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Poly[[dodecaaqua(μ_4-benzene-1,4-dicarboxylato)(μ_2-4,4′-bipyridine-κ^2N:N')dicerium(III)] bis(benzene-1,4-dicarboxylate)]

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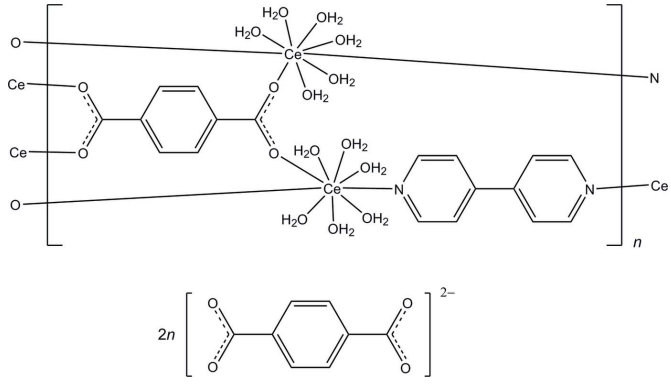
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.034; wR factor = 0.068; data-to-parameter ratio = 13.4.

The asymmetric unit of the title compound, {[$Ce_2(C_8H_4O_4)(C_{10}H_8N_2)(H_2O)_{12}](C_8H_4O_4)_2$}$_n$, consists of half a Ce^{III} cation, a quarter of a coordinated benzene-1,4-dicarboxylate (bdc^{2-}) dianion, a quarter of a 4,4′-bipyridine (bpy) molecule, three water molecules and a half of an uncoordinated benzene-1,4-dicarboxylate dianion. The Ce^{III} ion is located on a twofold rotation axis and exhibits a distorted trigonal prism square-face tricapped coordination geometry. The coordinated and uncoordinated bdc^{2-} ions and the bpy molecule lie about special positions of site symmetries 2/m, m and 2/m, respectively. The Ce^{III} ions are bridged by the bdc^{2-} and bpy ligands, giving a sheet structure parallel to the ac plane. The uncoordinated bdc^{2-} dianion exists between the sheets and links the sheets by intermolecular O—H···O hydrogen bonds between the uncoordinated bdc^{2-} and coordinated water molecules. A π–π stacking interaction between the uncoordinated bdc^{2-} dianion and the bpy ligand [centroid–centroid distance = 3.750 (4) Å] is also observed.

Related literature

For coordination polymers, see: Cheetham *et al.* (1999); Furukawa *et al.* (2010). For related host–guest systems, see: Kawata & Kitagawa (2002).



Experimental

Crystal data

$[Ce_2(C_8H_4O_4)(C_{10}H_8N_2)(H_2O)_{12}](C_8H_4O_4)_2$
M_r = 572.48
Orthorhombic, *Pnnm*
a = 6.112 (4) Å
b = 14.278 (8) Å
c = 22.395 (12) Å
V = 1954.3 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.40 mm^{-1}
T = 293 K
0.60 × 0.20 × 0.10 mm

Data collection

Rigaku Mercury70 diffractometer
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
T_{min} = 0.511, T_{max} = 0.787
14945 measured reflections
2246 independent reflections
2163 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.068
S = 1.39
2246 reflections
167 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ce1—O1	2.479 (3)	Ce1—O3^{i}	2.551 (3)
Ce1—O1^{i}	2.479 (3)	Ce1—O4	2.533 (3)
Ce1—O2	2.530 (3)	Ce1—O4^{i}	2.533 (3)
Ce1—O2^{i}	2.530 (3)	Ce1—N1	2.873 (5)
Ce1—O3	2.551 (3)		

Symmetry code: (i) $-x+2, -y, z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O5	0.84 (4)	1.93 (4)	2.754 (5)	167 (5)
O2—H3···O6^{ii}	0.84 (3)	1.90 (4)	2.725 (5)	166 (4)
O3—H4···O5	0.83 (5)	2.02 (5)	2.828 (4)	164 (6)
O3—H5···O6^{iii}	0.84 (5)	1.81 (5)	2.650 (4)	175 (6)
O4—H7···O5^{iv}	0.84 (4)	1.91 (4)	2.749 (5)	174 (6)

Symmetry codes: (ii) $x+1, y, z$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR2008* (Burla *et al.*, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2010); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5110).

