

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

 Poly[[μ -1,4-anhydroerythritolato-di- μ -aqua-sodium(I)] monohydrate]

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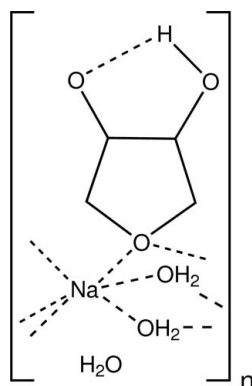
Received 31 October 2008; accepted 25 November 2008

 Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.032; wR factor = 0.086; data-to-parameter ratio = 14.4.

In the title compound, $[\text{Na}(\text{C}_4\text{H}_7\text{O}_3)(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}]_n$, the sodium ion is octahedrally coordinated by two bridging 1,4-anhydroerythritolate ligands, unexpectedly coordinated by the ring oxygen and four water ligands. This bonding pattern leads to one-dimensional antitactical polymeric chains along [010]. One of the exocyclic O atoms of the anhydroerythritolate group is an acceptor in four hydrogen bonds, giving further evidence that it is deprotonated.

Related literature

For the neutral 1,4-anhydroerythritole as a coordination ligand on sodium with either the hydroxyl groups coordinating sodium or a mixed coordination by both the ring oxygen and the hydroxyl groups, see: Ballard *et al.* (1974, 1976). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

 $[\text{Na}(\text{C}_4\text{H}_7\text{O}_3)(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$
 $M_r = 180.13$

 Monoclinic, $C2/c$
 $a = 23.155$ (6) Å
 $b = 6.0900$ (16) Å
 $c = 14.543$ (5) Å
 $\beta = 127.678$ (17)°
 $V = 1623.1$ (9) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.18$ mm⁻¹
 $T = 200$ (2) K
 $0.23 \times 0.20 \times 0.10$ mm

Data collection

 Oxford Diffraction XCalibur diffractometer
 Absorption correction: none
 6310 measured reflections

 1699 independent reflections
 1088 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.086$
 $S = 0.95$
 1699 reflections
 118 parameters
 9 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O2}-\text{H2} \cdots \text{O3}$	0.82	1.85	2.4367 (17)	127
$\text{O4}-\text{H41} \cdots \text{O3}^{\text{i}}$	0.839 (14)	1.939 (15)	2.7706 (17)	170.9 (17)
$\text{O4}-\text{H42} \cdots \text{O3}^{\text{ii}}$	0.883 (14)	1.827 (14)	2.7078 (19)	174.5 (18)
$\text{O6}-\text{H61} \cdots \text{O2}^{\text{ii}}$	0.877 (14)	1.940 (14)	2.813 (2)	173.1 (18)
$\text{O6}-\text{H62} \cdots \text{O5}^{\text{iii}}$	0.859 (14)	1.838 (14)	2.6903 (18)	171.0 (18)
$\text{O5}-\text{H51} \cdots \text{O3}^{\text{i}}$	0.842 (15)	1.825 (15)	2.6653 (18)	176 (2)
$\text{O5}-\text{H52} \cdots \text{O2}^{\text{iv}}$	0.828 (14)	2.131 (15)	2.958 (2)	177 (2)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP III* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

TK is indebted to the Hanns-Seidel Stiftung for a PhD grant funded by the German Bundesministerium für Bildung und Forschung.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2067).

References

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supplementary materials

Acta Cryst. (2008). E64, m1637 [doi:10.1107/S1600536808039640]

Poly[[μ -1,4-anhydroerythritolato-di- μ -aqua-sodium(I)] monohydrate]

T. Kerscher, P. Zeller, P. Mayer and P. Klüfers

Comment

The title compound was obtained as a byproduct in a reaction involving sodium hydroxide, anhydroerythritole and iron(II) chloride. .

Sodium is octahedrally coordinated by bridging anhydroerythritolate and water ligands. The anhydroerythritolate coordinates the sodium unexpectedly by its ring oxygen atom while the alkoxide group is stabilized by intramolecular hydrogen bonding from the hydroxyl group. The anhydroerythritolate contains a five-membered ring containing O1, C1, C2, C3 and C4 which can be described according to Cremer & Pople (1975) by the puckering parameters $q_2 = 0.3903 \text{ \AA}$ and $\Phi_2 = 180.9772$. The closest pucker descriptor is an envelope E_{O1} .

