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catena-Poly[[[triaqua(4,4′-bipyridine *N*,*N*′-dioxide-κ*O*)dichloridocerium(III)]-μ_2-4,4′-bipyridine *N*,*N*′-dioxide-κ^2O:*O*′] chloride monohydrate]

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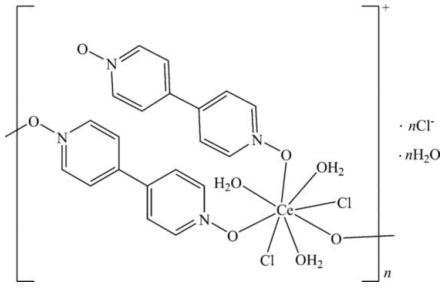
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.033; wR factor = 0.083; data-to-parameter ratio = 17.5.

In the title compound, $[CeCl_2(C_{10}H_8N_2O_2)_2(H_2O)_3]Cl\cdot H_2O$, each Ce^{III} atom is coordinated by six O atoms [Ce—O = 2.454 (3)–2.454 (3) Å] and two chloride ions [Ce—Cl = 2.8277 (9) and 2.8721 (9) Å] in a distorted tetragonal-antiprismatic geometry. One of the 4,4′-bipyridine *N*,*N*′-dioxide ligands acts as a bridging ligand while the other acts a terminal ligand, leading to the formation of a linear polymeric structure. In the crystal structure, adjacent polymeric chains are cross-linked by O—H···O and O—H···Cl hydrogen bonds, forming a three-dimensional network.

Related literature

For related literature, see: Hill *et al.* (2004); Kitagawa & Kitaura (2004); Long *et al.* (2000, 2001, 2002, 2004); Ma *et al.* (2005); Yaghi *et al.* (2003).



Experimental

Crystal data

$[CeCl_2(C_{10}H_8N_2O_2)_2(H_2O)_3]$-Cl·$H_2O$
M_r = 694.90
Triclinic, $P\overline{1}$
a = 8.6677 (1) Å
b = 10.4584 (3) Å
c = 14.7861 (3) Å
α = 83.362 (5)°
β = 73.027 (4)°
γ = 86.190 (6)°
V = 1272.63 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.16 mm^{-1}
T = 293 (2) K
0.45 × 0.22 × 0.10 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2004)
T_{min} = 0.444, T_{max} = 0.813
9756 measured reflections
5698 independent reflections
5315 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.084
S = 1.06
5698 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.31 e Å^{-3}
$\Delta\rho_{min}$ = −1.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O8	0.85	2.06	2.896 (3)	170
O5—H5B···O3^{i}	0.85	1.93	2.763 (4)	167
O6—H6A···O2^{ii}	0.85	1.90	2.716 (4)	161
O6—H6B···Cl2^{iii}	0.85	2.50	3.214 (3)	142
O7—H7A···O3^{iv}	0.85	1.95	2.778 (4)	164
O7—H7B···Cl3	0.85	2.17	3.014 (3)	176
O8—H8B···Cl3^{v}	0.85	2.32	3.059 (2)	145

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

Data collection: *CrystalClear* (Rigaku/MSC, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); 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: CI2363).

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supplementary materials

Acta Cryst. (2007). E**63**, m1430 [**doi:10.1107/S1600536807019010**]

catena-Poly[[[triaqua(4,4'-bipyridine *N*,*N*'-dioxide-*κO*)dichloridocerium(III)]-μ_2-4,4'-bipyridine *N*,*N*'-dioxide-κ^2*O*:*O*'] chloride monohydrate]

D.-Q. Yuan, F.-Y. Lian and M.-C. Hong

Comment

Recently, inorganic-organic coordination compounds attracted considerable attention due to their fascinating structure and potential applications as functional materials (Kitagawa & Kitaura, 2004; Yaghi *et al.*, 2003). Multidentate O-donor ligands have been employed extensively as organic spacers in the construction of extended networks. 4,4'-Bipyridine N,*N*'-dioxide (*L*), a typical bridge ligand, can coordinate to lanthanide metal ions in five possible modes, and generate some predicted, controlled structural frameworks, including one-dimensional chains, two-dimensional layer, and three-dimensional network (Hill *et al.*, 2004; Long *et al.*, 2000, 2001, 2002, 2004; Ma *et al.*, 2005). We report here the synthesis and crystal structure of the title compound, (I).

