

Cerium(III) dihydroxidohexaoxidotetra- borate chloride

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 Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{B}-\text{O}) = 0.007$ Å; R factor = 0.020; wR factor = 0.051; data-to-parameter ratio = 11.4.

The crystal structure of the title compound, $\text{Ce}[\text{B}_4\text{O}_6(\text{OH})_2]\text{Cl}$, is built from polyborate sheets parallel to the (001) plane. These sheets stack along the [001] direction and are linked by Ce atoms exhibiting an CeO_8Cl_2 coordination sphere. $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds additionally stabilize the structural set-up. The polyborate sheet is made up of zigzag borate chains running along the $[\bar{1}10]$ direction. These zigzag chains are interconnected by shared O-vertices, resulting in a two-dimensional layer with nine-membered rings. All B and O atoms (except for the terminal OH atoms) lie in the nearly planar sheets of polyborates, leading to their isotropic atomic displacement parameters being significantly smaller than usual. This may be attributed to the fact that the atomic displacement parameters correlate not only with their atomic masses but with their coordination environments also.

Related literature

For background to borate compounds and their applications, see: Burns *et al.* (1995); Chen *et al.* (1985); Zhao *et al.* (1990); Sun, Sun *et al.* (2010); Sun, Zhou *et al.* (2010). For isotopic structures, see: Belokoneva *et al.* (2002) for $\text{Ln}[\text{B}_4\text{O}_6(\text{OH})_2]\text{Cl}$ ($\text{Ln} = \text{Pr}, \text{Nd}$).

Experimental

Crystal data

$\text{Ce}[\text{B}_4\text{O}_6(\text{OH})_2]\text{Cl}$	$V = 689.8$ (2) Å ³
$M_r = 348.83$	$Z = 4$
Monoclinic, Cc	Mo $K\alpha$ radiation
$a = 6.5169$ (11) Å	$\mu = 7.00$ mm ⁻¹
$b = 11.245$ (2) Å	$T = 295$ K
$c = 9.7575$ (17) Å	$0.16 \times 0.07 \times 0.03$ mm
$\beta = 105.284$ (3)°	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2825 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2001)	1532 independent reflections
$T_{\min} = 0.401$, $T_{\max} = 0.818$	1523 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.020$	All H-atom parameters refined
$wR(F^2) = 0.051$	$\Delta\rho_{\max} = 0.53$ e Å ⁻³
$S = 1.00$	$\Delta\rho_{\min} = -1.64$ e Å ⁻³
1532 reflections	Absolute structure: Flack (1983),
134 parameters	716 Friedel pairs
10 restraints	Flack parameter: 0.034 (19)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O8}-\text{H1}\cdots\text{O1}^{\text{i}}$	0.82 (2)	2.43 (7)	2.859 (5)	114 (6)
$\text{O8}-\text{H1}\cdots\text{Cl1}^{\text{ii}}$	0.82 (2)	2.52 (5)	3.219 (4)	145 (7)
$\text{O7}-\text{H2}\cdots\text{O4}^{\text{ii}}$	0.83 (2)	2.13 (6)	2.860 (6)	148 (10)
$\text{O7}-\text{H2}\cdots\text{Cl1}^{\text{ii}}$	0.83 (2)	2.81 (11)	3.220 (4)	112 (9)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2011) and *ATOMS* (Dowty, 2004); 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: FJ2495).

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supporting information

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Cerium(III) dihydroxidohexaoxidotetraborate chloride

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S1. Comment

Borate compounds have been extensively studied due to their variety of fundamental building blocks and crystal structure types (Burns *et al.*, 1995), as well as their successful industry applications as nonlinear optical materials, *e.g.* β -Ba(B₂O₄) (BBO) (Chen *et al.*, 1985) and LiB₃O₅ (LBO) (Zhao *et al.*, 1990). Besides alkali metals and alkaline-earth metals (Sun, Sun *et al.*, 2010), rare-earth elements become highlighted with being introduced into the borate system in order to obtain multifunctional materials with the distinctive luminescence properties of rare-earth elements. Belokoneva *et al.* (2002) claimed that Ln(B₄O₆(OH)₂)Cl (Ln = Pr, Nd) exhibits excellent nonlinear optical properties. But the atomic coordinates of its cerium analogue have not been reported until now. Herein, we report the crystal structure of Ce(B₄O₆(OH)₂)Cl determined from single-crystal X-ray diffraction data, including the sites of hydrogen atoms.