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supplementary materials

Acta Cryst. (2012). E**68**, m643–m644 [doi:10.1107/S1600536812016388]

Poly[[dodecaaqua(μ_4-benzene-1,4-dicarboxylato)(μ_2-4,4′-bipyridine-κ^2N:N')dicerium(III)] bis(benzene-1,4-dicarboxylate)]

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Comment

The design of coordination polymers (CPs), also known as metal-organic frameworks (MOFs), have received considerable attention in recent years due to potential applications for sorption, catalysis, optical, magnetic materials and host-guest interactions (Cheetham *et al.*, 1999; Furukawa *et al.*, 2010; Kawata & Kitagawa, 2002). Here we report synthesis and single-crystal structure of the title compound.

The coordination polymer of the title compound, $\{[Ce_2(C_8H_4O_4)(C_{10}H_{10}N_2)(H_2O)_{12}](C_8H_4O_4)_2\}_n$, consists of Ce^{III} ions, bdc^{2-} dianions and bpy as bridging ligands, and water molecules. In the crystal, two types of bdc^{2-} dianions are found. One bdc^{2-} dianion coordinates to Ce^{III} ions and acts as a bridging ligand to form a two-dimensional network. The other is an uncoordinated bdc^{2-} dianion. Uncoordinated bdc^{2-} dianions are stabilized by intermolecular hydrogen bonds between the uncoordinated bdc^{2-} and coordinated water molecules and π–π stacking interactions between uncoordinated bdc^{2-} dianions and bridging ligands to give a three-dimensional network structure.

Experimental

An aqueous solution (5 ml) of cerium nitrate hexahydrate (0.81 g) was transferred to a glass tube, then an ethanol-water mixture (5 ml) of tetrabromoerephthalic acid (0.2 g), NaOH (0.08 g) and 4,4′-bpy (0.19 g) was poured into the glass tube without mixing the two solutions. Colorless crystals began to form at ambient temperature in 1 month. One of these crystals was used for X-ray crystallography.

Refinement

H atoms bonded to C atoms were introduced at the positions calculated theoretically (C—H = 0.93 Å) and treated as riding, with U_{iso}(H) = 1.2U_{eq}(C). H atoms of water molecules were located in a difference Fourier map and were refined isotropically with distance restraints of O—H = 0.84 (2) Å.

Computing details

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear* (Rigaku/MSC, 2005); data reduction: *CrystalClear* (Rigaku/MSC, 2005); program(s) used to solve structure: *SIR2008* (Burla *et al.*, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2010); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2010).

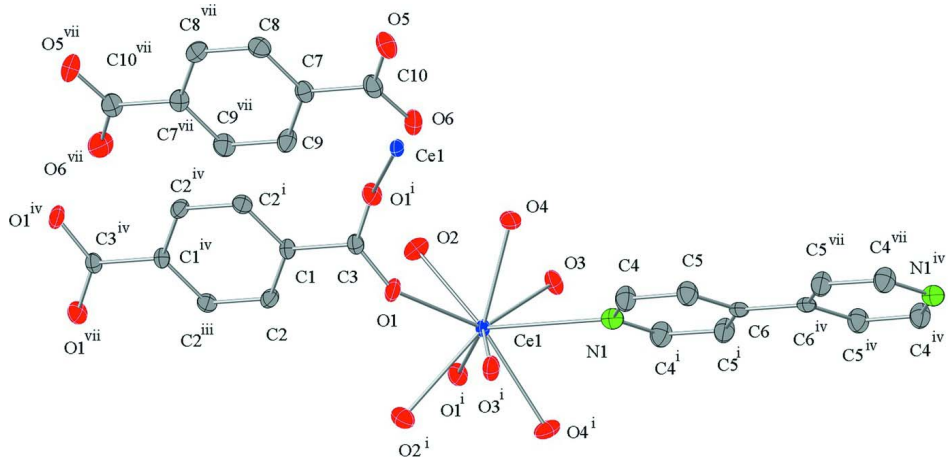

Figure 1

View of the title compound with atomic numbering scheme. Hydrogen atoms have been omitted for clarity. [Symmetry codes: (i) -*x* + 2, -*y*, *z*; (iii) *x*, *y*, -*z* + 1; (iv) -*x* + 2, -*y*, -*z*; (vii) *x*, *y*, -*z*.]