As illustrated in Fig. 1, in compound (I), each Ce^{III} atom is coordinated by six O atoms [Ce—O = 2.454 (3)–2.545 (3) Å] from three *L* ligands and three water molecules, and two chloride ions [Ce—Cl = 2.8277 (9) and 2.8721 (9) Å] in a distorted tetragonal antiprism geometry. The interesting feature of (I) is that the asymmetric unit contains two *L* ligands, which exhibit two different coordination modes. One of the *L* acts as a bridging ligand, linking two Ce^{III} ions, with a $Ce\cdots Ce^{i}$ distance of 13.1324 (8) Å [symmetry code: (i) $x + 1, y - 1, z$], and the other acts a terminal ligand. As a result of this coordination a linear polymeric chain is formed (Fig. 2), similar to that in *catena*-[bis(μ_2-4,4'-bipyridine *N*,*N*'-dioxide)-tris (nitrato)-terbium(III)] (Long *et al.*, 2002) but different from the wave-like chain in *catena*-[(μ_2-4,4'-bipyridine *N*,*N*'-dioxide)-(methanol)-\ tris(nitrato)-terbium(III)] (Long *et al.*, 2002). The pyridine rings in the *L* ligand are not coplanar; the dihedral angle between the N1- and N2-pyridine rings is 14.2 (2)° and that between the N3- and N4-pyridine rings is 10.5 (2)°.

In the polymeric chain, weak face-to face π-π interactions are observed between the adjacent bridging and terminal *L* ligands, with $Cg3\cdots Cg2^{i}$ and $Cg4\cdots Cg1^{i}$ distances of 3.596 (2) and 3.888 (2) Å, respectively (*Cg*1, *Cg*2, *Cg*3 and *Cg*4 denote the centroids of the N1/C1—C5, N2/C6—C10, N3/C11—C15 and N4/C16—C20 rings, respectively). The neighboring chains are cross-linked by O—H···O and O—H···Cl hydrogen bonds, involving three coordinated water molecules, one lattice water molecule, one uncoordinated chloride ion and the uncoordinated O atom of the *L* ligand (Table 1), forming a three-dimensional hydrogen-bonded network, as shown in Fig.3.

Experimental

A mixture of $CeCl_3\cdot 6H_2O$ (0.20 mmol), 4,4'-bipyridine N,*N*'-dioxide (0.40 mmol) and water (10 ml) was stirred at *ca* 323 K for 3 h and then filtered. The filtrate was kept at room temperature and yellow crystals of the title compound (yield 53%, based on Ce) were obtained after several days.

Refinement

The water H atoms were located in difference Fourier maps, and refined with O—H distances restrained at 0.85 Å and U_{iso} = 1.2U_{eq}(O). The remaining H atoms were positioned geometrically, with C—H = 0.93 Å, and were constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C)

Figures

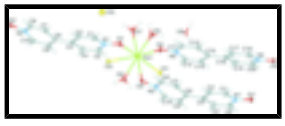


Fig. 1. Coordination environment of the Cerium atom in (I). Displacement ellipsoids are drawn at the 35% probability level. [Symmetry code: (i) *x* + 1, *y* − 1, *z*.]

Fig. 2. Part of the polymeric chain of (I). H atoms have been omitted for clarity. [Symmetry code: (i) *x* + 1, *y* − 1, *z*.]

Fig. 3. Part of the hydrogen-bonded (dashed lines) network in (I). [Symmetry codes: (i) *x* + 1, *y* − 1, *z*; (ii) *x* − 1, *y* + 1, *z*; (iii) −*x* − 1, −*y* + 2, −*z* + 2; (iv) −*x*, −*y* + 1, −*z* + 2; (v) −*x* + 1, −*y*, −*z* + 1; (vi) −*x*, −*y* + 1, −*z* + 1.]

catena-Poly[[[triaqua(4,4'-bipyridine *N*,*N*'-dioxide-κ*O*)dichloridocerium(III)]-μ_2-4,4'-bipyridine *N*,*N*'-dioxide-κ^2*O*:*O*'] chloride monohydrate]

Crystal data

$[CeCl_2(C_{10}H_8N_2O_2)_2(H_2O)_3]Cl·H_2O$	Z = 2
M_r = 694.90	F_{000} = 690
Triclinic, $P\overline{1}$	D_x = 1.813 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.6677 (1) Å	Cell parameters from 3563 reflections
b = 10.4584 (3) Å	θ = 2.3–27.5º
c = 14.7861 (3) Å	μ = 2.16 mm^{-1}
α = 83.362 (5)º	T = 293 (2) K
β = 73.027 (4)º	Prism, orange
γ = 86.190 (6)º	0.45 × 0.22 × 0.10 mm
V = 1272.63 (6) Å^3	