The crystal structure of Ce(B₄O₆(OH)₂)Cl is characterized as a layered structure of polyborate sheets parallel to (001) (Fig. 1 & 2). In the structure boron atoms have two types of polyhedral coordinations. One is 3-coordinated by oxygen atoms, forming a triangular planar [BO₃] group. The other is 4-coordinated to three O-atoms and one hydroxyl group to form a [BO₃(OH)] tetrahedron (Fig. 3). Both [BO₃] group and [BO₃(OH)] polyhedron link to three neighbouring borate groups *via* their common O-corners except for OH terminals. Two [BO₃(OH)] tetrahedra and two triangular planar [BO₃] groups compose a borate tetramer as a fundamental building block (FBB) (Fig. 2) (Burns *et al.*, 1995). The FBBs share their common oxygen vertices to form a zigzag borate chain running along the $[\bar{1}10]$ direction. The zigzag chains are further interconnected with each other by sharing their common O-corners, resulting in a two-dimensional layer with 9-membered rings within the layer. The 9-membered ring has a nearly equilateral (about 7.00 Å) triangular motif (Fig. 2). The Ce atoms just reside at the center of 9-membered rings and adopt a 10-coordination with the surrounding eight oxygen and two chlorine atoms, forming a 1-6-3 crown-shaped polyhedron (Fig. 2). The two-dimensional layers stack along the [001] direction and are linked by Ce and Cl atoms as well as hydrogen bonds to form the three-dimensional crystal structure (Fig. 1). It is interesting that all boron and oxygen atoms (except for OH terminals) lying in the nearly planar sheets of polyborates lead to their isotropic atomic parameters significantly smaller than as-expected usually. For example, the isotropic atomic parameters of boron atoms are distributed in the range of 0.0062 (10) to 0.0085 (10) Å², significantly smaller than that of chlorine atom (0.0130 (2) Å²). This may give a hint that the atomic displacement parameters correlate not only with their atomic masses but with their coordination environments also. However the standard uncertainties of atomic displacement parameters do have close correlation with their atomic masses of individual elements. As-observed in the title compound, standard uncertainties of atomic displacement parameters of all atoms distribute as-expected in the sequence of Ce, Cl, O, B and H, increasing while their atomic masses decrease.

S2. Experimental

The title compound, Ce(B₄O₆(OH)₂)Cl was synthesized by using a hydrothermal method during our systematically exploiting rare earth borates (Sun, Zhou *et al.*, 2010). Typically, a mixture of Ce₂O₃ (0.33 g), CrCl₃·6H₂O (0.80 g), H₃BO₃

(2.00 g) and 2 ml distilled water with molar ratio of Ce: Cl: B = 1: 9: 32 was prepared, and transferred into a Teflon-lined stainless-steel autoclave (30 ml in volume), then heated to and kept at 468 K for three days. Transparent, colorless crystals of the title compound were obtained by filtration, rinsed with distilled water several times, and dried in desiccators. Optical examination and powder X-ray diffraction (PXRD) analyses were used to identify the phases of the solid products.

S3. Refinement

The hydrogen positions were obtained from the difference Fourier map and refined *via* fixing the bond distance of $d(\text{OH}) = 0.82(2)\text{\AA}$ with the donor of coordinated oxygen atoms. Moreover a common variable was set for the isotropic atomic displacement parameters of all hydrogen atoms during the refinement.

