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Potassium bis(2-methyllactato)borate hemihydrate

Govindharajan Gokila,[a] Aravazhi Amalan Thiruvalluvar[b]* and Chidambaram Ramachandra Raja[a]

[a]Department of Physics, Government Arts College (Autonomous), Kumbakonam 612 002, Tamilnadu, India, and [b]Principal, Kunthavai Naacchiyaar Government Arts College for Women (Autonomous), Thanjavur 613 007, Tamilnadu, India. *Correspondence e-mail: thiruvalluvar.a@gmail.com

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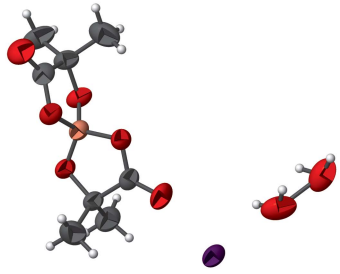
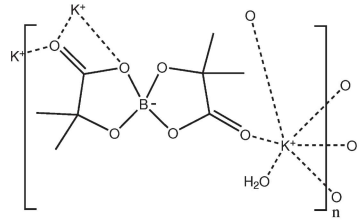
The asymmetric unit of the title organic–inorganic hybrid salt poly[aquabis[μ_3-bis(2-methyllactato)borato]dipotassium], $[K(C_8H_{12}BO_6)(H_2O)_{0.5}]_n$, consists of one bis(2-methyllactato)borate anion, one potassium cation and one water molecule that shows half occupancy due to disorder around a twofold rotation axis. The potassium cation is pseudo-octahedrally coordinated by five O atoms of four symmetry-related bis(2-methyllactato)borate ligands and by the half-occupied water molecule. O—H···O hydrogen bonds between the water molecule and one of the borate O atoms of the bis(2-methyllactato)borate ligand are present in the crystal structure.

3D view



Chemical scheme



Structure description

Lithium-based salts are used in the development of lithium-ion batteries. Allen *et al.* (2012) have reported the structure of lithium bis(2-methyllactato)borate monohydrate. In our investigations we have replaced lithium by another alkali cation, *i.e.* rubidium (Gokila *et al.*, 2019). In this context, we report here the growth and structural analysis of potassium bis(2-methyllactato)borate hemihydrate, prepared by the slow evaporation method. Whereas the lithium and rubidium salts crystallize in the space group *Pbca* with $Z = 8$ and $P2_1/n$ with $Z = 4$, respectively, the potassium title salt crystallizes in the space group $C2/c$ with $Z = 8$.

The asymmetric unit of the title compound consists of one bis(2-methyllactato)borate anion, a potassium cation and a water molecule (half occupancy) disordered about a twofold rotation axis (Fig. 1). The B—O distances (Table 1) are similar to that of the Rb analogue (Gokila *et al.*, 2019). The five-membered ring O2/C5/C6/O3/B1 adopts an envelope form on the O3 atom [puckering parameters $Q_2 = 0.177$ (3) Å, $\varphi_2 = 106.7$ (10)°] whereas the five-membered ring O4/C1/C2/O5/B1 is essentially planar (r.m.s. deviation

Table 1
Selected bond lengths (Å).

K1—O6	2.612 (2)	K1—O1^{iii}	3.101 (2)
K1—O5^{i}	2.6686 (19)	O2—B1	1.514 (4)
K1—O1^{ii}	2.674 (2)	O3—B1	1.425 (4)
K1—O2^{iii}	2.8460 (19)	O4—B1	1.498 (3)
K1—O7	2.851 (6)	O5—B1	1.427 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H1···O3^{iv}	0.83 (5)	2.49 (9)	2.870 (6)	109 (7)
O7—H2···O3^{i}	0.83 (5)	2.14 (6)	2.865 (7)	146 (6)

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

from the least-squares plane = 0.0196 Å). The dihedral angle between the above two five-membered ring planes is 89.36 (17)°. The potassium cation is pseudo-octahedrally coordinated by five O atoms from four bis(2-methyllactato)borate ligands (three monodentate, one chelating) and the half-occupied water molecule (Table 1). This arrangement leads to the formation of layers parallel to (001). In the crystal structure, these layers are linked by hydrogen bonds involving the water molecule and the O3 borate O atom (Fig. 2, Table 2).

