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Synthesis and crystal structure of $NaCsB_5O_8(OH)\cdot H_2O$

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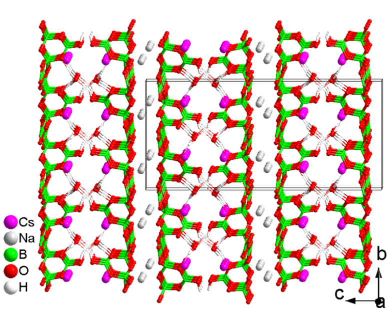
The solvothermal reaction of H_3BO_3, Cs_2CO_3, $NaBO_2\cdot 4H_2O$, formic acid and ethanol led to a new mixed alkali metal borate, $NaCsB_5O_8(OH)\cdot H_2O$, sodium caesium pentaborate hydroxide monohydrate. Its crystal structure contains pentaborate $[B_5O_{10}(OH)]^{6-}$ building units, and displays a layered structure containing nine-membered rings. The layers extend parallel to the *ab* plane and are stacked along the *c* axis. Na^+ and Cs^+ cations are situated between the layers and bond to oxygen atoms with coordination numbers of 7 and 10, respectively. The water molecule likewise occupies the interlayer space and is hydrogen-bonded to the layers, both as a donor and an acceptor.



1. Chemical context

Crystalline borates have been well recognized as promising ultraviolet and deep-ultraviolet nonlinear optical and birefringent materials (Zhang *et al.*, 2026; Li *et al.*, 2023*a*,*b*; Lu *et al.*, 2024; Ou *et al.*, 2025; Zou *et al.*, 2026). Borates exhibit a remarkably rich structural chemistry originating from the various coordination modes of boron to oxygen atoms: BO_3 triangles and BO_4 tetrahedra that can be interconnected via corner-sharing oxygen atoms to construct a variety of polyborate anions (Lin & Yang, 2011; Huang *et al.*, 2019; Chen *et al.*, 2024*b*). To date, more than 3900 borate compounds have been documented in the literature (Mutailipu *et al.*, 2021).

Pentaborates constitute a family of structurally rich borates, whose fundamental building units typically comprise two B_3O_3 rings that are nearly orthogonal to each other. The linkage modes between BO_4 tetrahedra and BO_3 triangles give rise to a series of pentaborate anions, including $[B_5O_{10}]^{5-}$, $[B_5O_{11}]^{7-}$, $[B_5O_{12}]^{9-}$, and $[B_5O_{14}]^{13-}$. Hydroxyl-functionalized pentaborate anions are also well-documented, such as $[B_5O_{10}(OH)]^{6-}$, $[B_5O_8(OH)_2]^{3-}$, $[B_5O_9(OH)_3]^{6-}$ and $[B_5O_6(OH)_4]^-$ (Wei *et al.*, 2014; Ding *et al.*, 2018). Moreover, extended crystalline frameworks of borates can be formed through condensation reactions accompanied by the elimination of water molecules (Li *et al.*, 2024; Shi *et al.*, 2019; Zhao *et al.*, 2022,2024; Chen *et al.*, 2024*a*; Wang *et al.*, 2025; Chen & Yang, 2024).

In this work, we present the solvothermal synthesis and single-crystal X-ray structure analysis of a novel mixed alkali-metal pentaborate, $NaCsB_5O_8(OH)\cdot H_2O$, (I).

2. Structural commentary

The asymmetric unit of (I) consists of one formula unit. The pentaborate $[B_5O_{10}(OH)]^{6-}$ building unit (Fig. 1) is constructed by the linkage of two BO_3 triangles (B4, B5), two BO_4 tetrahedra (B2, B3), and one $BO_2(OH)$ group (B1), with