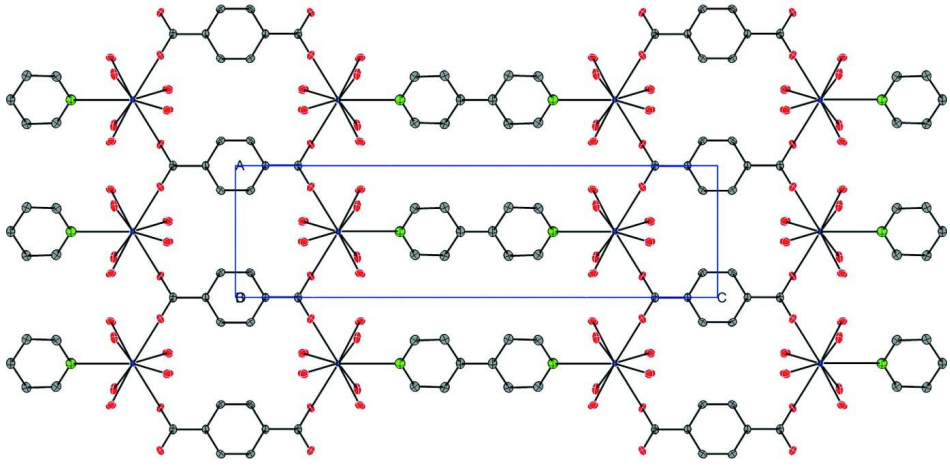

Figure 2

Packing diagram of the title compound, showing a sheet structure. Hydrogen atoms have been omitted for clarity.

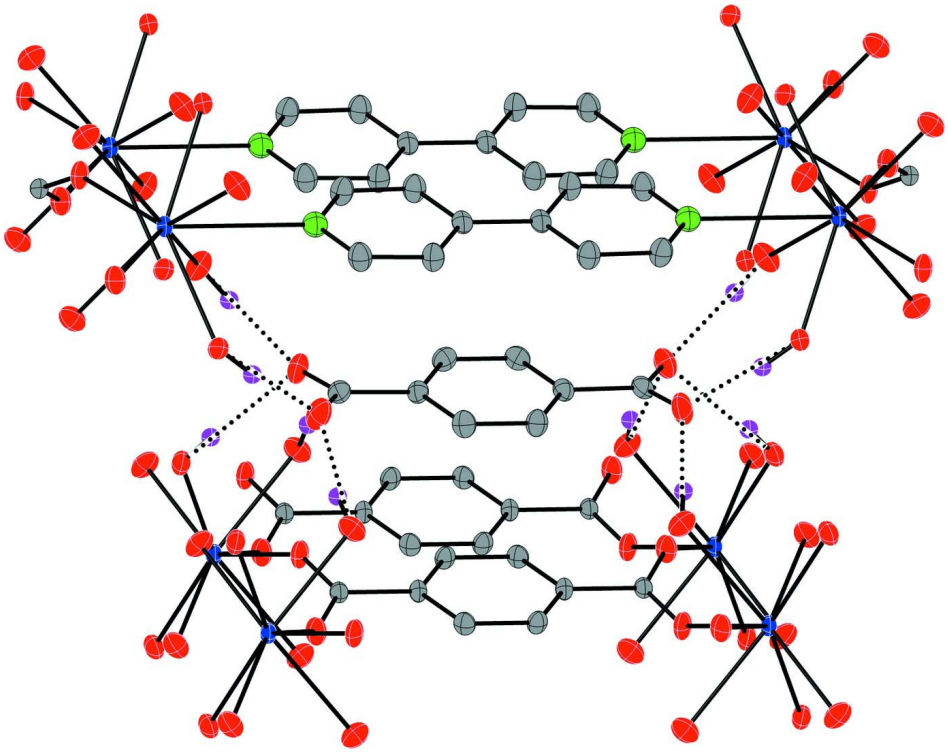

Figure 3

Hydrogen bonding interactions for the title compound. Hydrogen atoms and hydrogen bonding interactions are shown as purple color and dashed line, respectively.

