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Synthesis and crystal structure of $NaRbB_5O_8(OH)\cdot H_2O$

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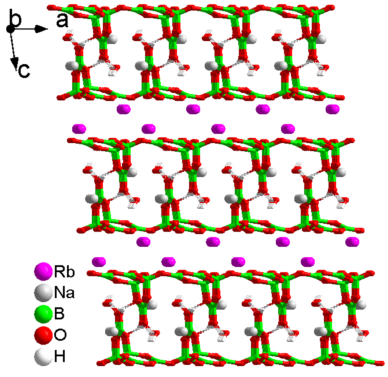
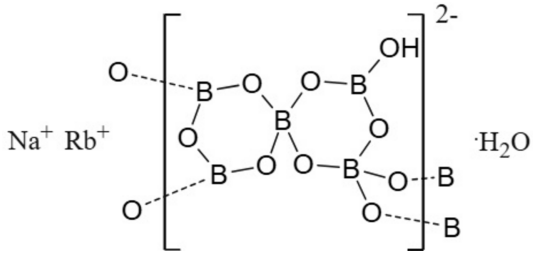
A new mixed alkali-metal borate, poly[[sodium rubidium [hydroxidoocta-μ-oxidopentaborate] monohydrate], $NaRbB_5O_8(OH)\cdot H_2O$, has been synthesized *via* a surfactant-thermal method using H_3BO_3, Rb_2CO_3, $Na_2SiO_3\cdot 9H_2O$, ethanediamine and poly(ethylene glycol)-400 as starting materials. It features a layered boron-oxide framework constructed from pentaborate $[B_5O_{10}(OH)]^{6-}$ building units. Adjacent single layers are interconnected to form double layers through hydrogen-bonding interactions. Na^+, Rb^+ cations and H_2O molecules are located in the voids of the framework.

1. Chemical context

Crystalline metal borates are widely recognized as promising non-linear optical materials in the ultraviolet region (Zhang *et al.*, 2026; Li *et al.*, 2023*a*,*b*,*c*; Lu *et al.*, 2024; Tian *et al.*, 2013; Chen *et al.*, 2024*a*, 2025; Wang *et al.*, 2017, 2025; Wei *et al.*, 2016; Yu *et al.*, 2017; Zhao *et al.*, 2025, 2026; Zou *et al.*, 2026*a*). Boron can adopt either three- or four-coordinate geometries with oxygen atoms. Corner-sharing oxygen linkages between planar BO_3 triangles and tetrahedral BO_4 units enable the construction of various polyborate anions (Mutailipu *et al.*, 2021), including $[B_3O_3(OH)_4]^-$, $[B_4O_5(OH)_4]^{2-}$, $[B_7O_{12}(OH)_{14}]^{7-}$, and $[B_{12}O_{18}(OH)_6]^{6-}$ (Lin *et al.*, 2011; Huang *et al.*, 2019; Chen *et al.*, 2024*c*). Pentaborate units typically serve as fundamental building blocks. Various arrangements of BO_3 triangles, BO_4 tetrahedra, as well as $[B_5O_n]$ (n= 10–12, 14) and hydroxylated $[B_5O_n(OH)_m]$ units, have been observed (Wei *et al.*, 2014; Ding *et al.*, 2018). These pentaborate anions are further interconnected to construct chains, layers, and three-dimensional frameworks with rich structural diversity (Li *et al.*, 2024; Shi *et al.*, 2019; Zhao *et al.*, 2022, 2024; Chen *et al.*, 2024*b*). In such crystal structures, alkali and alkaline-earth metal cations reside in interstitial voids to balance the overall charge of the polyborate anionic frameworks.





Borosilicates are new types of non-linear optical materials that combine different anionic groups (Ou *et al.*, 2025). Our

Table 1
Selected bond lengths (Å).

Rb1—O8^{i}	2.8044 (18)	B1—O2	1.365 (3)
Rb1—O6^{ii}	2.8777 (18)	B1—O1	1.386 (4)
Rb1—O4	2.9174 (17)	B2—O4	1.420 (3)
Rb1—O7^{ii}	2.9197 (17)	B2—O6^{vii}	1.474 (3)
Rb1—O4^{i}	2.9691 (17)	B2—O9^{viii}	1.495 (3)
Rb1—O5	3.0402 (19)	B2—O2	1.504 (3)
Rb1—O9^{ii}	3.0659 (19)	B3—O4	1.438 (3)
Rb1—O5^{iii}	3.0669 (17)	B3—O7	1.469 (3)
Rb1—O7	3.1981 (19)	B3—O5	1.493 (3)
Na1—O3	2.320 (2)	B3—O3	1.506 (3)
Na1—O10	2.328 (2)	B4—O5	1.344 (3)
Na1—O6	2.372 (2)	B4—O6	1.364 (3)
Na1—O10^{iv}	2.408 (3)	B4—O8^{ix}	1.392 (3)
Na1—O2^{v}	2.470 (2)	B5—O7	1.356 (3)
Na1—O1^{vi}	2.773 (3)	B5—O9	1.359 (3)
B1—O3	1.348 (4)	B5—O8	1.383 (3)

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

initial synthetic strategy was aimed at the exploration of new borosilicate crystals. However, the targeted borosilicate phase was not obtained under the applied synthetic conditions, and a pure borate compound was ultimately isolated instead. Herein, we report the synthesis and single-crystal structural characterization of a new mixed alkali-metal pentaborate, $NaRbB_5O_8(OH)\cdot H_2O$, (I).