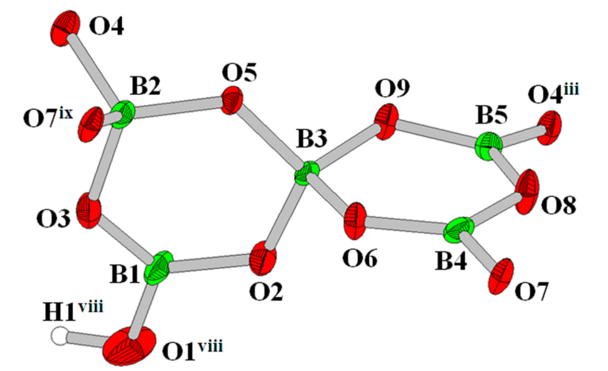


Figure 1
The $[B_5O_{10}(OH)]^{6-}$ building unit in (I) with displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, z$; (viii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (ix) $-x-\frac{1}{2}, y-\frac{1}{2}, z$.]

the B—O bond lengths falling in the range of 1.340 (8) to 1.502 (8) Å (Table 1). Furthermore, each $[B_5O_{10}(OH)]^{6-}$ unit links to four identical units, giving rise to a layered $^2_\infty[B_5O_8(OH)]^{2-}$ anion extending parallel to the *ab* plane featuring nine-membered rings (Fig. 2). The layers stack along the *c* axis in an ...*ABAB*... alternating fashion. The Na^+ cations, Cs^+ cations, and crystal water molecules reside in the interlayer space. The Na^+ cation is seven-coordinated in a highly distorted pentagonal–bipyramidal coordination environment, while the Cs^+ cation is ten-coordinated in a distorted pentagonal-prismatic coordination environment (Pinsky & Avnir, 1998), as shown in Fig. 3. The Na—O bond lengths range from 2.290 (5) to 2.654 (5) Å and the Cs—O bond lengths from 3.054 (4) to 3.604 (4) Å (Table 1).

A view of the crystal structure is given in Fig. 4. The extended structure is consolidated by hydrogen-bonding interactions between the hydroxy group (O1) and the water molecule (O10), and between the water molecule and the anionic framework (Table 2).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O10	0.91	1.90	2.683 (9)	143
O10—H10*A*···O3^{iii}	0.87	2.35	3.173 (13)	157
O10—H10*B*···O2^{ii}	0.87	1.95	2.796 (9)	165

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

Table 1
Selected bond lengths (Å).

Cs—O1^{i}	3.110 (5)	B1—O1^{viii}	1.382 (9)
Cs—O2	3.054 (4)	B1—O2	1.363 (8)
Cs—O2^{ii}	3.604 (4)	B1—O3	1.353 (9)
Cs—O3^{ii}	3.406 (5)	B2—O3	1.502 (8)
Cs—O3^{iii}	3.335 (4)	B2—O4	1.474 (8)
Cs—O4^{iii}	3.324 (4)	B2—O5	1.429 (8)
Cs—O6^{ii}	3.313 (4)	B2—O7^{ix}	1.493 (8)
Cs—O7^{iv}	3.356 (4)	B3—O2	1.478 (8)
Cs—O9	3.111 (4)	B3—O5	1.433 (8)
Cs—O10	3.407 (11)	B3—O6	1.493 (8)
Na—O4^{v}	2.652 (5)	B3—O9	1.480 (8)
Na—O5^{vi}	2.431 (5)	B4—O6	1.358 (8)
Na—O5	2.290 (5)	B4—O7	1.340 (8)
Na—O6^{vi}	2.457 (5)	B4—O8	1.408 (9)
Na—O7^{vii}	2.567 (5)	B5—O4^{iii}	1.340 (9)
Na—O8^{iv}	2.563 (5)	B5—O8	1.399 (8)
Na—O9	2.654 (5)	B5—O9	1.366 (8)

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

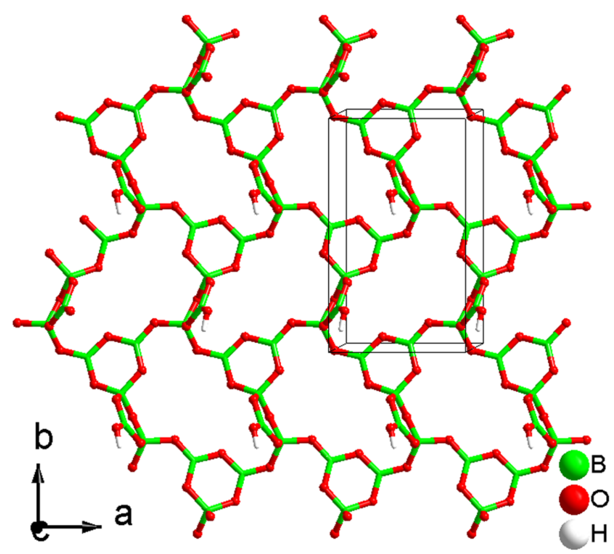


Figure 2
Formation of anionic layers extending parallel to the *ab* plane.