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M_r = 572.48
Orthorhombic, *Pnnm*
Hall symbol: -P 2 2n
a = 6.112 (4) Å
b = 14.278 (8) Å
c = 22.395 (12) Å
V = 1954.3 (18) Å^3
Z = 4
$F(000)$ = 1140.00
D_x = 1.946 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71070 Å
Cell parameters from 3992 reflections
θ = 3.1–27.5°
μ = 2.40 mm^{-1}
T = 293 K
Platelet, colorless
0.60 × 0.20 × 0.10 mm

Data collection

Rigaku Mercury70 diffractometer
Detector resolution: 7.314 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
T_{min} = 0.511, T_{max} = 0.787
14945 measured reflections
2246 independent reflections
2163 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.029
θ_{max} = 27.5°
h = −7→7
k = −18→18
l = −29→29

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.068$
$S = 1.39$
2246 reflections
167 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 7.6254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY
Refinement. Refinement was performed using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on F^2. *R*-factor (σt) are based on *F*. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating *R*-factor (σt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ce1	1.0000	0.0000	0.286968 (11)	0.01450 (9)
O1	0.6621 (5)	0.03486 (19)	0.34397 (11)	0.0229 (6)
O2	1.0784 (5)	0.1316 (2)	0.35957 (13)	0.0257 (6)
O3	0.8063 (5)	0.14579 (19)	0.24774 (12)	0.0234 (6)
O4	0.6817 (5)	−0.0885 (2)	0.24157 (13)	0.0259 (6)
O5	0.7801 (5)	0.2740 (2)	0.34373 (11)	0.0276 (7)
O6	0.4224 (6)	0.2508 (3)	0.34529 (12)	0.0331 (8)
N1	1.0000	0.0000	0.15870 (19)	0.0230 (10)
C1	0.5000	0.0000	0.4378 (2)	0.0152 (9)
C2	0.6884 (6)	0.0245 (3)	0.46904 (14)	0.0171 (8)
C3	0.5000	0.0000	0.37044 (19)	0.0152 (9)
C4	0.8241 (7)	0.0259 (3)	0.12810 (16)	0.0252 (9)
C5	0.8174 (7)	0.0271 (3)	0.06620 (16)	0.0244 (9)
C6	1.0000	0.0000	0.0334 (2)	0.0187 (10)
C7	0.6065 (7)	0.2588 (3)	0.43811 (15)	0.0182 (7)
C8	0.7943 (7)	0.2825 (3)	0.46897 (16)	0.0209 (8)
C9	0.4180 (7)	0.2347 (3)	0.46905 (15)	0.0218 (8)
C10	0.6024 (7)	0.2610 (3)	0.37083 (16)	0.0214 (8)
H1	0.8145	0.0410	0.4483	0.0206*
H2	0.983 (7)	0.174 (3)	0.361 (3)	0.041 (15)*
H3	1.197 (5)	0.160 (3)	0.353 (2)	0.030 (14)*
H4	0.778 (11)	0.188 (4)	0.272 (2)	0.07 (2)*
H5	0.848 (10)	0.176 (4)	0.2178 (18)	0.062 (19)*
H6	0.555 (5)	−0.094 (5)	0.255 (3)	0.059 (19)*
H7	0.684 (10)	−0.130 (3)	0.2149 (18)	0.053 (17)*
H8	0.6998	0.0439	0.1491	0.0303*
H9	0.6908	0.0461	0.0466	0.0293*
H10	0.9207	0.2984	0.4482	0.0251*
H11	0.2917	0.2186	0.4483	0.0262*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.01572 (15)	0.01786 (15)	0.00993 (13)	−0.00118 (11)	0.0000	0.0000
O1	0.0214 (14)	0.0323 (15)	0.0151 (12)	−0.0021 (12)	0.0063 (11)	−0.0001 (11)
O2	0.0233 (15)	0.0241 (15)	0.0296 (15)	0.0009 (13)	−0.0026 (13)	−0.0080 (12)
O3	0.0324 (17)	0.0219 (14)	0.0160 (13)	0.0043 (13)	0.0037 (12)	0.0031 (11)
O4	0.0189 (15)	0.0319 (16)	0.0269 (15)	−0.0084 (13)	0.0037 (12)	−0.0094 (12)
O5	0.0305 (17)	0.0330 (16)	0.0191 (13)	0.0052 (14)	0.0063 (12)	0.0056 (11)
O6	0.0366 (18)	0.0413 (18)	0.0215 (14)	−0.0084 (15)	−0.0094 (13)	0.0093 (13)
N1	0.024 (3)	0.022 (3)	0.023 (2)	−0.004 (3)	0.0000	0.0000
C1	0.017 (3)	0.017 (3)	0.011 (2)	0.001 (3)	0.0000	0.0000
C2	0.0144 (18)	0.0205 (19)	0.0165 (17)	−0.0018 (14)	0.0031 (14)	0.0010 (13)
C3	0.020 (3)	0.014 (3)	0.012 (2)	0.002 (3)	0.0000	0.0000
C4	0.023 (2)	0.033 (3)	0.0206 (18)	0.0004 (17)	0.0021 (15)	−0.0021 (15)
C5	0.023 (2)	0.031 (3)	0.0193 (18)	0.0004 (17)	−0.0021 (15)	−0.0005 (15)
C6	0.025 (3)	0.015 (3)	0.016 (3)	−0.009 (3)	0.0000	0.0000
C7	0.0205 (19)	0.0173 (18)	0.0167 (16)	0.0034 (15)	0.0002 (14)	0.0015 (13)
C8	0.017 (2)	0.0222 (19)	0.0233 (19)	−0.0012 (16)	0.0033 (15)	0.0021 (15)
C9	0.0181 (19)	0.027 (2)	0.0199 (18)	0.0009 (16)	−0.0045 (15)	0.0000 (15)
C10	0.029 (2)	0.0168 (18)	0.0184 (17)	0.0037 (16)	−0.0012 (15)	0.0026 (14)

