Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

The methanol sesquisolvate of sodium naproxen

Helene Kriegner,[a] Matthias Weil[a]* and Matthew J. Jones[b]

[a]Institute for Chemical Technologies and Analytics, Division of Structural Chemistry, TU Wien, Getreidemarkt 9/164-SC, A-1060 Vienna, Austria, and [b]Patheon Austria GmbH & Co KG, St.-Peter-Strasse 25, A-4020 Linz, Austria. *Correspondence e-mail: Matthias.Weil@tuwien.ac.at

Received 9 October 2018
Accepted 16 October 2018

Edited by C. Rizzoli, Universita degli Studi di Parma, Italy

Keywords: crystal structure; solvatomorphism; naproxen; methanol solvate; disorder.

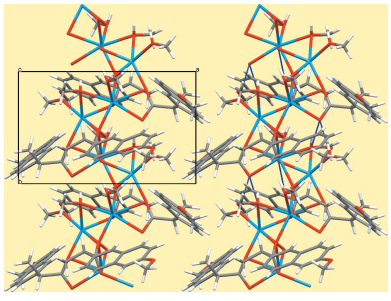
CCDC reference: 1873620

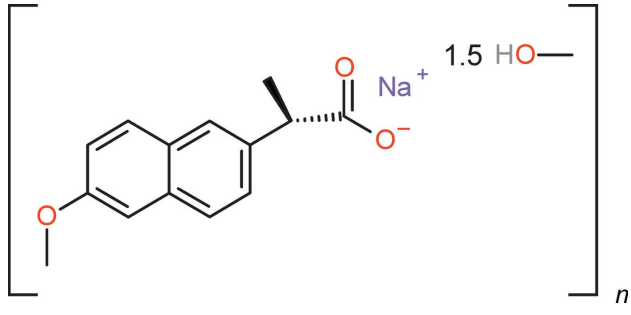
Supporting information: this article has supporting information at journals.iucr.org/e

The asymmetric unit of the methanol solvate of sodium naproxen, systematic name: sodium (2*S*)-2-(6-methoxynaphthalen-2-yl)propanoate methanol sesquisolvate, $Na^+\cdot C_{14}H_{13}O_3^-\cdot 1.5CH_3OH$, comprises two formula units of the molecular salt and three methanol molecules. One of the sodium cations exhibits a coordination number of six and is bonded to three carboxylate O atoms and three methanol OH groups whereas the second sodium cation has a coordination number of seven, defined by five carboxylate O atoms and two methanol OH groups. Both coordination polyhedra around the sodium cations are considerably distorted. The two types of cations are bridged into polymeric chains extending parallel to [010]. This arrangement is stabilized by intrachain O—H···O hydrogen bonds between methanol ligands as donor and carboxylate O atoms as acceptor groups. The hydrophobic 6-methoxynaphthyl moieties flank the hydrophilic sodium oxygen chains into ribbons parallel to [010]. There are no noticeable intermolecular interactions between these ribbons. One of the 6-methoxynaphthyl moieties is disordered over two sets of sites in a 0.723 (3):0.277 (3) ratio.

1. Chemical context

Naproxen, or (*S*)-2-(6-methoxynaphthalen-2-yl)propanoic acid, and in particular its better soluble sodium salt are non-steroidal anti-inflammatory drugs with pain-relieving and antipyretic properties. For a recent project on the crystallization of active pharmaceutical ingredients (APIs; Kovačič *et al.*, 2012), we used sodium naproxen as a model substance. During these investigations, we obtained the methanol sesquisolvate as a solvatomorph of sodium naproxen, $[Na(C_{14}H_{13}O_3)]\cdot 1.5CH_3OH$. Although a preliminary structure model of this compound has been reported as part of a PhD thesis (Chavez, 2009), it was never published or deposited in the Cambridge Structural Database (Groom *et al.*, 2016). We report here the precise crystal structure determination of $[Na(C_{14}H_{13}O_3)]\cdot 1.5CH_3OH$, (I), including disorder of one 6-methoxynaphthyl moiety that was not modelled in the preliminary study (Chavez, 2009).





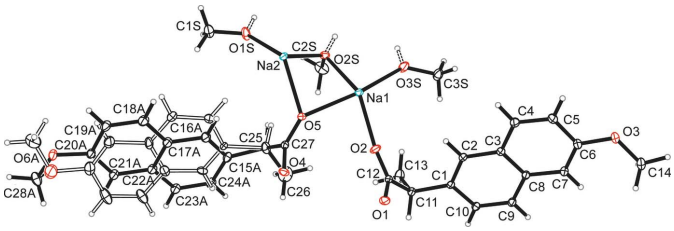


Figure 1
The asymmetric unit of (I) with displacement ellipsoids drawn at the 30% probability level. The minor disordered part *B* of one 6-methoxynaphthyl moiety is displayed with open bonds and without labelling of atoms.

