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Poly[[hexaaqua(μ_2-oxalato-κ^4O^1,O^2:$O^{1'},O^{2'}$)bis(μ_3-pyridine-2,4-dicarboxylato-κ^4N,O^1:$O^{1'}$:O^4)dicerium(III)] monohydrate]

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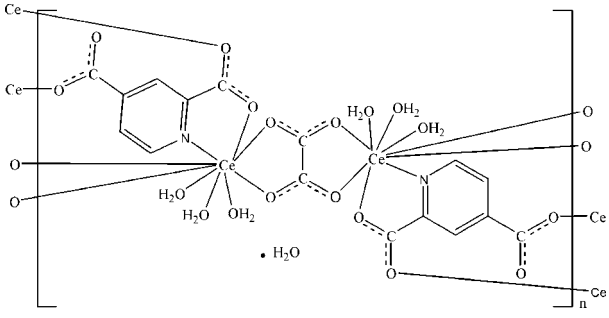
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; disorder in solvent or counterion; R factor = 0.028; wR factor = 0.081; data-to-parameter ratio = 15.1.

In the polymeric title compound, $\{[Ce_2(C_7H_3NO_4)_2(C_2O_4)(H_2O)_6]\cdot H_2O\}_n$, the Ce^{3+} cation is nine-coordinated in a distorted $CeNO_8$ tricapped trigonal–prismatic geometry, formed by three pyridine-2,4-dicarboxylate anions, one oxalate anion and three water molecules. The mid-point of the oxalate anion is located on an inversion center. The oxalate and pyridine-2,4-dicarboxylate anions bridge the Ce^{3+} cations, forming a two-dimensional polymeric complex parallel to (010). Intermolecular classical O—H···O hydrogen bonding and weak C—H···O hydrogen bonding are present in the crystal structure and π–π stacking [centroid–centroid distance = 3.558 (2) Å] is observed between parallel pyridine rings of adjacent molecules. The uncoordinated water molecule shows an occupancy of 0.5.

Related literature

For the isotypic La^{3+} complex, see: Shen & Lush (2011). For related pyridine-2,4-dicarboxylate complexes, see: Aghabozorg *et al.* (2011); Li *et al.* (2007); Wang *et al.* (2009).



Experimental

Crystal data

$[Ce_2(C_7H_3NO_4)_2(C_2O_4)(H_2O)_6]\cdot H_2O$
M_r = 824.58
Triclinic, $P\overline{1}$
a = 6.4160 (5) Å
b = 6.6486 (6) Å
c = 13.9920 (12) Å
α = 89.917 (1)°
β = 85.588 (1)°
γ = 73.676 (1)°
V = 570.98 (8) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 4.04 mm^{-1}
T = 294 K
0.30 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.639, T_{max} = 0.937
6072 measured reflections
2664 independent reflections
2416 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.081
S = 1.10
2664 reflections
177 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.75 e Å^{-3}
$\Delta\rho_{min}$ = −2.70 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ce—N1	2.684 (3)	Ce—O6^{iii}	2.515 (3)
Ce—O1^{i}	2.409 (4)	Ce—O7	2.568 (5)
Ce—O3^{ii}	2.505 (3)	Ce—O8	2.515 (4)
Ce—O4	2.511 (3)	Ce—O9	2.582 (5)
Ce—O5	2.508 (3)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O4^{ii}	0.86	2.03	2.879 (6)	171
O7—H7B···O10^{iv}	0.83	1.84	2.569 (10)	146
O8—H8A···O6^{v}	0.92	2.00	2.910 (5)	170
O8—H8B···O2^{vi}	0.86	1.84	2.655 (6)	159
O9—H9A···O6^{v}	0.99	2.01	2.987 (6)	169
O9—H9B···O10	0.84	1.93	2.440 (10)	118
O10—H10A···O5^{ii}	0.84	2.12	2.844 (9)	143
O10—H10A···O8^{ii}	0.84	2.39	2.913 (10)	121
O10—H10B···O9^{vii}	0.94	1.63	2.501 (11)	153
C5—H5A···O3^{ii}	0.93	2.46	3.131 (5)	129

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5400).

