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Poly[(μ_4-benzene-1,3,5-tricarboxylato)-bis(*N*,*N*-dimethylformamide)cerium(III)]

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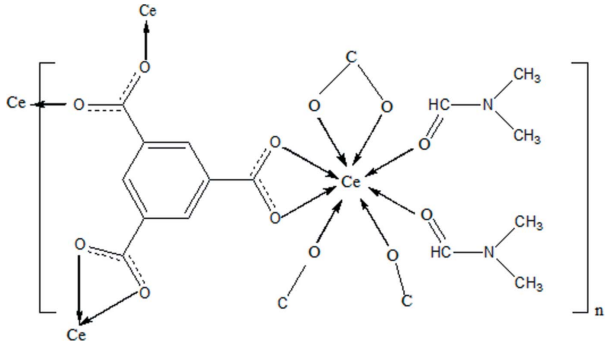
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.046; wR factor = 0.076; data-to-parameter ratio = 12.9.

The asymmetric unit of the title rare earth coordination polymer, $[Ce(C_9H_3O_6)(C_3H_7NO)_2]_n$, contains one eight-coordinated Ce^{3+} ion, one benzene-1,3,5-tricarboxylate (BTC) ligand and two coordinated *N*,*N*-dimethylformamide (DMF) molecules. The Ce^{3+} ion is coordinated by six O atoms from four carboxylate groups of the BTC ligands and by two O atoms from two terminal DMF molecules.

Related literature

Metal-organic framework (MOF) design and construction is currently a flourishing field of research owing to the intriguing molecular topologies and the potentially exploitable adsorption, catalytic, fluorescence, and magnetic properties, see: Chen *et al.* (2006); Serre *et al.* (2007); Zhang *et al.* (2007). As functional metal centers, rare earth metals are attracting increasing attention from synthesis chemists for their coordination properties and special chemical characteristics arising from 4f electrons and their propensity to form isostructural complexes, see: Thirumurugan *et al.* (2004); Long *et al.* (2001).



Experimental

Crystal data

$[Ce(C_9H_3O_6)(C_3H_7NO)_2]$
M_r = 493.43
Monoclinic, $P2_1/n$
a = 10.6994 (11) Å
b = 13.6773 (14) Å
c = 12.1961 (13) Å
β = 101.574 (2)°
V = 1748.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.65 mm^{-1}
T = 298 K
0.8 × 0.6 × 0.5 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.226, T_{max} = 0.351
9223 measured reflections
3087 independent reflections
2516 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.076
S = 1.02
3087 reflections
239 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.14 e Å^{-3}
$\Delta\rho_{min}$ = −1.05 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: QM2010).

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Poly[(μ_4-benzene-1,3,5-tricarboxylato)bis(*N*,*N*-dimethylformamide)cerium(III)]

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S1. Experimental

All reagents were of analytical grade. A mixture of cerium nitrate (40 mg, 0.10 mmol) and μ_3-benzene-*1,3,5*-tricarboxylate acid(H_3BTC) (10 mg, 0.05 mmol) was dissolved in *N,N*′-dimethylformamide (DMF) (10 mL) and isopropanol (2 mL) at room temperature, two drops of triethylamine was added, then some nitric acid(2M) was added utill the solution is clear. This mixture was placed in a 20 mL test tube. Then a small vial containing triethylamine (0.1 mL) and DMF (1.5 mL) was put in the test tube. The test tube was left undisturbed at room temprature for 15 days.

S2. Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å.