2. Structural commentary

The title compound crystallizes in the triclinic space group $P\overline{1}$. The asymmetric unit of (I) consists of five boron atoms, ten oxygen atoms, three hydrogen atoms, one Na^+ cation and one Rb^+ cation. As shown in Fig. 1, the fundamental building block of (I) is the $[B_5O_{10}(OH)]^{6-}$ unit, which is composed of two $[BO_3]$ triangles, two $[BO_4]$ tetrahedra and one $[BO_2(OH)]$ group. The B—O bond lengths fall in the range 1.344 (3)–1.506 (3) Å (Table 1). Each $[B_5O_{10}(OH)]^{6-}$ unit links to four adjacent equivalents, generating a two-dimensional layered structure containing nine-membered ring windows in the *ab* plane (Fig. 2).

Adjacent single layers are connected into double layers through O—H···O hydrogen-bonding interactions between the hydroxyl group (O1) and oxygen atom (O2) of the $[B_5O_{10}(OH)]^{6-}$ units. Hydrogen-bonding interactions also

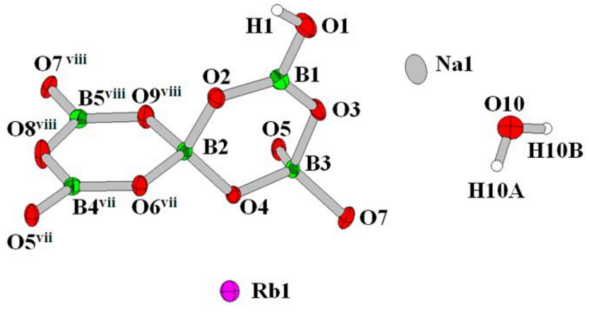


Figure 1
Structure of (I) with displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (vii) $x, y-1, z$; (viii) $x-1, y, z$].

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{x}	0.82	2.11	2.869 (3)	155
O10—H10*B*···O1^{iv}	0.84	2.16	2.916 (3)	151

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

exist between the water molecule (O10) and hydroxyl group (O1) in the anionic framework. The corresponding O···O hydrogen-bond distances range from 2.869 (3) to 2.916 (3) Å (Table 2). Its hydrogen-bonding interactions are highly analogous to those of the isotypic protonated borate $NaKB_5O_8(OH)\cdot H_2O$ (Li *et al.*, 2024). These hydrogen-bonded double layers further stack parallel to one another along the *c*

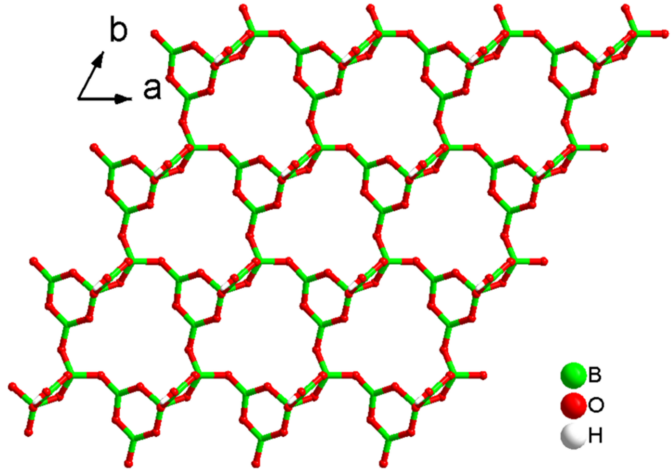


Figure 2
Two-dimensional layered structure of (I) in the *ab* plane.

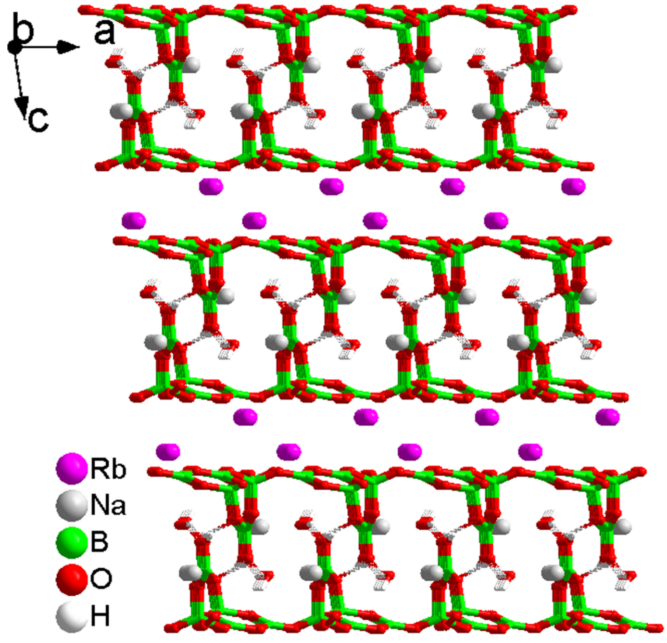


Figure 3
View of the three-dimensional packing structure of (I) along the *b* axis.

Table 3
Experimental details.