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supplementary materials

Acta Cryst. (2012). E**68**, m21-m22 [**doi:10.1107/S1600536811051956**]

Poly[[hexaaqua(μ_2-oxalato-$\kappa^4O^1,O^2:O^{1'},O^{2'}$)bis($\mu_3$-pyridine-2,4-dicarboxylato-$\kappa^4N,O^1:O^{1'}:O^4$)dicerium(III)] monohydrate]

F. M. Shen and S. F. Lush

Comment

The pyridine-2,4-dicarboxylic acid (pdcH2) has important coordination functions to metals by either carboxylate bridges between metal centers, to form dimeric complexes or tridentate (O, N, O') chelation to metal ions. Some pydc complexes have been reported (Li *et al.*, 2007; Wang *et al.*, 2009; Aghabozorg *et al.*, 2011).

The title complex is isomorphous with the La^{3+} complex (Shen & Lush, 2011). The Ce^{III} is nine-coordinated in a distorted tricapped trigonal prismatic geometry formed by N and O atoms from a pydc ligand, two O atoms from two pydc ligands, two O atoms from one oxalate ligand and three O atoms from coordinated water molecules (shown as Fig. 1, Table 1). The mid-point of the oxalate anion is located on an inversion center. The oxalate and pyridinedicarboxylate anions bridge the Ce^{3+} cations to form the polymeric complex (Fig. 2).

The crystal structure contains O—H···O and weak C—H···O hydrogen bonds. The π-π stacking between two pyridine rings of (pydc) anion fragments with centroids distance of 3.558 (2) Å (1 - *x*, 1 - *y*, 1 - *z*) are observed. The uncoordinated water molecule shows half-occupation.

Experimental

$Ce(NO_3)_3.6H2O$ (0.1086 g, 0.25 mmole), pydridine-2,4-dicarboxylic acid (0.0418 g, 0.25 mmol) and 4,4'-dipyridine (0.0464 g, 0.25 mmol) were mixed in 10 ml of deionized water. After stirring for 30 min, the mixture was placed in a 23 ml Teflon-lined reactor which was heated under autogenous pressure to 418 K for 48 h and then allowed to cool to room temperature. The colorless transparent single crystals were obtained in 35.6% yield (based on Ce).

Refinement

The site occupancy factor of the lattice water O10 was refined to 0.486 (15), and was set as 0.5 at the final cycles of refinement. Water H atoms were fixed in chemical sensible positions, thermal parameters were fixed as 0.08 $Å^2$. Other H atoms were positioned geometrically with C—H = 0.93 Å (aromatic) and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

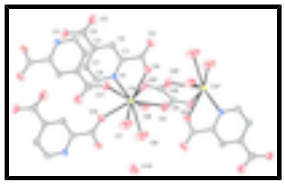

Fig. 1. View of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. All H atoms have been omitted for clarity. [Symmetry code: (i) *x* - 1, *y*, *z*; (ii) -*x* + 1, -*y* + 1, -*z* + 1; (iii) -*x* + 1, -*y* + 1, -*z* + 2.]

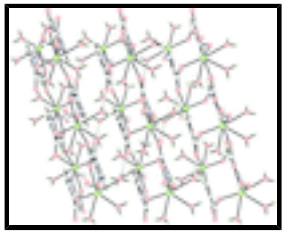

Fig. 2. The crystal packing of (I) viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

Poly[[hexaaqua(μ$_2$-oxalato- κ^4*O*^{1},*O*^{2}:*O*$^{1'}$,*O*$^{2'}$)bis(μ$_3$-pyridine- 2,4-dicarboxylato- κ^4*N*,*O*^{1}:*O*$^{1'}$:*O*^{4})dicerium(III)] monohydrate]