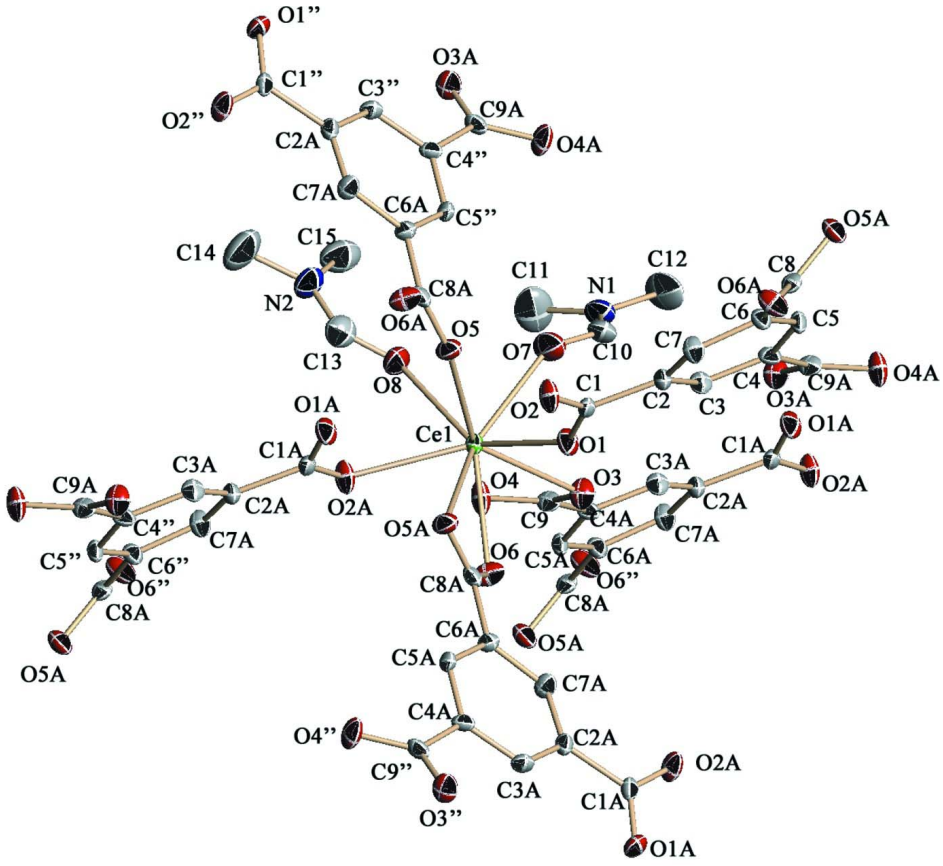

Figure 1

Coordination environment of Ce in the compound with nonhydrogen atoms represented by thermal ellipsoids draw at 30 % probability level.

Poly[(μ_4-benzene-1,3,5-tricarboxylato)bis(*N*,*N*- dimethylformamide)cerium(III)]

Crystal data

$[Ce(C_9H_3O_6)(C_3H_7NO)_2]$
$M_r = 493.43$
Monoclinic, $P2_1/n$
$a = 10.6994$ (11) Å
$b = 13.6773$ (14) Å
$c = 12.1961$ (13) Å
$\beta = 101.574$ (2)°
$V = 1748.5$ (3) Å^3
$Z = 4$
$F(000) = 972$
$D_x = 1.874$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\mu = 2.65$ mm^{-1}
$T = 298$ K
Rod, colorless
0.8 × 0.6 × 0.5 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.226$, $T_{max} = 0.351$
9223 measured reflections
3087 independent reflections
2516 reflections with $I > 2\sigma(I)$
$R_{int} = 0.059$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
$h = -9 \rightarrow 12$
$k = -16 \rightarrow 16$
$l = -13 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.076$
$S = 1.02$
3087 reflections
239 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0173P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.008$