The bridging ligands lead to a linear chain-like structure along [010] which resembles an antitactical polymer well known from organic chemistry.

Experimental

The title compound was obtained as a byproduct by the reaction of 40 mMol anhydroerythritol with 160 mMol sodiumhydroxide in 15 mL water at room temperature.

Upon standing for about 14 days at room temperature, colorless platelets of the title compound crystalized from the solution.

Refinement

Carbon hydrogen atoms and hydroxide hydrogen atoms were calculated in ideal geometry with $U(H)=1.2*U(C)$ for all C-bound hydrogen atoms and $U(H)=1.5*U(O)$ for the hydroxide hydrogen atom. The water-bound hydrogen atoms were found from the difference map, the O-H distances were fixed to 0.84 \AA and the H-H distances within the water molecules were fixed to 1.36 \AA .

Figures

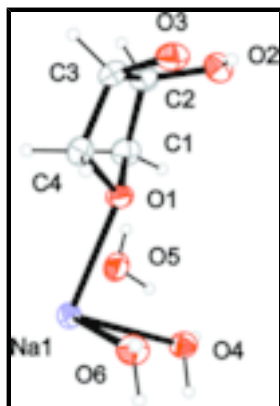


Fig. 1. The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

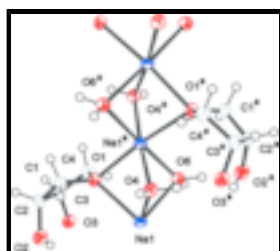


Fig. 2. Part of the antitactical polymer-like chain structure of the title compound along [010]. Symmetry code: (iii) $-x + 1/2, y - 1/2, -z + 1/2$.

Poly[[μ -1,4-anhydroerythritolato-di- μ -aqua-sodium(I)] monohydrate]

Crystal data

$[\text{Na}(\text{C}_4\text{H}_7\text{O}_3)(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}_1$

$M_r = 180.13$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 23.155\ (6)\ \text{\AA}$

$b = 6.0900\ (16)\ \text{\AA}$

$c = 14.543\ (5)\ \text{\AA}$

$\beta = 127.678\ (17)^\circ$

$V = 1623.1\ (9)\ \text{\AA}^3$

$Z = 8$

$F_{000} = 768$

$D_x = 1.474\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2600 reflections

$\theta = 3.8\text{--}26.5^\circ$

$\mu = 0.18\ \text{mm}^{-1}$

$T = 200\ (2)\ \text{K}$

Platelet, colourless

$0.23 \times 0.20 \times 0.10\ \text{mm}$

Data collection

Oxford Diffraction KappaCCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 200\ (2)\ \text{K}$

ω scans

Absorption correction: none

1088 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\text{max}} = 26.5^\circ$

$\theta_{\text{min}} = 4.2^\circ$

$h = -21 \rightarrow 28$

$k = -7 \rightarrow 6$

6310 measured reflections
1699 independent reflections

$l = -17 \rightarrow 18$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.032$