Crystal data

$[Ce_2(C_7H_3NO_4)_2(C_2O_4)(H_2O)_6]\cdot H_2O$	$Z = 1$
$M_r = 824.58$	$F(000) = 398$
Triclinic, $P\overline{1}$	$D_x = 2.398$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.4160$ (5) Å	Cell parameters from 4490 reflections
$b = 6.6486$ (6) Å	$\theta = 2.5$–$25.0°$
$c = 13.9920$ (12) Å	$\mu = 4.04$ mm^{-1}
$\alpha = 89.917$ (1)°	$T = 294$ K
$\beta = 85.588$ (1)°	Columnar, colorless
$\gamma = 73.676$ (1)°	0.30 × 0.10 × 0.10 mm
$V = 570.98$ (8) Å^3	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	2664 independent reflections
Radiation source: fine-focus sealed tube	2416 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.030$
Detector resolution: 9 pixels mm^{-1}	$\theta_{max} = 27.8°$, $\theta_{min} = 1.5°$
φ and ω scans	$h = -8 \rightarrow 8$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$k = -8 \rightarrow 8$
$T_{min} = 0.639$, $T_{max} = 0.937$	$l = -18 \rightarrow 18$
6072 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
$R[F^2 > 2\sigma(F^2)] = 0.028$	H-atom parameters constrained
$wR(F^2) = 0.081$	$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.4154P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.019$
2664 reflections	$\Delta\rho_{max} = 2.75$ e Å^{-3}
177 parameters	$\Delta\rho_{min} = -2.70$ e Å^{-3}
0 restraints	Extinction correction: *SHELXTL* (Sheldrick, 2008), $FC^*=KFC[1+0.001XFC^2\Lambda^3/SIN(2\Theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0071 (15)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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)
Ce	0.36484 (3)	0.33000 (3)	0.80343 (1)	0.0198 (1)	
O1	0.7620 (6)	0.3463 (6)	0.2798 (2)	0.0356 (11)	
O2	1.0901 (6)	0.2177 (7)	0.3373 (3)	0.0438 (13)	
O3	1.0817 (5)	0.2746 (6)	0.7009 (2)	0.0350 (10)	
O4	0.7595 (5)	0.3214 (7)	0.7822 (2)	0.0380 (13)	
O5	0.5054 (7)	0.2476 (5)	0.9655 (2)	0.0408 (13)	
O6	0.5773 (6)	0.3678 (5)	1.1047 (2)	0.0360 (10)	
O7	0.0036 (8)	0.5134 (8)	0.8992 (4)	0.0729 (14)	
O8	0.5654 (6)	−0.0533 (6)	0.7844 (3)	0.0419 (11)	
O9	0.1789 (8)	0.0870 (8)	0.8994 (4)	0.0729 (14)	
N1	0.5723 (5)	0.2600 (6)	0.6274 (2)	0.0208 (9)	
C1	0.7770 (7)	0.2748 (6)	0.6150 (3)	0.0218 (11)	
C2	0.5683 (7)	0.2406 (7)	0.4556 (3)	0.0248 (11)	
C3	0.7772 (7)	0.2622 (7)	0.4439 (3)	0.0227 (11)	
C4	0.8836 (7)	0.2747 (7)	0.5250 (3)	0.0251 (11)	
C5	0.4745 (7)	0.2392 (7)	0.5484 (3)	0.0256 (12)	

C6	0.8875 (8)	0.2745 (7)	0.3451 (3)	0.0275 (12)	
C7	0.8828 (7)	0.2921 (7)	0.7052 (3)	0.0246 (11)	
C8	0.5247 (7)	0.3884 (6)	1.0201 (3)	0.0237 (11)	
O10	−0.1094 (13)	−0.0862 (13)	0.9223 (7)	0.050 (3)	0.500
H2A	0.49300	0.22740	0.40290	0.039 (15)*	
H4A	1.02630	0.28290	0.51910	0.0300*	
H5A	0.33490	0.22280	0.55600	0.0300*	
H7A	−0.07800	0.47060	0.86320	0.0800*	
H7B	−0.02500	0.63680	0.88280	0.0800*	
H8A	0.53670	−0.16200	0.81820	0.0800*	
H8B	0.65420	−0.09500	0.73490	0.0800*	
H9A	0.24360	−0.06740	0.89420	0.0800*	
H9B	0.06500	0.09050	0.87300	0.0800*	
H10A	−0.21970	0.00790	0.90760	0.0800*	0.500
H10B	−0.12520	−0.12960	0.98560	0.0800*	0.500