$\Delta\rho_{max} = 1.14$ e Å^{-3}
$\Delta\rho_{min} = -1.05$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ce1	0.62306 (3)	1.03609 (3)	0.39566 (3)	0.01481 (11)
C1	0.6993 (6)	0.9240 (4)	0.6584 (5)	0.0170 (15)
C2	0.8218 (6)	0.8724 (4)	0.7133 (6)	0.0188 (15)
C3	0.9313 (6)	0.8882 (4)	0.6695 (5)	0.0189 (15)
H3	0.9285	0.9309	0.6096	0.023*
C4	1.0448 (6)	0.8403 (4)	0.7153 (5)	0.0174 (15)
C5	1.0469 (6)	0.7730 (4)	0.7994 (5)	0.0179 (15)
H5	1.1210	0.7378	0.8264	0.021*
C6	0.9388 (6)	0.7571 (4)	0.8446 (5)	0.0178 (15)
C7	0.8280 (6)	0.8097 (4)	0.8014 (5)	0.0206 (15)
H7	0.7567	0.8018	0.8334	0.025*
C8	0.9393 (6)	0.6846 (5)	0.9368 (6)	0.0184 (15)
C9	0.8386 (6)	1.1342 (4)	0.3310 (6)	0.0189 (15)
C10	0.8855 (7)	0.8868 (5)	0.3589 (7)	0.0347 (19)
H10	0.9423	0.8752	0.4260	0.042*
C11	0.8492 (8)	0.9013 (7)	0.1589 (7)	0.068 (3)
H11A	0.7749	0.9368	0.1690	0.102*
H11B	0.8236	0.8408	0.1212	0.102*
H11C	0.8959	0.9396	0.1148	0.102*
C12	1.0614 (7)	0.8523 (6)	0.2683 (8)	0.061 (3)
H12A	1.1029	0.9018	0.2327	0.091*
H12B	1.0622	0.7915	0.2290	0.091*
H12C	1.1057	0.8444	0.3445	0.091*
C13	0.4387 (8)	0.9287 (5)	0.1597 (7)	0.038 (2)
H13	0.3729	0.9378	0.1982	0.046*

