H2A	0.9900	C43—C44	1.447 (3)

C2—H2B	0.9900	C45—C46	1.402 (4)
C3—C8	1.394 (3)	C45—H45	0.9500
C3—C4	1.395 (3)	C46—C47	1.369 (5)
C4—C5	1.387 (5)	C46—H46	0.9500
C4—H4	0.9500	C47—C48	1.406 (5)
C5—C6	1.376 (6)	C47—H47	0.9500
C5—H5	0.9500	C48—C56	1.410 (3)
C6—C7	1.372 (5)	C48—C49	1.428 (5)
C6—H6	0.9500	C49—C50	1.348 (5)
C7—C8	1.398 (3)	C49—H49	0.9500
C7—H7	0.9500	C50—C51	1.441 (4)
C8—C9	1.505 (3)	C50—H50	0.9500
C9—C10	1.538 (3)	C51—C52	1.392 (5)
C9—H9A	0.9900	C51—C55	1.409 (4)
C9—H9B	0.9900	C52—C53	1.367 (4)
C11—C12	1.529 (3)	C52—H52	0.9500
C12—C13	1.517 (3)	C53—C54	1.399 (4)
C12—H12A	0.9900	C53—H53	0.9500
C12—H12B	0.9900	C54—H54	0.9500
C13—C14	1.390 (3)	C55—C56	1.439 (4)
C13—C18	1.401 (3)	O11—H01A	0.82 (3)
C14—C15	1.388 (3)	O11—H01B	0.82 (3)
C14—H14	0.9500	O12—O13	2.624 (6)
C15—C16	1.377 (4)	O12—H02A	0.80 (3)
C15—H15	0.9500	O12—H02B	0.83 (6)
C16—C17	1.399 (4)	O10—C58	1.446 (3)
C16—H16	0.9500	O10—H10	0.8400
C17—C18	1.390 (3)	C58—C57	1.504 (3)
C17—H17	0.9500	C58—H58A	0.9900
C18—C19	1.509 (3)	C58—H58B	0.9900
C19—C20	1.531 (3)	C57—H57A	0.9800
C19—H19A	0.9900	C57—H57B	0.9800
C19—H19B	0.9900	C57—H57C	0.9800
O9—Cd1—O5	94.96 (7)	C16—C17—H17	119.4
O9—Cd1—O2	155.26 (6)	C17—C18—C13	118.9 (2)
O5—Cd1—O2	102.44 (7)	C17—C18—C19	119.8 (2)
O9—Cd1—N1	103.79 (7)	C13—C18—C19	121.3 (2)
O5—Cd1—N1	81.95 (7)	C18—C19—C20	112.13 (18)
O2—Cd1—N1	96.01 (6)	C18—C19—H19A	109.2
O9—Cd1—N2	80.43 (7)	C20—C19—H19A	109.2
O5—Cd1—N2	149.43 (7)	C18—C19—H19B	109.2
O2—Cd1—N2	92.79 (6)	C20—C19—H19B	109.2
N1—Cd1—N2	70.09 (6)	H19A—C19—H19B	107.9
O9—Cd1—O1	100.71 (6)	O8—C20—O7	125.1 (2)
O5—Cd1—O1	130.02 (7)	O8—C20—C19	119.4 (2)
O2—Cd1—O1	54.58 (5)	O7—C20—C19	115.5 (2)
N1—Cd1—O1	137.32 (6)	N1—C21—C22	123.0 (2)
N2—Cd1—O1	80.34 (6)	N1—C21—H21	118.5
O9—Cd1—O6	88.46 (8)	C22—C21—H21	118.5