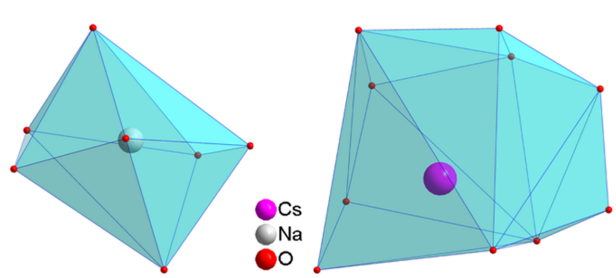


Figure 3
The coordination polyhedra around Na^+ and Cs^+ cations.

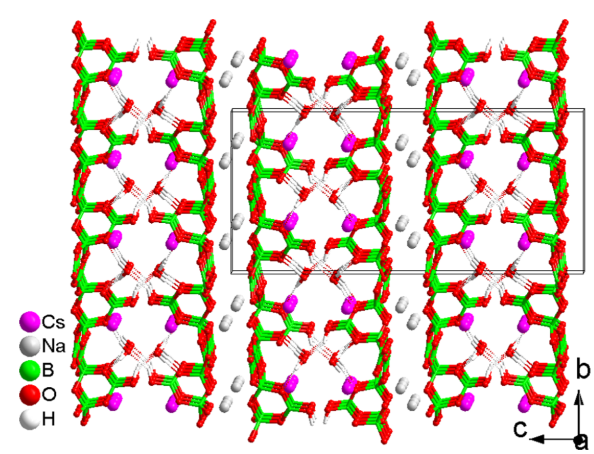


Figure 4
The crystal structure of (I) in a view along the *a* axis. Hydrogen-bonding interactions are shown as dashed lines; bonds to the cations are not shown for clarity.

3. Database survey

A search of the Inorganic Crystal Structure Database (ICSD, version 5.6.0, updated January 2026; Zagorac *et al.*, 2019) for alkali metal compounds with the $[B_5O_8(OH)]^{2-}$ anion returned seven hits: $NaKB_5O_8(OH)\cdot H_2O$ (triclinic, $P\bar{1}$; Li *et al.*, 2024), $LiRbB_5O_8(OH)\cdot H_2O$ (monoclinic, $P2_1/n$: Shi *et al.*, 2019), $K_2B_5O_8(OH)\cdot 2H_2O$ (orthorhombic, $Pna2_1$; Shi *et al.*, 2019), $Rb_2B_5O_8(OH)$ (orthorhombic, $Pca2_1$; Qiu *et al.*, 2021), $LiCsB_5O_8(OH)\cdot H_2O$ (monoclinic, $P2_1/c$; Chen *et al.*, 2017), $LiKB_5O_8(OH)\cdot 1.5H_2O$ (orthorhombic, $C222_1$; Li & Yang, 2019), and $Na_2B_5O_8(OH)\cdot 2H_2O$ (orthorhombic, $Pna2_1$; Corazza *et al.*, 1975, Wang *et al.*, 2009). Compared with compound (I), the seven compounds adopt a similar layered structure and share the same $[B_5O_{10}(OH)]^{6-}$ building unit, but they contain different alkali metal ions and possess different space groups, making (I) unique.