2. Structural commentary

The asymmetric unit of (I) is displayed in Fig. 1 and comprises two Na^+ cations, two naproxate anions (one of which shows disorder of the 6-methoxynaphthyl moiety) and three methanol molecules (Z' = 2). Na1 is bound to six oxygen atoms, three of them originating from methanol OH groups and three from monodentate carboxylate groups (O2; O5; O4^{i}; for symmetry codes, see: Table 1). The Na1—O bond lengths are not uniformly distributed, revealing a distorted [5 + 1] coordination with five shorter bonds between 2.2355 (14) and 2.4403 (14) Å and one significantly longer bond of 2.856 (2) Å to the OH group of a methanol molecule. In comparison, the coordination sphere of Na2 is enlarged to seven coordination partners, two of them from methanol OH groups, four from two chelating carboxylate groups (O1^{i},O2^{i}; O4^{i},O5^{i}) and one from a monodentate carboxylate group (O5). The Na2—O distances are somewhat more evenly distributed and range from 2.3418 (13) to 2.5983 (14) Å. Nevertheless, the resulting coordination polyhedron around Na2 is likewise distorted. Details of the Na—O coordination spheres are depicted in Fig. 2. The bond-valence sums (Brown, 2002) of 1.24 and 1.17 valence units for Na1 and Na2, respectively, are higher than expected and point to some strain in the structure.

Table 1
Selected bond lengths (Å).

Na1—O2	2.2355 (14)	Na2—O1*S*	2.3667 (15)
Na1—O3*S*	2.3003 (15)	Na2—O4^{i}	2.4635 (13)
Na1—O5	2.3604 (13)	Na2—O2*S*	2.4748 (14)
Na1—O2*S*	2.3838 (14)	Na2—O1^{i}	2.5394 (14)
Na1—O4^{i}	2.4403 (14)	Na2—O2^{i}	2.5459 (15)
Na1—O1*S*^{ii}	2.856 (2)	Na2—O5^{i}	2.5983 (14)
Na2—O5	2.3418 (13)		

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

The two sodium cations are bridged by the O1*S* and O2*S* methanol OH groups and by carboxylate atoms O2, O4 and O5 into zigzag chains extending parallel to [010]. The third methanol molecule is terminally bound to Na1. The hydrophobic 6-methoxynaphthyl moieties flank the hydrophilic $[Na—O]_n$ chains, leading to the formation of ribbons along the chain direction (Fig. 3). The methoxy groups attached to the naphthyl rings are twisted slightly out of the aromatic plane, with dihedral angles of 6.42 (18)° for ring (C1–C10) and methoxy group O3–C14, and 5.2 (3)° for ring (C15*A*–C24*A*) and methoxy group O6*A*–C28*A*.

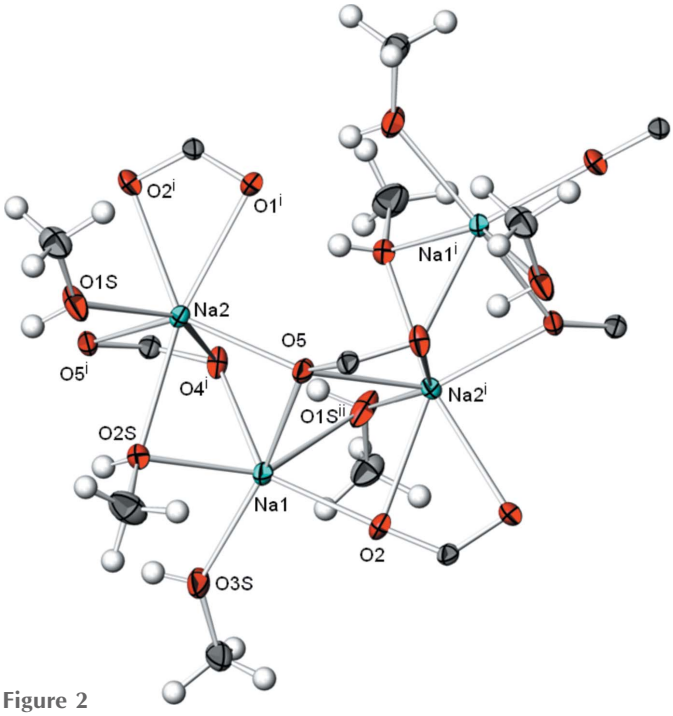


Figure 2
Part of the crystal structure of (I) emphasizing the coordination environments of the two Na^+ cations. Displacement ellipsoids are drawn at the 50% probability level. Symmetry codes refer to Table 1.

3. Supramolecular features

Intrachain O—H···O hydrogen bonding interactions of medium strength [Table 2, Fig. 3(right)] between methanol molecules and carboxylate O atoms stabilize the arrangement within the ribbons. Oxygen atom O1, which is not a bridging atom in the $[Na—O]_n$ chain and which has a comparatively long Na—O bond, is the acceptor of two hydrogen bonds.

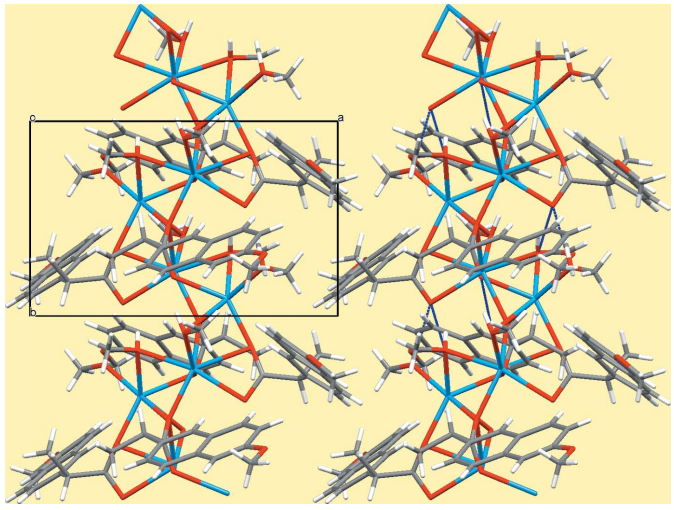


Figure 3
The crystal structure of (I) in a projection along [001]. O—H···O hydrogen bonds within a ribbon are displayed in blue on the right hand side. For clarity, only the major part *A* of the disordered 6-methoxynaphthyl moiety is shown.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1S—H1S···O4^{iii}	0.84 (2)	1.90 (2)	2.6756 (18)	153 (3)
O2S—H2S···O1^{iii}	0.83 (2)	2.06 (2)	2.8331 (18)	156 (3)
O3S—H3S···O1^{iii}	0.79 (2)	1.94 (2)	2.7226 (19)	172 (3)

Symmetry code: (iii) $x, y-1, z$.