C14	0.2840 (8)	0.8444 (6)	0.0187 (8)	0.068 (3)
H14A	0.2850	0.7743	0.0206	0.102*
H14B	0.2575	0.8662	−0.0573	0.102*
H14C	0.2255	0.8684	0.0627	0.102*
C15	0.5082 (8)	0.8594 (6)	0.0012 (7)	0.053 (2)
H15A	0.5838	0.8965	0.0303	0.080*
H15B	0.4775	0.8761	−0.0759	0.080*
H15C	0.5278	0.7909	0.0072	0.080*
N1	0.9291 (6)	0.8814 (4)	0.2665 (6)	0.0356 (16)
N2	0.4117 (6)	0.8815 (4)	0.0643 (5)	0.0374 (16)
O1	0.7104 (4)	0.9890 (3)	0.5883 (4)	0.0250 (11)
O2	0.5978 (4)	0.9001 (3)	0.6867 (4)	0.0263 (11)
O3	0.8522 (4)	1.1009 (3)	0.4277 (4)	0.0268 (11)
O4	0.7289 (4)	1.1428 (3)	0.2671 (4)	0.0289 (12)
O5	0.5116 (4)	0.8900 (3)	0.4415 (4)	0.0241 (11)
O6	0.6335 (4)	1.1973 (3)	0.4976 (4)	0.0270 (12)
O7	0.7738 (5)	0.9063 (3)	0.3633 (4)	0.0406 (14)
O8	0.5433 (4)	0.9618 (4)	0.2023 (4)	0.0342 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.01096 (19)	0.01648 (19)	0.0170 (2)	−0.00043 (18)	0.00285 (13)	−0.00011 (19)
C1	0.012 (4)	0.018 (4)	0.019 (4)	0.001 (3)	−0.001 (3)	−0.005 (3)
C2	0.012 (4)	0.017 (4)	0.026 (4)	0.001 (3)	0.000 (3)	−0.002 (3)
C3	0.020 (4)	0.016 (3)	0.021 (4)	−0.001 (3)	0.004 (3)	0.006 (3)
C4	0.020 (4)	0.011 (3)	0.021 (4)	−0.001 (3)	0.005 (3)	0.002 (3)
C5	0.010 (4)	0.017 (4)	0.025 (4)	0.000 (3)	−0.001 (3)	0.004 (3)
C6	0.016 (4)	0.015 (4)	0.022 (4)	0.002 (3)	0.003 (3)	0.003 (3)
C7	0.016 (4)	0.026 (4)	0.021 (4)	0.001 (3)	0.005 (3)	0.005 (3)
C8	0.013 (4)	0.016 (4)	0.026 (4)	−0.005 (3)	0.003 (3)	−0.002 (3)
C9	0.015 (4)	0.015 (4)	0.029 (4)	−0.004 (3)	0.009 (3)	0.000 (3)
C10	0.032 (5)	0.024 (4)	0.047 (6)	0.007 (4)	0.004 (4)	−0.011 (4)
C11	0.068 (7)	0.096 (8)	0.037 (6)	0.023 (6)	0.006 (5)	−0.025 (6)
C12	0.032 (5)	0.060 (6)	0.097 (8)	0.011 (4)	0.029 (5)	−0.020 (6)
C13	0.044 (5)	0.041 (5)	0.029 (5)	0.003 (4)	0.004 (4)	0.001 (4)
C14	0.069 (7)	0.071 (7)	0.053 (7)	−0.018 (5)	−0.014 (5)	−0.015 (5)
C15	0.075 (7)	0.043 (5)	0.039 (6)	−0.004 (4)	0.006 (5)	−0.006 (4)
N1	0.029 (4)	0.030 (4)	0.049 (5)	0.005 (3)	0.011 (3)	−0.013 (3)
N2	0.043 (4)	0.040 (4)	0.024 (4)	−0.005 (3)	−0.004 (3)	−0.005 (3)
O1	0.023 (3)	0.024 (3)	0.025 (3)	0.002 (2)	−0.002 (2)	0.010 (2)
O2	0.012 (3)	0.039 (3)	0.029 (3)	0.003 (2)	0.005 (2)	0.008 (2)
O3	0.021 (3)	0.036 (3)	0.026 (3)	−0.002 (2)	0.008 (2)	0.004 (2)
O4	0.012 (3)	0.042 (3)	0.032 (3)	0.003 (2)	0.003 (2)	0.009 (2)
O5	0.019 (3)	0.019 (3)	0.035 (3)	−0.004 (2)	0.007 (2)	−0.007 (2)
O6	0.030 (3)	0.025 (3)	0.030 (3)	−0.008 (2)	0.016 (2)	−0.007 (2)
O7	0.028 (3)	0.036 (3)	0.060 (4)	0.003 (2)	0.015 (3)	−0.012 (3)
O8	0.031 (3)	0.036 (3)	0.031 (3)	0.002 (3)	−0.002 (2)	−0.011 (3)