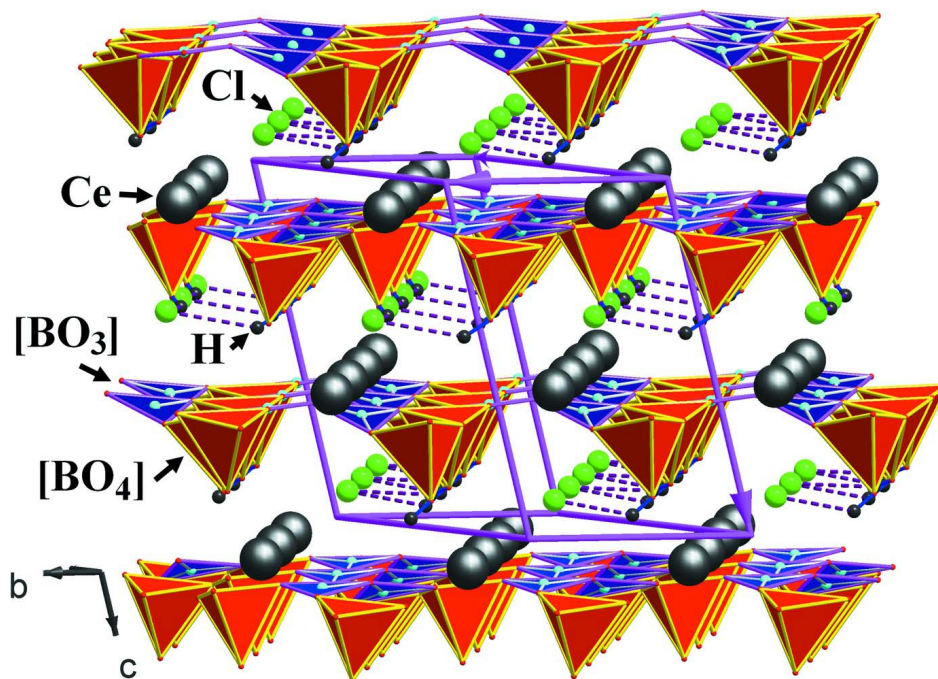
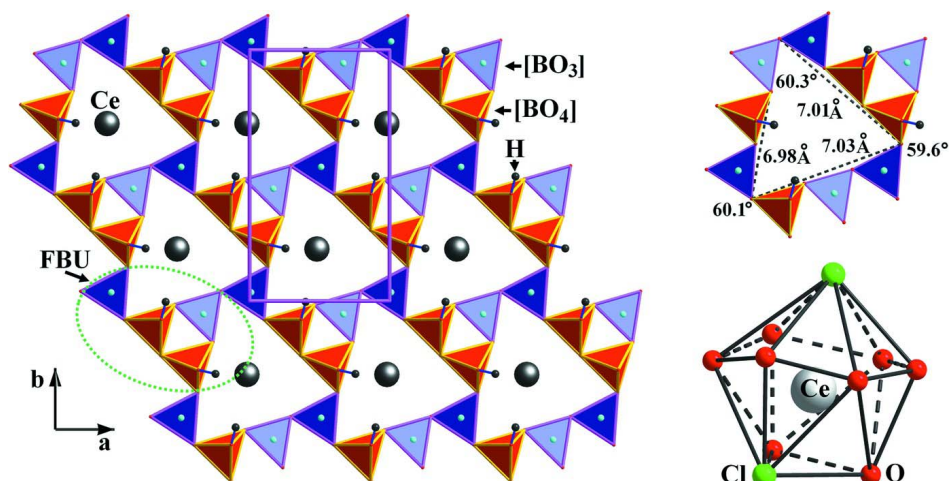
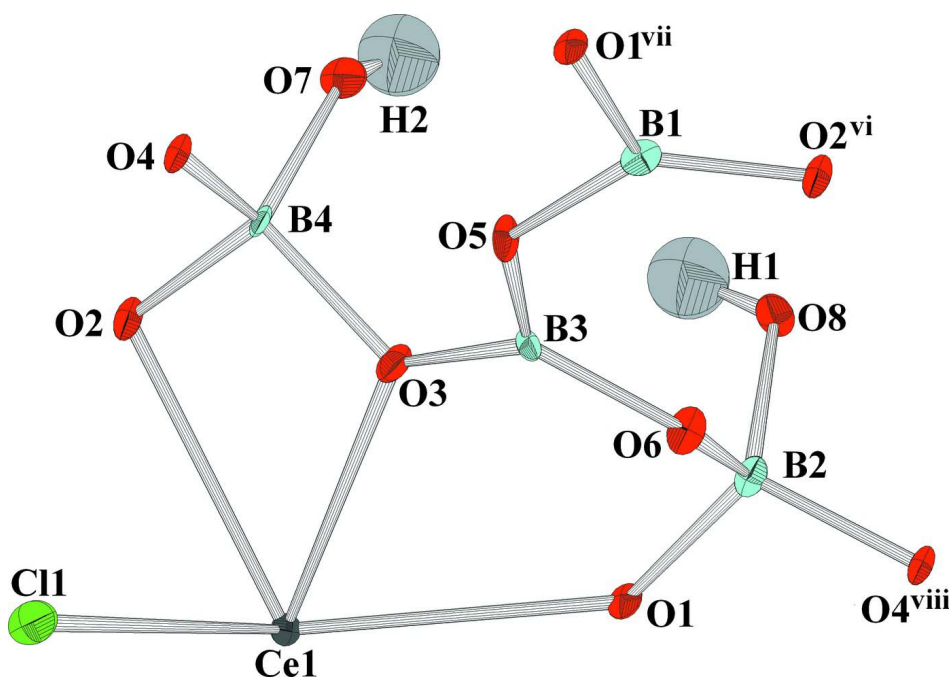