Data collection

Rigaku Mercury CCD diffractometer	5698 independent reflections
Radiation source: fine-focus sealed tube	5315 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
Detector resolution: 14.6306 pixels mm^{-1}	θ_{max} = 27.5º

T = 293(2) K

ω scans

Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2004)

T_{min} = 0.444, T_{max} = 0.813

9756 measured reflections

θ_{min} = 2.3°

h = −11→10

k = −13→9

l = −19→19

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.033

$wR(F^2)$ = 0.084

S = 1.06

5698 reflections

325 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 2.1096P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 1.31 e Å^{-3}

$\Delta\rho_{min}$ = −1.13 e Å^{-3}

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}
Ce1	0.00594 (2)	0.441087 (16)	0.796133 (12)	0.01936 (7)
Cl1	−0.11177 (11)	0.19676 (8)	0.88064 (7)	0.03122 (19)
Cl2	0.09043 (12)	0.67876 (8)	0.84625 (6)	0.03285 (19)
Cl3	0.10399 (16)	0.85283 (13)	0.58040 (9)	0.0563 (3)
O1	−0.2380 (4)	0.5682 (3)	0.7862 (2)	0.0387 (7)
O2	−0.8044 (3)	1.3811 (2)	0.8983 (2)	0.0350 (6)
O3	0.7408 (4)	−0.5185 (3)	0.5485 (2)	0.0378 (6)
O4	0.2428 (3)	0.3201 (3)	0.6970 (2)	0.0373 (6)
O5	−0.1189 (4)	0.3598 (3)	0.6824 (2)	0.0464 (8)
H5A	−0.0935	0.2845	0.6653	0.056*
H5B	−0.1466	0.3972	0.6351	0.056*
O6	−0.1698 (3)	0.4586 (3)	0.96565 (18)	0.0332 (6)