As noted above, individual features in the crystal structure of rubidium bis(2-methyllactato)borate monohydrate (Gokila *et al.*, 2019) are very similar to those of the title compound, with the rubidium cation in a likewise pseudo-octahedral coordination sphere defined by five O atoms from four bis(2-methyllactato)borate ligands and by a fully occupied water molecule.

Synthesis and crystallization

The title compound was synthesized by reacting 2-methyllactic acid, boric acid and potassium carbonate (molar ratio 4:2:1) in

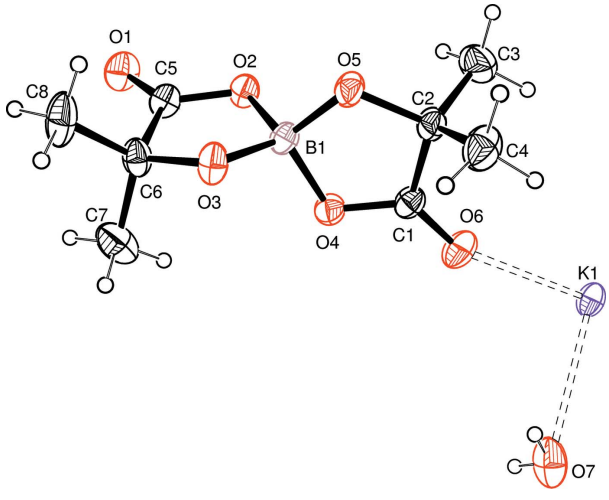


Figure 1
A view of the asymmetric unit of the title compound showing the atom numbering with displacement ellipsoids drawn at the 25% probability level.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[K(C_8H_{12}BO_6)(H_2O)_{0.5}]$
M_r	263.09
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	296
a, *b*, *c* (Å)	12.3919 (7), 10.7917 (6), 19.9794 (12)
β (°)	103.138 (2)
V (Å^3)	2601.9 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.42
Crystal size (mm)	0.15 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker Kappa APEX3 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.689, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32254, 2474, 1904
R_{int}	0.063
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.611
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.119, 1.16
No. of reflections	2474
No. of parameters	164
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.25

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

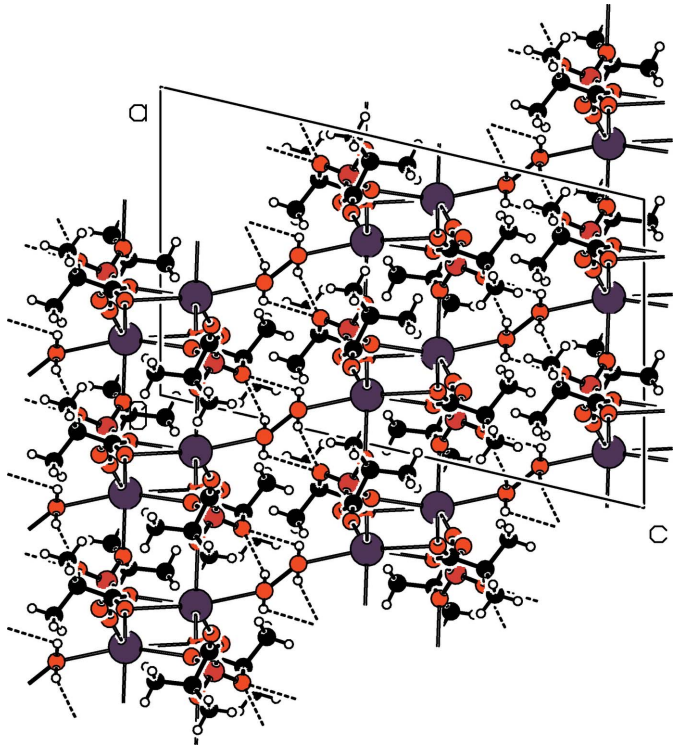


Figure 2
Packing diagram of the title compound viewed along the *b* axis. Dashed lines indicate O—H···O hydrogen bonds.

double-distilled water. Slow evaporation of the solvent yielded good quality crystals in a period of about 50 days.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The occupancy of the O atom of the water molecule (O7) was refined freely and converged with a value close to 0.5. For the final refinement it was constrained to 0.5.

