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catena-Poly[[[pentaaquacerium(III)]-μ-pyridine-2,4,6-tricarboxylato-$\kappa^4N,O^2,O^6:O^{6'}$] tetrahydrate]

Shahzad Sharif,[a] Islam Ullah Khan,[a] Samia Zaheer[a] and Seik Weng Ng[b,c]*

[a]Materials Chemistry Laboratory, Department of Chemistry, GC University, Lahore, Pakistan, [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [c]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia
Correspondence e-mail: seikweng@um.edu.my

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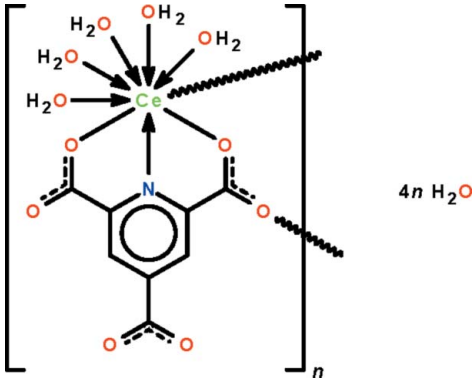
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.033; wR factor = 0.078; data-to-parameter ratio = 16.3.

The Ce^{III} atom in the title compound, $\{[Ce(C_8H_2NO_6)(H_2O)_5]\cdot 4H_2O\}_n$, is N,O,O'-chelated by the carboxylate trianion and is coordinated by five water molecules; a carboxyl O atom from an adjacent trianion bridges the Ce^{III} atom, resulting in a chain running along the a axis. The nine atoms surrounding the metal atom comprise a tricapped trigonal-prismatic polyhedron. The coordinated and lattice water molecules interact with each other and with the carboxyl O atoms by O—H···O hydrogen bonds, generating a three-dimensional network.

Related literature

For the isotypic Sm^{III}, Eu^{III}, Tb^{III} and Ho^{III} analogs, see: Wang *et al.* (2007). For the synthesis of 2,4,6-pyridinetricarboxylic acid, see: Syper *et al.* (1980).



Experimental

Crystal data

$[Ce(C_8H_2NO_6)(H_2O)_5]\cdot 4H_2O$
M_r = 510.37
Orthorhombic, $Pna2_1$
a = 6.8437 (3) Å
b = 13.3207 (5) Å
c = 17.9045 (7) Å
V = 1632.23 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.87 mm^{-1}
T = 293 K
0.21 × 0.06 × 0.04 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.584, T_{max} = 0.894
19512 measured reflections
3690 independent reflections
3336 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.078
S = 1.07
3690 reflections
226 parameters
25 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}
Absolute structure: Flack (1983), 1757 Friedel pairs
Flack parameter: −0.05 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H12···O6w^{i}	0.84	2.00	2.789 (7)	157
O1w—H11···O5^{ii}	0.84	2.00	2.723 (7)	144
O2w—H21···O3^{iii}	0.84	2.05	2.762 (7)	142
O2w—H22···O6w	0.84	2.31	2.699 (7)	109
O3w—H31···O9w	0.84	1.89	2.710 (10)	165
O4w—H41···O4^{ii}	0.84	2.03	2.693 (7)	136
O4w—H42···O4^{iii}	0.84	2.02	2.713 (7)	139
O5w—H52···O7w	0.84	2.25	2.762 (9)	119
O6w—H61···O1^{iv}	0.84	2.04	2.751 (7)	142
O6w—H62···O8w^{ii}	0.84	2.09	2.825 (9)	146
O7w—H71···O3^{iv}	0.84	1.99	2.818 (9)	169
O7w—H72···O8w^{v}	0.84	2.36	3.169 (10)	162
O8w—H81···O5	0.84	2.22	2.778 (8)	124
O8w—H82···O9w	0.84	2.45	2.756 (11)	103
O9w—H91···O4w^{vi}	0.84	2.29	2.895 (9)	130

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

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2011); data reduction: *SAINT*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5510).