H6A	−0.1812	0.5220	0.9984	0.040*
H6B	−0.1465	0.3917	0.9983	0.040*
O7	0.1258 (4)	0.5682 (2)	0.63959 (18)	0.0385 (7)
H7B	0.1148	0.6482	0.6236	0.046*
H7A	0.1731	0.5393	0.5867	0.046*
O8	−0.0742 (3)	0.10277 (19)	0.62206 (14)	0.0154 (4)
H8A	−0.0028	0.0725	0.6485	0.018*
H8B	−0.0526	0.0870	0.5645	0.018*
N1	−0.3048 (4)	0.6797 (3)	0.8165 (2)	0.0291 (7)
N2	−0.7157 (4)	1.2713 (3)	0.8993 (2)	0.0271 (6)
N3	0.3114 (4)	0.2040 (3)	0.6792 (2)	0.0259 (6)
N4	0.6763 (4)	−0.4033 (3)	0.5714 (2)	0.0284 (6)
C1	−0.2279 (5)	0.7893 (4)	0.7815 (3)	0.0357 (9)
H1	−0.1242	0.7867	0.7399	0.043*
C2	−0.4516 (5)	0.6817 (4)	0.8794 (3)	0.0416 (10)
H2	−0.5020	0.6048	0.9059	0.050*
C3	−0.3012 (5)	0.9058 (4)	0.8068 (3)	0.0335 (8)
H3	−0.2455	0.9810	0.7825	0.040*
C4	−0.5281 (5)	0.7971 (4)	0.9050 (3)	0.0394 (10)
H4	−0.6304	0.7972	0.9483	0.047*
C5	−0.4557 (4)	0.9133 (3)	0.8673 (2)	0.0236 (7)
C6	−0.5413 (4)	1.0395 (3)	0.8856 (2)	0.0232 (7)
C7	−0.4733 (4)	1.1541 (3)	0.8356 (3)	0.0299 (8)
H7	−0.3675	1.1530	0.7966	0.036*
C8	−0.6954 (4)	1.0496 (4)	0.9479 (3)	0.0297 (8)
H8	−0.7416	0.9769	0.9859	0.036*
C9	−0.5622 (5)	1.2680 (4)	0.8442 (3)	0.0320 (8)
H9	−0.5157	1.3437	0.8114	0.038*
C10	−0.7813 (5)	1.1658 (4)	0.9543 (3)	0.0313 (8)
H10	−0.8841	1.1712	0.9966	0.038*
C11	0.4609 (5)	0.1976 (4)	0.6179 (3)	0.0304 (8)
H11	0.5140	0.2728	0.5895	0.037*
C12	0.2344 (4)	0.0960 (3)	0.7219 (3)	0.0282 (7)
H12	0.1312	0.1022	0.7637	0.034*
C13	0.5353 (4)	0.0786 (3)	0.5975 (3)	0.0290 (7)
H13	0.6372	0.0748	0.5540	0.035*
C14	0.3065 (4)	−0.0234 (4)	0.7045 (3)	0.0276 (7)
H14	0.2523	−0.0971	0.7355	0.033*
C15	0.4602 (4)	−0.0351 (3)	0.6406 (2)	0.0231 (7)
C16	0.5370 (4)	−0.1637 (3)	0.6185 (2)	0.0246 (7)
C17	0.6976 (5)	−0.1775 (4)	0.5648 (3)	0.0343 (8)
H17	0.7603	−0.1053	0.5437	0.041*
C18	0.4512 (5)	−0.2754 (4)	0.6482 (3)	0.0338 (8)
H18	0.3443	−0.2705	0.6851	0.041*
C19	0.7645 (5)	−0.2979 (4)	0.5423 (3)	0.0361 (9)
H19	0.8719	−0.3057	0.5067	0.043*
C20	0.5208 (5)	−0.3933 (4)	0.6241 (3)	0.0368 (9)
H20	0.4602	−0.4668	0.6443	0.044*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.02181 (11)	0.01415 (10)	0.02068 (10)	0.00357 (7)	−0.00417 (7)	−0.00329 (6)
Cl1	0.0306 (4)	0.0229 (4)	0.0348 (4)	−0.0044 (3)	−0.0010 (4)	−0.0006 (3)
Cl2	0.0440 (5)	0.0219 (4)	0.0313 (4)	−0.0052 (4)	−0.0082 (4)	−0.0018 (3)
Cl3	0.0570 (7)	0.0563 (7)	0.0524 (7)	−0.0063 (6)	−0.0124 (6)	0.0020 (6)
O1	0.0418 (16)	0.0312 (14)	0.0461 (16)	0.0220 (12)	−0.0178 (13)	−0.0154 (12)
O2	0.0448 (16)	0.0252 (13)	0.0402 (15)	0.0187 (12)	−0.0205 (13)	−0.0144 (11)
O3	0.0529 (17)	0.0228 (13)	0.0358 (14)	0.0162 (12)	−0.0107 (13)	−0.0102 (11)
O4	0.0410 (16)	0.0239 (13)	0.0414 (15)	0.0138 (12)	−0.0041 (12)	−0.0098 (11)
O5	0.078 (2)	0.0238 (13)	0.0532 (18)	0.0115 (14)	−0.0437 (18)	−0.0115 (13)
O6	0.0428 (15)	0.0281 (13)	0.0260 (13)	0.0021 (11)	−0.0042 (11)	−0.0084 (10)
O7	0.0617 (19)	0.0198 (12)	0.0246 (13)	0.0018 (12)	0.0009 (12)	−0.0012 (10)
O8	0.0277 (11)	0.0113 (9)	0.0100 (9)	−0.0060 (8)	−0.0094 (8)	0.0005 (7)
N1	0.0283 (15)	0.0276 (15)	0.0313 (15)	0.0147 (12)	−0.0096 (13)	−0.0084 (12)
N2	0.0329 (16)	0.0223 (14)	0.0302 (15)	0.0113 (12)	−0.0149 (13)	−0.0112 (12)
N3	0.0283 (15)	0.0237 (14)	0.0255 (14)	0.0099 (12)	−0.0070 (12)	−0.0096 (11)
N4	0.0368 (17)	0.0217 (14)	0.0265 (14)	0.0096 (12)	−0.0098 (13)	−0.0063 (12)
C1	0.0287 (19)	0.033 (2)	0.035 (2)	0.0093 (16)	0.0029 (16)	0.0026 (16)
C2	0.033 (2)	0.0256 (19)	0.057 (3)	−0.0006 (16)	0.0026 (19)	−0.0050 (18)
C3	0.0281 (19)	0.0261 (18)	0.038 (2)	0.0042 (15)	0.0001 (16)	0.0053 (15)
C4	0.0263 (19)	0.0262 (19)	0.055 (3)	0.0031 (15)	0.0064 (17)	−0.0089 (17)
C5	0.0246 (16)	0.0227 (16)	0.0233 (16)	0.0061 (13)	−0.0077 (13)	−0.0023 (13)
C6	0.0228 (16)	0.0239 (16)	0.0229 (15)	0.0047 (13)	−0.0074 (13)	−0.0036 (13)
C7	0.0231 (17)	0.0258 (18)	0.040 (2)	0.0023 (14)	−0.0086 (15)	−0.0034 (15)
C8	0.0294 (18)	0.0284 (18)	0.0264 (17)	0.0065 (15)	−0.0031 (14)	0.0006 (14)
C9	0.033 (2)	0.0234 (17)	0.041 (2)	−0.0006 (15)	−0.0128 (17)	−0.0020 (15)
C10	0.0299 (19)	0.035 (2)	0.0257 (17)	0.0105 (16)	−0.0047 (14)	−0.0058 (15)
C11	0.0308 (19)	0.0241 (17)	0.0305 (18)	0.0030 (14)	−0.0012 (15)	−0.0013 (14)
C12	0.0239 (17)	0.0266 (17)	0.0324 (18)	0.0036 (14)	−0.0037 (14)	−0.0104 (14)
C13	0.0246 (17)	0.0265 (17)	0.0313 (18)	0.0064 (14)	−0.0009 (14)	−0.0069 (14)
C14	0.0261 (17)	0.0249 (17)	0.0308 (18)	0.0006 (14)	−0.0053 (14)	−0.0067 (14)
C15	0.0228 (16)	0.0217 (16)	0.0255 (16)	0.0037 (13)	−0.0075 (13)	−0.0069 (13)
C16	0.0260 (17)	0.0212 (16)	0.0267 (16)	0.0038 (13)	−0.0072 (14)	−0.0065 (13)
C17	0.0250 (18)	0.0266 (18)	0.049 (2)	0.0024 (15)	−0.0045 (16)	−0.0122 (17)
C18	0.0271 (19)	0.0249 (18)	0.042 (2)	0.0018 (15)	0.0017 (16)	−0.0047 (16)
C19	0.0257 (18)	0.031 (2)	0.048 (2)	0.0072 (15)	−0.0038 (17)	−0.0124 (17)
C20	0.038 (2)	0.0220 (18)	0.044 (2)	0.0005 (16)	−0.0013 (17)	−0.0039 (16)