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x190202 [https://doi.org/10.1107/S2414314619002025]

Potassium bis(2-methyllactato)borate hemihydrate

Govindharajan Gokila, Aravazhi Amalan Thiruvalluvar and Chidambaram Ramachandra Raja

Poly[aquabis[μ_3-bis(2-methyllactato)borato]dipotassium] [$K(C_8H_{12}BO_6)(H_2O)_{0.5}$]

Crystal data

$[K(C_8H_{12}BO_6)(H_2O)_{0.5}]$
M_r = 263.09
Monoclinic, $C2/c$
a = 12.3919 (7) Å
b = 10.7917 (6) Å
c = 19.9794 (12) Å
β = 103.138 (2)°
V = 2601.9 (3) Å^3
Z = 8
$F(000)$ = 1096
D_x = 1.343 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9798 reflections
θ = 3.0–25.6°
μ = 0.42 mm^{-1}
T = 296 K
Block, colourless
0.15 × 0.15 × 0.10 mm

Data collection

Bruker Kappa APEX3 CMOS diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.689, T_{max} = 0.745
32254 measured reflections
2474 independent reflections
1904 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 25.7°, θ_{min} = 3.4°
h = −15→15
k = −13→13
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.119
S = 1.16
2474 reflections
164 parameters
3 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 3.8042P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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.

Refinement. H atoms of the water molecule were discernable from difference Fourier maps and were refined with a distance constraint of d(O—H) = 0.85 (2) Å and U_{iso}(H) = 1.2U_{eq}(O).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
K1	0.15628 (5)	1.09153 (6)	0.42734 (4)	0.0506 (2)	
C1	0.2944 (2)	0.7909 (3)	0.39898 (15)	0.0472 (7)	
C2	0.4166 (2)	0.7875 (3)	0.43384 (15)	0.0487 (7)	
C3	0.4309 (3)	0.8111 (4)	0.51015 (18)	0.0821 (12)	
H3A	0.392100	0.748541	0.529535	0.123*	
H3B	0.401517	0.891143	0.517026	0.123*	
H3C	0.508280	0.808381	0.532212	0.123*	
C4	0.4813 (3)	0.8766 (3)	0.3993 (2)	0.0771 (11)	
H4A	0.557938	0.875484	0.423076	0.116*	
H4B	0.452259	0.958795	0.400604	0.116*	
H4C	0.474846	0.851963	0.352400	0.116*	
C5	0.3054 (2)	0.3895 (3)	0.40145 (15)	0.0480 (7)	
C6	0.3190 (3)	0.4065 (3)	0.32830 (15)	0.0528 (7)	
C7	0.2039 (3)	0.4120 (4)	0.28002 (19)	0.0860 (12)	
H7A	0.210978	0.433095	0.234536	0.129*	
H7B	0.160035	0.473708	0.296120	0.129*	
H7C	0.168503	0.332713	0.279131	0.129*	
C8	0.3929 (4)	0.3084 (3)	0.3078 (2)	0.0838 (12)	
H8A	0.465638	0.313788	0.337303	0.126*	
H8B	0.397454	0.321471	0.261032	0.126*	
H8C	0.362369	0.227842	0.312210	0.126*	
O1	0.27906 (19)	0.2950 (2)	0.42639 (12)	0.0672 (6)	
O2	0.32499 (16)	0.49337 (17)	0.43563 (9)	0.0484 (5)	
O3	0.37049 (17)	0.52461 (17)	0.33094 (10)	0.0528 (5)	
O4	0.26098 (15)	0.68262 (17)	0.37398 (10)	0.0485 (5)	
O5	0.44883 (15)	0.66399 (17)	0.42278 (11)	0.0524 (5)	
O6	0.23570 (19)	0.8815 (2)	0.39470 (13)	0.0689 (6)	
B1	0.3552 (3)	0.5923 (3)	0.38934 (17)	0.0426 (7)	
O7	0.0564 (5)	1.1217 (5)	0.2850 (3)	0.0830 (16)	0.5
H1	0.116 (3)	1.085 (6)	0.287 (5)	0.100*	0.5
H2	0.003 (4)	1.075 (5)	0.284 (4)	0.100*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0514 (4)	0.0405 (3)	0.0654 (4)	0.0067 (3)	0.0246 (3)	−0.0010 (3)
C1	0.0494 (16)	0.0434 (16)	0.0519 (17)	0.0089 (13)	0.0180 (13)	0.0010 (13)
C2	0.0488 (16)	0.0394 (14)	0.0575 (18)	0.0062 (13)	0.0112 (13)	−0.0071 (13)
C3	0.089 (3)	0.087 (3)	0.064 (2)	0.012 (2)	0.004 (2)	−0.023 (2)
C4	0.060 (2)	0.059 (2)	0.114 (3)	−0.0066 (17)	0.022 (2)	0.005 (2)
C5	0.0484 (16)	0.0454 (16)	0.0549 (17)	−0.0027 (13)	0.0219 (13)	0.0039 (14)
C6	0.070 (2)	0.0454 (16)	0.0492 (17)	−0.0095 (15)	0.0264 (15)	−0.0073 (14)
C7	0.096 (3)	0.102 (3)	0.057 (2)	−0.028 (2)	0.011 (2)	−0.006 (2)
C8	0.124 (3)	0.055 (2)	0.091 (3)	−0.002 (2)	0.063 (3)	−0.0203 (19)
O1	0.0784 (16)	0.0540 (13)	0.0759 (15)	−0.0148 (12)	0.0314 (12)	0.0125 (11)