There are no notable intermolecular interactions between adjacent ribbons involving the outer hydrophobic parts. It seems that cohesion of the ribbons is dominated by van der Waals forces only.

4. Database survey

The crystal structure of naproxen, *i.e.* the free acid (±)2-(6-methoxy-2-naphthyl)propionic acid, was reported by Ravikumar *et al.* (1985). A search in the Cambridge Structural Database (CSD version 5.39, November 2017, update 3, May 2018; Groom *et al.*, 2016) for the sodium salt and its hydrates revealed six entries: anhydrous sodium naproxen, [Na($C_{14}H_{13}O_3$)] (Kim *et al.*, 2004), sodium naproxen monohydrate [Na($C_{14}H_{13}O_3$)]·H_2O (Kim *et al.*, 1990), two forms of sodium naproxen dihydrate [Na($C_{14}H_{13}O_3$)]·2H_2O (Bond *et al.*, 2014), and sodium naproxen heminonahydrate [Na($C_{14}H_{13}O_3$)]·4.5H_2O (Burgess *et al.*, 2012) that was subsequently reinterpreted as a disordered tetrahydrate [Na($C_{14}H_{13}O_3$)]·4H_2O (Bond *et al.*, 2013). The structural motif of ribbons formed between sodium cations and oxygen atoms is likewise found in all anhydrous and hydrous sodium naproxen structures.

Only one methanol solvate of naproxen is deposited in the CSD. However, this is an Na salt of naproxen with an additional free acid molecule, *viz.* sodium hydrogen bis(naproxate) methanol disolvate, [Na($C_{14}H_{13}O_3$)($C_{14}H_{14}O_3$)]·2CH_3OH (Perumalla & Sun, 2012). A homologous series of alcohol solvates of sodium naproxen obtained as polycrystalline powders and without structure determinations was reported by Chavez *et al.* (2010). During these investigations, another methanol solvate of sodium naproxen was reported with only one methanol molecule per formula unit (Chavez, 2009; Burgess *et al.*, 2012).

5. Synthesis and crystallization

Crystals of sodium naproxen methanol sesquisolvate were grown by slow crystallization in methanol. Polycrystalline anhydrous sodium naproxen was dissolved in methanol to yield a solution 20% in weight of the salt. 0.5 ml of this solution were heated to 338 K and slowly cooled down to room temperature (298 K) over the course of 130 min (cooling rate 0.3 K min^{-1}). Colourless parallelepipeds with edge lengths of up to 1 cm were obtained. A suitable fragment was broken from a larger specimen for the X-ray diffraction experiment.

Table 3
Experimental details.

Crystal data	
Chemical formula	$Na^+·C_{14}H_{13}O_3^-·1.5CH_3OH$
M_r	300.30
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	100
a, b, c (Å)	12.6776 (9), 7.9675 (6), 15.1932 (11)
β (°)	95.7559 (19)
V (Å^3)	1526.91 (19)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.12
Crystal size (mm)	0.45 × 0.45 × 0.35
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.675, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32667, 11521, 10262
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.767
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.105, 1.02
No. of reflections	11521
No. of parameters	508
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.43, −0.24
Absolute structure	Flack x determined using 4468 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.07 (8)

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2017* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2008), *ATOMS* (Dowty, 2006) and *XP* in *SHELXTL* (Sheldrick, 2008), *publCIF* (Westrip, 2010).

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 3. The structure model obtained with *SHELXT* (Sheldrick, 2015*a*) was very similar to the preliminary model of Chavez (2009) from 173 K data using Cu K_α radiation. After placing all atoms with full occupancy in the asymmetric unit, elongated displacement parameters of atoms of one of the 6-methoxynaphthyl moieties and conspicuous electron density peaks in the vicinity of these atoms were found. This model converged with $R[F^2 > 2\sigma(F^2)] = 0.08$ and $wR(F^2) = 0.23$. Consideration of disorder over two sets of sites for this fragment led to more spherical atoms and much better reliability factors (Table 3). The refined occupancy ratio of the two disordered parts is 0.723 (3):0.277 (3) for major part *A*: minor part *B*. The positions of C-bound H atoms were calculated and refined using a riding model, with C—H = 0.93–0.98 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms. H atoms bound to methanol O atoms were clearly discernible from difference maps. They were refined with distance restraints of 0.85±2 Å and free U_{iso}(H) values. The absolute structure was determined on the basis of the current

data set (Table 3), revealing that the usual (*S*) enantiomer is present.

Reflections (100) and (001) were obstructed by the beam stop and were omitted from the refinement.

Lattice parameters refined from single-crystal room temperature X-ray data are a = 12.8458 (9), b = 8.0235 (6), c = 15.3012 (11) Å, β = 94.898 (2)°.

References

Bond, A. D., Cornett, C., Larsen, F. H., Qu, H., Raijada, D. & Rantanen, J. (2013). *Cryst. Growth Des.* **13**, 3665–3671.