H atoms treated by a mixture of independent and constrained refinement

$wR(F^2) = 0.086$

$$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2]$$

where $P = (F_o^2 + 2F_c^2)/3$

$S = 0.95$

$(\Delta/\sigma)_{\max} < 0.001$

1699 reflections

$\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$

118 parameters

$\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

9 restraints

Extinction correction: none

Primary atom site location: structure-invariant direct methods

Special details

Refinement. Carbon hydrogen atoms and hydroxide hydrogen atoms were calculated in ideal geometry with $U(\text{H})=1.2*U(\text{C})$ for all C-bound hydrogen atoms and $U(\text{H})=1.5*U(\text{O})$ for the hydroxide hydrogen atom. The water-bound hydrogen atoms were found from the difference map, the O-H distances were restrained to 0.84 Å and the H-H distances within the water molecules were restrained to 1.36 Å.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Na1	0.24809 (3)	0.43051 (10)	0.24000 (5)	0.0238 (2)
O1	0.16736 (6)	0.16529 (17)	0.09168 (9)	0.0238 (3)
O2	0.05729 (6)	-0.21567 (19)	-0.03931 (10)	0.0322 (3)
H2	0.0846	-0.2907	-0.0445	0.048*
O3	0.14255 (6)	-0.19459 (18)	-0.08460 (9)	0.0295 (3)
O4	0.24091 (7)	0.19528 (18)	0.36644 (10)	0.0261 (3)
H41	0.2075 (8)	0.196 (3)	0.3733 (15)	0.039*
H42	0.2796 (8)	0.222 (3)	0.4385 (13)	0.039*
O6	0.34457 (6)	0.18090 (18)	0.30154 (10)	0.0285 (3)
H61	0.3781 (9)	0.212 (3)	0.3752 (12)	0.043*
H62	0.3710 (10)	0.123 (3)	0.2850 (14)	0.043*
C1	0.09012 (9)	0.1596 (3)	0.03391 (15)	0.0288 (4)
H11	0.0686	0.3080	0.0067	0.035*
H12	0.0801	0.1041	0.0868	0.035*
C2	0.05911 (9)	0.0052 (3)	-0.06810 (14)	0.0282 (4)
H1	0.0097	0.0547	-0.1367	0.034*
C3	0.11567 (9)	0.0160 (3)	-0.09473 (14)	0.0272 (4)
H3	0.0922	0.0765	-0.1742	0.033*
C4	0.17244 (9)	0.1743 (3)	-0.00250 (14)	0.0284 (4)

supplementary materials

H43	0.2218	0.1304	0.0251	0.034*
H44	0.1626	0.3251	-0.0343	0.034*
O5	0.06903 (7)	0.4653 (2)	0.23361 (12)	0.0439 (4)
H51	0.0915 (10)	0.384 (3)	0.2926 (14)	0.066*
H52	0.0326 (9)	0.400 (3)	0.1783 (15)	0.066*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0278 (4)	0.0183 (4)	0.0225 (4)	-0.0002 (3)	0.0140 (3)	-0.0003 (3)
O1	0.0232 (7)	0.0270 (6)	0.0190 (6)	-0.0019 (5)	0.0116 (5)	-0.0015 (5)
O2	0.0308 (7)	0.0304 (7)	0.0336 (7)	-0.0053 (5)	0.0188 (6)	-0.0022 (5)
O3	0.0292 (7)	0.0322 (7)	0.0242 (7)	0.0002 (5)	0.0149 (6)	-0.0048 (5)
O4	0.0268 (7)	0.0304 (7)	0.0229 (7)	-0.0016 (6)	0.0160 (6)	-0.0025 (5)
O6	0.0269 (7)	0.0299 (7)	0.0281 (7)	0.0016 (5)	0.0165 (6)	-0.0036 (5)
C1	0.0238 (10)	0.0310 (10)	0.0292 (10)	0.0037 (7)	0.0149 (8)	0.0005 (8)
C2	0.0202 (9)	0.0307 (10)	0.0232 (9)	0.0007 (8)	0.0079 (8)	0.0013 (8)
C3	0.0282 (9)	0.0310 (10)	0.0180 (9)	0.0006 (8)	0.0119 (8)	0.0017 (7)
C4	0.0332 (10)	0.0290 (10)	0.0248 (10)	-0.0031 (8)	0.0186 (9)	0.0014 (7)
O5	0.0361 (8)	0.0447 (9)	0.0349 (8)	-0.0085 (6)	0.0136 (7)	0.0117 (6)

Geometric parameters (\AA , $^\circ$)