Geometric parameters (Å, °)

Ce1—O1	2.454 (3)	C2—H2	0.93
Ce1—O5	2.498 (3)	C3—C5	1.380 (5)
Ce1—O7	2.504 (3)	C3—H3	0.93
Ce1—O4	2.508 (3)	C4—C5	1.386 (5)
Ce1—O2^{i}	2.544 (3)	C4—H4	0.93

Ce1—O6	2.545 (3)	C5—C6	1.484 (4)
Ce1—Cl1	2.8277 (9)	C6—C8	1.389 (5)
Ce1—Cl2	2.8721 (9)	C6—C7	1.402 (5)
O1—N1	1.332 (4)	C7—C9	1.373 (5)
O2—N2	1.340 (4)	C7—H7	0.93
O3—N4	1.332 (4)	C8—C10	1.380 (5)
O4—N3	1.336 (4)	C8—H8	0.93
O5—H5A	0.85	C9—H9	0.93
O5—H5B	0.85	C10—H10	0.93
O6—H6A	0.85	C11—C13	1.387 (5)
O6—H6B	0.85	C11—H11	0.93
O7—H7B	0.85	C12—C14	1.377 (5)
O7—H7A	0.85	C12—H12	0.93
O8—H8A	0.85	C13—C15	1.389 (5)
O8—H8B	0.85	C13—H13	0.93
N1—C1	1.337 (5)	C14—C15	1.397 (5)
N1—C2	1.340 (5)	C14—H14	0.93
N2—C9	1.343 (5)	C15—C16	1.488 (4)
N2—C10	1.344 (5)	C16—C18	1.384 (5)
N3—C12	1.345 (5)	C16—C17	1.395 (5)
N3—C11	1.350 (5)	C17—C19	1.385 (5)
N4—C19	1.339 (5)	C17—H17	0.93
N4—C20	1.350 (5)	C18—C20	1.374 (5)
C1—C3	1.375 (5)	C18—H18	0.93
C1—H1	0.93	C19—H19	0.93
C2—C4	1.375 (5)	C20—H20	0.93
O1—Ce1—O5	68.28 (9)	N1—C2—H2	119.9
O1—Ce1—O7	82.33 (10)	C4—C2—H2	119.9
O5—Ce1—O7	74.47 (10)	C1—C3—C5	121.3 (4)
O1—Ce1—O4	141.78 (10)	C1—C3—H3	119.3
O5—Ce1—O4	79.52 (10)	C5—C3—H3	119.3
O7—Ce1—O4	69.30 (9)	C2—C4—C5	121.3 (4)
O1—Ce1—O2^{i}	144.12 (9)	C2—C4—H4	119.4
O5—Ce1—O2^{i}	144.07 (8)	C5—C4—H4	119.4
O7—Ce1—O2^{i}	115.80 (10)	C3—C5—C4	116.3 (3)
O4—Ce1—O2^{i}	73.45 (9)	C3—C5—C6	121.1 (3)
O1—Ce1—O6	72.90 (9)	C4—C5—C6	122.5 (3)
O5—Ce1—O6	117.92 (10)	C8—C6—C7	116.8 (3)
O7—Ce1—O6	143.72 (8)	C8—C6—C5	122.1 (3)
O4—Ce1—O6	143.38 (9)	C7—C6—C5	120.9 (3)
O2^{i}—Ce1—O6	75.39 (9)	C9—C7—C6	120.2 (3)
O1—Ce1—Cl1	103.72 (8)	C9—C7—H7	119.9
O5—Ce1—Cl1	74.42 (8)	C6—C7—H7	119.9
O7—Ce1—Cl1	143.21 (6)	C10—C8—C6	121.1 (4)
O4—Ce1—Cl1	86.13 (7)	C10—C8—H8	119.5
O2^{i}—Ce1—Cl1	80.49 (7)	C6—C8—H8	119.5
O6—Ce1—Cl1	70.10 (6)	N2—C9—C7	120.8 (4)