Geometric parameters (Å, º)

Ce1—O1	2.434 (4)	C9—O3	1.245 (8)
Ce1—O5	2.448 (4)	C9—O4	1.278 (7)
Ce1—O7	2.483 (5)	C9—C4^{iii}	1.511 (8)
Ce1—O6	2.522 (4)	C10—O7	1.236 (7)
Ce1—O2^{i}	2.531 (4)	C10—N1	1.306 (9)
Ce1—O8	2.553 (5)	C10—H10	0.9300
Ce1—O3	2.562 (4)	C11—N1	1.441 (10)
Ce1—O4	2.565 (4)	C11—H11A	0.9600
Ce1—O5^{i}	2.862 (4)	C11—H11B	0.9600
Ce1—C9	2.910 (6)	C11—H11C	0.9600
Ce1—C8^{ii}	3.049 (6)	C12—N1	1.466 (8)
Ce1—Ce1^{i}	4.1322 (7)	C12—H12A	0.9600
C1—O2	1.247 (7)	C12—H12B	0.9600
C1—O1	1.256 (7)	C12—H12C	0.9600
C1—C2	1.520 (8)	C13—O8	1.222 (8)
C2—C7	1.367 (8)	C13—N2	1.311 (9)
C2—C3	1.399 (8)	C13—H13	0.9300
C3—C4	1.394 (8)	C14—N2	1.459 (9)
C3—H3	0.9300	C14—H14A	0.9600
C4—C5	1.374 (8)	C14—H14B	0.9600
C4—C9^{iii}	1.511 (8)	C14—H14C	0.9600
C5—C6	1.394 (8)	C15—N2	1.438 (9)
C5—H5	0.9300	C15—H15A	0.9600
C6—C7	1.397 (8)	C15—H15B	0.9600
C6—C8	1.498 (8)	C15—H15C	0.9600
C7—H7	0.9300	O2—Ce1^{i}	2.531 (4)
C8—O6^{iv}	1.236 (7)	O5—C8^{vi}	1.276 (7)
C8—O5^{v}	1.276 (7)	O5—Ce1^{i}	2.862 (4)
C8—Ce1^{iv}	3.049 (6)	O6—C8^{ii}	1.236 (7)
O1—Ce1—O5	70.96 (14)	C4—C3—H3	119.9
O1—Ce1—O7	80.11 (16)	C2—C3—H3	119.9
O5—Ce1—O7	79.29 (15)	C5—C4—C3	119.8 (6)
O1—Ce1—O6	77.59 (14)	C5—C4—C9^{iii}	122.9 (6)
O5—Ce1—O6	125.18 (13)	C3—C4—C9^{iii}	117.3 (6)
O7—Ce1—O6	137.51 (16)	C4—C5—C6	120.6 (6)
O1—Ce1—O2^{i}	128.43 (14)	C4—C5—H5	119.7
O5—Ce1—O2^{i}	85.03 (14)	C6—C5—H5	119.7
O7—Ce1—O2^{i}	140.18 (16)	C5—C6—C7	118.7 (6)
O6—Ce1—O2^{i}	80.79 (15)	C5—C6—C8	121.4 (5)
O1—Ce1—O8	141.15 (15)	C7—C6—C8	119.9 (5)
O5—Ce1—O8	78.37 (15)	C2—C7—C6	121.5 (6)
O7—Ce1—O8	71.08 (16)	C2—C7—H7	119.2
O6—Ce1—O8	140.98 (15)	C6—C7—H7	119.2
O2^{i}—Ce1—O8	70.00 (14)	O6^{iv}—C8—O5^{v}	122.6 (6)
O1—Ce1—O3	76.95 (14)	O6^{iv}—C8—C6	119.1 (6)