Bond, A. D., Cornett, C., Larsen, F. H., Qu, H., Raijada, D. & Rantanen, J. (2014). *IUCrJ*, **1**, 328–337.

Brown, I. D. (2002). *The Chemical Bond in Inorganic Chemistry: The Bond Valence Model*. Oxford University Press.

Bruker (2017). *APEX3* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Burgess, K. M. N., Perras, F. A., Lebrun, A., Messner-Henning, E., Korobkov, I. & Bryce, D. L. (2012). *J. Pharm. Sci.* **101**, 2930–2940.

Chavez, K. J. (2009). *Crystallization of pseudopolymorphic forms of sodium naproxen in mixed solvent systems.* Ph. D. Thesis, Georgia Institute of Technology, USA.

Chavez, K. J., Guevara, M. & Rousseau, R. W. (2010). *Cryst. Growth Des.* **10**, 3372–3377.

Dowty, E. (2006). *ATOMS for Windows*. Shape Software, Kingsport, Tennessee, USA.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Kim, Y. B., Park, I. Y. & Lah, W. R. (1990). *Arch. Pharm. Res.* **13**, 166–173.

Kim, Y.-s., VanDerveer, D., Rousseau, R. W. & Wilkinson, A. P. (2004). *Acta Cryst.* E**60**, m419–m420.

Kovačič, B., Vrečer, F. & Planinšek, O. (2012). *Acta Pharm.* **62**, 1–14.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.

Perumalla, S. R. & Sun, C. C. (2012). *CrystEngComm*, **14**, 3851–3853.

Ravikumar, K., Rajan, S. S., Pattabhi, V. & Gabe, E. J. (1985). *Acta Cryst.* C**41**, 280–282.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2018). E**74**, 1624-1627 [https://doi.org/10.1107/S2056989018014652]

The methanol sesquisolvate of sodium naproxen

Helene Kriegner, Matthias Weil and Matthew J. Jones

Computing details

Data collection: *APEX3* (Bruker, 2017); cell refinement: *SAINT* (Bruker, 2017); data reduction: *SAINT* (Bruker, 2017); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2008), *ATOMS* (Dowty, 2006) and *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Sodium (2*S*)-2-(6-methoxynaphthalen-2-yl)propanoate methanol sesquisolvate

Crystal data

$Na^+ \cdot C_{14}H_{13}O_3^- \cdot 1.5CH_4O$
$M_r = 300.30$
Monoclinic, $P2_1$
$a = 12.6776$ (9) Å
$b = 7.9675$ (6) Å
$c = 15.1932$ (11) Å
$\beta = 95.7559$ (19)°
$V = 1526.91$ (19) Å^3
$Z = 4$
$F(000) = 636$
$D_x = 1.306$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9943 reflections
$\theta = 2.5$–38.0°
$\mu = 0.12$ mm^{-1}
$T = 100$ K
Block, colourless
0.45 × 0.45 × 0.35 mm

Data collection

Bruker APEXII CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
$T_{min} = 0.675$, $T_{max} = 0.747$
32667 measured reflections
11521 independent reflections
10262 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 33.0°$, $\theta_{min} = 2.2°$
$h = -16 \rightarrow 19$
$k = -12 \rightarrow 12$
$l = -23 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.105$
$S = 1.02$
11521 reflections
508 parameters
4 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2 + 0.2474P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Absolute structure: Flack *x* determined using 4468 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.07 (8)

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}	Occ. (<1)
Na1	0.35919 (5)	0.41121 (8)	0.55421 (5)	0.01949 (13)	
Na2	0.53085 (5)	0.27034 (8)	0.43935 (4)	0.01651 (12)	
O1	0.30172 (10)	0.93243 (15)	0.58392 (9)	0.0234 (2)	
O2	0.27973 (11)	0.66163 (15)	0.55460 (10)	0.0259 (3)	
O3	0.09118 (12)	0.70972 (19)	1.09131 (8)	0.0282 (3)	
O4	0.46523 (10)	0.79820 (14)	0.39887 (8)	0.0209 (2)	
O5	0.44988 (10)	0.53419 (14)	0.44218 (8)	0.0194 (2)	
C1	0.09928 (11)	0.80698 (17)	0.67179 (9)	0.0141 (2)	
C2	0.16031 (12)	0.71291 (19)	0.73342 (10)	0.0167 (2)	
H2	0.218745	0.651509	0.715525	0.020*	
C3	0.13817 (12)	0.7053 (2)	0.82309 (10)	0.0177 (3)	
C4	0.20276 (15)	0.6122 (2)	0.88774 (11)	0.0245 (3)	
H4	0.259778	0.546767	0.870353	0.029*	
C5	0.18346 (15)	0.6161 (2)	0.97496 (12)	0.0255 (3)	
H5	0.227230	0.553456	1.017487	0.031*	
C6	0.09883 (15)	0.7127 (2)	1.00203 (11)	0.0228 (3)	
C7	0.03229 (13)	0.7995 (2)	0.94124 (10)	0.0205 (3)	
H7	−0.025886	0.860850	0.959611	0.025*	
C8	0.05126 (12)	0.79659 (19)	0.85034 (10)	0.0173 (3)	
C9	−0.01335 (12)	0.8878 (2)	0.78550 (10)	0.0187 (3)	
H9	−0.073439	0.946900	0.801972	0.022*	
C10	0.00991 (12)	0.89198 (19)	0.69887 (10)	0.0171 (3)	
H10	−0.034925	0.953119	0.656440	0.020*	
C11	0.12458 (12)	0.82248 (19)	0.57623 (10)	0.0164 (2)	
H11	0.104366	0.938450	0.555788	0.020*	
C12	0.24397 (12)	0.80296 (18)	0.57028 (10)	0.0161 (2)	
C13	0.05919 (15)	0.6995 (3)	0.51580 (12)	0.0306 (4)	
H13A	0.077854	0.584172	0.533647	0.046*	
H13B	0.074224	0.717156	0.454462	0.046*	
H13C	−0.016427	0.718215	0.520568	0.046*	
C14	0.0128 (2)	0.8144 (3)	1.12363 (13)	0.0371 (5)	
H14A	0.025640	0.931340	1.107814	0.056*	
H14B	0.016201	0.804060	1.188131	0.056*	
H14C	−0.057606	0.779923	1.097220	0.056*	
C27	0.43419 (12)	0.64886 (19)	0.38570 (10)	0.0168 (3)	
C26	0.2643 (2)	0.6973 (4)	0.29275 (16)	0.0477 (6)	
H26A	0.275881	0.818801	0.290702	0.072*	
H26B	0.228868	0.669292	0.345285	0.072*	
H26C	0.219732	0.661993	0.239531	0.072*	