O2	0.0640 (12)	0.0447 (11)	0.0418 (10)	0.0017 (9)	0.0231 (9)	0.0006 (9)
O3	0.0756 (14)	0.0422 (11)	0.0522 (12)	−0.0075 (10)	0.0384 (11)	−0.0040 (9)
O4	0.0395 (10)	0.0466 (11)	0.0583 (12)	0.0044 (9)	0.0089 (9)	−0.0035 (9)
O5	0.0405 (11)	0.0397 (10)	0.0752 (14)	0.0069 (8)	0.0092 (9)	−0.0081 (10)
O6	0.0674 (14)	0.0531 (13)	0.0881 (17)	0.0248 (11)	0.0218 (12)	−0.0003 (12)
B1	0.0435 (16)	0.0383 (15)	0.0492 (18)	0.0034 (14)	0.0177 (14)	0.0007 (14)
O7	0.112 (4)	0.074 (3)	0.082 (3)	−0.023 (3)	0.061 (3)	−0.024 (3)

Geometric parameters (Å, º)

K1—O6	2.612 (2)	C4—H4C	0.9600
K1—O5^{i}	2.6686 (19)	C5—O1	1.212 (3)
K1—O1^{ii}	2.674 (2)	C5—O2	1.307 (3)
K1—O2^{iii}	2.8460 (19)	C5—C6	1.520 (4)
K1—O7	2.851 (6)	C6—O3	1.421 (3)
K1—O1^{iii}	3.101 (2)	C6—C8	1.515 (4)
K1—C5^{iii}	3.351 (3)	C6—C7	1.530 (5)
K1—K1^{iv}	4.7390 (13)	C7—H7A	0.9600
K1—H1	2.74 (9)	C7—H7B	0.9600
K1—H2	3.05 (7)	C7—H7C	0.9600
C1—O6	1.210 (3)	C8—H8A	0.9600
C1—O4	1.301 (3)	C8—H8B	0.9600
C1—C2	1.517 (4)	C8—H8C	0.9600
C2—O5	1.423 (3)	O2—B1	1.514 (4)
C2—C4	1.515 (4)	O3—B1	1.425 (4)
C2—C3	1.516 (4)	O4—B1	1.498 (3)
C3—H3A	0.9600	O5—B1	1.427 (4)
C3—H3B	0.9600	O7—O7^{v}	1.738 (13)
C3—H3C	0.9600	O7—H1	0.83 (2)
C4—H4A	0.9600	O7—H2	0.83 (2)
C4—H4B	0.9600		