Na1—O4 ⁱ	2.3544 (13)	O4—H42	0.883 (14)
Na1—O6	2.3787 (14)	O6—Na1 ⁱⁱ	2.3893 (14)
Na1—O6 ⁱ	2.3893 (14)	O6—H61	0.877 (14)
Na1—O1	2.4139 (13)	O6—H62	0.859 (14)
Na1—O4	2.4155 (14)	C1—C2	1.516 (2)
Na1—O1 ⁱ	2.4517 (14)	C1—H11	0.9900
Na1—Na1 ⁱ	3.0550 (8)	C1—H12	0.9900
Na1—Na1 ⁱⁱ	3.0550 (8)	C2—C3	1.578 (2)
O1—C1	1.438 (2)	C2—H1	1.0000
O1—C4	1.445 (2)	C3—C4	1.517 (2)
O1—Na1 ⁱⁱ	2.4517 (14)	C3—H3	1.0000
O2—C2	1.417 (2)	C4—H43	0.9900
O2—H2	0.8200	C4—H44	0.9900
O3—C3	1.394 (2)	O5—H51	0.842 (15)
O4—Na1 ⁱⁱ	2.3544 (13)	O5—H52	0.828 (14)
O4—H41	0.839 (14)		
?...?	?		
O4 ⁱ —Na1—O6	103.35 (5)	Na1 ⁱⁱ —O4—H41	124.1 (12)
O4 ⁱ —Na1—O6 ⁱ	80.67 (5)	Na1—O4—H41	125.9 (13)
O6—Na1—O6 ⁱ	174.07 (3)	Na1 ⁱⁱ —O4—H42	117.9 (12)
O4 ⁱ —Na1—O1	101.92 (5)	Na1—O4—H42	107.6 (12)
O6—Na1—O1	86.84 (5)	H41—O4—H42	101.5 (14)
O6 ⁱ —Na1—O1	96.65 (5)	Na1—O6—Na1 ⁱⁱ	79.69 (4)

O4 ⁱ —Na1—O4	172.80 (5)	Na1—O6—H61	104.5 (12)
O6—Na1—O4	79.65 (5)	Na1 ⁱⁱ —O6—H61	115.6 (13)
O6 ⁱ —Na1—O4	95.86 (5)	Na1—O6—H62	145.5 (12)
O1—Na1—O4	84.69 (5)	Na1 ⁱⁱ —O6—H62	110.5 (13)
O4 ⁱ —Na1—O1 ⁱ	85.17 (5)	H61—O6—H62	100.4 (15)
O6—Na1—O1 ⁱ	90.22 (5)	O1—C1—C2	105.23 (13)
O6 ⁱ —Na1—O1 ⁱ	85.75 (5)	O1—C1—H11	110.7
O1—Na1—O1 ⁱ	172.78 (4)	C2—C1—H11	110.7
O4—Na1—O1 ⁱ	88.30 (5)	O1—C1—H12	110.7
O4 ⁱ —Na1—Na1 ⁱ	51.06 (3)	C2—C1—H12	110.7
O6—Na1—Na1 ⁱ	129.44 (5)	H11—C1—H12	108.8
O6 ⁱ —Na1—Na1 ⁱ	50.00 (3)	O2—C2—C1	112.42 (14)
O1—Na1—Na1 ⁱ	135.52 (4)	O2—C2—C3	106.92 (13)
O4—Na1—Na1 ⁱ	122.01 (4)	C1—C2—C3	104.28 (13)
O1 ⁱ —Na1—Na1 ⁱ	50.56 (3)	O2—C2—H1	111.0
O4 ⁱ —Na1—Na1 ⁱⁱ	137.46 (4)	C1—C2—H1	111.0
O6—Na1—Na1 ⁱⁱ	50.31 (3)	C3—C2—H1	111.0
O6 ⁱ —Na1—Na1 ⁱⁱ	129.01 (4)	O3—C3—C4	113.69 (14)
O1—Na1—Na1 ⁱⁱ	51.66 (3)	O3—C3—C2	108.65 (13)
O4—Na1—Na1 ⁱⁱ	49.30 (3)	C4—C3—C2	102.13 (13)
O1 ⁱ —Na1—Na1 ⁱⁱ	121.82 (4)	O3—C3—H3	110.7
Na1 ⁱ —Na1—Na1 ⁱⁱ	170.73 (4)	C4—C3—H3	110.7
C1—O1—C4	103.87 (12)	C2—C3—H3	110.7
C1—O1—Na1	123.05 (9)	O1—C4—C3	106.58 (13)
C4—O1—Na1	110.75 (9)	O1—C4—H43	110.4
C1—O1—Na1 ⁱⁱ	121.20 (10)	C3—C4—H43	110.4
C4—O1—Na1 ⁱⁱ	119.37 (9)	O1—C4—H44	110.4
Na1—O1—Na1 ⁱⁱ	77.78 (4)	C3—C4—H44	110.4
C2—O2—H2	109.7	H43—C4—H44	108.6
Na1 ⁱⁱ —O4—Na1	79.64 (4)	H51—O5—H52	109.6 (19)
O4 ⁱ —Na1—O1—C1	-98.09 (11)	Na1 ⁱ —Na1—O4—Na1 ⁱⁱ	-175.97 (5)
O6—Na1—O1—C1	158.92 (11)	O4 ⁱ —Na1—O6—Na1 ⁱⁱ	-141.91 (5)
O6 ⁱ —Na1—O1—C1	-16.27 (12)	O1—Na1—O6—Na1 ⁱⁱ	-40.40 (4)
O4—Na1—O1—C1	79.03 (12)	O4—Na1—O6—Na1 ⁱⁱ	44.77 (4)
Na1 ⁱ —Na1—O1—C1	-52.67 (13)	O1 ⁱ —Na1—O6—Na1 ⁱⁱ	133.00 (5)
Na1 ⁱⁱ —Na1—O1—C1	119.44 (12)	Na1 ⁱ —Na1—O6—Na1 ⁱⁱ	167.97 (6)
O4 ⁱ —Na1—O1—C4	25.43 (10)	C4—O1—C1—C2	41.42 (15)
O6—Na1—O1—C4	-77.55 (10)	Na1—O1—C1—C2	168.00 (9)
O6 ⁱ —Na1—O1—C4	107.26 (10)	Na1 ⁱⁱ —O1—C1—C2	-96.32 (14)
O4—Na1—O1—C4	-157.45 (10)	O1—C1—C2—O2	90.07 (16)
Na1 ⁱ —Na1—O1—C4	70.85 (11)	O1—C1—C2—C3	-25.39 (17)