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supporting information

Acta Cryst. (2012). E**68**, m624–m625 [doi:10.1107/S1600536812015887]

catena-Poly[[[pentaaquacerium(III)]-μ-pyridine-2,4,6-tricarboxylato-$\kappa^4N,O^2,O^6:O^{6'}$] tetrahydrate]

Shahzad Sharif, Islam Ullah Khan, Samia Zaheer and Seik Weng Ng

S1. Comment

Some lanthanide coordination polymers of 2,4,6-pyridinetricarboxylic acid exhibit photoluminescence; the Sm, Eu, Tb and Ho derivatives are isostructural pentaaqua-coordinated tetrahydrates having the rare-earth atoms in tricapped trigonal prismatic geometries (Wang *et al.*, 2007). The cerium analog is also isostructural; The Ce(III) atom in $Ce(H_2O)_5(C_8H_2NO_6)\cdot 4H_2O$ (Scheme I, Fig. 1) is *N*,*O*,*O*′-chelated by the carboxylate trianion and is coordinated by five water molecules. A carboxyl O atom from an adjacent trianion results in a chain running along the *a*-axis of the orthorhombic unit cell. The nine atoms surrounding the metal atom comprises a tricapped trigonal prismatic polyhedron (Fig. 2). The coordinated and lattice water molecules interact by themselves and with the carboxyl O-atoms by O–H···O hydrogen bonds to generate a three-dimensional network (Table 1).

S2. Experimental

Pyridinetricarboxylic acid was synthesized by using a reported method (Syper *et al.*, 1980). The compound (0.110 g, 0.5 mmol) was dissolved in water (7 ml) and added to a solution of cerium nitrate (0.054 g. 0.5 mmol) dissolved in 50% aqueous methanol (5 ml). The solution was heated for a hour, and then set aside for the growth of yellow prisms. These appeared after three weeks. mixture was refluxed for two hours. Yellow prisms like crystals were obtained after three weeks.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C).

The water H-atoms were placed in chemically sensible positions on the basis of hydrogen bonds (O–H 0.8 Å); their temperature factors were fixed ats 1.5 times those of the parent O-atoms.

The anisotropic temperature factors of the O-atoms of the lattice water molecules were restrained to be nearly isotropic.

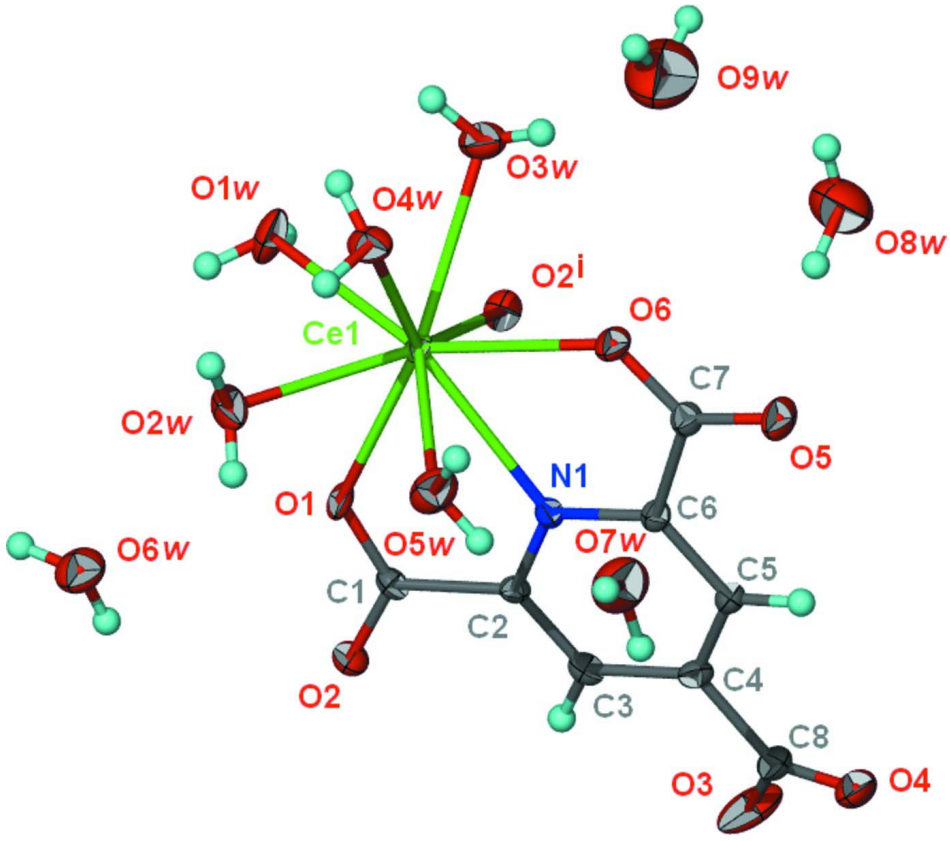

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the formular unit of polymeric $Ce(H_2O)_5(C_8H_2NO_6)\cdot 4H_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