C25	0.37115 (15)	0.6064 (2)	0.29702 (11)	0.0256 (3)	
H25A	0.357320	0.482859	0.295488	0.031*	0.723 (3)
H25B	0.352875	0.484963	0.302090	0.031*	0.277 (3)
C15A	0.4275 (3)	0.6512 (5)	0.2181 (2)	0.0216 (6)	0.723 (3)
C16A	0.5293 (2)	0.5923 (4)	0.21714 (16)	0.0245 (5)	0.723 (3)
H16A	0.561067	0.532294	0.266975	0.029*	0.723 (3)
C17A	0.5886 (2)	0.6187 (3)	0.14351 (18)	0.0227 (5)	0.723 (3)
C18A	0.6929 (2)	0.5558 (4)	0.14182 (16)	0.0274 (5)	0.723 (3)
H18A	0.725846	0.496607	0.191447	0.033*	0.723 (3)
C19A	0.7463 (2)	0.5801 (4)	0.06897 (16)	0.0265 (5)	0.723 (3)
H19A	0.815841	0.535976	0.068427	0.032*	0.723 (3)
C20A	0.6998 (2)	0.6698 (4)	−0.00588 (19)	0.0205 (5)	0.723 (3)
C21A	0.59938 (19)	0.7341 (3)	−0.00630 (14)	0.0218 (5)	0.723 (3)
H21A	0.568545	0.795556	−0.055962	0.026*	0.723 (3)
C22A	0.5413 (3)	0.7079 (5)	0.0688 (2)	0.0212 (6)	0.723 (3)
C23A	0.43633 (19)	0.7676 (3)	0.07052 (14)	0.0231 (5)	0.723 (3)
H23A	0.403419	0.827833	0.021220	0.028*	0.723 (3)
C24A	0.3816 (2)	0.7395 (3)	0.14262 (16)	0.0241 (5)	0.723 (3)
H24A	0.311058	0.780256	0.141984	0.029*	0.723 (3)
C28A	0.7197 (2)	0.7553 (5)	−0.1545 (2)	0.0315 (6)	0.723 (3)
H28A	0.656366	0.692641	−0.177536	0.047*	0.723 (3)
H28B	0.772161	0.751836	−0.197667	0.047*	0.723 (3)
H28C	0.700449	0.872125	−0.143910	0.047*	0.723 (3)
O6A	0.76404 (16)	0.6807 (3)	−0.07288 (12)	0.0237 (4)	0.723 (3)
O1S	0.50266 (14)	0.08627 (18)	0.31699 (10)	0.0341 (3)	
C1S	0.55409 (18)	0.0686 (3)	0.24025 (14)	0.0322 (4)	
H1S1	0.587260	0.175409	0.226716	0.048*	
H1S2	0.502388	0.036587	0.190801	0.048*	
H1S3	0.608648	−0.018496	0.249473	0.048*	
O2S	0.34838 (10)	0.17528 (15)	0.45724 (8)	0.0205 (2)	
C2S	0.25390 (17)	0.1708 (3)	0.39960 (16)	0.0391 (5)	
H2S1	0.195993	0.128143	0.431475	0.059*	
H2S2	0.263523	0.096897	0.349473	0.059*	
H2S3	0.236603	0.284294	0.377843	0.059*	
O3S	0.24271 (15)	0.24954 (18)	0.62435 (13)	0.0412 (4)	
C3S	0.16678 (18)	0.2742 (3)	0.68361 (15)	0.0337 (4)	
H3S1	0.202144	0.285994	0.743672	0.051*	
H3S2	0.118646	0.177752	0.681302	0.051*	
H3S3	0.126265	0.376335	0.667452	0.051*	
O6B	0.7222 (7)	0.7340 (10)	−0.1082 (7)	0.050 (2)	0.277 (3)
C15B	0.4588 (7)	0.6105 (10)	0.2265 (5)	0.0158 (13)	0.277 (3)
C24B	0.5534 (7)	0.5183 (10)	0.2415 (5)	0.0313 (16)	0.277 (3)
H24B	0.566878	0.454601	0.294247	0.038*	0.277 (3)
C23B	0.6268 (7)	0.5193 (10)	0.1806 (6)	0.0365 (18)	0.277 (3)
H23B	0.689893	0.454986	0.191046	0.044*	0.277 (3)
C22B	0.6085 (6)	0.6161 (9)	0.1022 (5)	0.0292 (15)	0.277 (3)
C21B	0.6837 (7)	0.6204 (10)	0.0362 (6)	0.0324 (17)	0.277 (3)
H21B	0.747181	0.556454	0.043704	0.039*	0.277 (3)