O6—K1—O5^{i}	131.34 (7)	O1—C5—O2	122.9 (3)
O6—K1—O1^{ii}	117.60 (8)	O1—C5—C6	126.6 (3)
O5^{i}—K1—O1^{ii}	107.73 (7)	O2—C5—C6	110.5 (2)
O6—K1—O2^{iii}	90.45 (7)	O1—C5—K1^{iii}	67.72 (17)
O5^{i}—K1—O2^{iii}	89.68 (6)	O2—C5—K1^{iii}	56.47 (13)
O1^{ii}—K1—O2^{iii}	110.43 (7)	C6—C5—K1^{iii}	162.42 (19)
O6—K1—O7	87.30 (12)	O3—C6—C8	110.0 (3)
O5^{i}—K1—O7	74.69 (12)	O3—C6—C5	102.7 (2)
O1^{ii}—K1—O7	91.02 (11)	C8—C6—C5	112.4 (3)
O2^{iii}—K1—O7	156.71 (12)	O3—C6—C7	109.6 (3)
O6—K1—O1^{iii}	123.14 (7)	C8—C6—C7	113.0 (3)
O5^{i}—K1—O1^{iii}	87.54 (6)	C5—C6—C7	108.7 (3)
O1^{ii}—K1—O1^{iii}	69.93 (7)	C6—C7—H7A	109.5
O2^{iii}—K1—O1^{iii}	43.41 (6)	C6—C7—H7B	109.5
O7—K1—O1^{iii}	148.82 (11)	H7A—C7—H7B	109.5
O6—K1—C5^{iii}	109.51 (7)	C6—C7—H7C	109.5

O5^{i}—K1—C5^{iii}	85.92 (7)	H7A—C7—H7C	109.5
O1^{ii}—K1—C5^{iii}	90.47 (7)	H7B—C7—H7C	109.5
O2^{iii}—K1—C5^{iii}	22.50 (6)	C6—C8—H8A	109.5
O7—K1—C5^{iii}	160.05 (12)	C6—C8—H8B	109.5
O1^{iii}—K1—C5^{iii}	21.20 (6)	H8A—C8—H8B	109.5
O6—K1—K1^{iv}	128.25 (6)	C6—C8—H8C	109.5
O5^{i}—K1—K1^{iv}	98.26 (5)	H8A—C8—H8C	109.5
O1^{ii}—K1—K1^{iv}	37.93 (5)	H8B—C8—H8C	109.5
O2^{iii}—K1—K1^{iv}	73.83 (4)	C5—O1—K1^{vi}	154.3 (2)
O7—K1—K1^{iv}	124.74 (10)	C5—O1—K1^{iii}	91.08 (19)
O1^{iii}—K1—K1^{iv}	32.00 (4)	K1^{vi}—O1—K1^{iii}	110.07 (7)
C5^{iii}—K1—K1^{iv}	52.73 (5)	C5—O2—B1	109.2 (2)
O6—C1—O4	124.4 (3)	C5—O2—K1^{iii}	101.03 (16)
O6—C1—C2	125.0 (3)	B1—O2—K1^{iii}	146.83 (16)
O4—C1—C2	110.6 (2)	C6—O3—B1	110.4 (2)
O5—C2—C4	109.1 (2)	C1—O4—B1	109.9 (2)
O5—C2—C3	109.9 (3)	C2—O5—B1	110.7 (2)
C4—C2—C3	113.5 (3)	C2—O5—K1^{vii}	124.83 (16)
O5—C2—C1	103.7 (2)	B1—O5—K1^{vii}	122.08 (15)
C4—C2—C1	110.6 (3)	C1—O6—K1	159.7 (2)
C3—C2—C1	109.5 (3)	O3—B1—O5	114.6 (2)
C2—C3—H3A	109.5	O3—B1—O4	114.1 (2)
C2—C3—H3B	109.5	O5—B1—O4	104.8 (2)
H3A—C3—H3B	109.5	O3—B1—O2	103.6 (2)
C2—C3—H3C	109.5	O5—B1—O2	112.6 (2)
H3A—C3—H3C	109.5	O4—B1—O2	107.1 (2)
H3B—C3—H3C	109.5	O7^{v}—O7—K1	152.9 (4)
C2—C4—H4A	109.5	O7^{v}—O7—H1	125 (6)
C2—C4—H4B	109.5	K1—O7—H1	74 (7)
H4A—C4—H4B	109.5	O7^{v}—O7—H2	60 (6)
C2—C4—H4C	109.5	K1—O7—H2	96 (6)
H4A—C4—H4C	109.5	H1—O7—H2	114 (4)
H4B—C4—H4C	109.5		