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce	0.0191 (2)	0.0294 (2)	0.0134 (1)	−0.0113 (1)	−0.0006 (1)	0.0005 (1)
O1	0.0380 (19)	0.044 (2)	0.0238 (16)	−0.0092 (16)	−0.0055 (14)	0.0092 (14)
O2	0.0270 (18)	0.064 (3)	0.0303 (19)	0.0011 (17)	0.0068 (15)	0.0078 (17)
O3	0.0199 (15)	0.061 (2)	0.0274 (17)	−0.0163 (15)	−0.0040 (13)	−0.0028 (15)
O4	0.0268 (17)	0.075 (3)	0.0185 (15)	−0.0250 (17)	−0.0004 (13)	−0.0012 (16)
O5	0.074 (3)	0.0266 (17)	0.0225 (16)	−0.0142 (17)	−0.0080 (17)	−0.0003 (13)
O6	0.058 (2)	0.0306 (17)	0.0222 (16)	−0.0141 (16)	−0.0143 (15)	0.0071 (13)
O7	0.055 (2)	0.061 (2)	0.088 (3)	−0.0018 (16)	0.0304 (19)	0.0251 (19)
O8	0.048 (2)	0.0333 (19)	0.041 (2)	−0.0115 (16)	0.0176 (17)	−0.0007 (15)
O9	0.055 (2)	0.061 (2)	0.088 (3)	−0.0018 (16)	0.0304 (19)	0.0251 (19)
N1	0.0174 (16)	0.0268 (17)	0.0193 (16)	−0.0077 (13)	−0.0030 (13)	0.0001 (13)
C1	0.0197 (19)	0.024 (2)	0.022 (2)	−0.0068 (16)	−0.0017 (15)	0.0017 (15)
C2	0.028 (2)	0.030 (2)	0.0179 (19)	−0.0099 (17)	−0.0049 (16)	−0.0011 (16)
C3	0.024 (2)	0.025 (2)	0.0162 (18)	−0.0024 (16)	−0.0005 (15)	0.0042 (15)
C4	0.0172 (19)	0.035 (2)	0.022 (2)	−0.0057 (17)	−0.0003 (16)	0.0045 (17)
C5	0.022 (2)	0.031 (2)	0.026 (2)	−0.0110 (17)	−0.0029 (16)	0.0014 (17)
C6	0.033 (2)	0.029 (2)	0.017 (2)	−0.0045 (18)	0.0037 (17)	−0.0004 (16)
C7	0.0196 (19)	0.033 (2)	0.025 (2)	−0.0129 (17)	−0.0041 (16)	0.0032 (17)
C8	0.028 (2)	0.023 (2)	0.0189 (19)	−0.0052 (16)	−0.0027 (16)	0.0009 (15)
O10	0.037 (4)	0.042 (4)	0.072 (6)	−0.010 (3)	−0.013 (4)	0.009 (4)

Geometric parameters (Å, °)

Ce—N1	2.684 (3)	O8—H8B	0.8600
Ce—O1^{i}	2.409 (4)	O9—H9B	0.8400
Ce—O3^{ii}	2.505 (3)	O9—H9A	0.9900
Ce—O4	2.511 (3)	O10—H10A	0.8400
Ce—O5	2.508 (3)	O10—H10B	0.9400
Ce—O6^{iii}	2.515 (3)	N1—C5	1.338 (5)