Figure 1

Crystal structure of $\text{Ce}(\text{B}_4\text{O}_6(\text{OH})_2)\text{Cl}$. ([BO₄] drawn in red tetrahedra; [BO₃] in blue triangular groups; Ce in black spheres; Cl in green spheres; H in small black balls).


Figure 2

Left: a two-dimensional sheet with 9-membered rings, the fundamental building block (FBU) marked by a dash-line ellipse; Right upper: a 9-membered ring with a nearly equilateral triangular motif; Right down: coordination environment of Ce in a 1-6-3 crown-shaped polyhedron.


Figure 3

Coordination environment of metal atoms, with displacement ellipsoids drawn at the 50% probability level (symmetry codes: (vi) $x-1/2, y-1/2, z$; (vii) $x-1, y, z$; (viii) $x+1/2, y-1/2, z$)

Cerium(III) dihydroxidohexaoxidotetraborate chloride

Crystal data

$\text{Ce}[\text{B}_4\text{O}_6(\text{OH})_2]\text{Cl}$

$M_r = 348.83$

Monoclinic, Cc

Hall symbol: $C-2yc$

$a = 6.5169(11) \text{ \AA}$

$b = 11.245(2) \text{ \AA}$

$c = 9.7575$ (17) Å
 $\beta = 105.284$ (3)°
 $V = 689.8$ (2) Å³
 $Z = 4$
 $F(000) = 644$
 $D_x = 3.359$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2825 reflections
 $\theta = 3.6$ – 28.0 °
 $\mu = 7.00$ mm⁻¹
 $T = 295$ K
 Prism, colorless
 $0.16 \times 0.07 \times 0.03$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 1800 images, $\varphi = 0, 90, 180$ °, $\chi = 54.74$ °,
 $\Delta\omega = 0.3$ °, Exp time: 15 s. scans
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\min} = 0.401$, $T_{\max} = 0.818$

2825 measured reflections
 1532 independent reflections
 1523 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$
 $\theta_{\max} = 28.0$ °, $\theta_{\min} = 3.6$ °
 $h = -8 \rightarrow 8$
 $k = -14 \rightarrow 14$
 $l = -12 \rightarrow 12$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.020$
 $wR(F^2) = 0.051$
 $S = 1.00$
 1532 reflections
 134 parameters
 10 restraints
 Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
 Hydrogen site location: difference Fourier map
 All H-atom parameters refined
 $w = 1/[\sigma^2(F_o^2) + (0.0285P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.53$ e Å⁻³
 $\Delta\rho_{\min} = -1.64$ e Å⁻³
 Absolute structure: Flack (1983), 716 Friedel pairs
 Absolute structure parameter: 0.034 (19)

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ce1	0.98063 (4)	0.706775 (17)	0.56430 (4)	0.00585 (8)
Cl1	0.6202 (2)	0.82445 (12)	0.37031 (14)	0.0130 (2)
B1	0.1685 (9)	0.4466 (5)	0.6439 (6)	0.0073 (10)
B2	0.8287 (9)	0.4064 (5)	0.6939 (6)	0.0085 (10)
B3	0.5112 (9)	0.5338 (5)	0.6256 (6)	0.0068 (10)
B4	0.5809 (9)	0.7447 (5)	0.7169 (6)	0.0062 (10)
O1	0.9639 (5)	0.4852 (3)	0.6324 (3)	0.0076 (7)