O6—C1—C2—O5	−177.6 (3)	O6—C1—O4—B1	−179.5 (3)
O4—C1—C2—O5	2.3 (3)	C2—C1—O4—B1	0.7 (3)
O6—C1—C2—C4	−60.7 (4)	C4—C2—O5—B1	−122.4 (3)
O4—C1—C2—C4	119.1 (3)	C3—C2—O5—B1	112.6 (3)
O6—C1—C2—C3	65.1 (4)	C1—C2—O5—B1	−4.4 (3)
O4—C1—C2—C3	−115.0 (3)	C4—C2—O5—K1^{vii}	40.3 (3)
O1—C5—C6—O3	−169.1 (3)	C3—C2—O5—K1^{vii}	−84.7 (3)
O2—C5—C6—O3	11.7 (3)	C1—C2—O5—K1^{vii}	158.28 (16)
K1^{iii}—C5—C6—O3	−27.9 (8)	O4—C1—O6—K1	147.2 (5)
O1—C5—C6—C8	−51.0 (4)	C2—C1—O6—K1	−33.0 (8)
O2—C5—C6—C8	129.9 (3)	C6—O3—B1—O5	141.7 (3)
K1^{iii}—C5—C6—C8	90.2 (7)	C6—O3—B1—O4	−97.4 (3)
O1—C5—C6—C7	74.9 (4)	C6—O3—B1—O2	18.6 (3)
O2—C5—C6—C7	−104.3 (3)	C2—O5—B1—O3	130.7 (3)

K1^{iii}—C5—C6—C7	−143.9 (6)	K1^{vii}—O5—B1—O3	−32.6 (3)
O2—C5—O1—K1^{vi}	133.4 (4)	C2—O5—B1—O4	4.8 (3)
C6—C5—O1—K1^{vi}	−45.7 (6)	K1^{vii}—O5—B1—O4	−158.41 (15)
K1^{iii}—C5—O1—K1^{vi}	146.1 (5)	C2—O5—B1—O2	−111.2 (3)
O2—C5—O1—K1^{iii}	−12.7 (3)	K1^{vii}—O5—B1—O2	85.5 (2)
C6—C5—O1—K1^{iii}	168.2 (3)	C1—O4—B1—O3	−129.5 (2)
O1—C5—O2—B1	−179.8 (3)	C1—O4—B1—O5	−3.3 (3)
C6—C5—O2—B1	−0.6 (3)	C1—O4—B1—O2	116.4 (2)
K1^{iii}—C5—O2—B1	166.1 (2)	C5—O2—B1—O3	−10.8 (3)
O1—C5—O2—K1^{iii}	14.1 (3)	K1^{iii}—O2—B1—O3	143.6 (2)
C6—C5—O2—K1^{iii}	−166.6 (2)	C5—O2—B1—O5	−135.1 (2)
C8—C6—O3—B1	−138.6 (3)	K1^{iii}—O2—B1—O5	19.3 (4)
C5—C6—O3—B1	−18.8 (3)	C5—O2—B1—O4	110.2 (2)
C7—C6—O3—B1	96.6 (3)	K1^{iii}—O2—B1—O4	−95.4 (3)

Symmetry codes: (i) *x*−1/2, *y*+1/2, *z*; (ii) *x*, *y*+1, *z*; (iii) −*x*+1/2, −*y*+3/2, −*z*+1; (iv) −*x*+1/2, −*y*+5/2, −*z*+1; (v) −*x*, *y*, −*z*+1/2; (vi) *x*, *y*−1, *z*; (vii) *x*+1/2, *y*−1/2, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H1···O3^{viii}	0.83 (5)	2.49 (9)	2.870 (6)	109 (7)
O7—H2···O3^{i}	0.83 (5)	2.14 (6)	2.865 (7)	146 (6)

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