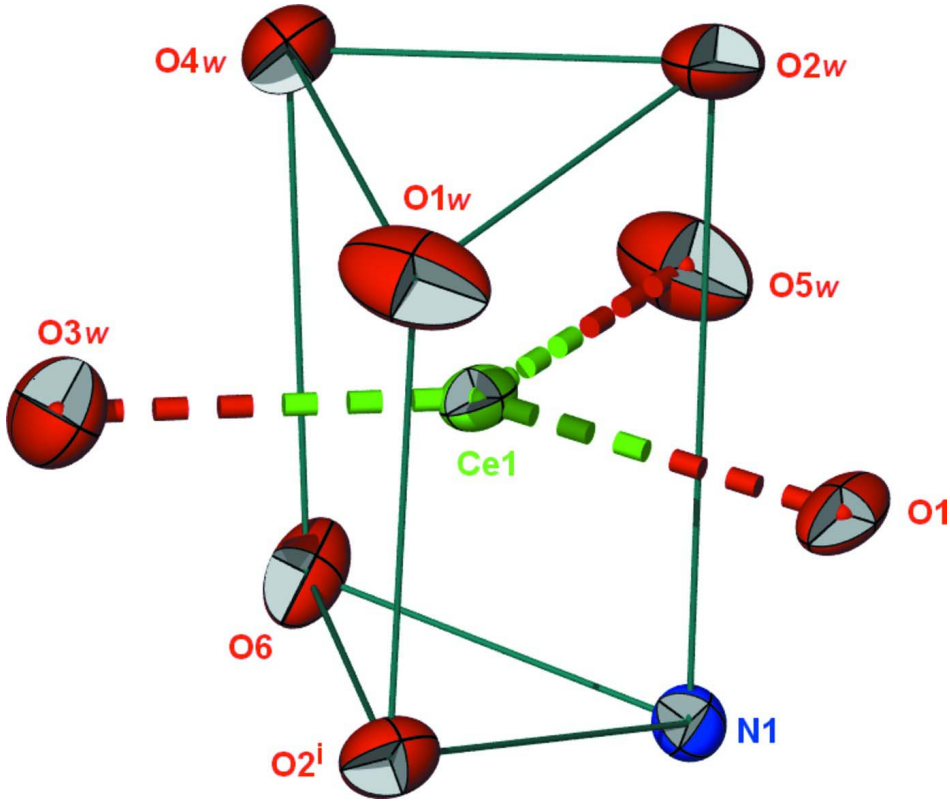

Figure 2

Tricapped trigonal prismatic geometry of the Ce(III) atom in $Ce(H_2O)_5(C_8H_2NO_6)\cdot 4H_2O$.

catena-Poly[[[pentaaquacerium(III)]-μ-pyridine-2,4,6-tricarboxylato- κ^4N,\<i>O^2,O^6:O$^{6'}$)] tetrahydrate]