C20B	0.6611 (8)	0.7178 (12)	−0.0363 (6)	0.0355 (19)	0.277 (3)
C19B	0.5698 (8)	0.8163 (13)	−0.0498 (5)	0.045 (2)	0.277 (3)
H19B	0.558921	0.887368	−0.100039	0.054*	0.277 (3)
C18B	0.4966 (7)	0.8096 (12)	0.0097 (5)	0.0380 (18)	0.277 (3)
H18B	0.432892	0.872406	−0.001075	0.046*	0.277 (3)
C16B	0.4398 (6)	0.7027 (8)	0.1519 (4)	0.0204 (11)	0.277 (3)
H16B	0.375346	0.763864	0.142336	0.024*	0.277 (3)
C17B	0.5134 (9)	0.7109 (14)	0.0874 (7)	0.027 (2)	0.277 (3)
C28B	0.7973 (8)	0.6136 (14)	−0.1092 (8)	0.049 (2)	0.277 (3)
H28D	0.854049	0.635146	−0.061943	0.073*	0.277 (3)
H28E	0.826577	0.614705	−0.166515	0.073*	0.277 (3)
H28F	0.765540	0.503621	−0.099974	0.073*	0.277 (3)
H3S	0.256 (3)	0.155 (3)	0.615 (2)	0.049 (9)*	
H1S	0.478 (2)	−0.009 (3)	0.3271 (18)	0.033 (7)*	
H2S	0.350 (2)	0.090 (3)	0.4883 (18)	0.039 (8)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0218 (3)	0.0118 (3)	0.0264 (3)	0.0010 (2)	0.0102 (2)	0.0011 (2)
Na2	0.0174 (3)	0.0133 (3)	0.0193 (3)	0.0021 (2)	0.0045 (2)	−0.0010 (2)
O1	0.0205 (5)	0.0154 (5)	0.0356 (7)	−0.0030 (4)	0.0100 (5)	0.0017 (4)
O2	0.0260 (6)	0.0152 (5)	0.0384 (7)	0.0048 (4)	0.0118 (5)	−0.0042 (5)
O3	0.0387 (7)	0.0308 (6)	0.0159 (5)	0.0053 (6)	0.0077 (5)	0.0033 (5)
O4	0.0310 (6)	0.0131 (4)	0.0182 (5)	−0.0021 (4)	0.0003 (4)	0.0015 (4)
O5	0.0235 (5)	0.0130 (4)	0.0231 (5)	0.0036 (4)	0.0089 (4)	0.0029 (4)
C1	0.0133 (6)	0.0129 (5)	0.0164 (6)	−0.0020 (4)	0.0033 (4)	−0.0023 (5)
C2	0.0167 (6)	0.0164 (6)	0.0173 (6)	0.0027 (5)	0.0033 (5)	−0.0008 (5)
C3	0.0188 (6)	0.0177 (6)	0.0168 (6)	0.0021 (5)	0.0028 (5)	0.0000 (5)
C4	0.0274 (8)	0.0264 (8)	0.0201 (7)	0.0093 (6)	0.0042 (6)	0.0024 (6)
C5	0.0299 (9)	0.0273 (8)	0.0195 (7)	0.0075 (7)	0.0030 (6)	0.0048 (6)
C6	0.0290 (8)	0.0232 (7)	0.0169 (6)	0.0001 (6)	0.0053 (6)	0.0010 (6)
C7	0.0231 (7)	0.0215 (7)	0.0177 (6)	0.0012 (5)	0.0062 (5)	−0.0010 (5)
C8	0.0184 (6)	0.0174 (6)	0.0166 (6)	−0.0002 (5)	0.0042 (5)	−0.0015 (5)
C9	0.0176 (6)	0.0201 (6)	0.0189 (6)	0.0026 (5)	0.0045 (5)	−0.0015 (5)
C10	0.0148 (6)	0.0184 (6)	0.0180 (6)	0.0006 (5)	0.0019 (5)	−0.0010 (5)
C11	0.0154 (6)	0.0184 (6)	0.0156 (6)	0.0014 (5)	0.0028 (5)	−0.0012 (5)
C12	0.0177 (6)	0.0145 (6)	0.0170 (6)	0.0016 (5)	0.0061 (5)	0.0011 (5)
C13	0.0248 (8)	0.0434 (10)	0.0236 (8)	−0.0100 (8)	0.0023 (6)	−0.0124 (7)
C14	0.0542 (13)	0.0394 (11)	0.0200 (8)	0.0117 (10)	0.0146 (8)	0.0036 (7)
C27	0.0203 (7)	0.0154 (6)	0.0156 (6)	0.0000 (5)	0.0053 (5)	−0.0014 (5)
C26	0.0367 (12)	0.0679 (17)	0.0352 (11)	0.0031 (12)	−0.0127 (9)	−0.0064 (11)
C25	0.0326 (9)	0.0282 (8)	0.0162 (7)	−0.0105 (7)	0.0036 (6)	−0.0049 (6)
C15A	0.0222 (16)	0.0255 (15)	0.0171 (11)	0.0012 (11)	0.0022 (10)	−0.0058 (11)
C16A	0.0302 (14)	0.0296 (13)	0.0134 (9)	0.0069 (10)	0.0002 (8)	−0.0005 (9)
C17A	0.0248 (11)	0.0295 (12)	0.0133 (10)	0.0081 (9)	−0.0008 (8)	0.0013 (8)
C18A	0.0286 (12)	0.0351 (13)	0.0178 (10)	0.0134 (10)	−0.0007 (8)	0.0027 (9)
C19A	0.0256 (12)	0.0337 (13)	0.0201 (10)	0.0108 (10)	0.0019 (9)	0.0002 (9)