4. Synthesis and crystallization

A mixture of H_3BO_3 (0.3710 g, 6 mmol), Cs_2CO_3 (0.3258 g, 1 mmol), $NaBO_2\cdot 4H_2O$ (0.1378 g, 1 mmol), formic acid (0.25 ml) and ethanol (4 ml) was sealed in a 30 ml Teflon-lined autoclave at 453 K for 6 d and then cooled to room temperature. Colorless crystals of (I) were obtained by filtration, washed with distilled water, and dried in air.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms bonded to O atoms were positioned geometrically and refined using a riding model [$O_{hydroxyl}$—H = 0.91 Å and O_{water}—H = 0.87 Å, $U_{iso}(H) = 1.5 U_{eq}(O)$]. O10 of the water molecule exhibits relatively large displacement parameters, suggesting the presence of potential positional disorder. In the current structure refinement, O10 was modeled as a single site.

Table 3
Experimental details.

Crystal data	
Chemical formula	$NaCsB_5O_8(OH)\cdot H_2O$
M_r	372.97
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	152
a, *b*, *c* (Å)	6.5803 (3), 11.2304 (6), 24.3738 (12)
V (Å^3)	1801.21 (15)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	4.20
Crystal size (mm)	0.18 × 0.18 × 0.16
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.49, 0.51
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21866, 1643, 1228
R_{int}	0.125
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.091, 1.02
No. of reflections	1643
No. of parameters	154
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.14, −1.24

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SIR2004* (Burla *et al.*, 2007), *SHELXL* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

Funding information

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supporting information

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Synthesis and crystal structure of $NaCsB_5O_8(OH)\cdot H_2O$

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Computing details

Sodium caesium pentaborate hydroxide monohydrate

Crystal data

$NaCsB_5O_8(OH)\cdot H_2O$
M_r = 372.97
Orthorhombic, *Pbca*
a = 6.5803 (3) Å
b = 11.2304 (6) Å
c = 24.3738 (12) Å
V = 1801.21 (15) Å^3
Z = 8
F(000) = 1392
D_x = 2.751 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 3085 reflections
θ = 3.3–24.8°
μ = 4.20 mm^{-1}
T = 152 K
Block, colorless
0.18 × 0.18 × 0.16 mm