Crystal data

$[Ce(C_8H_2NO_6)(H_2O)_5]\cdot 4H_2O$
$M_r = 510.37$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 6.8437$ (3) Å
$b = 13.3207$ (5) Å
$c = 17.9045$ (7) Å
$V = 1632.23$ (11) Å^3
$Z = 4$
$F(000) = 1012$
$D_x = 2.077$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7136 reflections
$\theta = 3.1$–$28.2°$
$\mu = 2.87$ mm^{-1}
$T = 293$ K
Prism, yellow
0.21 × 0.06 × 0.04 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.584$, $T_{max} = 0.894$
19512 measured reflections
3690 independent reflections
3336 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -8\rightarrow5$
$k = -17\rightarrow16$
$l = -23\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.078$
$S = 1.07$
3690 reflections
226 parameters
25 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
$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2 + 6.9973P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.68$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-3}
Absolute structure: Flack (1983), 1757 Friedel pairs
Absolute structure parameter: −0.05 (2)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ce1	0.48574 (3)	0.464973 (17)	0.49983 (4)	0.01583 (8)
O1	0.5984 (6)	0.2872 (3)	0.5134 (2)	0.0230 (10)
O2	0.6815 (6)	0.1363 (3)	0.4705 (2)	0.0245 (9)
O3	0.5476 (11)	0.0845 (5)	0.1892 (4)	0.0538 (19)
O4	0.6142 (9)	0.2190 (4)	0.1212 (3)	0.0446 (14)
O5	0.4457 (8)	0.5584 (3)	0.2552 (3)	0.0346 (11)
O6	0.4253 (7)	0.5458 (3)	0.3787 (2)	0.0279 (9)
O1w	0.3428 (7)	0.4311 (4)	0.6266 (3)	0.0392 (12)
H11	0.4322	0.4136	0.6560	0.059*
H12	0.2597	0.3850	0.6233	0.059*
O2w	0.7604 (7)	0.4543 (3)	0.5942 (3)	0.0336 (11)
H21	0.7783	0.5110	0.6135	0.050*
H22	0.8633	0.4356	0.5727	0.050*
O3w	0.1808 (6)	0.5787 (4)	0.5174 (3)	0.0368 (13)
H31	0.1733	0.6194	0.4817	0.055*
H32	0.1907	0.6105	0.5577	0.055*
O4w	0.5804 (7)	0.6370 (3)	0.5462 (3)	0.0308 (10)
H41	0.5090	0.6528	0.5826	0.046*
H42	0.6977	0.6360	0.5600	0.046*
O5w	0.8185 (7)	0.5032 (4)	0.4421 (3)	0.0386 (11)
H51	0.8272	0.5650	0.4335	0.058*
H52	0.8305	0.4712	0.4019	0.058*
O6w	1.0103 (8)	0.3123 (4)	0.6438 (3)	0.0423 (13)
H61	1.0118	0.2610	0.6165	0.063*
H62	0.9898	0.2961	0.6884	0.063*
O7w	0.9175 (12)	0.5539 (6)	0.2974 (4)	0.0593 (19)
H71	0.9540	0.5066	0.2697	0.089*
H72	1.0053	0.5977	0.3007	0.089*
O8w	0.2199 (9)	0.7304 (5)	0.2708 (4)	0.0668 (18)
H81	0.3388	0.7149	0.2686	0.100*
H82	0.1979	0.7848	0.2931	0.100*
O9w	0.1128 (17)	0.7295 (6)	0.4192 (5)	0.113 (3)