Crystal data	
Chemical formula	$NaRbB_5O_8(OH)\cdot H_2O$
M_r	325.53
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	287
a, b, c (Å)	6.6580 (4), 6.6744 (4), 11.5322 (6)
α, β, γ (°)	79.094 (2), 77.508 (2), 60.492 (2)
V (Å^3)	433.37 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.80
Crystal size (mm)	0.13 × 0.12 × 0.10
Data collection	
Diffractometer	Bruker APEXII area detector
Absorption correction	Empirical (using intensity measurements) (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.48, 0.56
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9111, 1985, 1863
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.026, 0.065, 1.08
No. of reflections	1985
No. of parameters	155
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.87, −0.42

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

axis. Na^+ ions and water molecules reside in the interlayer voids within the double layers, whereas Rb^+ ions occupy the voids between adjacent double layers. The Na^+ and Rb^+ ions are six- and nine-coordinated, respectively, with Na—O distances of 2.320 (2)–2.773 (3) Å and Rb—O distances of 2.8044 (18)–3.1981 (19) Å (Table 1). These cations occupy the voids of the framework to maintain overall charge balance (Fig. 3).

3. Database survey

An online search of the Inorganic Crystal Structure Database (ICSD, version 5.6.0, updated January 2026, Zagorac *et al.*, 2019) for alkali-metal compounds incorporating the $[B_5O_{10}(OH)]^{6-}$ moiety returned seven hits: $NaKB_5O_8(OH)\cdot H_2O$ (triclinic, $P\overline{1}$ space group; Li *et al.*, 2024), $LiRbB_5O_8(OH)\cdot H_2O$ (monoclinic, $P2_1/n$ space group; Shi *et al.*, 2019), $K_2B_5O_8(OH)\cdot 2H_2O$ (orthorhombic, $Pna2_1$ space group; Shi *et al.*, 2019), $Rb_2B_5O_8(OH)$ (orthorhombic, $Pca2_1$ space group; Qiu *et al.*, 2021), $LiCsB_5O_8(OH)\cdot H_2O$ (monoclinic, $P2_1/c$ space group; Chen *et al.*, 2017), $LiKB_5O_8(OH)\cdot 1.5H_2O$ (orthorhombic, $C222_1$ space group; Li *et al.*, 2019), and $Na_2B_5O_8(OH)\cdot 2H_2O$ (orthorhombic, $Pna2_1$ space group; Wang *et al.*, 2009). In addition, we have recently reported another pentaborate, $NaCsB_5O_8(OH)\cdot H_2O$ (orthorhombic, *Pbca* space group; Zou *et al.*, 2026*b*). Compound (I) is isostructural with $NaKB_5O_8(OH)\cdot H_2O$, and they share the same space group and similar cell parameters. The other seven reported compounds share similar layered structural features and the common $[B_5O_{10}(OH)]^{6-}$ building unit. Differences in alkali metal cations and space groups lead to the structural uniqueness of compound (I).

4. Synthesis and crystallization

A mixture of H_3BO_3 (0.6183 g, 10 mmol), Rb_2CO_3 (0.2308 g, 1 mmol), $Na_2SiO_3\cdot 9H_2O$ (0.2842 g, 1 mmol), ethanediamine (1 ml), and poly(ethylene glycol)-400 (4 ml) was sealed in a 30 ml Teflon-lined bomb at 453 K for 6 days and then cooled to room temperature over 6 hours. 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 = 0.82 Å and O_{water}—H = 0.84 Å, U_{iso}(H) = 1.2 U_{eq}(O)].

Acknowledgements

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Computing details

Poly[[sodium rubidium [hydroxidoocta-μ-oxidopentaborate] monohydrate]

Crystal data

$NaRbB_5O_8(OH)\cdot H_2O$
M_r = 325.53
Triclinic, $P\overline{1}$
a = 6.6580 (4) Å
b = 6.6744 (4) Å
c = 11.5322 (6) Å
α = 79.094 (2)°
β = 77.508 (2)°
γ = 60.492 (2)°
V = 433.37 (4) Å^3
Z = 2
$F(000)$ = 312
D_x = 2.495 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5543 reflections
θ = 3.5–27.5°
μ = 5.80 mm^{-1}
T = 287 K
Block, clear colourless
0.13 × 0.12 × 0.10 mm