Data collection

Bruker APEXII CCD diffractometer
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.49, T_{max} = 0.51
21866 measured reflections
1643 independent reflections
1228 reflections with $I > 2\sigma(I)$
R_{int} = 0.125
θ_{max} = 25.3°, θ_{min} = 3.3°
$h = -7\rightarrow7$
$k = -13\rightarrow13$
$l = -29\rightarrow29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.091
S = 1.02
1643 reflections
154 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0194P)^2 + 20.4113P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.14 e Å^{-3}
$\Delta\rho_{min}$ = −1.24 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cs	0.54972 (7)	0.30565 (5)	0.66570 (2)	0.03814 (19)
Na	0.2006 (4)	0.1934 (2)	0.48463 (11)	0.0257 (6)
B1	0.0294 (12)	0.1797 (6)	0.6701 (3)	0.0197 (16)
B2	−0.1027 (11)	0.1034 (6)	0.5815 (3)	0.0141 (16)
B3	0.0647 (11)	0.3085 (6)	0.5883 (3)	0.0129 (14)
B4	−0.0397 (12)	0.5207 (6)	0.5698 (3)	0.0157 (15)
B5	0.3167 (11)	0.4635 (6)	0.5607 (3)	0.0150 (16)
O1	0.9171 (9)	0.6659 (5)	0.7755 (2)	0.0392 (15)
H1	0.942046	0.588286	0.767268	0.059*
O2	0.0920 (7)	0.2845 (4)	0.64744 (18)	0.0181 (10)
O3	−0.0829 (7)	0.0978 (4)	0.64290 (18)	0.0203 (11)
O4	−0.0143 (6)	−0.0079 (4)	0.56023 (18)	0.0165 (10)
O5	−0.0124 (6)	0.2079 (4)	0.55865 (16)	0.0123 (9)
O6	−0.0868 (6)	0.4071 (4)	0.58409 (19)	0.0163 (10)
O7	−0.1763 (6)	0.6090 (4)	0.56782 (18)	0.0158 (10)
O8	0.1635 (7)	0.5496 (4)	0.5576 (2)	0.0213 (11)
O9	0.2635 (7)	0.3464 (4)	0.56586 (18)	0.0158 (10)
O10	0.946 (2)	0.4776 (7)	0.7082 (3)	0.132 (5)
H10A	0.875861	0.521456	0.685701	0.198*
H10B	1.007984	0.426560	0.687130	0.198*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs	0.0248 (3)	0.0548 (4)	0.0349 (3)	0.0060 (3)	−0.0028 (2)	0.0119 (3)
Na	0.0267 (15)	0.0213 (14)	0.0289 (15)	0.0020 (13)	0.0117 (12)	0.0023 (13)
B1	0.029 (4)	0.008 (3)	0.022 (4)	0.002 (3)	−0.002 (4)	−0.002 (3)
B2	0.019 (4)	0.009 (3)	0.015 (4)	0.001 (3)	−0.001 (3)	−0.001 (3)
B3	0.013 (3)	0.008 (3)	0.017 (3)	0.001 (3)	0.005 (3)	−0.003 (3)
B4	0.017 (4)	0.012 (4)	0.018 (4)	0.002 (3)	0.003 (3)	−0.005 (3)
B5	0.019 (4)	0.012 (4)	0.014 (4)	0.002 (3)	0.001 (3)	0.001 (3)
O1	0.065 (4)	0.033 (3)	0.019 (3)	0.015 (3)	−0.017 (3)	−0.004 (2)
O2	0.021 (2)	0.013 (2)	0.020 (2)	−0.0034 (19)	−0.0026 (19)	0.0007 (19)
O3	0.026 (3)	0.015 (2)	0.021 (2)	−0.007 (2)	0.000 (2)	0.003 (2)
O4	0.013 (2)	0.011 (2)	0.026 (2)	0.0023 (18)	−0.002 (2)	−0.0011 (19)
O5	0.013 (2)	0.010 (2)	0.014 (2)	−0.0036 (18)	−0.0017 (17)	−0.0006 (18)
O6	0.010 (2)	0.010 (2)	0.029 (3)	0.0003 (18)	0.0034 (19)	0.003 (2)
O7	0.010 (2)	0.008 (2)	0.029 (3)	−0.0007 (18)	−0.001 (2)	−0.0024 (19)
O8	0.013 (2)	0.009 (2)	0.042 (3)	0.0019 (19)	0.002 (2)	0.005 (2)
O9	0.013 (2)	0.010 (2)	0.024 (2)	−0.0016 (18)	−0.002 (2)	0.0010 (19)
O10	0.268 (15)	0.052 (5)	0.075 (6)	−0.006 (7)	0.057 (8)	−0.033 (5)

Geometric parameters (Å, º)