H91	0.1622	0.7812	0.4383	0.169*
H92	−0.0087	0.7384	0.4195	0.169*
N1	0.5422 (7)	0.3589 (3)	0.3789 (3)	0.0167 (9)
C1	0.6225 (7)	0.2232 (4)	0.4618 (3)	0.0174 (11)
C2	0.5789 (8)	0.2597 (4)	0.3837 (3)	0.0159 (10)
C3	0.5835 (8)	0.1987 (4)	0.3213 (4)	0.0205 (11)
H3	0.6024	0.1298	0.3262	0.025*
C4	0.5595 (8)	0.2415 (4)	0.2508 (3)	0.0201 (11)
C5	0.5308 (8)	0.3449 (4)	0.2457 (3)	0.0192 (11)
H5	0.5228	0.3763	0.1994	0.023*
C6	0.5142 (7)	0.4002 (4)	0.3112 (3)	0.0172 (10)
C7	0.4583 (8)	0.5113 (4)	0.3140 (3)	0.0199 (11)
C8	0.5716 (9)	0.1763 (5)	0.1811 (4)	0.0272 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.02002 (12)	0.01382 (12)	0.01366 (12)	−0.00054 (9)	−0.0016 (3)	−0.0023 (2)
O1	0.041 (2)	0.0170 (17)	0.011 (3)	0.0042 (15)	−0.0039 (16)	−0.0025 (15)
O2	0.029 (2)	0.019 (2)	0.025 (2)	0.0062 (16)	−0.0011 (17)	0.0015 (16)
O3	0.082 (5)	0.035 (3)	0.045 (4)	−0.009 (3)	0.024 (3)	−0.021 (3)
O4	0.067 (4)	0.043 (3)	0.024 (3)	0.027 (3)	0.005 (2)	0.000 (2)
O5	0.058 (3)	0.027 (2)	0.019 (2)	0.011 (2)	0.003 (2)	0.0068 (19)
O6	0.043 (2)	0.021 (2)	0.019 (2)	0.0103 (19)	0.0019 (19)	−0.0015 (17)
O1w	0.040 (3)	0.062 (3)	0.016 (2)	−0.012 (2)	0.0009 (19)	0.000 (2)
O2w	0.038 (3)	0.030 (2)	0.033 (3)	0.003 (2)	−0.019 (2)	−0.010 (2)
O3w	0.033 (2)	0.040 (3)	0.038 (4)	0.0065 (19)	0.0004 (19)	−0.012 (2)
O4w	0.032 (2)	0.025 (2)	0.036 (3)	0.0027 (18)	−0.004 (2)	−0.0116 (19)
O5w	0.031 (2)	0.051 (3)	0.033 (3)	−0.006 (2)	0.005 (2)	−0.007 (2)
O6w	0.055 (3)	0.034 (3)	0.038 (3)	0.004 (2)	0.003 (2)	−0.007 (2)
O7w	0.065 (4)	0.065 (4)	0.048 (4)	0.003 (3)	0.010 (3)	0.003 (3)
O8w	0.057 (4)	0.067 (4)	0.077 (4)	0.014 (3)	−0.002 (3)	0.001 (3)
O9w	0.172 (8)	0.076 (5)	0.090 (5)	0.046 (5)	−0.008 (6)	−0.014 (4)
N1	0.018 (2)	0.016 (2)	0.017 (2)	0.0018 (17)	−0.0022 (17)	−0.0001 (18)
C1	0.015 (2)	0.014 (3)	0.023 (3)	−0.0001 (19)	−0.002 (2)	0.002 (2)
C2	0.017 (2)	0.013 (2)	0.018 (3)	0.0021 (19)	0.000 (2)	−0.002 (2)
C3	0.018 (3)	0.018 (3)	0.026 (3)	0.001 (2)	−0.001 (2)	0.001 (2)
C4	0.018 (2)	0.022 (3)	0.020 (3)	0.003 (2)	0.004 (2)	−0.002 (2)
C5	0.021 (3)	0.022 (3)	0.015 (3)	0.003 (2)	0.000 (2)	−0.001 (2)
C6	0.018 (2)	0.019 (3)	0.015 (3)	−0.0012 (19)	0.001 (2)	0.001 (2)
C7	0.024 (3)	0.018 (3)	0.018 (3)	0.001 (2)	0.001 (2)	0.003 (2)
C8	0.028 (3)	0.034 (3)	0.020 (3)	0.006 (3)	−0.004 (2)	−0.010 (3)

Geometric parameters (Å, º)

Ce1—O6	2.456 (4)	O4w—H42	0.8399
Ce1—O1	2.502 (4)	O5w—H51	0.8400
Ce1—O1w	2.512 (5)	O5w—H52	0.8399

Ce1—O4w	2.523 (4)	O6w—H61	0.8399
Ce1—O2w	2.532 (4)	O6w—H62	0.8401
Ce1—O2^{i}	2.536 (4)	O7w—H71	0.8399
Ce1—O5w	2.552 (5)	O7w—H72	0.8401
Ce1—O3w	2.598 (4)	O8w—H81	0.8400
Ce1—N1	2.615 (5)	O8w—H82	0.8400
O1—C1	1.268 (6)	O9w—H91	0.8400
O2—C1	1.237 (6)	O9w—H92	0.8399
O2—Ce1^{ii}	2.536 (4)	N1—C6	1.344 (7)
O3—C8	1.242 (9)	N1—C2	1.347 (7)
O4—C8	1.249 (8)	C1—C2	1.509 (8)
O5—C7	1.228 (7)	C2—C3	1.383 (8)
O6—C7	1.266 (7)	C3—C4	1.394 (8)
O1w—H11	0.8399	C3—H3	0.9300
O1w—H12	0.8400	C4—C5	1.395 (8)
O2w—H21	0.8399	C4—C8	1.523 (8)
O2w—H22	0.8400	C5—C6	1.390 (8)
O3w—H31	0.8401	C5—H5	0.9300
O3w—H32	0.8399	C6—C7	1.530 (8)
O4w—H41	0.8401		