O1—Ce1—Cl2	82.29 (7)	N2—C9—H9	119.6
O5—Ce1—Cl2	140.34 (7)	C7—C9—H9	119.6
O7—Ce1—Cl2	75.80 (7)	N2—C10—C8	119.8 (3)
O4—Ce1—Cl2	113.29 (7)	N2—C10—H10	120.1
O2^{i}—Ce1—Cl2	73.59 (6)	C8—C10—H10	120.1
O6—Ce1—Cl2	74.96 (6)	N3—C11—C13	119.8 (3)
Cl1—Ce1—Cl2	140.64 (3)	N3—C11—H11	120.1
N1—O1—Ce1	134.5 (2)	C13—C11—H11	120.1
N2—O2—Ce1^{ii}	125.79 (19)	N3—C12—C14	120.7 (3)
N3—O4—Ce1	145.4 (2)	N3—C12—H12	119.6
Ce1—O5—H5A	119.7	C14—C12—H12	119.6
Ce1—O5—H5B	132.0	C11—C13—C15	121.2 (3)
H5A—O5—H5B	101.3	C11—C13—H13	119.4
Ce1—O6—H6A	128.0	C15—C13—H13	119.4
Ce1—O6—H6B	105.8	C12—C14—C15	120.7 (3)
H6A—O6—H6B	108.1	C12—C14—H14	119.7
Ce1—O7—H7B	129.1	C15—C14—H14	119.7
Ce1—O7—H7A	127.5	C13—C15—C14	116.8 (3)
H7B—O7—H7A	102.5	C13—C15—C16	122.0 (3)
H8A—O8—H8B	113.1	C14—C15—C16	121.2 (3)
O1—N1—C1	120.0 (3)	C18—C16—C17	116.6 (3)
O1—N1—C2	119.6 (3)	C18—C16—C15	121.6 (3)
C1—N1—C2	120.4 (3)	C17—C16—C15	121.8 (3)
O2—N2—C9	119.2 (3)	C19—C17—C16	120.6 (4)
O2—N2—C10	120.0 (3)	C19—C17—H17	119.7
C9—N2—C10	120.8 (3)	C16—C17—H17	119.7
O4—N3—C12	120.9 (3)	C20—C18—C16	121.4 (4)
O4—N3—C11	118.3 (3)	C20—C18—H18	119.3
C12—N3—C11	120.8 (3)	C16—C18—H18	119.3
O3—N4—C19	120.5 (3)	N4—C19—C17	120.8 (4)
O3—N4—C20	119.4 (3)	N4—C19—H19	119.6
C19—N4—C20	120.1 (3)	C17—C19—H19	119.6
N1—C1—C3	120.4 (3)	N4—C20—C18	120.5 (4)
N1—C1—H1	119.8	N4—C20—H20	119.7
C3—C1—H1	119.8	C18—C20—H20	119.7
N1—C2—C4	120.2 (4)		
O5—Ce1—O1—N1	−168.3 (4)	C8—C6—C7—C9	−4.6 (5)
O7—Ce1—O1—N1	−92.1 (3)	C5—C6—C7—C9	171.5 (3)
O4—Ce1—O1—N1	−133.7 (3)	C7—C6—C8—C10	4.8 (5)
O2^{i}—Ce1—O1—N1	32.2 (4)	C5—C6—C8—C10	−171.2 (3)
O6—Ce1—O1—N1	61.1 (3)	O2—N2—C9—C7	−173.0 (3)
Cl1—Ce1—O1—N1	124.9 (3)	C10—N2—C9—C7	6.3 (5)
Cl2—Ce1—O1—N1	−15.5 (3)	C6—C7—C9—N2	−0.8 (6)
O1—Ce1—O4—N3	−108.8 (4)	O2—N2—C10—C8	173.3 (3)
O5—Ce1—O4—N3	−76.3 (4)	C9—N2—C10—C8	−6.0 (5)
O7—Ce1—O4—N3	−153.5 (4)	C6—C8—C10—N2	0.3 (6)
O2^{i}—Ce1—O4—N3	79.8 (4)	O4—N3—C11—C13	−179.7 (3)
O6—Ce1—O4—N3	47.0 (5)	C12—N3—C11—C13	1.1 (5)