O5—Cd1—O6	53.06 (6)	C23—C22—C21	119.2 (2)
O2—Cd1—O6	88.12 (7)	C23—C22—H22	120.4
N1—Cd1—O6	134.45 (6)	C21—C22—H22	120.4
N2—Cd1—O6	155.23 (6)	C22—C23—C24	119.1 (2)
O1—Cd1—O6	80.08 (6)	C22—C23—H23	120.4
O9—Cd1—C1	127.90 (7)	C24—C23—H23	120.4
O5—Cd1—C1	119.58 (7)	C32—C24—C23	117.8 (2)
O2—Cd1—C1	27.37 (6)	C32—C24—C25	119.9 (2)
N1—Cd1—C1	117.77 (7)	C23—C24—C25	122.3 (2)
N2—Cd1—C1	85.39 (6)	C26—C25—C24	120.7 (2)
O1—Cd1—C1	27.23 (6)	C26—C25—H25	119.6
O6—Cd1—C1	84.13 (7)	C24—C25—H25	119.6
$O7^{i}$—Cd2—O3	96.07 (6)	C25—C26—C27	120.8 (2)
$O7^{i}$—Cd2—N3	82.72 (6)	C25—C26—H26	119.6
O3—Cd2—N3	128.91 (6)	C27—C26—H26	119.6
$O7^{i}$—Cd2—N6	123.74 (7)	C31—C27—C28	117.4 (2)
O3—Cd2—N6	81.73 (6)	C31—C27—C26	120.0 (2)
N3—Cd2—N6	139.90 (7)	C28—C27—C26	122.5 (2)
$O7^{i}$—Cd2—N4	148.45 (7)	C29—C28—C27	119.2 (2)
O3—Cd2—N4	90.95 (6)	C29—C28—H28	120.4
N3—Cd2—N4	69.16 (6)	C27—C28—H28	120.4
N6—Cd2—N4	87.67 (7)	C28—C29—C30	119.3 (2)
$O7^{i}$—Cd2—N5	88.72 (7)	C28—C29—H29	120.3
O3—Cd2—N5	146.51 (7)	C30—C29—H29	120.3
N3—Cd2—N5	84.56 (7)	N2—C30—C29	123.1 (2)
N6—Cd2—N5	68.34 (7)	N2—C30—H30	118.5
N4—Cd2—N5	102.12 (6)	C29—C30—H30	118.5
C1—O1—Cd1	88.85 (13)	N2—C31—C27	122.6 (2)
C1—O2—Cd1	94.08 (14)	N2—C31—C32	118.2 (2)
C10—O3—Cd2	120.91 (14)	C27—C31—C32	119.2 (2)
C11—O5—Cd1	98.65 (15)	N1—C32—C24	122.3 (2)
C11—O6—Cd1	85.81 (16)	N1—C32—C31	118.5 (2)
C20—O7—$Cd2^{ii}$	121.04 (15)	C24—C32—C31	119.2 (2)
Cd1—O9—H9AO	122 (2)	N3—C33—C34	123.0 (2)
Cd1—O9—H9BO	115 (2)	N3—C33—H33	118.5
H9AO—O9—H9BO	118 (3)	C34—C33—H33	118.5
C21—N1—C32	118.5 (2)	C35—C34—C33	119.4 (2)
C21—N1—Cd1	124.41 (17)	C35—C34—H34	120.3
C32—N1—Cd1	117.07 (14)	C33—C34—H34	120.3
C30—N2—C31	118.3 (2)	C34—C35—C36	119.3 (2)
C30—N2—Cd1	125.61 (17)	C34—C35—H35	120.4
C31—N2—Cd1	116.00 (14)	C36—C35—H35	120.4
C33—N3—C44	118.0 (2)	C35—C36—C44	117.9 (2)
C33—N3—Cd2	123.73 (15)	C35—C36—C37	122.2 (2)
C44—N3—Cd2	117.61 (14)	C44—C36—C37	119.8 (2)
C42—N4—C43	118.0 (2)	C38—C37—C36	120.2 (2)
C42—N4—Cd2	126.33 (18)	C38—C37—H37	119.9
C43—N4—Cd2	115.59 (14)	C36—C37—H37	119.9