O6—Ce1—O1	123.53 (13)	Ce1—O2w—H22	109.5
O6—Ce1—O1w	144.17 (17)	H21—O2w—H22	109.5
O1—Ce1—O1w	82.09 (16)	Ce1—O3w—H31	109.5
O6—Ce1—O4w	86.32 (15)	Ce1—O3w—H32	109.5
O1—Ce1—O4w	138.49 (14)	H31—O3w—H32	109.5
O1w—Ce1—O4w	88.02 (17)	Ce1—O4w—H41	109.4
O6—Ce1—O2w	137.65 (17)	Ce1—O4w—H42	109.1
O1—Ce1—O2w	69.70 (14)	H41—O4w—H42	109.5
O1w—Ce1—O2w	71.10 (17)	Ce1—O5w—H51	109.4
O4w—Ce1—O2w	68.94 (14)	Ce1—O5w—H52	109.5
O6—Ce1—O2^{i}	84.95 (15)	H51—O5w—H52	109.5
O1—Ce1—O2^{i}	76.68 (13)	H61—O6w—H62	110.3
O1w—Ce1—O2^{i}	76.83 (15)	H71—O7w—H72	110.5
O4w—Ce1—O2^{i}	139.67 (14)	H81—O8w—H82	114.1
O2w—Ce1—O2^{i}	135.89 (16)	H91—O9w—H92	106.3
O6—Ce1—O5w	72.86 (17)	C6—N1—C2	119.1 (5)
O1—Ce1—O5w	87.32 (17)	C6—N1—Ce1	120.3 (4)
O1w—Ce1—O5w	138.51 (17)	C2—N1—Ce1	120.3 (3)
O4w—Ce1—O5w	73.92 (17)	O2—C1—O1	125.5 (5)
O2w—Ce1—O5w	67.60 (18)	O2—C1—C2	118.9 (5)
O2^{i}—Ce1—O5w	139.01 (16)	O1—C1—C2	115.6 (4)
O6—Ce1—O3w	73.51 (15)	N1—C2—C3	121.9 (5)
O1—Ce1—O3w	141.96 (15)	N1—C2—C1	114.4 (4)
O1w—Ce1—O3w	71.48 (17)	C3—C2—C1	123.7 (5)
O4w—Ce1—O3w	68.68 (14)	C2—C3—C4	119.2 (5)
O2w—Ce1—O3w	123.26 (15)	C2—C3—H3	120.4
O2^{i}—Ce1—O3w	71.08 (13)	C4—C3—H3	120.4

O5w—Ce1—O3w	130.50 (17)	C3—C4—C5	118.7 (5)
O6—Ce1—N1	62.00 (14)	C3—C4—C8	120.1 (5)
O1—Ce1—N1	61.53 (13)	C5—C4—C8	121.1 (5)
O1w—Ce1—N1	135.14 (16)	C6—C5—C4	118.6 (5)
O4w—Ce1—N1	136.56 (16)	C6—C5—H5	120.7
O2w—Ce1—N1	114.37 (15)	C4—C5—H5	120.7
O2^{i}—Ce1—N1	70.25 (14)	N1—C6—C5	122.2 (5)
O5w—Ce1—N1	68.94 (16)	N1—C6—C7	113.8 (5)
O3w—Ce1—N1	122.29 (14)	C5—C6—C7	124.1 (5)
C1—O1—Ce1	127.3 (3)	O5—C7—O6	125.9 (5)
C1—O2—Ce1^{ii}	142.4 (4)	O5—C7—C6	118.9 (5)
C7—O6—Ce1	128.2 (4)	O6—C7—C6	115.1 (5)
Ce1—O1w—H11	109.4	O3—C8—O4	125.4 (7)
Ce1—O1w—H12	109.4	O3—C8—C4	117.3 (6)
H11—O1w—H12	109.5	O4—C8—C4	117.2 (6)
Ce1—O2w—H21	109.4		