supplementary materials

Na1 ⁱⁱ —Na1—O1—C4	-117.04 (10)	O2—C2—C3—O3	1.87 (17)
O4 ⁱ —Na1—O1—Na1 ⁱⁱ	142.47 (5)	C1—C2—C3—O3	121.13 (14)
O6—Na1—O1—Na1 ⁱⁱ	39.48 (4)	O2—C2—C3—C4	-118.55 (14)
O6 ⁱ —Na1—O1—Na1 ⁱⁱ	-135.70 (5)	C1—C2—C3—C4	0.71 (16)
O4—Na1—O1—Na1 ⁱⁱ	-40.41 (4)	C1—O1—C4—C3	-41.55 (15)
Na1 ⁱ —Na1—O1—Na1 ⁱⁱ	-172.11 (6)	Na1—O1—C4—C3	-175.52 (10)
O6—Na1—O4—Na1 ⁱⁱ	-45.63 (4)	Na1 ⁱⁱ —O1—C4—C3	97.14 (13)
O6 ⁱ —Na1—O4—Na1 ⁱⁱ	138.29 (5)	O3—C3—C4—O1	-92.61 (16)
O1—Na1—O4—Na1 ⁱⁱ	42.12 (4)	C2—C3—C4—O1	24.23 (16)
O1 ⁱ —Na1—O4—Na1 ⁱⁱ	-136.17 (5)		

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

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O2—H2 \cdots O3	0.82	1.85	2.4367 (17)	127
O4—H41 \cdots O3 ⁱⁱⁱ	0.839 (14)	1.939 (15)	2.7706 (17)	170.9 (17)
O4—H42 \cdots O3 ⁱ	0.883 (14)	1.827 (14)	2.7078 (19)	174.5 (18)
O6—H61 \cdots O2 ⁱ	0.877 (14)	1.940 (14)	2.813 (2)	173.1 (18)
O6—H62 \cdots O5 ⁱⁱ	0.859 (14)	1.838 (14)	2.6903 (18)	171.0 (18)
O5—H51 \cdots O3 ⁱⁱⁱ	0.842 (15)	1.825 (15)	2.6653 (18)	176 (2)
O5—H52 \cdots O2 ^{iv}	0.828 (14)	2.131 (15)	2.958 (2)	177 (2)