C20A	0.0186 (11)	0.0251 (11)	0.0181 (11)	0.0053 (9)	0.0029 (9)	0.0005 (9)
C21A	0.0214 (10)	0.0288 (11)	0.0145 (9)	0.0053 (8)	−0.0010 (8)	−0.0008 (8)
C22A	0.0202 (15)	0.0287 (13)	0.0138 (14)	0.0072 (12)	−0.0026 (10)	−0.0001 (11)
C23A	0.0207 (10)	0.0309 (11)	0.0169 (9)	0.0081 (9)	−0.0025 (7)	0.0006 (8)
C24A	0.0232 (12)	0.0299 (12)	0.0187 (9)	0.0040 (10)	−0.0004 (8)	−0.0030 (8)
C28A	0.0321 (14)	0.0450 (16)	0.0169 (10)	−0.0077 (11)	−0.0006 (10)	0.0056 (11)
O6A	0.0191 (8)	0.0346 (10)	0.0178 (8)	0.0078 (7)	0.0040 (6)	0.0033 (7)
O1S	0.0552 (9)	0.0230 (6)	0.0274 (6)	−0.0187 (6)	0.0211 (6)	−0.0076 (5)
C1S	0.0385 (11)	0.0342 (10)	0.0251 (8)	−0.0100 (8)	0.0094 (7)	−0.0034 (7)
O2S	0.0200 (5)	0.0151 (5)	0.0267 (6)	−0.0003 (4)	0.0033 (4)	0.0007 (4)
C2S	0.0284 (10)	0.0434 (12)	0.0436 (11)	−0.0081 (9)	−0.0065 (8)	0.0083 (10)
O3S	0.0528 (10)	0.0150 (6)	0.0630 (11)	−0.0036 (6)	0.0417 (8)	−0.0020 (6)
C3S	0.0402 (10)	0.0241 (8)	0.0405 (10)	−0.0074 (8)	0.0214 (8)	−0.0073 (8)
O6B	0.051 (5)	0.037 (4)	0.064 (6)	−0.009 (3)	0.025 (4)	−0.009 (4)
C15B	0.018 (4)	0.014 (3)	0.016 (3)	0.003 (2)	0.006 (3)	−0.002 (2)
C24B	0.037 (4)	0.030 (3)	0.029 (3)	0.015 (3)	0.012 (3)	0.012 (3)
C23B	0.037 (4)	0.033 (4)	0.043 (4)	0.016 (3)	0.021 (3)	0.009 (3)
C22B	0.045 (4)	0.024 (3)	0.022 (3)	−0.011 (3)	0.017 (3)	−0.009 (2)
C21B	0.039 (4)	0.024 (3)	0.036 (4)	−0.007 (3)	0.015 (3)	−0.009 (3)
C20B	0.044 (5)	0.030 (4)	0.035 (4)	−0.016 (4)	0.016 (4)	−0.015 (3)
C19B	0.056 (5)	0.059 (6)	0.019 (3)	−0.025 (5)	0.001 (3)	0.006 (3)
C18B	0.044 (4)	0.050 (5)	0.020 (3)	−0.008 (4)	−0.001 (3)	0.012 (3)
C16B	0.023 (3)	0.019 (2)	0.018 (2)	0.003 (2)	−0.006 (2)	0.0044 (19)
C17B	0.040 (6)	0.022 (3)	0.021 (4)	−0.009 (4)	0.008 (3)	−0.004 (3)
C28B	0.031 (4)	0.051 (5)	0.063 (6)	−0.006 (4)	−0.002 (4)	0.013 (5)

Geometric parameters (Å, º)

Na1—O2	2.2355 (14)	C16A—C17A	1.424 (4)
Na1—O3S	2.3003 (15)	C16A—H16A	0.9500
Na1—O5	2.3604 (13)	C17A—C18A	1.417 (4)
Na1—O2S	2.3838 (14)	C17A—C22A	1.420 (4)
Na1—O4^{i}	2.4403 (14)	C18A—C19A	1.368 (4)
Na1—O1S^{ii}	2.856 (2)	C18A—H18A	0.9500
Na2—O5	2.3418 (13)	C19A—C20A	1.420 (4)
Na2—O1S	2.3667 (15)	C19A—H19A	0.9500
Na2—O4^{i}	2.4635 (13)	C20A—O6A	1.368 (3)
Na2—O2S	2.4748 (14)	C20A—C21A	1.372 (3)
Na2—O1^{i}	2.5394 (14)	C21A—C22A	1.434 (4)
Na2—O2^{i}	2.5459 (15)	C21A—H21A	0.9500
Na2—O5^{i}	2.5983 (14)	C22A—C23A	1.416 (4)
O1—C12	1.2700 (19)	C23A—C24A	1.373 (3)
O2—C12	1.2457 (18)	C23A—H23A	0.9500
O3—C6	1.3698 (19)	C24A—H24A	0.9500
O3—C14	1.422 (3)	C28A—O6A	1.437 (3)
O4—C27	1.2629 (18)	C28A—H28A	0.9800
O5—C27	1.2555 (19)	C28A—H28B	0.9800
C1—C2	1.375 (2)	C28A—H28C	0.9800