Ce—O7	2.568 (5)	N1—C1	1.343 (6)
Ce—O8	2.515 (4)	C1—C4	1.386 (6)
Ce—O9	2.582 (5)	C1—C7	1.498 (6)
O1—C6	1.268 (6)	C2—C3	1.385 (7)
O2—C6	1.244 (7)	C2—C5	1.390 (6)
O3—C7	1.245 (6)	C3—C6	1.517 (6)
O4—C7	1.268 (5)	C3—C4	1.383 (6)
O5—C8	1.248 (5)	C8—C8^{iii}	1.543 (5)
O6—C8	1.253 (5)	C2—H2A	0.9300
O7—H7B	0.8300	C4—H4A	0.9300
O7—H7A	0.8600	C5—H5A	0.9300
O8—H8A	0.9200		
O4—Ce—O5	74.74 (12)	Ce—O5—C8	121.3 (3)
O4—Ce—O7	142.54 (15)	Ce^{iii}—O6—C8	120.9 (3)
O4—Ce—O8	75.62 (14)	Ce—O7—H7B	105.00
O4—Ce—O9	130.01 (15)	H7A—O7—H7B	99.00
O4—Ce—N1	61.02 (10)	Ce—O7—H7A	96.00
O3^{ii}—Ce—O4	137.32 (10)	Ce—O8—H8A	127.00
O1^{i}—Ce—O4	94.76 (13)	H8A—O8—H8B	113.00
O4—Ce—O6^{iii}	70.50 (13)	Ce—O8—H8B	119.00
O5—Ce—O7	84.31 (15)	Ce—O9—H9A	120.00
O5—Ce—O8	78.05 (12)	H9A—O9—H9B	96.00
O5—Ce—O9	67.22 (15)	Ce—O9—H9B	107.00
O5—Ce—N1	130.72 (12)	H10A—O10—H10B	112.00
O3^{ii}—Ce—O5	141.57 (12)	Ce—N1—C5	123.6 (3)
O1^{i}—Ce—O5	132.71 (11)	Ce—N1—C1	118.7 (2)
O5—Ce—O6^{iii}	64.05 (10)	C1—N1—C5	117.1 (3)
O7—Ce—O8	130.23 (15)	N1—C1—C4	122.5 (4)
O7—Ce—O9	64.30 (16)	N1—C1—C7	115.4 (4)
O7—Ce—N1	144.66 (14)	C4—C1—C7	122.1 (4)
O3^{ii}—Ce—O7	76.31 (14)	C3—C2—C5	118.1 (4)
O1^{i}—Ce—O7	76.97 (15)	C2—C3—C6	121.4 (4)
O6^{iii}—Ce—O7	72.47 (15)	C4—C3—C6	120.3 (4)
O8—Ce—O9	65.94 (15)	C2—C3—C4	118.3 (4)
O8—Ce—N1	71.24 (12)	C1—C4—C3	119.8 (4)
O3^{ii}—Ce—O8	89.53 (13)	N1—C5—C2	124.1 (4)
O1^{i}—Ce—O8	144.86 (12)	O1—C6—O2	127.1 (4)
O6^{iii}—Ce—O8	134.19 (12)	O2—C6—C3	116.8 (4)
O9—Ce—N1	127.54 (14)	O1—C6—C3	116.0 (4)
O3^{ii}—Ce—O9	74.47 (14)	O4—C7—C1	116.2 (4)
O1^{i}—Ce—O9	134.92 (15)	O3—C7—C1	119.4 (4)
O6^{iii}—Ce—O9	116.36 (14)	O3—C7—O4	124.4 (4)
O3^{ii}—Ce—N1	76.35 (10)	O5—C8—O6	126.7 (4)
O1^{i}—Ce—N1	74.55 (11)	O5—C8—C8^{iii}	116.7 (4)
O6^{iii}—Ce—N1	114.97 (11)	O6—C8—C8^{iii}	116.6 (4)

