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ISSN 2414-3146

Sodium bis(2-methyllactato)borate

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Received 24 April 2019
Accepted 29 April 2019

Edited by M. Weil, Vienna University of Technology, Austria

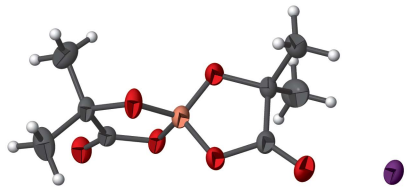
Keywords: crystal structure; inorganic–organic hybrid material; borate.

CCDC reference: 1912840

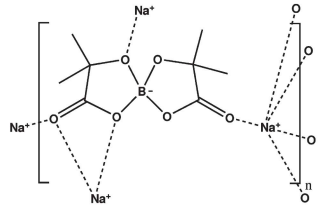
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title organic–inorganic hybrid salt, poly[[μ_4-bis(2-methyllactato)borato]sodium], $[Na(C_8H_{12}BO_6)]_n$, comprises a sodium cation and a bis(2-methyllactato)borate anion. The sodium cation exhibits a [4 + 1] coordination by borate and carbonyl O atoms of the bis(2-methyllactato)borate anion, leading to a three-dimensional polymeric structure.

3D view



Chemical scheme



Structure description

Alkaline cations such as lithium, potassium and sodium, together with different anions, are used in the development of rechargeable batteries. Allen *et al.* (2012) have reported the structure of lithium bis(2-methyllactato)borate monohydrate. In our current investigation we have replaced lithium by sodium and report here the growth and structural analysis of sodium bis(2-methyllactato)borate, $[Na(C_8H_{12}BO_6)]_n$, prepared by the slow evaporation method. Whereas other alkaline bis(2-methyllactato)borate salts crystallize as hydrates (Li as a monohydrate, Allen *et al.*, 2012; K as a hemihydrate, Gokila *et al.*, 2019*a*; Rb as a monohydrate; Golika *et al.*, 2019*b*), the title sodium salt is anhydrous.

The asymmetric unit of the title compound comprises a sodium cation and a bis(2-methyllactato)borate anion (Fig. 1). The sodium cation is surrounded in a pseudo-tetrahedral manner by four O atoms (O1, O4^{i}, O6^{iii} and O6^{ii}; for symmetry codes: see Table 1) at short distances. The τ_4 descriptor (Yang *et al.*, 2007) amounts to 0.81 (extreme forms 0 for ideal square-planar and 1 for ideal tetrahedral coordination). However, the coordination sphere around Na1 is augmented by a fifth O atom (O5^{iii}) at a considerably longer distances (Table 1). In the anion, the five-membered ring O2/C1/C2/O3/B1 is essentially planar [r.m.s. deviation 0.0312 Å, with the greatest deviation for O3 of 0.045 (1) Å], whereas ring O4/C6/C5/O5/B1 has a conformation between planar and an envelope form [puckering parameters Q_2 = 0.1015 (17) Å, φ_2 = 172.9 (9)°]. The dihedral

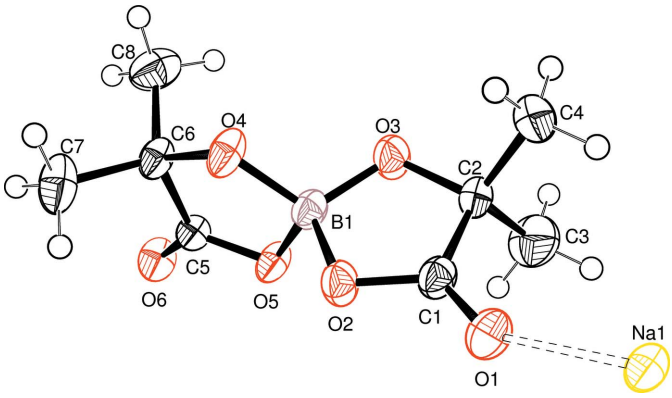


Figure 1
A view of the asymmetric unit of the title compound showing the atom numbering with displacement ellipsoids drawn at the 50% probability level.

angle between these two rings is 89.81 (9)°. The packing of the three-dimensional polymeric crystal structure is shown in Fig. 2.