Cl1—Ce1—O4—N3	−1.5 (4)	O4—N3—C12—C14	−179.0 (3)
Cl2—Ce1—O4—N3	143.1 (4)	C11—N3—C12—C14	0.2 (5)
Ce1—O1—N1—C1	64.5 (5)	N3—C11—C13—C15	−1.6 (6)
Ce1—O1—N1—C2	−117.8 (4)	N3—C12—C14—C15	−1.1 (5)
Ce1^{ii}—O2—N2—C9	94.6 (4)	C11—C13—C15—C14	0.7 (5)
Ce1^{ii}—O2—N2—C10	−84.7 (4)	C11—C13—C15—C16	179.1 (3)
Ce1—O4—N3—C12	5.9 (6)	C12—C14—C15—C13	0.6 (5)
Ce1—O4—N3—C11	−173.3 (3)	C12—C14—C15—C16	−177.8 (3)
O1—N1—C1—C3	175.0 (4)	C13—C15—C16—C18	−168.2 (4)
C2—N1—C1—C3	−2.7 (6)	C14—C15—C16—C18	10.2 (5)
O1—N1—C2—C4	−174.3 (4)	C13—C15—C16—C17	10.0 (5)
C1—N1—C2—C4	3.4 (7)	C14—C15—C16—C17	−171.7 (3)
N1—C1—C3—C5	−0.9 (6)	C18—C16—C17—C19	0.6 (6)
N1—C2—C4—C5	−0.6 (7)	C15—C16—C17—C19	−177.7 (4)
C1—C3—C5—C4	3.5 (6)	C17—C16—C18—C20	−1.1 (6)
C1—C3—C5—C6	−172.9 (4)	C15—C16—C18—C20	177.2 (4)
C2—C4—C5—C3	−2.8 (6)	O3—N4—C19—C17	179.0 (4)
C2—C4—C5—C6	173.5 (4)	C20—N4—C19—C17	−0.7 (6)
C3—C5—C6—C8	−178.5 (3)	C16—C17—C19—N4	0.3 (6)
C4—C5—C6—C8	5.3 (5)	O3—N4—C20—C18	−179.5 (4)
C3—C5—C6—C7	5.6 (5)	C19—N4—C20—C18	0.2 (6)
C4—C5—C6—C7	−170.5 (4)	C16—C18—C20—N4	0.7 (7)

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*
O5—H5A···O8	0.85	2.06	2.896 (3)	170
O5—H5B···O3^{ii}	0.85	1.93	2.763 (4)	167
O6—H6A···O2^{iii}	0.85	1.90	2.716 (4)	161
O6—H6B···Cl2^{iv}	0.85	2.50	3.214 (3)	142
O7—H7A···O3^{v}	0.85	1.95	2.778 (4)	164
O7—H7B···Cl3	0.85	2.17	3.014 (3)	176
O8—H8B···Cl3^{vi}	0.85	2.32	3.059 (2)	145