Geometric parameters (Å, º)

Ce1—O1	2.479 (3)	C5—C6	1.391 (5)
Ce1—O1^{i}	2.479 (3)	C6—C6^{iv}	1.496 (7)
Ce1—O2	2.530 (3)	C7—C8	1.382 (6)
Ce1—O2^{i}	2.530 (3)	C7—C9	1.388 (6)
Ce1—O3	2.551 (3)	C7—C10	1.507 (5)
Ce1—O3^{i}	2.551 (3)	C8—C8^{iii}	1.390 (6)
Ce1—O4	2.533 (3)	C9—C9^{iii}	1.386 (5)
Ce1—O4^{i}	2.533 (3)	O2—H2	0.84 (4)
Ce1—N1	2.873 (5)	O2—H3	0.84 (4)
O1—C3	1.257 (4)	O3—H4	0.83 (5)
O5—C10	1.258 (5)	O3—H5	0.84 (5)
O6—C10	1.248 (5)	O4—H6	0.84 (4)
N1—C4	1.327 (5)	O4—H7	0.84 (4)
N1—C4^{i}	1.327 (5)	C2—H1	0.930
C1—C2	1.392 (5)	C4—H8	0.930
C1—C2^{ii}	1.392 (5)	C5—H9	0.930
C1—C3	1.509 (7)	C8—H10	0.930
C2—C2^{iii}	1.387 (5)	C9—H11	0.930
C4—C5	1.387 (6)		
C5···C7^{v}	3.532 (6)	C6···C8^{vi}	3.589 (4)
C5···C9^{v}	3.544 (6)	C7···C2	3.453 (6)
C6···C7^{v}	3.562 (4)	C7···C5^{vii}	3.532 (6)
C6···C7^{vi}	3.562 (4)	C7···C6^{vii}	3.562 (4)
C6···C8^{v}	3.589 (4)	C8···C6^{vii}	3.589 (4)