Data collection

Bruker APEXII area detector diffractometer
ω scans
Absorption correction: empirical (using intensity measurements) (SADABS; Krause *et al.*, 2015)
T_{min} = 0.48, T_{max} = 0.56
9111 measured reflections
1985 independent reflections
1863 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.5°, θ_{min} = 3.5°
h = −8→8
k = −8→8
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.065
S = 1.08
1985 reflections
155 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0306P)^2 + 0.5265P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}
Extinction correction: SHELXL2014/7 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.005 (2)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Rb1	−0.15536 (4)	0.31899 (4)	0.42548 (2)	0.01816 (11)
Na1	−0.1957 (2)	0.6023 (2)	0.90050 (11)	0.0262 (3)
B1	−0.3018 (5)	0.1647 (5)	0.9121 (3)	0.0167 (6)
B2	−0.3654 (5)	0.0470 (5)	0.7382 (3)	0.0126 (5)
B3	−0.1935 (5)	0.3118 (4)	0.7072 (2)	0.0111 (5)
B4	−0.4410 (5)	0.7519 (5)	0.6765 (3)	0.0133 (5)
B5	0.2491 (5)	0.1475 (5)	0.6798 (3)	0.0147 (5)
O1	−0.3247 (4)	0.1631 (4)	1.03462 (18)	0.0266 (5)
H1	−0.3758	0.0744	1.0684	0.040*
O2	−0.3634 (3)	0.0278 (3)	0.87005 (16)	0.0172 (4)
O3	−0.2273 (3)	0.3071 (3)	0.84093 (16)	0.0182 (4)
O4	−0.2045 (3)	0.1225 (3)	0.67186 (15)	0.0118 (3)
O5	−0.3820 (3)	0.5345 (3)	0.66024 (17)	0.0152 (4)
O6	−0.2980 (3)	0.8115 (3)	0.71344 (16)	0.0136 (4)
O7	0.0306 (3)	0.3107 (3)	0.66079 (17)	0.0156 (4)
O8	0.3356 (3)	−0.0786 (3)	0.6563 (2)	0.0228 (4)
O9	0.3882 (3)	0.2091 (3)	0.71832 (18)	0.0182 (4)
O10	0.1852 (4)	0.5348 (4)	0.8910 (2)	0.0294 (5)
H10A	0.2601	0.4538	0.8343	0.044*
H10B	0.2258	0.6376	0.8853	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb1	0.01984 (15)	0.01750 (15)	0.02004 (15)	−0.01100 (11)	−0.00189 (9)	−0.00294 (9)
Na1	0.0329 (6)	0.0231 (6)	0.0287 (6)	−0.0154 (5)	−0.0134 (5)	0.0009 (5)
B1	0.0189 (14)	0.0152 (13)	0.0169 (14)	−0.0080 (11)	−0.0038 (11)	−0.0020 (11)
B2	0.0103 (12)	0.0104 (12)	0.0178 (14)	−0.0050 (10)	−0.0016 (10)	−0.0032 (10)
B3	0.0115 (12)	0.0082 (11)	0.0152 (13)	−0.0055 (10)	−0.0022 (10)	−0.0017 (10)
B4	0.0115 (12)	0.0122 (12)	0.0154 (13)	−0.0046 (10)	−0.0017 (10)	−0.0026 (10)
B5	0.0139 (13)	0.0120 (12)	0.0173 (14)	−0.0053 (11)	−0.0024 (10)	−0.0022 (10)
O1	0.0438 (13)	0.0338 (12)	0.0146 (9)	−0.0283 (10)	−0.0024 (9)	−0.0025 (8)
O2	0.0234 (9)	0.0200 (9)	0.0151 (9)	−0.0161 (8)	−0.0012 (7)	−0.0016 (7)
O3	0.0284 (10)	0.0197 (9)	0.0151 (9)	−0.0173 (8)	−0.0033 (8)	−0.0034 (7)
O4	0.0125 (8)	0.0102 (8)	0.0147 (8)	−0.0068 (7)	−0.0012 (6)	−0.0023 (6)
O5	0.0119 (8)	0.0094 (8)	0.0261 (10)	−0.0039 (7)	−0.0071 (7)	−0.0037 (7)
O6	0.0113 (8)	0.0086 (8)	0.0217 (9)	−0.0039 (7)	−0.0049 (7)	−0.0024 (7)
O7	0.0093 (8)	0.0107 (8)	0.0274 (10)	−0.0052 (7)	−0.0034 (7)	−0.0006 (7)
O8	0.0148 (9)	0.0124 (9)	0.0439 (13)	−0.0032 (7)	−0.0137 (8)	−0.0074 (8)

O9	0.0120 (9)	0.0107 (8)	0.0321 (11)	−0.0028 (7)	−0.0057 (7)	−0.0072 (7)
O10	0.0274 (11)	0.0318 (12)	0.0292 (12)	−0.0139 (9)	−0.0003 (9)	−0.0078 (9)

Geometric parameters (Å, º)

Rb1—O8^{i}	2.8044 (18)	B2—Rb1^{i}	3.482 (3)
Rb1—O6^{ii}	2.8777 (18)	B3—O4	1.438 (3)
Rb1—O4	2.9174 (17)	B3—O7	1.469 (3)
Rb1—O7^{ii}	2.9197 (17)	B3—O5	1.493 (3)
Rb1—O4^{i}	2.9691 (17)	B3—O3	1.506 (3)
Rb1—O5	3.0402 (19)	B4—O5	1.344 (3)
Rb1—O9^{ii}	3.0659 (19)	B4—O6	1.364 (3)
Rb1—O5^{iii}	3.0669 (17)	B4—O8^{ix}	1.392 (3)
Rb1—B3	3.197 (3)	B4—Rb1^{iii}	3.415 (3)
Rb1—O7	3.1981 (19)	B4—Rb1^{ii}	3.703 (3)
Rb1—B5^{ii}	3.323 (3)	B5—O7	1.356 (3)
Rb1—B4^{iii}	3.415 (3)	B5—O9	1.359 (3)
Na1—O3	2.320 (2)	B5—O8	1.383 (3)
Na1—O10	2.328 (2)	B5—Rb1^{ii}	3.323 (3)
Na1—O6	2.372 (2)	O1—Na1^{vi}	2.773 (3)
Na1—O10^{iv}	2.408 (3)	O1—H1	0.8200
Na1—O2^{v}	2.470 (2)	O2—Na1^{vii}	2.470 (2)
Na1—O1^{vi}	2.773 (3)	O4—Rb1^{i}	2.9691 (17)
Na1—B2^{v}	3.017 (3)	O5—Rb1^{iii}	3.0669 (17)
Na1—B4	3.095 (3)	O6—B2^{v}	1.474 (3)
Na1—Na1^{iv}	3.438 (2)	O6—Rb1^{ii}	2.8778 (18)
Na1—Rb1^{ii}	4.0661 (13)	O7—Rb1^{ii}	2.9197 (17)
Na1—H10A	2.6638	O8—B4^{x}	1.393 (3)
B1—O3	1.348 (4)	O8—Rb1^{i}	2.8043 (18)
B1—O2	1.365 (3)	O9—B2^{xi}	1.495 (3)
B1—O1	1.386 (4)	O9—Rb1^{ii}	3.0659 (19)
B2—O4	1.420 (3)	O10—Na1^{iv}	2.408 (3)
B2—O6^{vii}	1.474 (3)	O10—Rb1^{ii}	3.618 (2)
B2—O9^{viii}	1.495 (3)	O10—H10A	0.8343
B2—O2	1.504 (3)	O10—H10B	0.8397
B2—Na1^{vii}	3.017 (3)		