O2	0.7362 (6)	0.8358 (3)	0.6858 (4)	0.0086 (7)
O3	0.6294 (6)	0.6361 (3)	0.6426 (4)	0.0093 (7)
O4	0.3652 (6)	0.7819 (3)	0.6635 (4)	0.0068 (7)
O5	0.2933 (6)	0.5383 (3)	0.6124 (4)	0.0087 (7)
O6	0.6027 (6)	0.4259 (3)	0.6207 (4)	0.0086 (7)
O7	0.6335 (7)	0.7247 (3)	0.8706 (4)	0.0116 (7)
O8	0.8688 (6)	0.4269 (3)	0.8477 (4)	0.0101 (7)
H1	0.894 (13)	0.495 (3)	0.876 (7)	0.04 (2)*
H2	0.731 (13)	0.706 (6)	0.940 (7)	0.04 (2)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.00577 (12)	0.00558 (12)	0.00601 (12)	0.00003 (13)	0.00121 (8)	0.00002 (14)
Cl1	0.0132 (6)	0.0155 (6)	0.0094 (6)	0.0047 (5)	0.0012 (5)	-0.0001 (5)
B1	0.004 (2)	0.009 (2)	0.009 (3)	-0.0008 (19)	0.001 (2)	-0.002 (2)
B2	0.009 (3)	0.006 (2)	0.009 (3)	0.001 (2)	0.002 (2)	-0.001 (2)
B3	0.011 (3)	0.005 (2)	0.005 (2)	0.001 (2)	0.0029 (19)	0.0021 (19)
B4	0.009 (3)	0.003 (2)	0.006 (2)	0.003 (2)	0.002 (2)	-0.0001 (19)
O1	0.0040 (16)	0.0072 (16)	0.0124 (17)	0.0020 (13)	0.0036 (14)	0.0006 (13)
O2	0.0079 (18)	0.0045 (16)	0.0131 (19)	0.0007 (14)	0.0025 (14)	-0.0005 (14)
O3	0.0083 (18)	0.0063 (15)	0.0145 (18)	0.0011 (14)	0.0055 (14)	-0.0014 (14)
O4	0.0061 (17)	0.0036 (16)	0.0105 (19)	0.0009 (12)	0.0015 (14)	-0.0010 (12)
O5	0.0046 (16)	0.0042 (15)	0.0180 (18)	-0.0009 (13)	0.0041 (14)	0.0023 (14)
O6	0.0027 (15)	0.0077 (14)	0.0138 (17)	-0.0020 (13)	-0.0004 (13)	-0.0019 (13)
O7	0.0091 (19)	0.0155 (17)	0.0097 (19)	0.0059 (15)	0.0017 (15)	0.0023 (15)
O8	0.0161 (18)	0.0084 (17)	0.0048 (17)	-0.0029 (14)	0.0007 (14)	-0.0010 (13)

Geometric parameters (Å, °)

Ce1—O7 ⁱ	2.480 (4)	B1—O5	1.396 (6)
Ce1—O8 ⁱⁱ	2.539 (4)	B2—O4 ^{viii}	1.464 (6)
Ce1—O4 ⁱⁱⁱ	2.579 (4)	B2—O8	1.472 (6)
Ce1—O1	2.589 (3)	B2—O6	1.474 (6)
Ce1—O6 ^{iv}	2.603 (3)	B2—O1	1.483 (7)
Ce1—O2	2.654 (4)	B3—O6	1.359 (6)
Ce1—O3	2.716 (4)	B3—O3	1.370 (6)
Ce1—O5 ⁱⁱⁱ	2.731 (3)	B3—O5	1.392 (7)
Ce1—Cl1 ^v	2.9041 (14)	B4—O4	1.427 (6)
Ce1—Cl1	2.9168 (14)	B4—O7	1.465 (6)
B1—O2 ^{vi}	1.349 (6)	B4—O3	1.496 (6)
B1—O1 ^{vii}	1.378 (6)	B4—O2	1.526 (7)
O7 ⁱ —Ce1—O8 ⁱⁱ	68.55 (12)	O8 ⁱⁱ —Ce1—Cl1	73.91 (9)
O7 ⁱ —Ce1—O4 ⁱⁱⁱ	68.81 (13)	O4 ⁱⁱⁱ —Ce1—Cl1	129.17 (8)
O8 ⁱⁱ —Ce1—O4 ⁱⁱⁱ	122.93 (12)	O1—Ce1—Cl1	121.47 (8)
O7 ⁱ —Ce1—O1	123.18 (11)	O6 ^{iv} —Ce1—Cl1	81.76 (8)
O8 ⁱⁱ —Ce1—O1	67.76 (11)	O2—Ce1—Cl1	64.30 (8)