O6—Ce1—O1—C1	−4.4 (5)	Ce1^{ii}—O2—C1—C2	105.5 (6)
O1w—Ce1—O1—C1	148.5 (5)	Ce1—O1—C1—O2	178.7 (4)
O4w—Ce1—O1—C1	−133.6 (4)	Ce1—O1—C1—C2	0.4 (7)
O2w—Ce1—O1—C1	−138.8 (5)	C6—N1—C2—C3	−1.8 (8)
O2^{i}—Ce1—O1—C1	70.2 (4)	Ce1—N1—C2—C3	171.2 (4)
O5w—Ce1—O1—C1	−71.7 (5)	C6—N1—C2—C1	175.7 (5)
O3w—Ce1—O1—C1	102.7 (5)	Ce1—N1—C2—C1	−11.3 (6)
N1—Ce1—O1—C1	−4.3 (4)	O2—C1—C2—N1	−171.1 (5)
O1—Ce1—O6—C7	−6.2 (6)	O1—C1—C2—N1	7.3 (7)
O1w—Ce1—O6—C7	−135.7 (5)	O2—C1—C2—C3	6.3 (8)
O4w—Ce1—O6—C7	142.8 (5)	O1—C1—C2—C3	−175.2 (5)
O2w—Ce1—O6—C7	90.0 (5)	N1—C2—C3—C4	3.4 (8)
O2^{i}—Ce1—O6—C7	−76.6 (5)	C1—C2—C3—C4	−173.9 (5)
O5w—Ce1—O6—C7	68.5 (5)	C2—C3—C4—C5	−0.3 (8)
O3w—Ce1—O6—C7	−148.3 (5)	C2—C3—C4—C8	177.7 (5)
N1—Ce1—O6—C7	−6.3 (5)	C3—C4—C5—C6	−4.2 (8)
O6—Ce1—N1—C6	1.1 (4)	C8—C4—C5—C6	177.8 (5)
O1—Ce1—N1—C6	−178.8 (4)	C2—N1—C6—C5	−3.0 (8)
O1w—Ce1—N1—C6	141.2 (4)	Ce1—N1—C6—C5	−176.0 (4)
O4w—Ce1—N1—C6	−47.1 (5)	C2—N1—C6—C7	175.5 (5)
O2w—Ce1—N1—C6	−131.6 (4)	Ce1—N1—C6—C7	2.6 (6)
O2^{i}—Ce1—N1—C6	96.0 (4)	C4—C5—C6—N1	6.0 (8)
O5w—Ce1—N1—C6	−80.1 (4)	C4—C5—C6—C7	−172.4 (5)
O3w—Ce1—N1—C6	45.3 (4)	Ce1—O6—C7—O5	−171.5 (5)
O6—Ce1—N1—C2	−171.8 (5)	Ce1—O6—C7—C6	9.8 (7)
O1—Ce1—N1—C2	8.3 (4)	N1—C6—C7—O5	173.9 (5)
O1w—Ce1—N1—C2	−31.7 (5)	C5—C6—C7—O5	−7.6 (8)
O4w—Ce1—N1—C2	140.1 (4)	N1—C6—C7—O6	−7.4 (7)
O2w—Ce1—N1—C2	55.5 (4)	C5—C6—C7—O6	171.1 (5)
O2^{i}—Ce1—N1—C2	−76.9 (4)	C3—C4—C8—O3	19.8 (9)
O5w—Ce1—N1—C2	107.0 (4)	C5—C4—C8—O3	−162.2 (7)

O3w—Ce1—N1—C2	−127.5 (4)	C3—C4—C8—O4	−156.7 (6)
Ce1^{ii}—O2—C1—O1	−72.8 (9)	C5—C4—C8—O4	21.2 (9)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H12···O6*w*^{iii}	0.84	2.00	2.789 (7)	157
O1*w*—H11···O5^{iv}	0.84	2.00	2.723 (7)	144
O2*w*—H21···O3^{v}	0.84	2.05	2.762 (7)	142
O2*w*—H22···O6*w*	0.84	2.31	2.699 (7)	109
O3*w*—H31···O9*w*	0.84	1.89	2.710 (10)	165
O4*w*—H41···O4^{iv}	0.84	2.03	2.693 (7)	136
O4*w*—H42···O4^{v}	0.84	2.02	2.713 (7)	139
O5*w*—H52···O7*w*	0.84	2.25	2.762 (9)	119
O6*w*—H61···O1^{ii}	0.84	2.04	2.751 (7)	142
O6*w*—H62···O8*w*^{iv}	0.84	2.09	2.825 (9)	146
O7*w*—H71···O3^{ii}	0.84	1.99	2.818 (9)	169
O7*w*—H72···O8*w*^{vi}	0.84	2.36	3.169 (10)	162
O8*w*—H81···O5	0.84	2.22	2.778 (8)	124
O8*w*—H82···O9*w*	0.84	2.45	2.756 (11)	103
O9*w*—H91···O4*w*^{vii}	0.84	2.29	2.895 (9)	130

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