O8^{i}—Rb1—O6^{ii}	105.39 (5)	Na1^{iv}—Na1—Rb1^{ii}	106.24 (5)
O8^{i}—Rb1—O4	93.14 (6)	O3—Na1—H10A	99.4
O6^{ii}—Rb1—O4	120.87 (5)	O10—Na1—H10A	17.6
O8^{i}—Rb1—O7^{ii}	139.14 (6)	O6—Na1—H10A	94.4
O6^{ii}—Rb1—O7^{ii}	63.54 (5)	O10^{iv}—Na1—H10A	97.8
O4—Rb1—O7^{ii}	126.94 (5)	O2^{v}—Na1—H10A	103.5
O8^{i}—Rb1—O4^{i}	65.68 (5)	O1^{vi}—Na1—H10A	169.4
O6^{ii}—Rb1—O4^{i}	48.12 (5)	B2^{v}—Na1—H10A	97.7
O4—Rb1—O4^{i}	96.20 (4)	B4—Na1—H10A	109.6
O7^{ii}—Rb1—O4^{i}	111.32 (5)	Na1^{iv}—Na1—H10A	56.6
O8^{i}—Rb1—O5	119.37 (6)	Rb1^{ii}—Na1—H10A	50.7

O6^{ii}—Rb1—O5	132.86 (5)	O3—B1—O2	123.4 (2)
O4—Rb1—O5	47.21 (5)	O3—B1—O1	118.3 (2)
O7^{ii}—Rb1—O5	88.93 (5)	O2—B1—O1	118.2 (2)
O4^{i}—Rb1—O5	141.35 (5)	O4—B2—O6^{vii}	111.0 (2)
O8^{i}—Rb1—O9^{ii}	100.57 (5)	O4—B2—O9^{viii}	113.1 (2)
O6^{ii}—Rb1—O9^{ii}	94.20 (5)	O6^{vii}—B2—O9^{viii}	110.6 (2)
O4—Rb1—O9^{ii}	137.30 (5)	O4—B2—O2	111.0 (2)
O7^{ii}—Rb1—O9^{ii}	46.02 (5)	O6^{vii}—B2—O2	104.7 (2)
O4^{i}—Rb1—O9^{ii}	126.34 (5)	O9^{viii}—B2—O2	106.1 (2)
O5—Rb1—O9^{ii}	91.62 (5)	O4—B2—Na1^{vii}	120.06 (16)
O8^{i}—Rb1—O5^{iii}	46.44 (5)	O6^{vii}—B2—Na1^{vii}	50.58 (11)
O6^{ii}—Rb1—O5^{iii}	128.56 (5)	O9^{viii}—B2—Na1^{vii}	126.80 (17)
O4—Rb1—O5^{iii}	104.92 (5)	O2—B2—Na1^{vii}	54.58 (11)
O7^{ii}—Rb1—O5^{iii}	107.34 (5)	O4—B2—Rb1^{i}	57.43 (11)
O4^{i}—Rb1—O5^{iii}	108.89 (5)	O6^{vii}—B2—Rb1^{i}	54.13 (11)
O5—Rb1—O5^{iii}	94.80 (5)	O9^{viii}—B2—Rb1^{i}	137.87 (17)
O9^{ii}—Rb1—O5^{iii}	61.34 (5)	O2—B2—Rb1^{i}	115.65 (15)
O8^{i}—Rb1—B3	118.10 (7)	Na1^{vii}—B2—Rb1^{i}	77.10 (6)
O6^{ii}—Rb1—B3	117.20 (6)	O4—B3—O7	112.4 (2)
O4—Rb1—B3	26.71 (6)	O4—B3—O5	109.14 (19)
O7^{ii}—Rb1—B3	100.64 (6)	O7—B3—O5	107.95 (19)
O4^{i}—Rb1—B3	113.99 (6)	O4—B3—O3	111.7 (2)
O5—Rb1—B3	27.55 (6)	O7—B3—O3	107.32 (19)
O9^{ii}—Rb1—B3	117.66 (6)	O5—B3—O3	108.17 (19)
O5^{iii}—Rb1—B3	114.24 (6)	O4—B3—Rb1	65.75 (12)
O8^{i}—Rb1—O7	138.07 (5)	O7—B3—Rb1	76.77 (13)
O6^{ii}—Rb1—O7	91.65 (5)	O5—B3—Rb1	70.37 (12)
O4—Rb1—O7	46.24 (4)	O3—B3—Rb1	175.90 (16)
O7^{ii}—Rb1—O7	82.76 (5)	O5—B4—O6	123.9 (2)
O4^{i}—Rb1—O7	103.24 (5)	O5—B4—O8^{ix}	116.5 (2)
O5—Rb1—O7	45.07 (4)	O6—B4—O8^{ix}	119.6 (2)
O9^{ii}—Rb1—O7	116.34 (5)	O5—B4—Na1	93.79 (16)
O5^{iii}—Rb1—O7	139.24 (5)	O6—B4—Na1	46.49 (12)
B3—Rb1—O7	26.56 (6)	O8^{ix}—B4—Na1	131.13 (18)
O8^{i}—Rb1—B5^{ii}	124.32 (6)	O5—B4—Rb1^{iii}	63.74 (13)
O6^{ii}—Rb1—B5^{ii}	83.61 (6)	O6—B4—Rb1^{iii}	172.23 (18)
O4—Rb1—B5^{ii}	129.51 (6)	O8^{ix}—B4—Rb1^{iii}	52.91 (12)
O7^{ii}—Rb1—B5^{ii}	23.98 (6)	Na1—B4—Rb1^{iii}	138.69 (10)
O4^{i}—Rb1—B5^{ii}	127.99 (6)	O5—B4—Rb1^{ii}	94.43 (15)
O5—Rb1—B5^{ii}	83.11 (6)	O6—B4—Rb1^{ii}	43.80 (12)
O9^{ii}—Rb1—B5^{ii}	24.12 (6)	O8^{ix}—B4—Rb1^{ii}	135.22 (17)
O5^{iii}—Rb1—B5^{ii}	84.63 (6)	Na1—B4—Rb1^{ii}	72.86 (6)
B3—Rb1—B5^{ii}	103.94 (7)	Rb1^{iii}—B4—Rb1^{ii}	138.55 (9)
O7—Rb1—B5^{ii}	95.01 (6)	O7—B5—O9	119.4 (2)
O8^{i}—Rb1—B4^{iii}	23.33 (6)	O7—B5—O8	121.0 (2)
O6^{ii}—Rb1—B4^{iii}	119.67 (6)	O9—B5—O8	119.5 (2)
O4—Rb1—B4^{iii}	99.01 (6)	O7—B5—Rb1^{ii}	61.07 (13)
O7^{ii}—Rb1—B4^{iii}	125.52 (6)	O9—B5—Rb1^{ii}	67.26 (14)