O1^{i}—Ce—O3^{ii}	74.72 (12)	C5—C2—H2A	121.00
O3^{ii}—Ce—O6^{iii}	136.22 (12)	C3—C2—H2A	121.00
O1^{i}—Ce—O6^{iii}	68.95 (11)	C1—C4—H4A	120.00
Ce^{i}—O1—C6	138.2 (3)	C3—C4—H4A	120.00
Ce^{iv}—O3—C7	140.1 (3)	N1—C5—H5A	118.00
Ce—O4—C7	127.9 (3)	C2—C5—H5A	118.00
O5—Ce—O4—C7	158.0 (4)	N1—Ce—O1^{i}—C6^{i}	73.5 (5)
O7—Ce—O4—C7	−143.7 (4)	O4—Ce—O6^{iii}—C8^{iii}	−87.9 (4)
O8—Ce—O4—C7	76.7 (4)	O5—Ce—O6^{iii}—C8^{iii}	−5.9 (3)
O9—Ce—O4—C7	116.9 (4)	O7—Ce—O6^{iii}—C8^{iii}	86.3 (4)
N1—Ce—O4—C7	0.5 (4)	O8—Ce—O6^{iii}—C8^{iii}	−43.3 (4)
O3^{ii}—Ce—O4—C7	3.6 (5)	O9—Ce—O6^{iii}—C8^{iii}	37.9 (4)
O1^{i}—Ce—O4—C7	−68.9 (4)	N1—Ce—O6^{iii}—C8^{iii}	−130.9 (3)
O6^{iii}—Ce—O4—C7	−134.6 (4)	Ce^{i}—O1—C6—O2	−76.7 (7)
O4—Ce—O5—C8	80.8 (4)	Ce^{i}—O1—C6—C3	101.7 (5)
O7—Ce—O5—C8	−67.9 (4)	Ce^{iv}—O3—C7—O4	−12.4 (8)
O8—Ce—O5—C8	158.9 (4)	Ce^{iv}—O3—C7—C1	168.6 (3)
O9—Ce—O5—C8	−132.4 (4)	Ce—O4—C7—O3	−174.5 (3)
N1—Ce—O5—C8	106.9 (4)	Ce—O4—C7—C1	4.5 (6)
O3^{ii}—Ce—O5—C8	−127.4 (4)	Ce—O5—C8—O6	174.3 (4)
O1^{i}—Ce—O5—C8	−1.5 (5)	Ce—O5—C8—C8^{iii}	−4.7 (6)
O6^{iii}—Ce—O5—C8	5.4 (4)	Ce^{iii}—O6—C8—O5	175.0 (4)
O4—Ce—N1—C1	−6.1 (3)	Ce^{iii}—O6—C8—C8^{iii}	−6.0 (5)
O4—Ce—N1—C5	−176.6 (4)	Ce—N1—C1—C4	−169.4 (3)
O5—Ce—N1—C1	−35.2 (4)	Ce—N1—C1—C7	10.5 (5)
O5—Ce—N1—C5	154.3 (3)	C5—N1—C1—C4	1.7 (6)
O7—Ce—N1—C1	135.9 (3)	C5—N1—C1—C7	−178.4 (4)
O7—Ce—N1—C5	−34.6 (5)	Ce—N1—C5—C2	168.0 (3)
O8—Ce—N1—C1	−89.7 (3)	C1—N1—C5—C2	−2.7 (7)
O8—Ce—N1—C5	99.8 (4)	N1—C1—C4—C3	1.0 (6)
O9—Ce—N1—C1	−126.2 (3)	C7—C1—C4—C3	−178.8 (4)
O9—Ce—N1—C5	63.3 (4)	N1—C1—C7—O3	169.2 (4)
O3^{ii}—Ce—N1—C1	176.1 (3)	N1—C1—C7—O4	−9.8 (6)
O3^{ii}—Ce—N1—C5	5.6 (3)	C4—C1—C7—O3	−11.0 (6)
O1^{i}—Ce—N1—C1	98.5 (3)	C4—C1—C7—O4	170.0 (4)
O1^{i}—Ce—N1—C5	−72.0 (3)	C5—C2—C3—C4	2.0 (6)
O6^{iii}—Ce—N1—C1	41.2 (3)	C5—C2—C3—C6	−177.4 (4)
O6^{iii}—Ce—N1—C5	−129.3 (3)	C3—C2—C5—N1	0.9 (7)
O4—Ce—O3^{ii}—C7^{ii}	−172.6 (4)	C2—C3—C4—C1	−2.8 (7)
O5—Ce—O3^{ii}—C7^{ii}	49.5 (6)	C6—C3—C4—C1	176.5 (4)
O7—Ce—O3^{ii}—C7^{ii}	−12.4 (5)	C2—C3—C6—O1	27.1 (6)
O8—Ce—O3^{ii}—C7^{ii}	119.4 (5)	C2—C3—C6—O2	−154.4 (5)