Synthesis and crystallization

The title compound was synthesized by reacting 2-methyllactic acid, boric acid and sodium carbonate (molar ratio 4:2:1) in double-distilled water. Slow evaporation of the solvent yielded good quality crystals over a period of about three months.

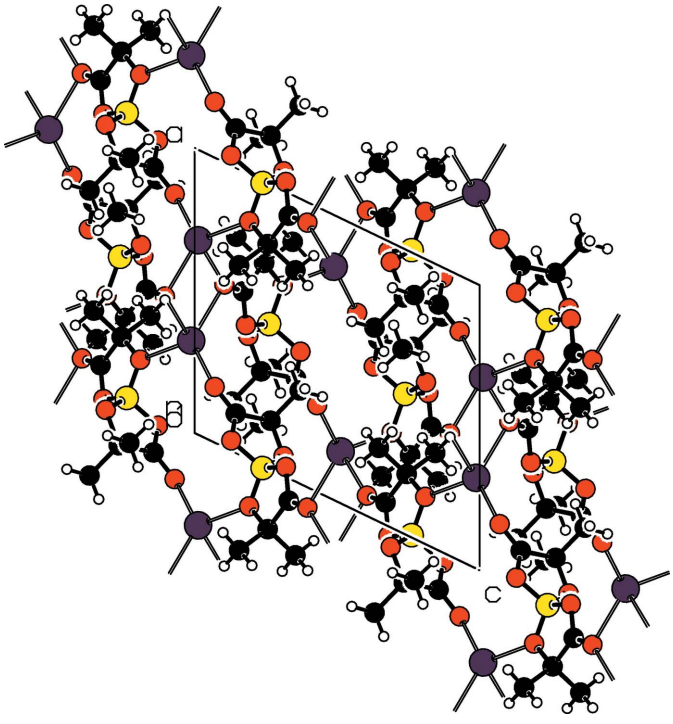


Figure 2
Packing diagram of the title compound viewed along the *b* axis.

Table 1
Selected bond lengths (Å).

Na1—O1	2.2262 (12)	O5—B1	1.528 (2)
Na1—O4^{i}	2.2733 (12)	O4—B1	1.447 (2)
Na1—O6^{ii}	2.3149 (12)	O2—B1	1.492 (2)
Na1—O6^{iii}	2.3880 (13)	O3—B1	1.417 (2)
Na1—O5^{iii}	2.8768 (12)		

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Na(C_8H_{12}BO_6)]$
M_r	237.98
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	10.1398 (5), 10.8359 (6), 11.2588 (5)
β (°)	115.687 (3)
V (Å^3)	1114.80 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.15
Crystal size (mm)	0.20 × 0.20 × 0.15
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.711, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23270, 2425, 1844
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.096, 1.04
No. of reflections	2425
No. of parameters	145
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.25

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *ORTEP-3 for Windows* (Farrugia, 2012), *SHELXL2018* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors thank the Sophisticated Analytical Instrument Facility (SAIF), Indian Institute of Technology Madras (IITM), Chennai 600 036, Tamilnadu, India, for the single-crystal X-ray diffraction data.

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full crystallographic data

IUCrData (2019). **4**, x190593 [https://doi.org/10.1107/S2414314619005935]

Sodium bis(2-methyllactato)borate

Govindharajan Gokila, Aravazhi Amalan Thiruvalluvar and Chidambaram Ramachandra Raja

Poly[[μ_4-bis(2-methyllactato)borato]sodium]