O5—Ce1—O3	137.95 (14)	O5^{v}—C8—C6	118.3 (5)
O7—Ce1—O3	68.89 (15)	O6^{iv}—C8—Ce1^{iv}	53.7 (3)
O6—Ce1—O3	71.07 (14)	O5^{v}—C8—Ce1^{iv}	69.4 (3)
O2^{i}—Ce1—O3	136.88 (14)	C6—C8—Ce1^{iv}	167.4 (4)
O8—Ce1—O3	114.27 (14)	O3—C9—O4	122.0 (6)
O1—Ce1—O4	127.54 (14)	O3—C9—C4^{iii}	119.4 (6)
O5—Ce1—O4	153.98 (15)	O4—C9—C4^{iii}	118.5 (6)
O7—Ce1—O4	85.95 (15)	O3—C9—Ce1	61.5 (3)
O6—Ce1—O4	79.79 (14)	O4—C9—Ce1	61.7 (3)
O2^{i}—Ce1—O4	93.02 (14)	C4^{iii}—C9—Ce1	165.2 (4)
O8—Ce1—O4	76.61 (15)	O7—C10—N1	124.5 (8)
O3—Ce1—O4	50.97 (14)	O7—C10—H10	117.8
O1—Ce1—O5^{i}	64.72 (13)	N1—C10—H10	117.8
O5—Ce1—O5^{i}	78.09 (14)	N1—C11—H11A	109.5
O7—Ce1—O5^{i}	142.78 (15)	N1—C11—H11B	109.5
O6—Ce1—O5^{i}	47.78 (12)	H11A—C11—H11B	109.5
O2^{i}—Ce1—O5^{i}	66.03 (13)	N1—C11—H11C	109.5
O8—Ce1—O5^{i}	131.33 (13)	H11A—C11—H11C	109.5
O3—Ce1—O5^{i}	111.80 (13)	H11B—C11—H11C	109.5
O4—Ce1—O5^{i}	124.65 (13)	N1—C12—H12A	109.5
O1—Ce1—C9	102.23 (17)	N1—C12—H12B	109.5
O5—Ce1—C9	152.48 (15)	H12A—C12—H12B	109.5
O7—Ce1—C9	73.23 (16)	N1—C12—H12C	109.5
O6—Ce1—C9	76.78 (15)	H12A—C12—H12C	109.5
O2^{i}—Ce1—C9	117.46 (17)	H12B—C12—H12C	109.5
O8—Ce1—C9	93.97 (17)	O8—C13—N2	125.4 (7)
O3—Ce1—C9	25.29 (16)	O8—C13—H13	117.3
O4—Ce1—C9	26.02 (16)	N2—C13—H13	117.3
O5^{i}—Ce1—C9	124.18 (15)	N2—C14—H14A	109.5
O1—Ce1—C8^{ii}	67.83 (15)	N2—C14—H14B	109.5
O5—Ce1—C8^{ii}	102.05 (15)	H14A—C14—H14B	109.5
O7—Ce1—C8^{ii}	145.03 (17)	N2—C14—H14C	109.5
O6—Ce1—C8^{ii}	23.26 (14)	H14A—C14—H14C	109.5
O2^{i}—Ce1—C8^{ii}	73.98 (16)	H14B—C14—H14C	109.5
O8—Ce1—C8^{ii}	143.82 (16)	N2—C15—H15A	109.5
O3—Ce1—C8^{ii}	89.90 (15)	N2—C15—H15B	109.5
O4—Ce1—C8^{ii}	102.32 (16)	H15A—C15—H15B	109.5
O5^{i}—Ce1—C8^{ii}	24.66 (13)	N2—C15—H15C	109.5
C9—Ce1—C8^{ii}	99.56 (17)	H15A—C15—H15C	109.5
O1—Ce1—Ce1^{i}	60.72 (10)	H15B—C15—H15C	109.5
O5—Ce1—Ce1^{i}	42.67 (9)	C10—N1—C11	121.7 (7)
O7—Ce1—Ce1^{i}	116.20 (11)	C10—N1—C12	120.9 (7)
O6—Ce1—Ce1^{i}	82.87 (9)	C11—N1—C12	117.3 (6)
O2^{i}—Ce1—Ce1^{i}	70.56 (10)	C13—N2—C15	121.6 (7)
O8—Ce1—Ce1^{i}	109.76 (11)	C13—N2—C14	122.2 (7)
O3—Ce1—Ce1^{i}	134.19 (10)	C15—N2—C14	116.2 (7)
O4—Ce1—Ce1^{i}	157.85 (10)	C1—O1—Ce1	140.8 (4)
O5^{i}—Ce1—Ce1^{i}	35.43 (8)	C1—O2—Ce1^{i}	126.5 (4)

C9—Ce1—Ce1^{i}	156.13 (14)	C9—O3—Ce1	93.2 (4)
C8^{ii}—Ce1—Ce1^{i}	59.61 (12)	C9—O4—Ce1	92.3 (4)
O2—C1—O1	125.5 (6)	C8^{vi}—O5—Ce1	164.1 (4)
O2—C1—C2	118.6 (6)	C8^{vi}—O5—Ce1^{i}	85.9 (3)
O1—C1—C2	115.9 (5)	Ce1—O5—Ce1^{i}	101.90 (14)
C7—C2—C3	119.0 (6)	C8^{ii}—O6—Ce1	103.0 (4)
C7—C2—C1	122.6 (5)	C10—O7—Ce1	145.6 (4)
C3—C2—C1	118.3 (6)	C13—O8—Ce1	130.4 (5)
C4—C3—C2	120.2 (6)		

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x+3/2, y+1/2, -z+3/2$; (iii) $-x+2, -y+2, -z+1$; (iv) $-x+3/2, y-1/2, -z+3/2$; (v) $x+1/2, -y+3/2, z+1/2$; (vi) $x-1/2, -y+3/2, z-1/2$.