Cs—B1^{i}	3.461 (8)	Na—O7^{viii}	2.567 (5)
Cs—B5	3.470 (7)	Na—O8^{iv}	2.563 (5)
Cs—O1^{ii}	3.110 (5)	Na—O9	2.654 (5)
Cs—O2	3.054 (4)	B1—O1^{ix}	1.382 (9)
Cs—O2^{i}	3.604 (4)	B1—O2	1.363 (8)
Cs—O3^{i}	3.406 (5)	B1—O3	1.353 (9)
Cs—O3^{iii}	3.335 (4)	B2—O3	1.502 (8)
Cs—O4^{iii}	3.324 (4)	B2—O4	1.474 (8)
Cs—O6^{i}	3.313 (4)	B2—O5	1.429 (8)
Cs—O7^{iv}	3.356 (4)	B2—O7^{x}	1.493 (8)
Cs—O9	3.111 (4)	B3—O2	1.478 (8)
Cs—O10	3.407 (11)	B3—O5	1.433 (8)
Cs—H10A	3.2737	B3—O6	1.493 (8)
Cs—H10B	3.3482	B3—O9	1.480 (8)
Na—Na^{v}	3.606 (2)	B4—O6	1.358 (8)
Na—Na^{vi}	3.606 (2)	B4—O7	1.340 (8)
Na—B2^{v}	3.080 (8)	B4—O8	1.408 (9)
Na—B3	2.975 (7)	B5—O4^{iii}	1.340 (9)
Na—B3^{v}	2.983 (8)	B5—O8	1.399 (8)
Na—O4^{vii}	2.652 (5)	B5—O9	1.366 (8)
Na—O5^{v}	2.431 (5)	O1—H1	0.9089
Na—O5	2.290 (5)	O10—H10A	0.8700
Na—O6^{v}	2.457 (5)	O10—H10B	0.8700
O1^{ii}—Cs—O2^{i}	90.19 (13)	O5—B2—O3	112.8 (5)
O1^{ii}—Cs—O3^{iii}	129.45 (12)	O5—B2—O4	113.3 (5)
O1^{ii}—Cs—O3^{i}	75.20 (13)	O5—B2—O7^{x}	106.4 (5)
O1^{ii}—Cs—O4^{iii}	171.26 (12)	O7^{x}—B2—O3	108.0 (5)
O1^{ii}—Cs—O6^{i}	129.75 (14)	O2—B3—O6	106.4 (5)
O1^{ii}—Cs—O7^{iv}	105.19 (12)	O2—B3—O9	107.8 (5)
O1^{ii}—Cs—O9	142.17 (14)	O5—B3—O2	113.0 (5)
O1^{ii}—Cs—O10	88.33 (19)	O5—B3—O6	108.3 (5)
O2—Cs—O1^{ii}	98.94 (14)	O5—B3—O9	110.7 (5)
O2—Cs—O2^{i}	162.45 (15)	O9—B3—O6	110.6 (5)
O2—Cs—O3^{iii}	96.71 (11)	O6—B4—O8	119.2 (6)
O2—Cs—O3^{i}	128.53 (11)	O7—B4—O6	123.4 (6)
O2—Cs—O4^{iii}	82.37 (11)	O7—B4—O8	117.4 (6)
O2—Cs—O6^{i}	130.64 (11)	O4^{iii}—B5—O8	122.2 (6)
O2—Cs—O7^{iv}	95.17 (11)	O4^{iii}—B5—O9	118.7 (6)
O2—Cs—O9	45.61 (12)	O9—B5—O8	119.1 (6)
O2—Cs—O10	147.53 (19)	B1^{xi}—O1—Cs^{xii}	138.7 (4)
O3^{i}—Cs—O2^{i}	39.82 (10)	B1^{xi}—O1—Cs^{xi}	78.1 (4)
O3^{iii}—Cs—O2^{i}	88.83 (11)	B1^{xi}—O1—H1	105.9
O3^{iii}—Cs—O3^{i}	126.91 (7)	Cs—O2—Cs^{xiii}	162.45 (15)
O3^{iii}—Cs—O7^{iv}	120.85 (11)	B1—O2—Cs^{xiii}	73.0 (4)
O3^{i}—Cs—O10	83.94 (19)	B1—O2—Cs	107.8 (4)