Crystal data

$[Na(C_8H_{12}BO_6)]$
M_r = 237.98
Monoclinic, $P2_1/n$
a = 10.1398 (5) Å
b = 10.8359 (6) Å
c = 11.2588 (5) Å
β = 115.687 (3)°
V = 1114.80 (10) Å^3
Z = 4
$F(000)$ = 496
D_x = 1.418 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6833 reflections
θ = 2.8–24.0°
μ = 0.15 mm^{-1}
T = 296 K
Block, colourless
0.20 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.711, T_{max} = 0.746
23270 measured reflections
2425 independent reflections
1844 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.0°, θ_{min} = 2.3°
h = −12→12
k = −13→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.096
S = 1.04
2425 reflections
145 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.3964P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Na1	0.18199 (6)	0.45991 (6)	0.51222 (6)	0.03053 (18)
O5	0.46526 (11)	0.77164 (10)	0.18007 (11)	0.0313 (3)
O4	0.66535 (11)	0.65000 (11)	0.30890 (12)	0.0350 (3)
O2	0.46401 (12)	0.66651 (10)	0.37142 (11)	0.0324 (3)
O3	0.43130 (13)	0.54882 (11)	0.18818 (12)	0.0369 (3)
O6	0.57136 (12)	0.90904 (11)	0.10432 (11)	0.0366 (3)
O1	0.30453 (14)	0.57492 (12)	0.42985 (13)	0.0444 (3)
C5	0.57869 (16)	0.81707 (14)	0.16973 (15)	0.0261 (3)
C6	0.71409 (16)	0.74006 (15)	0.24391 (15)	0.0286 (4)
C1	0.36231 (17)	0.58448 (15)	0.35573 (16)	0.0301 (4)
C2	0.32873 (17)	0.50650 (15)	0.23385 (17)	0.0312 (4)
C7	0.83631 (19)	0.81732 (18)	0.34405 (19)	0.0463 (5)
H7A	0.867862	0.877269	0.299050	0.069*
H7B	0.801478	0.858795	0.400292	0.069*
H7C	0.917013	0.764826	0.396243	0.069*
C4	0.3549 (2)	0.37084 (17)	0.2705 (2)	0.0456 (5)
H4A	0.285302	0.342945	0.301244	0.068*
H4B	0.343855	0.323734	0.194535	0.068*
H4C	0.452253	0.360107	0.338941	0.068*
C8	0.7591 (2)	0.67706 (19)	0.1464 (2)	0.0482 (5)
H8A	0.791616	0.738048	0.103218	0.072*
H8B	0.837097	0.620028	0.192549	0.072*
H8C	0.676838	0.633343	0.081969	0.072*
B1	0.50800 (19)	0.65314 (17)	0.26160 (18)	0.0283 (4)
C3	0.1733 (2)	0.5293 (2)	0.1311 (2)	0.0565 (6)
H3A	0.105661	0.500202	0.163653	0.085*
H3B	0.158845	0.616150	0.113199	0.085*
H3C	0.157003	0.486080	0.051534	0.085*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0254 (3)	0.0345 (4)	0.0338 (4)	0.0025 (3)	0.0148 (3)	0.0069 (3)
O5	0.0213 (5)	0.0356 (6)	0.0378 (6)	0.0034 (4)	0.0135 (5)	0.0119 (5)
O4	0.0239 (6)	0.0373 (7)	0.0439 (7)	0.0033 (5)	0.0147 (5)	0.0217 (5)
O2	0.0357 (6)	0.0326 (6)	0.0334 (6)	−0.0093 (5)	0.0194 (5)	−0.0019 (5)
O3	0.0419 (7)	0.0385 (7)	0.0406 (7)	−0.0120 (5)	0.0274 (6)	−0.0075 (5)
O6	0.0341 (6)	0.0336 (6)	0.0399 (7)	0.0028 (5)	0.0140 (5)	0.0173 (5)
O1	0.0528 (8)	0.0449 (8)	0.0536 (8)	−0.0071 (6)	0.0401 (7)	0.0007 (6)
C5	0.0258 (7)	0.0270 (8)	0.0257 (8)	0.0010 (6)	0.0113 (6)	0.0038 (6)
C6	0.0230 (7)	0.0302 (8)	0.0325 (8)	0.0015 (6)	0.0120 (7)	0.0127 (7)
C1	0.0283 (8)	0.0294 (8)	0.0359 (9)	0.0004 (6)	0.0171 (7)	0.0062 (7)
C2	0.0272 (8)	0.0316 (9)	0.0379 (9)	−0.0057 (7)	0.0172 (7)	−0.0021 (7)
C7	0.0315 (9)	0.0516 (12)	0.0443 (11)	−0.0089 (8)	0.0058 (8)	0.0130 (9)
C4	0.0492 (11)	0.0326 (10)	0.0636 (13)	−0.0076 (8)	0.0326 (10)	−0.0041 (9)

C8	0.0500 (11)	0.0490 (12)	0.0569 (12)	0.0128 (9)	0.0338 (10)	0.0137 (10)
B1	0.0254 (8)	0.0307 (10)	0.0316 (9)	0.0000 (7)	0.0151 (8)	0.0054 (7)
C3	0.0344 (10)	0.0682 (15)	0.0542 (13)	−0.0007 (10)	0.0074 (9)	−0.0095 (11)