O9—Ce—O3^{ii}—C7^{ii}	54.3 (5)	C4—C3—C6—O1	−152.3 (4)
N1—Ce—O3^{ii}—C7^{ii}	−169.8 (5)	C4—C3—C6—O2	26.3 (6)
O4—Ce—O1^{i}—C6^{i}	131.6 (5)	O5—C8—C8^{iii}—O5^{iii}	−180.0 (5)
O5—Ce—O1^{i}—C6^{i}	−154.8 (4)	O5—C8—C8^{iii}—O6^{iii}	−0.9 (6)
O7—Ce—O1^{i}—C6^{i}	−85.4 (5)	O6—C8—C8^{iii}—O5^{iii}	0.9 (6)
O8—Ce—O1^{i}—C6^{i}	60.0 (6)	O6—C8—C8^{iii}—O6^{iii}	180.0 (4)
O9—Ce—O1^{i}—C6^{i}	−54.6 (5)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7A···O4^{ii}	0.86	2.03	2.879 (6)	171.00
O7—H7B···O10^{v}	0.83	1.84	2.569 (10)	146.00
O8—H8A···O6^{vi}	0.92	2.00	2.910 (5)	170.00
O8—H8B···O2^{vii}	0.86	1.84	2.655 (6)	159.00
O9—H9A···O6^{vi}	0.99	2.01	2.987 (6)	169.00
O9—H9B···O10	0.84	1.93	2.440 (10)	118.00
O10—H10A···O5^{ii}	0.84	2.12	2.844 (9)	143.00
O10—H10A···O8^{ii}	0.84	2.39	2.913 (10)	121.00
O10—H10B···O9^{viii}	0.94	1.63	2.501 (11)	153.00
C5—H5A···O3^{ii}	0.93	2.46	3.131 (5)	129.

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

Fig. 1

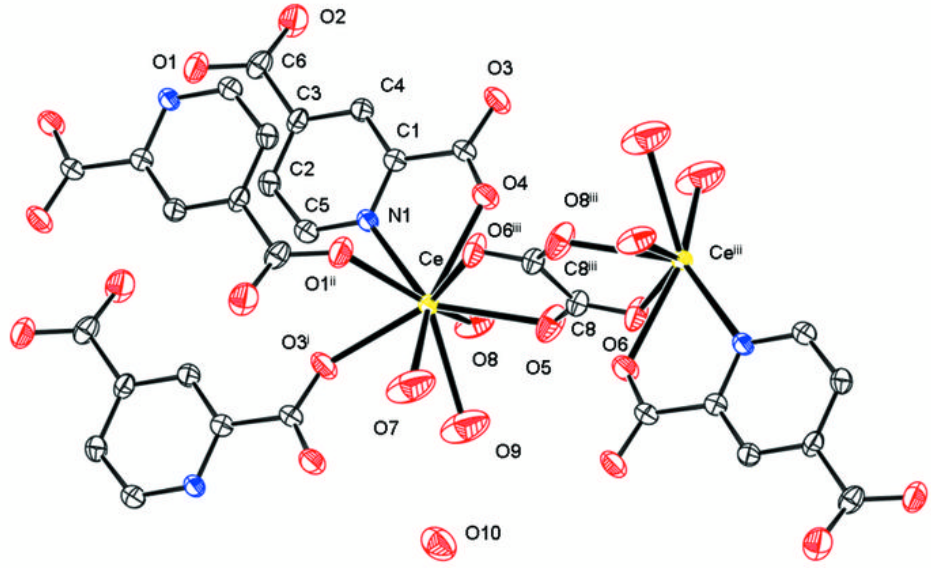
O2
O1
C6
C3
C4
O3
C1
C2
O4
C5
N1
O8iii
O6iii
Ce
C8iii
Ceiii
O1ii
C8
O3i
O8
O5
O6
O7
O9
O10

Fig. 2