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

Fig. 1

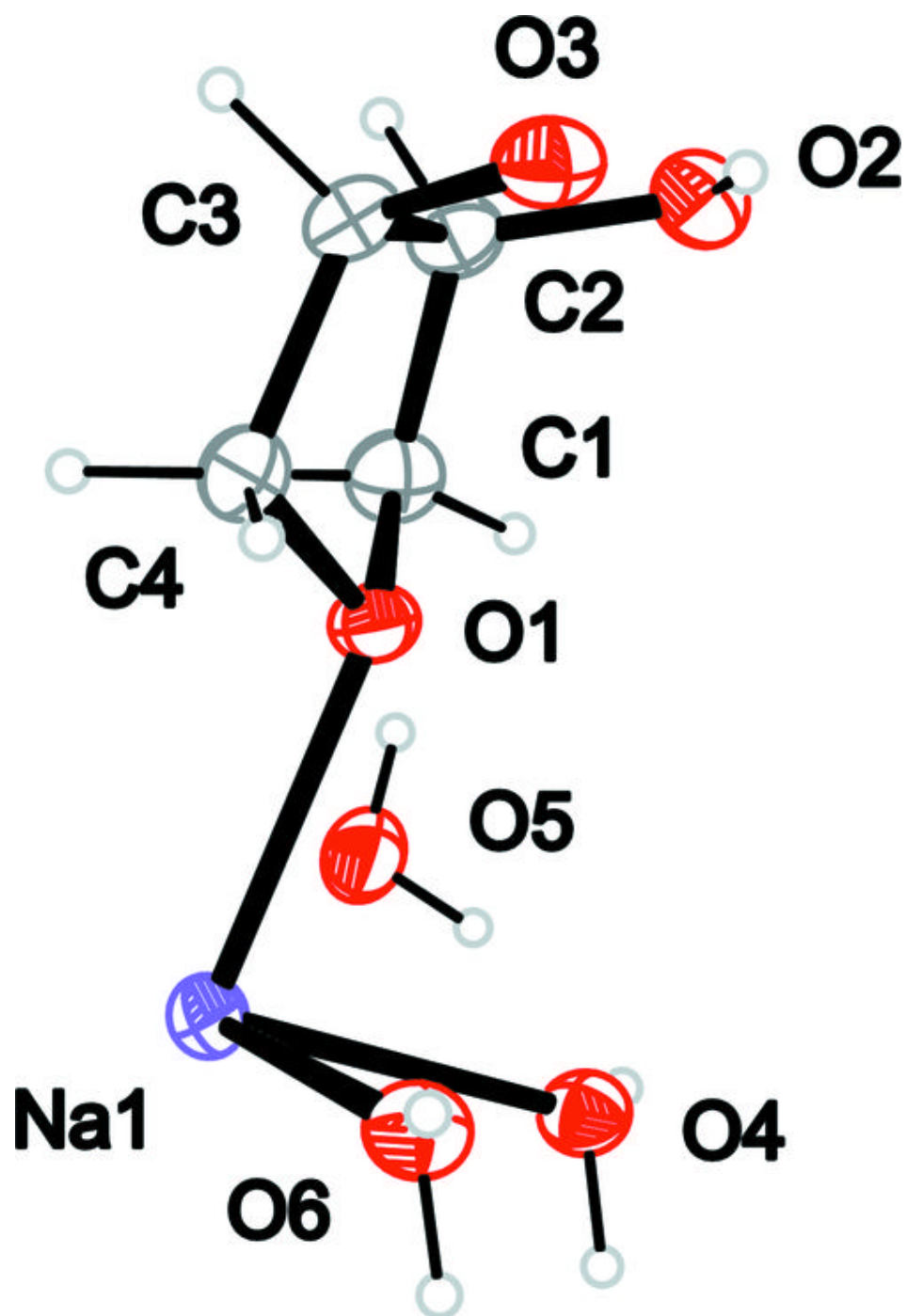


Fig. 2