Geometric parameters (Å, º)

Na1—O1	2.2262 (12)	C6—C7	1.515 (2)
Na1—O4^{i}	2.2733 (12)	C6—C8	1.521 (2)
Na1—O6^{ii}	2.3149 (12)	C1—C2	1.519 (2)
Na1—O6^{iii}	2.3880 (13)	C2—C3	1.518 (3)
Na1—O5^{iii}	2.8768 (12)	C2—C4	1.519 (3)
Na1—C5^{iii}	2.9808 (16)	C7—H7A	0.9600
Na1—Na1^{iv}	3.6840 (12)	C7—H7B	0.9600
O5—C5	1.3019 (18)	C7—H7C	0.9600
O5—B1	1.528 (2)	C4—H4A	0.9600
O4—C6	1.4302 (18)	C4—H4B	0.9600
O4—B1	1.447 (2)	C4—H4C	0.9600
O2—C1	1.3141 (18)	C8—H8A	0.9600
O2—B1	1.492 (2)	C8—H8B	0.9600
O3—B1	1.417 (2)	C8—H8C	0.9600
O3—C2	1.4211 (18)	C3—H3A	0.9600
O6—C5	1.2221 (18)	C3—H3B	0.9600
O1—C1	1.2141 (19)	C3—H3C	0.9600
C5—C6	1.512 (2)		
O1—Na1—O4^{i}	111.94 (5)	O4—C6—C8	109.95 (14)
O1—Na1—O6^{ii}	108.03 (5)	C5—C6—C8	109.50 (13)
O4^{i}—Na1—O6^{ii}	101.58 (5)	C7—C6—C8	112.37 (14)
O1—Na1—O6^{iii}	124.20 (5)	O1—C1—O2	123.35 (16)
O4^{i}—Na1—O6^{iii}	121.54 (5)	O1—C1—C2	125.97 (15)
O6^{ii}—Na1—O6^{iii}	76.88 (4)	O2—C1—C2	110.68 (13)
O1—Na1—O5^{iii}	106.55 (5)	O3—C2—C3	110.67 (15)
O4^{i}—Na1—O5^{iii}	103.13 (5)	O3—C2—C4	109.96 (13)
O6^{ii}—Na1—O5^{iii}	125.30 (4)	C3—C2—C4	111.50 (15)
O6^{iii}—Na1—O5^{iii}	48.62 (3)	O3—C2—C1	103.57 (12)
O1—Na1—C5^{iii}	119.55 (5)	C3—C2—C1	110.47 (14)
O4^{i}—Na1—C5^{iii}	113.41 (5)	C4—C2—C1	110.40 (14)
O6^{ii}—Na1—C5^{iii}	99.72 (4)	C6—C7—H7A	109.5
O6^{iii}—Na1—C5^{iii}	23.11 (4)	C6—C7—H7B	109.5
O5^{iii}—Na1—C5^{iii}	25.60 (4)	H7A—C7—H7B	109.5
O1—Na1—Na1^{iv}	123.97 (4)	C6—C7—H7C	109.5
O4^{i}—Na1—Na1^{iv}	117.72 (4)	H7A—C7—H7C	109.5
O6^{ii}—Na1—Na1^{iv}	39.15 (3)	H7B—C7—H7C	109.5
O6^{iii}—Na1—Na1^{iv}	37.73 (3)	C2—C4—H4A	109.5
O5^{iii}—Na1—Na1^{iv}	86.25 (3)	C2—C4—H4B	109.5
C5^{iii}—Na1—Na1^{iv}	60.65 (3)	H4A—C4—H4B	109.5
C5—O5—B1	109.88 (11)	C2—C4—H4C	109.5
C5—O5—Na1^{v}	81.67 (8)	H4A—C4—H4C	109.5