O4^{i}—Rb1—B4^{iii}	87.64 (6)	O8—B5—Rb1^{ii}	147.58 (19)
O5—Rb1—B4^{iii}	107.45 (6)	B1—O1—Na1^{vi}	102.67 (17)
O9^{ii}—Rb1—B4^{iii}	81.07 (6)	B1—O1—H1	109.5
O5^{iii}—Rb1—B4^{iii}	23.13 (6)	Na1^{vi}—O1—H1	68.7
B3—Rb1—B4^{iii}	117.84 (7)	B1—O2—B2	118.9 (2)
O7—Rb1—B4^{iii}	143.96 (6)	B1—O2—Na1^{vii}	128.30 (17)
B5^{ii}—Rb1—B4^{iii}	105.15 (7)	B2—O2—Na1^{vii}	95.68 (14)
O3—Na1—O10	114.72 (9)	B1—O3—B3	120.6 (2)
O3—Na1—O6	87.80 (7)	B1—O3—Na1	126.20 (17)
O10—Na1—O6	102.94 (8)	B3—O3—Na1	112.48 (14)
O3—Na1—O10^{iv}	97.54 (8)	B2—O4—B3	120.1 (2)
O10—Na1—O10^{iv}	86.93 (9)	B2—O4—Rb1	132.21 (15)
O6—Na1—O10^{iv}	165.69 (9)	B3—O4—Rb1	87.55 (13)
O3—Na1—O2^{v}	139.94 (8)	B2—O4—Rb1^{i}	98.80 (13)
O10—Na1—O2^{v}	94.71 (8)	B3—O4—Rb1^{i}	133.22 (14)
O6—Na1—O2^{v}	58.24 (6)	Rb1—O4—Rb1^{i}	83.80 (4)
O10^{iv}—Na1—O2^{v}	111.23 (8)	B4—O5—B3	129.0 (2)
O3—Na1—O1^{vi}	90.30 (8)	B4—O5—Rb1	124.85 (16)
O10—Na1—O1^{vi}	154.55 (9)	B3—O5—Rb1	82.08 (13)
O6—Na1—O1^{vi}	81.58 (7)	B4—O5—Rb1^{iii}	93.13 (14)
O10^{iv}—Na1—O1^{vi}	85.11 (8)	B3—O5—Rb1^{iii}	135.15 (14)
O2^{v}—Na1—O1^{vi}	66.05 (7)	Rb1—O5—Rb1^{iii}	85.20 (5)
O3—Na1—B2^{v}	115.13 (8)	B4—O6—B2^{v}	124.4 (2)
O10—Na1—B2^{v}	97.70 (9)	B4—O6—Na1	108.88 (16)
O6—Na1—B2^{v}	28.69 (7)	B2^{v}—O6—Na1	100.73 (14)
O10^{iv}—Na1—B2^{v}	140.75 (9)	B4—O6—Rb1^{ii}	117.06 (15)
O2^{v}—Na1—B2^{v}	29.74 (7)	B2^{v}—O6—Rb1^{ii}	101.35 (13)
O1^{vi}—Na1—B2^{v}	74.11 (7)	Na1—O6—Rb1^{ii}	101.09 (6)
O3—Na1—B4	66.83 (7)	B5—O7—B3	129.6 (2)
O10—Na1—B4	122.57 (9)	B5—O7—Rb1^{ii}	94.94 (15)
O6—Na1—B4	24.64 (7)	B3—O7—Rb1^{ii}	132.55 (14)
O10^{iv}—Na1—B4	150.00 (9)	B5—O7—Rb1	119.02 (16)
O2^{v}—Na1—B4	74.63 (7)	B3—O7—Rb1	76.67 (13)
O1^{vi}—Na1—B4	70.18 (7)	Rb1^{ii}—O7—Rb1	97.24 (5)
B2^{v}—Na1—B4	48.48 (8)	B5—O8—B4^{x}	121.5 (2)
O3—Na1—Na1^{iv}	112.03 (7)	B5—O8—Rb1^{i}	134.67 (16)
O10—Na1—Na1^{iv}	44.38 (6)	B4^{x}—O8—Rb1^{i}	103.76 (15)
O6—Na1—Na1^{iv}	146.14 (8)	B5—O9—B2^{xi}	124.3 (2)
O10^{iv}—Na1—Na1^{iv}	42.55 (6)	B5—O9—Rb1^{ii}	88.62 (15)
O2^{v}—Na1—Na1^{iv}	108.01 (7)	B2^{xi}—O9—Rb1^{ii}	133.40 (15)
O1^{vi}—Na1—Na1^{iv}	123.50 (7)	Na1—O10—Na1^{iv}	93.07 (9)
B2^{v}—Na1—Na1^{iv}	129.28 (8)	Na1—O10—Rb1^{ii}	83.25 (7)
B4—Na1—Na1^{iv}	166.20 (8)	Na1^{iv}—O10—Rb1^{ii}	172.67 (9)
O3—Na1—Rb1^{ii}	90.67 (6)	Na1—O10—H10A	104.6
O10—Na1—Rb1^{ii}	62.09 (6)	Na1^{iv}—O10—H10A	125.6
O6—Na1—Rb1^{ii}	43.99 (5)	Rb1^{ii}—O10—H10A	50.0
O10^{iv}—Na1—Rb1^{ii}	148.42 (7)	Na1—O10—H10B	125.3
O2^{v}—Na1—Rb1^{ii}	79.34 (5)	Na1^{iv}—O10—H10B	101.5