O1—Ce1—O1^{i}	118.00 (9)	C2—C1—C2^{ii}	119.7 (4)
O1—Ce1—O2	71.20 (10)	C2—C1—C3	120.2 (2)
O1—Ce1—O2^{i}	70.15 (10)	C2^{ii}—C1—C3	120.2 (2)
O1—Ce1—O3	68.08 (10)	C1—C2—C2^{iii}	120.2 (4)
O1—Ce1—O3^{i}	136.72 (9)	O1—C3—O1^{ii}	123.7 (4)
O1—Ce1—O4	70.53 (10)	O1—C3—C1	118.1 (2)
O1—Ce1—O4^{i}	138.31 (10)	O1^{ii}—C3—C1	118.1 (2)
O1—Ce1—N1	121.00 (7)	N1—C4—C5	122.9 (4)
O1^{i}—Ce1—O2	70.15 (10)	C4—C5—C6	120.1 (4)
O1^{i}—Ce1—O2^{i}	71.20 (10)	C5—C6—C5^{i}	116.2 (4)
O1^{i}—Ce1—O3	136.72 (9)	C5—C6—C6^{iv}	121.9 (3)
O1^{i}—Ce1—O3^{i}	68.08 (10)	C5^{i}—C6—C6^{iv}	121.9 (3)
O1^{i}—Ce1—O4	138.31 (10)	C8—C7—C9	120.0 (4)
O1^{i}—Ce1—O4^{i}	70.53 (10)	C8—C7—C10	120.6 (4)
O1^{i}—Ce1—N1	121.00 (7)	C9—C7—C10	119.4 (4)
O2—Ce1—O2^{i}	100.03 (11)	C7—C8—C8^{iii}	120.0 (4)
O2—Ce1—O3	72.74 (10)	C7—C9—C9^{iii}	120.0 (4)
O2—Ce1—O3^{i}	137.67 (10)	O5—C10—O6	123.9 (4)
O2—Ce1—O4	140.68 (10)	O5—C10—C7	118.1 (4)
O2—Ce1—O4^{i}	75.06 (10)	O6—C10—C7	118.1 (4)
O2—Ce1—N1	129.99 (7)	Ce1—O2—H2	115 (3)
O2^{i}—Ce1—O3	137.67 (10)	Ce1—O2—H3	114 (3)
O2^{i}—Ce1—O3^{i}	72.74 (10)	H2—O2—H3	104 (4)
O2^{i}—Ce1—O4	75.06 (10)	Ce1—O3—H4	117 (4)
O2^{i}—Ce1—O4^{i}	140.68 (10)	Ce1—O3—H5	124 (4)
O2^{i}—Ce1—N1	129.99 (7)	H4—O3—H5	102 (5)
O3—Ce1—O3^{i}	139.71 (9)	Ce1—O4—H6	128 (4)
O3—Ce1—O4	84.96 (10)	Ce1—O4—H7	128 (4)
O3—Ce1—O4^{i}	79.12 (10)	H6—O4—H7	102 (6)
O3—Ce1—N1	69.85 (7)	C1—C2—H1	119.897
O3^{i}—Ce1—O4	79.12 (10)	C2^{iii}—C2—H1	119.930
O3^{i}—Ce1—O4^{i}	84.96 (10)	N1—C4—H8	118.556
O3^{i}—Ce1—N1	69.85 (7)	C5—C4—H8	118.540
O4—Ce1—O4^{i}	132.66 (10)	C4—C5—H9	119.957
O4—Ce1—N1	66.33 (7)	C6—C5—H9	119.991
O4^{i}—Ce1—N1	66.33 (7)	C7—C8—H10	119.995
Ce1—O1—C3	145.08 (19)	C8^{iii}—C8—H10	119.992
Ce1—N1—C4	121.1 (3)	C7—C9—H11	120.023
Ce1—N1—C4^{i}	121.1 (3)	C9^{iii}—C9—H11	120.026
C4—N1—C4^{i}	117.8 (4)		

O1—Ce1—O1^{i}—C3^{viii}	−84.2 (3)	O4^{i}—Ce1—N1—C4^{i}	51.94 (8)
O1^{i}—Ce1—O1—C3	−84.2 (3)	Ce1—O1—C3—O1^{ii}	−75.3 (4)
O2—Ce1—O1—C3	−138.3 (3)	Ce1—O1—C3—C1	104.7 (4)
O2^{i}—Ce1—O1—C3	−29.7 (3)	Ce1—N1—C4—C5	179.8 (2)
O3—Ce1—O1—C3	143.3 (4)	Ce1—N1—C4^{i}—C5^{i}	179.8 (2)
O3^{i}—Ce1—O1—C3	2.8 (4)	C4—N1—C4^{i}—C5^{i}	−0.2 (5)
O4—Ce1—O1—C3	50.9 (3)	C4^{i}—N1—C4—C5	−0.2 (5)
O4^{i}—Ce1—O1—C3	−175.9 (3)	C2—C1—C2^{ii}—C2^{ix}	0.0 (4)