O3^{iii}—Cs—O10	56.14 (19)	B1—O2—B3	121.0 (5)
O4^{iii}—Cs—O2^{i}	90.89 (10)	B3—O2—Cs	104.4 (3)
O4^{iii}—Cs—O3^{i}	110.81 (11)	B3—O2—Cs^{xiii}	89.3 (3)
O4^{iii}—Cs—O3^{iii}	41.92 (11)	Cs^{iv}—O3—Cs^{xiii}	133.91 (14)
O4^{iii}—Cs—O7^{iv}	83.23 (11)	B1—O3—Cs^{xiii}	80.9 (4)
O4^{iii}—Cs—O10	86.08 (18)	B1—O3—Cs^{iv}	123.5 (4)
O6^{i}—Cs—O2^{i}	39.98 (10)	B1—O3—B2	120.4 (5)
O6^{i}—Cs—O3^{iii}	60.94 (11)	B2—O3—Cs^{xiii}	94.1 (3)
O6^{i}—Cs—O3^{i}	68.00 (10)	B2—O3—Cs^{iv}	102.3 (3)
O6^{i}—Cs—O4^{iii}	50.92 (10)	Na^{vii}—O4—Cs^{iv}	77.98 (12)
O6^{i}—Cs—O7^{iv}	67.69 (10)	B2—O4—Cs^{iv}	103.5 (3)
O6^{i}—Cs—O10	55.57 (16)	B2—O4—Na^{vii}	129.0 (4)
O7^{iv}—Cs—O2^{i}	67.85 (10)	B5^{iv}—O4—Cs^{iv}	84.8 (4)
O7^{iv}—Cs—O3^{i}	42.00 (11)	B5^{iv}—O4—Na^{vii}	105.3 (4)
O7^{iv}—Cs—O10	113.51 (17)	B5^{iv}—O4—B2	125.7 (5)
O9—Cs—O2^{i}	120.84 (11)	Na—O5—Na^{vi}	99.56 (15)
O9—Cs—O3^{iii}	76.38 (11)	B2—O5—Na	120.2 (4)
O9—Cs—O3^{i}	113.76 (11)	B2—O5—Na^{vi}	102.8 (4)
O9—Cs—O4^{iii}	42.26 (11)	B2—O5—B3	126.7 (5)
O9—Cs—O6^{i}	85.23 (11)	B3—O5—Na	103.7 (4)
O9—Cs—O7^{iv}	72.01 (11)	B3—O5—Na^{vi}	97.7 (4)
O9—Cs—O10	128.16 (18)	Na^{vi}—O6—Cs^{xiii}	80.81 (13)
O4^{vii}—Na—O9	152.63 (17)	B3—O6—Cs^{xiii}	100.7 (3)
O5—Na—O4^{vii}	95.63 (17)	B3—O6—Na^{vi}	94.9 (3)
O5^{v}—Na—O4^{vii}	122.56 (17)	B4—O6—Cs^{xiii}	129.9 (4)
O5—Na—O5^{v}	141.70 (14)	B4—O6—Na^{vi}	112.7 (4)
O5—Na—O6^{v}	156.68 (19)	B4—O6—B3	124.2 (5)
O5^{v}—Na—O6^{v}	58.07 (15)	Na^{viii}—O7—Cs^{iii}	78.48 (12)
O5—Na—O7^{viii}	107.02 (17)	B2^{xiv}—O7—Cs^{iii}	96.3 (3)
O5^{v}—Na—O7^{viii}	55.78 (14)	B2^{xiv}—O7—Na^{viii}	95.0 (3)
O5^{v}—Na—O8^{iv}	108.50 (17)	B4—O7—Cs^{iii}	107.2 (4)
O5—Na—O8^{iv}	73.26 (16)	B4—O7—Na^{viii}	134.4 (4)
O5—Na—O9	57.44 (15)	B4—O7—B2^{xiv}	127.9 (5)
O5^{v}—Na—O9	84.67 (16)	B4—O8—Na^{iii}	128.6 (4)
O6^{v}—Na—O4^{vii}	67.76 (15)	B5—O8—Na^{iii}	102.8 (4)
O6^{v}—Na—O7^{viii}	95.33 (16)	B5—O8—B4	120.9 (5)
O6^{v}—Na—O8^{iv}	89.14 (17)	Na—O9—Cs	125.63 (16)
O6^{v}—Na—O9	135.81 (18)	B3—O9—Cs	101.8 (3)
O7^{viii}—Na—O4^{vii}	116.43 (17)	B3—O9—Na	87.2 (3)
O7^{viii}—Na—O9	79.70 (15)	B5—O9—Cs	93.3 (4)
O8^{iv}—Na—O4^{vii}	87.28 (16)	B5—O9—Na	126.5 (4)
O8^{iv}—Na—O7^{viii}	155.80 (18)	B5—O9—B3	122.5 (5)
O8^{iv}—Na—O9	80.57 (16)	Cs—O10—Cs^{xv}	95.6 (2)
O2—B1—O1^{ix}	114.1 (6)	Cs^{xv}—O10—H10A	156.6
O3—B1—O1^{ix}	122.2 (6)	Cs—O10—H10A	73.9
O3—B1—O2	123.6 (6)	Cs—O10—H10B	78.8

O4—B2—O3	106.3 (5)	Cs^{xv}—O10—H10B	93.4
O4—B2—O7^{x}	109.9 (5)	H10A—O10—H10B	104.5

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O10	0.91	1.90	2.683 (9)	143
O10—H10*A*···O3^{iii}	0.87	2.35	3.173 (13)	157
O10—H10*B*···O2^{i}	0.87	1.95	2.796 (9)	165

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