O4 ⁱⁱⁱ —Ce1—O1	108.75 (10)	O3—Ce1—C11	73.81 (8)
O7 ⁱ —Ce1—O6 ^{iv}	72.87 (12)	O5 ⁱⁱⁱ —Ce1—C11	149.66 (8)
O8 ⁱⁱ —Ce1—O6 ^{iv}	137.83 (11)	C11 ^v —Ce1—C11	134.62 (5)
O4 ⁱⁱⁱ —Ce1—O6 ^{iv}	53.00 (10)	Ce1 ^{ix} —C11—Ce1	126.35 (5)
O1—Ce1—O6 ^{iv}	152.63 (11)	O2 ^{vi} —B1—O1 ^{vii}	123.2 (5)
O7 ⁱ —Ce1—O2	125.41 (12)	O2 ^{vi} —B1—O5	125.8 (5)
O8 ⁱⁱ —Ce1—O2	128.40 (12)	O1 ^{vii} —B1—O5	110.9 (4)
O4 ⁱⁱⁱ —Ce1—O2	106.95 (11)	O4 ^{viii} —B2—O8	111.2 (4)
O1—Ce1—O2	109.92 (11)	O4 ^{viii} —B2—O6	103.8 (4)
O6 ^{iv} —Ce1—O2	64.77 (11)	O8—B2—O6	110.9 (4)
O7 ⁱ —Ce1—O3	147.45 (13)	O4 ^{viii} —B2—O1	110.1 (4)
O8 ⁱⁱ —Ce1—O3	89.01 (12)	O8—B2—O1	110.8 (4)
O4 ⁱⁱⁱ —Ce1—O3	142.92 (12)	O6—B2—O1	109.9 (4)
O1—Ce1—O3	63.28 (10)	O6—B3—O3	121.1 (5)
O6 ^{iv} —Ce1—O3	116.78 (11)	O6—B3—O5	118.4 (5)
O2—Ce1—O3	52.04 (11)	O3—B3—O5	120.6 (4)
O7 ⁱ —Ce1—O5 ⁱⁱⁱ	85.14 (13)	O4—B4—O7	111.1 (4)
O8 ⁱⁱ —Ce1—O5 ⁱⁱⁱ	76.69 (11)	O4—B4—O3	112.1 (4)
O4 ⁱⁱⁱ —Ce1—O5 ⁱⁱⁱ	63.61 (10)	O7—B4—O3	110.4 (4)
O1—Ce1—O5 ⁱⁱⁱ	50.80 (10)	O4—B4—O2	111.9 (4)
O6 ^{iv} —Ce1—O5 ⁱⁱⁱ	116.61 (11)	O7—B4—O2	108.6 (4)
O2—Ce1—O5 ⁱⁱⁱ	144.19 (12)	O3—B4—O2	102.5 (4)
O3—Ce1—O5 ⁱⁱⁱ	113.23 (11)	B1 ⁱⁱⁱ —O1—B2	116.4 (4)
O7 ⁱ —Ce1—C11 ^v	137.84 (10)	B1 ^{iv} —O2—B4	119.9 (4)
O8 ⁱⁱ —Ce1—C11 ^v	136.70 (9)	B3—O3—B4	124.1 (4)
O4 ⁱⁱⁱ —Ce1—C11 ^v	69.13 (9)	B4—O4—B2 ^x	113.8 (4)
O1—Ce1—C11 ^v	69.06 (8)	B3—O5—B1	126.3 (4)
O6 ^{iv} —Ce1—C11 ^v	84.35 (8)	B3—O6—B2	120.5 (4)
O2—Ce1—C11 ^v	70.67 (8)	B4—O7—H2	143 (8)
O3—Ce1—C11 ^v	74.57 (8)	Ce1 ^{xi} —O7—H2	80 (8)
O5 ⁱⁱⁱ —Ce1—C11 ^v	73.87 (8)	B2—O8—H1	117 (5)
O7 ⁱ —Ce1—C11	77.35 (10)	Ce1 ^{xii} —O8—H1	107 (5)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O8—H1 \cdots O1 ^{xii}	0.82 (2)	2.43 (7)	2.859 (5)	114 (6)
O8—H1 \cdots C11 ^v	0.82 (2)	2.52 (5)	3.219 (4)	145 (7)
O7—H2 \cdots O4 ^v	0.83 (2)	2.13 (6)	2.860 (6)	148 (10)
O7—H2 \cdots C11 ^v	0.83 (2)	2.81 (11)	3.220 (4)	112 (9)

Symmetry codes: (v) $x+1/2, -y+3/2, z+1/2$; (xii) $x, -y+1, z+1/2$.