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

Fig. 1

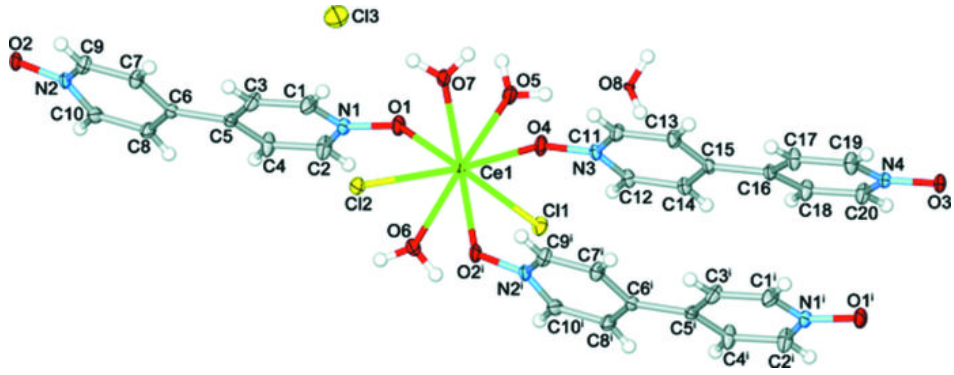

Cl3
O2
C9
C7
N2
C10
C8
C6
C5
C3
C1
C4
C2
N1
O1
O7
O5
O4
Ce1
Cl2
Cl1
O6
O2i
C9i
C7i
N2i
C10i
C8i
C6i
C5i
C3i
C1i
C4i
C2i
N1i
O1i
O8
C11
N3
C13
C12
C14
C15
C16
C17
C19
C18
C20
N4
O3

Fig. 2

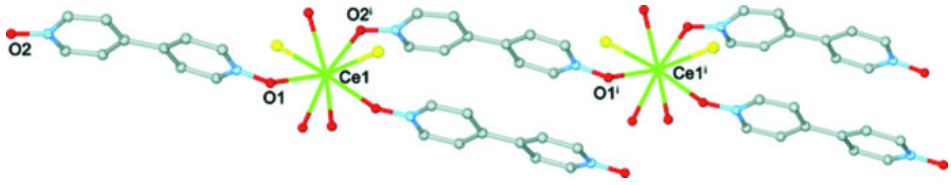
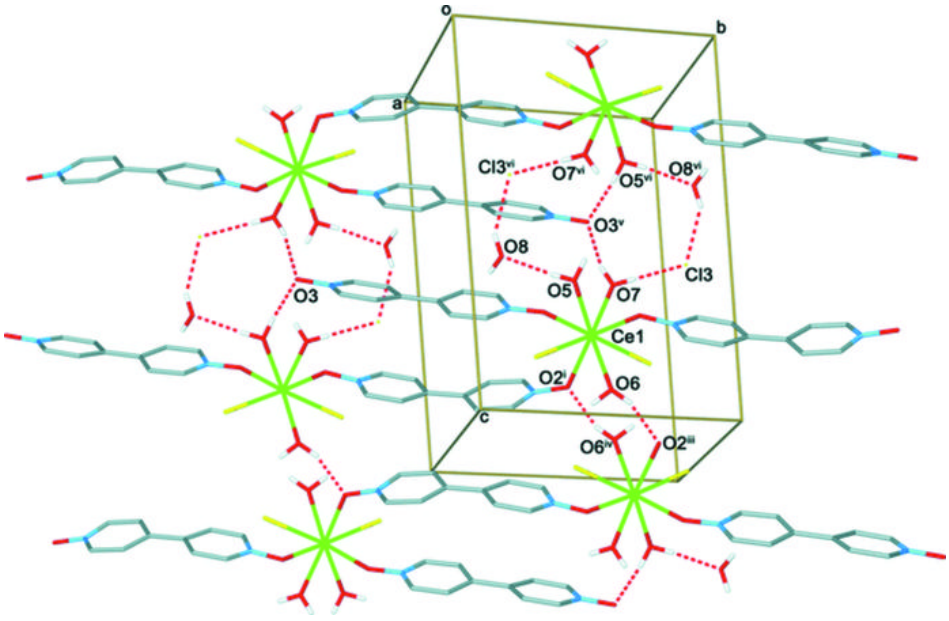


Fig. 3


o
b
a
c
Cl3vi
O7vi
O5vi
O8vi
O3v
O8
O5
O7
Cl3
O3
Ce1
O2i
O6
O6iv
O2iii