O1^{vi}—Na1—Rb1^{ii}	125.46 (6)	Rb1^{ii}—O10—H10B	85.8
B2^{v}—Na1—Rb1^{ii}	56.58 (6)	H10A—O10—H10B	108.3
B4—Na1—Rb1^{ii}	60.48 (6)		
O3—B1—O1—Na1^{vi}	106.2 (2)	Rb1^{iii}—B4—O5—Rb1	86.33 (13)
O2—B1—O1—Na1^{vi}	−71.6 (3)	Rb1^{ii}—B4—O5—Rb1	−56.82 (15)
O3—B1—O2—B2	−4.5 (4)	O6—B4—O5—Rb1^{iii}	−178.1 (2)
O1—B1—O2—B2	173.2 (2)	O8^{ix}—B4—O5—Rb1^{iii}	3.4 (2)
O3—B1—O2—Na1^{vii}	121.0 (2)	Na1—B4—O5—Rb1^{iii}	143.78 (7)
O1—B1—O2—Na1^{vii}	−61.3 (3)	Rb1^{ii}—B4—O5—Rb1^{iii}	−143.15 (6)
O4—B2—O2—B1	27.4 (3)	O4—B3—O5—B4	176.8 (2)
O6^{vii}—B2—O2—B1	147.2 (2)	O7—B3—O5—B4	−60.8 (3)
O9^{viii}—B2—O2—B1	−95.9 (3)	O3—B3—O5—B4	55.0 (3)
Na1^{vii}—B2—O2—B1	140.1 (2)	Rb1—B3—O5—B4	−129.0 (2)
Rb1^{i}—B2—O2—B1	90.3 (2)	O4—B3—O5—Rb1	−54.17 (17)
O4—B2—O2—Na1^{vii}	−112.69 (17)	O7—B3—O5—Rb1	68.22 (16)
O6^{vii}—B2—O2—Na1^{vii}	7.12 (18)	O3—B3—O5—Rb1	−175.95 (17)
O9^{viii}—B2—O2—Na1^{vii}	124.07 (16)	O4—B3—O5—Rb1^{iii}	20.8 (3)
Rb1^{i}—B2—O2—Na1^{vii}	−49.79 (13)	O7—B3—O5—Rb1^{iii}	143.17 (16)
O2—B1—O3—B3	−3.8 (4)	O3—B3—O5—Rb1^{iii}	−101.0 (2)
O1—B1—O3—B3	178.5 (2)	Rb1—B3—O5—Rb1^{iii}	74.95 (16)
O2—B1—O3—Na1	165.68 (19)	O5—B4—O6—B2^{v}	−176.3 (2)
O1—B1—O3—Na1	−12.0 (4)	O8^{ix}—B4—O6—B2^{v}	2.1 (4)
O4—B3—O3—B1	−11.5 (3)	Na1—B4—O6—B2^{v}	−118.2 (3)
O7—B3—O3—B1	−135.1 (2)	Rb1^{ii}—B4—O6—B2^{v}	128.1 (3)
O5—B3—O3—B1	108.7 (2)	O5—B4—O6—Na1	−58.2 (3)
O4—B3—O3—Na1	177.71 (15)	O8^{ix}—B4—O6—Na1	120.3 (2)
O7—B3—O3—Na1	54.1 (2)	Rb1^{ii}—B4—O6—Na1	−113.76 (15)
O5—B3—O3—Na1	−62.1 (2)	O5—B4—O6—Rb1^{ii}	55.6 (3)
O6^{vii}—B2—O4—B3	−161.2 (2)	O8^{ix}—B4—O6—Rb1^{ii}	−126.0 (2)
O9^{viii}—B2—O4—B3	73.8 (3)	Na1—B4—O6—Rb1^{ii}	113.76 (15)
O2—B2—O4—B3	−45.2 (3)	O9—B5—O7—B3	−127.1 (3)
Na1^{vii}—B2—O4—B3	−105.5 (2)	O8—B5—O7—B3	55.3 (4)
Rb1^{i}—B2—O4—B3	−153.0 (2)	Rb1^{ii}—B5—O7—B3	−162.2 (3)
O6^{vii}—B2—O4—Rb1	81.4 (2)	O9—B5—O7—Rb1^{ii}	35.1 (3)
O9^{viii}—B2—O4—Rb1	−43.6 (3)	O8—B5—O7—Rb1^{ii}	−142.5 (2)
O2—B2—O4—Rb1	−162.63 (13)	O9—B5—O7—Rb1	136.2 (2)
Na1^{vii}—B2—O4—Rb1	137.07 (12)	O8—B5—O7—Rb1	−41.4 (3)
Rb1^{i}—B2—O4—Rb1	89.59 (15)	Rb1^{ii}—B5—O7—Rb1	101.11 (12)
O6^{vii}—B2—O4—Rb1^{i}	−8.2 (2)	O4—B3—O7—B5	−60.4 (3)
O9^{viii}—B2—O4—Rb1^{i}	−133.16 (18)	O5—B3—O7—B5	179.2 (2)
O2—B2—O4—Rb1^{i}	107.78 (17)	O3—B3—O7—B5	62.8 (3)
Na1^{vii}—B2—O4—Rb1^{i}	47.47 (16)	Rb1—B3—O7—B5	−116.8 (2)
O7—B3—O4—B2	158.4 (2)	O4—B3—O7—Rb1^{ii}	144.03 (15)
O5—B3—O4—B2	−81.9 (3)	O5—B3—O7—Rb1^{ii}	23.6 (3)
O3—B3—O4—B2	37.6 (3)	O3—B3—O7—Rb1^{ii}	−92.7 (2)
Rb1—B3—O4—B2	−138.8 (2)	Rb1—B3—O7—Rb1^{ii}	87.61 (16)
O7—B3—O4—Rb1	−62.82 (18)	O4—B3—O7—Rb1	56.42 (17)