B1—O5—Na1^{v}	165.39 (9)	H4B—C4—H4C	109.5
C6—O4—B1	111.48 (11)	C6—C8—H8A	109.5
C6—O4—Na1^{i}	123.86 (9)	C6—C8—H8B	109.5
B1—O4—Na1^{i}	123.86 (9)	H8A—C8—H8B	109.5
C1—O2—B1	108.78 (12)	C6—C8—H8C	109.5
B1—O3—C2	110.42 (12)	H8A—C8—H8C	109.5
C5—O6—Na1^{vi}	148.81 (11)	H8B—C8—H8C	109.5
C5—O6—Na1^{v}	106.82 (10)	O3—B1—O4	115.76 (14)
Na1^{vi}—O6—Na1^{v}	103.12 (4)	O3—B1—O2	105.97 (12)
C1—O1—Na1	148.96 (12)	O4—B1—O2	112.04 (14)
O6—C5—O5	122.47 (14)	O3—B1—O5	112.26 (14)
O6—C5—C6	125.92 (14)	O4—B1—O5	102.78 (12)
O5—C5—C6	111.59 (12)	O2—B1—O5	107.90 (13)
O6—C5—Na1^{v}	50.08 (8)	C2—C3—H3A	109.5
O5—C5—Na1^{v}	72.73 (8)	C2—C3—H3B	109.5
C6—C5—Na1^{v}	171.45 (10)	H3A—C3—H3B	109.5
O4—C6—C5	103.11 (11)	C2—C3—H3C	109.5
O4—C6—C7	110.41 (13)	H3A—C3—H3C	109.5
C5—C6—C7	111.11 (14)	H3B—C3—H3C	109.5

Na1^{vi}—O6—C5—O5	−170.73 (14)	B1—O3—C2—C4	−125.15 (15)
Na1^{v}—O6—C5—O5	−7.54 (19)	B1—O3—C2—C1	−7.18 (17)
Na1^{vi}—O6—C5—C6	7.2 (3)	O1—C1—C2—O3	−176.35 (16)
Na1^{v}—O6—C5—C6	170.42 (13)	O2—C1—C2—O3	4.00 (17)
Na1^{vi}—O6—C5—Na1^{v}	−163.2 (2)	O1—C1—C2—C3	65.1 (2)
B1—O5—C5—O6	176.78 (15)	O2—C1—C2—C3	−114.54 (16)
Na1^{v}—O5—C5—O6	6.05 (15)	O1—C1—C2—C4	−58.7 (2)
B1—O5—C5—C6	−1.44 (18)	O2—C1—C2—C4	121.67 (15)
Na1^{v}—O5—C5—C6	−172.17 (12)	C2—O3—B1—O4	132.54 (14)
B1—O5—C5—Na1^{v}	170.74 (11)	C2—O3—B1—O2	7.69 (17)
B1—O4—C6—C5	10.23 (17)	C2—O3—B1—O5	−109.88 (14)
Na1^{i}—O4—C6—C5	−159.78 (10)	C6—O4—B1—O3	111.76 (16)
B1—O4—C6—C7	129.00 (15)	Na1^{i}—O4—B1—O3	−78.23 (17)
Na1^{i}—O4—C6—C7	−41.01 (18)	C6—O4—B1—O2	−126.57 (14)
B1—O4—C6—C8	−106.45 (16)	Na1^{i}—O4—B1—O2	43.44 (18)
Na1^{i}—O4—C6—C8	83.53 (15)	C6—O4—B1—O5	−10.99 (17)
O6—C5—C6—O4	176.60 (15)	Na1^{i}—O4—B1—O5	159.02 (9)
O5—C5—C6—O4	−5.25 (17)	C1—O2—B1—O3	−5.00 (17)
O6—C5—C6—C7	58.3 (2)	C1—O2—B1—O4	−132.13 (14)
O5—C5—C6—C7	−123.53 (15)	C1—O2—B1—O5	115.44 (14)
O6—C5—C6—C8	−66.4 (2)	C5—O5—B1—O3	−117.61 (14)
O5—C5—C6—C8	111.76 (15)	Na1^{v}—O5—B1—O3	23.2 (4)
Na1—O1—C1—O2	−157.82 (16)	C5—O5—B1—O4	7.45 (17)
Na1—O1—C1—C2	22.6 (3)	Na1^{v}—O5—B1—O4	148.3 (3)
B1—O2—C1—O1	−179.09 (16)	C5—O5—B1—O2	125.98 (13)

B1—O2—C1—C2	0.58 (17)	Na1^{v}—O5—B1—O2	−93.2 (4)
B1—O3—C2—C3	111.22 (16)		

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