C45—N5—C56	118.8 (2)	C37—C38—C39	121.7 (2)
C45—N5—Cd2	124.48 (17)	C37—C38—H38	119.1
C56—N5—Cd2	116.65 (17)	C39—C38—H38	119.1
C54—N6—C55	118.0 (2)	C43—C39—C40	117.0 (2)
C54—N6—Cd2	124.04 (16)	C43—C39—C38	119.9 (2)
C55—N6—Cd2	117.99 (17)	C40—C39—C38	123.1 (2)
O1—C1—O2	122.4 (2)	C41—C40—C39	119.6 (2)
O1—C1—C2	119.8 (2)	C41—C40—H40	120.2
O2—C1—C2	117.8 (2)	C39—C40—H40	120.2
O1—C1—Cd1	63.93 (11)	C40—C41—C42	119.3 (2)
O2—C1—Cd1	58.55 (11)	C40—C41—H41	120.4
C2—C1—Cd1	175.33 (17)	C42—C41—H41	120.4
C3—C2—C1	112.04 (19)	N4—C42—C41	123.0 (3)
C3—C2—H2A	109.2	N4—C42—H42	118.5
C1—C2—H2A	109.2	C41—C42—H42	118.5
C3—C2—H2B	109.2	N4—C43—C39	123.1 (2)
C1—C2—H2B	109.2	N4—C43—C44	118.24 (19)
H2A—C2—H2B	107.9	C39—C43—C44	118.6 (2)
C8—C3—C4	118.9 (2)	N3—C44—C36	122.5 (2)
C8—C3—C2	121.8 (2)	N3—C44—C43	117.9 (2)
C4—C3—C2	119.2 (2)	C36—C44—C43	119.6 (2)
C5—C4—C3	121.0 (3)	N5—C45—C46	123.0 (3)
C5—C4—H4	119.5	N5—C45—H45	118.5
C3—C4—H4	119.5	C46—C45—H45	118.5
C6—C5—C4	119.9 (3)	C47—C46—C45	118.5 (3)
C6—C5—H5	120.1	C47—C46—H46	120.8
C4—C5—H5	120.1	C45—C46—H46	120.8
C7—C6—C5	119.7 (3)	C46—C47—C48	120.3 (3)
C7—C6—H6	120.2	C46—C47—H47	119.9
C5—C6—H6	120.2	C48—C47—H47	119.9
C6—C7—C8	121.5 (3)	C47—C48—C56	117.0 (3)
C6—C7—H7	119.2	C47—C48—C49	123.2 (3)
C8—C7—H7	119.2	C56—C48—C49	119.7 (3)
C3—C8—C7	119.0 (2)	C50—C49—C48	121.9 (3)
C3—C8—C9	121.2 (2)	C50—C49—H49	119.0
C7—C8—C9	119.7 (2)	C48—C49—H49	119.0
C8—C9—C10	111.10 (18)	C49—C50—C51	119.9 (3)
C8—C9—H9A	109.4	C49—C50—H50	120.0
C10—C9—H9A	109.4	C51—C50—H50	120.0
C8—C9—H9B	109.4	C52—C51—C55	118.1 (3)
C10—C9—H9B	109.4	C52—C51—C50	122.4 (3)
H9A—C9—H9B	108.0	C55—C51—C50	119.6 (3)
O4—C10—O3	124.9 (2)	C53—C52—C51	119.8 (3)
O4—C10—C9	120.84 (19)	C53—C52—H52	120.1
O3—C10—C9	114.27 (19)	C51—C52—H52	120.1
O6—C11—O5	122.4 (2)	C52—C53—C54	118.7 (3)
O6—C11—C12	119.2 (2)	C52—C53—H53	120.6
O5—C11—C12	118.4 (2)	C54—C53—H53	120.6
C13—C12—C11	111.20 (19)	N6—C54—C53	123.5 (3)