O5—B3—O4—Rb1	56.89 (17)	O5—B3—O7—Rb1	−63.97 (16)
O3—B3—O4—Rb1	176.48 (17)	O3—B3—O7—Rb1	179.65 (17)
O7—B3—O4—Rb1^{i}	16.3 (3)	O7—B5—O8—B4^{x}	−179.4 (2)
O5—B3—O4—Rb1^{i}	136.02 (16)	O9—B5—O8—B4^{x}	3.0 (4)
O3—B3—O4—Rb1^{i}	−104.4 (2)	Rb1^{ii}—B5—O8—B4^{x}	96.7 (4)
Rb1—B3—O4—Rb1^{i}	79.14 (15)	O7—B5—O8—Rb1^{i}	−1.6 (4)
O6—B4—O5—B3	18.6 (4)	O9—B5—O8—Rb1^{i}	−179.15 (17)
O8^{ix}—B4—O5—B3	−159.9 (2)	Rb1^{ii}—B5—O8—Rb1^{i}	−85.5 (4)
Na1—B4—O5—B3	−19.5 (3)	O7—B5—O9—B2^{xi}	−177.7 (2)
Rb1^{iii}—B4—O5—B3	−163.3 (3)	O8—B5—O9—B2^{xi}	−0.1 (4)
Rb1^{ii}—B4—O5—B3	53.5 (3)	Rb1^{ii}—B5—O9—B2^{xi}	−144.7 (2)
O6—B4—O5—Rb1	−91.7 (3)	O7—B5—O9—Rb1^{ii}	−33.1 (2)
O8^{ix}—B4—O5—Rb1	89.8 (3)	O8—B5—O9—Rb1^{ii}	144.5 (2)
Na1—B4—O5—Rb1	−129.89 (11)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{xii}	0.82	2.11	2.869 (3)	155
O10—H10*B*···O1^{iv}	0.84	2.16	2.916 (3)	151

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