O1—Ce1—N1—C4	5.40 (8)	C2^{ii}—C1—C2—C2^{iii}	0.0 (4)
O1—Ce1—N1—C4^{i}	−174.60 (8)	C2—C1—C3—O1	−9.77 (16)
N1—Ce1—O1—C3	95.8 (3)	C2—C1—C3—O1^{ii}	170.23 (16)
O2—Ce1—O1^{i}—C3^{viii}	−29.7 (3)	C2^{ii}—C1—C3—O1	170.23 (16)
O2^{i}—Ce1—O1^{i}—C3^{viii}	−138.3 (3)	C2^{ii}—C1—C3—O1^{ii}	−9.77 (16)
O3—Ce1—O1^{i}—C3^{viii}	2.8 (4)	C1—C2—C2^{iii}—C1^{ix}	0.0 (5)
O3^{i}—Ce1—O1^{i}—C3^{viii}	143.3 (4)	N1—C4—C5—C6	0.4 (6)
O4—Ce1—O1^{i}—C3^{viii}	−175.9 (3)	C4—C5—C6—C5^{i}	−0.2 (4)
O4^{i}—Ce1—O1^{i}—C3^{viii}	50.9 (3)	C4—C5—C6—C6^{iv}	179.8 (3)
O1^{i}—Ce1—N1—C4	−174.60 (8)	C5—C6—C6^{iv}—C5^{iv}	180.00 (19)
O1^{i}—Ce1—N1—C4^{i}	5.40 (8)	C5—C6—C6^{iv}—C5^{x}	0.00 (19)
N1—Ce1—O1^{i}—C3^{viii}	95.8 (3)	C5^{i}—C6—C6^{iv}—C5^{iv}	0.00 (19)
O2—Ce1—N1—C4	−85.35 (10)	C8—C7—C9—C9^{iii}	0.2 (6)
O2—Ce1—N1—C4^{i}	94.65 (10)	C9—C7—C8—C8^{iii}	−0.2 (6)
O2^{i}—Ce1—N1—C4	94.65 (10)	C8—C7—C10—O5	8.2 (6)
O2^{i}—Ce1—N1—C4^{i}	−85.35 (10)	C8—C7—C10—O6	−170.9 (4)
O3—Ce1—N1—C4	−41.42 (8)	C10—C7—C8—C8^{iii}	178.4 (3)
O3—Ce1—N1—C4^{i}	138.58 (8)	C9—C7—C10—O5	−173.2 (4)
O3^{i}—Ce1—N1—C4	138.58 (8)	C9—C7—C10—O6	7.6 (5)
O3^{i}—Ce1—N1—C4^{i}	−41.42 (8)	C10—C7—C9—C9^{iii}	−178.4 (3)
O4—Ce1—N1—C4	51.94 (8)	C7—C8—C8^{iii}—C7^{iii}	0.0 (6)
O4—Ce1—N1—C4^{i}	−128.06 (8)	C7—C9—C9^{iii}—C7^{iii}	0.0 (6)
O4^{i}—Ce1—N1—C4	−128.06 (8)		

Symmetry codes: (i) −*x*+2, −*y*, *z*; (ii) −*x*+1, −*y*, *z*; (iii) *x*, *y*, −*z*+1; (iv) −*x*+2, −*y*, −*z*; (v) *x*+1/2, −*y*+1/2, −*z*+1/2; (vi) −*x*+3/2, *y*−1/2, −*z*+1/2; (vii) *x*−1/2, −*y*+1/2, −*z*+1/2; (viii) *x*+1, *y*, *z*; (ix) −*x*+1, −*y*, −*z*+1; (x) *x*, *y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O5	0.84 (4)	1.93 (4)	2.754 (5)	167 (5)
O2—H3···O6^{viii}	0.84 (3)	1.90 (4)	2.725 (5)	166 (4)
O3—H4···O5	0.83 (5)	2.02 (5)	2.828 (4)	164 (6)
O3—H5···O6^{v}	0.84 (5)	1.81 (5)	2.650 (4)	175 (6)
O4—H7···O5^{vi}	0.84 (4)	1.91 (4)	2.749 (5)	174 (6)

Symmetry codes: (v) *x*+1/2, −*y*+1/2, −*z*+1/2; (vi) −*x*+3/2, *y*−1/2, −*z*+1/2; (viii) *x*+1, *y*, *z*.