C13—C12—H12A	109.4	N6—C54—H54	118.2
C11—C12—H12A	109.4	C53—C54—H54	118.2
C13—C12—H12B	109.4	N6—C55—C51	121.9 (3)
C11—C12—H12B	109.4	N6—C55—C56	118.0 (2)
H12A—C12—H12B	108.0	C51—C55—C56	120.0 (2)
C14—C13—C18	119.6 (2)	N5—C56—C48	122.4 (3)
C14—C13—C12	119.6 (2)	N5—C56—C55	118.9 (2)
C18—C13—C12	120.8 (2)	C48—C56—C55	118.7 (2)
C15—C14—C13	120.8 (2)	H01A—O11—H01B	105 (4)
C15—C14—H14	119.6	O13—O12—H02A	119 (3)
C13—C14—H14	119.6	O13—O12—H02B	128 (5)
C16—C15—C14	120.1 (2)	H02A—O12—H02B	110 (5)
C16—C15—H15	120.0	O10—C58—C57	112.6 (3)
C14—C15—H15	120.0	O10—C58—H58A	109.1
C15—C16—C17	119.4 (2)	C57—C58—H58A	109.1
C15—C16—H16	120.3	O10—C58—H58B	109.1
C17—C16—H16	120.3	C57—C58—H58B	109.1
C18—C17—C16	121.1 (2)	H58A—C58—H58B	107.8
C18—C17—H17	119.4		

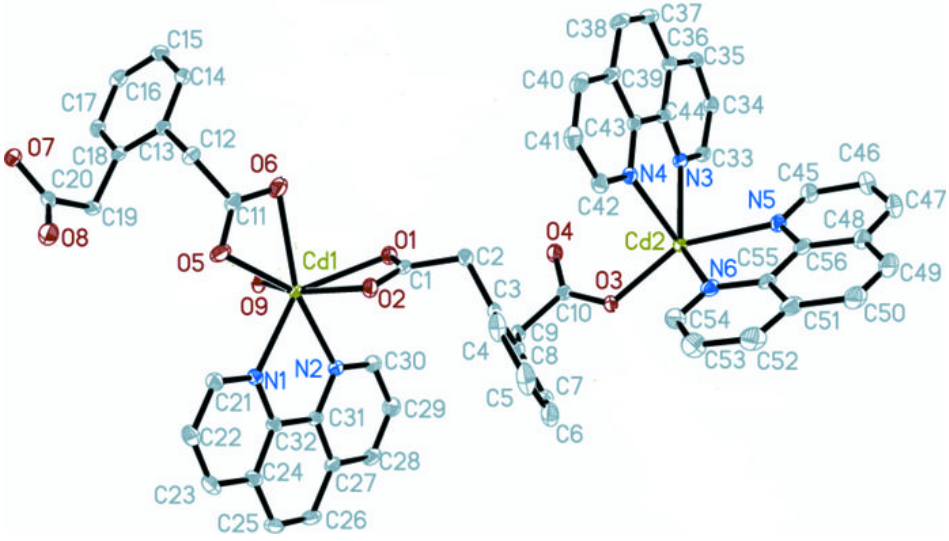
Symmetry codes: (i) *x*−1, *y*+1, *z*; (ii) *x*+1, *y*−1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9—H9BO···O1^{iii}	0.81 (3)	1.92 (3)	2.713 (2)	167 (4)
O9—H9AO···O4^{iii}	0.81 (3)	1.88 (3)	2.678 (2)	164 (3)
O11—H01B···O3^{ii}	0.82 (3)	2.07 (3)	2.860 (3)	161 (4)
O11—H01A···O8	0.82 (3)	1.92 (3)	2.732 (3)	170 (5)
O12—H02A···O10	0.80 (3)	2.22 (3)	2.844 (5)	136 (3)
O12—H02B···O11^{iv}	0.83 (6)	1.98 (5)	2.776 (4)	161 (6)
O10—H10···O6^{v}	0.84	1.91	2.745 (5)	174

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

Fig. 1


C15
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N4
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C46
N5
C47
C48
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C55
C56
C49
N6
C54
C51
C50
C53
C52

Fig. 2