C1—C10	1.416 (2)	O1S—C1S	1.399 (2)
C1—C11	1.523 (2)	O1S—H1S	0.84 (2)
C2—C3	1.420 (2)	C1S—H1S1	0.9800
C2—H2	0.9500	C1S—H1S2	0.9800
C3—C8	1.416 (2)	C1S—H1S3	0.9800
C3—C4	1.423 (2)	O2S—C2S	1.411 (2)
C4—C5	1.372 (2)	O2S—H2S	0.83 (2)
C4—H4	0.9500	C2S—H2S1	0.9800
C5—C6	1.415 (2)	C2S—H2S2	0.9800
C5—H5	0.9500	C2S—H2S3	0.9800
C6—C7	1.373 (2)	O3S—C3S	1.396 (2)
C7—C8	1.426 (2)	O3S—H3S	0.79 (2)
C7—H7	0.9500	C3S—H3S1	0.9800
C8—C9	1.417 (2)	C3S—H3S2	0.9800
C9—C10	1.378 (2)	C3S—H3S3	0.9800
C9—H9	0.9500	O6B—C28B	1.352 (13)
C10—H10	0.9500	O6B—C20B	1.408 (11)
C11—C13	1.529 (2)	C15B—C16B	1.352 (10)
C11—C12	1.533 (2)	C15B—C24B	1.405 (11)
C11—H11	1.0000	C24B—C23B	1.376 (10)
C13—H13A	0.9800	C24B—H24B	0.9500
C13—H13B	0.9800	C23B—C22B	1.417 (11)
C13—H13C	0.9800	C23B—H23B	0.9500
C14—H14A	0.9800	C22B—C17B	1.421 (15)
C14—H14B	0.9800	C22B—C21B	1.452 (11)
C14—H14C	0.9800	C21B—C20B	1.355 (14)
C27—C25	1.534 (2)	C21B—H21B	0.9500
C26—C25	1.532 (3)	C20B—C19B	1.396 (16)
C26—H26A	0.9800	C19B—C18B	1.359 (12)
C26—H26B	0.9800	C19B—H19B	0.9500
C26—H26C	0.9800	C18B—C17B	1.417 (13)
C25—C15A	1.499 (4)	C18B—H18B	0.9500
C25—C15B	1.620 (8)	C16B—C17B	1.421 (11)
C25—H25A	1.0000	C16B—H16B	0.9500
C25—H25B	1.0000	C28B—H28D	0.9800
C15A—C16A	1.375 (4)	C28B—H28E	0.9800
C15A—C24A	1.420 (4)	C28B—H28F	0.9800

O2—Na1—O3S	100.84 (6)	C26—C25—C15B	128.7 (3)
O2—Na1—O5	83.32 (5)	C27—C25—C15B	104.2 (3)
O3S—Na1—O5	161.49 (7)	C15A—C25—H25A	108.2
O2—Na1—O2S	135.03 (6)	C26—C25—H25A	108.2
O3S—Na1—O2S	81.08 (5)	C27—C25—H25A	108.2
O5—Na1—O2S	83.32 (5)	C26—C25—H25B	104.5
O2—Na1—O4^{i}	136.61 (6)	C27—C25—H25B	104.5
O3S—Na1—O4^{i}	105.50 (6)	C15B—C25—H25B	104.5
O5—Na1—O4^{i}	82.41 (5)	C16A—C15A—C24A	118.0 (3)
O2S—Na1—O4^{i}	83.33 (4)	C16A—C15A—C25	116.8 (3)

O2—Na1—O1S^{ii}	78.92 (5)	C24A—C15A—C25	125.0 (3)
O3S—Na1—O1S^{ii}	109.52 (6)	C15A—C16A—C17A	121.9 (3)
O5—Na1—O1S^{ii}	88.96 (5)	C15A—C16A—H16A	119.1
O2S—Na1—O1S^{ii}	143.32 (5)	C17A—C16A—H16A	119.1
O4^{i}—Na1—O1S^{ii}	60.08 (4)	C18A—C17A—C22A	118.8 (3)
O5—Na2—O1S	122.60 (6)	C18A—C17A—C16A	121.9 (2)
O5—Na2—O4^{i}	82.29 (4)	C22A—C17A—C16A	119.2 (3)
O1S—Na2—O4^{i}	145.68 (5)	C19A—C18A—C17A	120.2 (2)
O5—Na2—O2S	81.75 (4)	C19A—C18A—H18A	119.9
O1S—Na2—O2S	80.06 (5)	C17A—C18A—H18A	119.9
O4^{i}—Na2—O2S	81.00 (5)	C18A—C19A—C20A	121.3 (2)
O5—Na2—O1^{i}	85.41 (4)	C18A—C19A—H19A	119.3
O1S—Na2—O1^{i}	105.56 (5)	C20A—C19A—H19A	119.3
O4^{i}—Na2—O1^{i}	99.18 (5)	O6A—C20A—C21A	126.4 (3)
O2S—Na2—O1^{i}	167.02 (5)	O6A—C20A—C19A	113.4 (2)
O5—Na2—O2^{i}	135.92 (5)	C21A—C20A—C19A	120.1 (2)
O1S—Na2—O2^{i}	83.41 (6)	C20A—C21A—C22A	119.5 (3)
O4^{i}—Na2—O2^{i}	94.01 (5)	C20A—C21A—H21A	120.3
O2S—Na2—O2^{i}	141.32 (5)	C22A—C21A—H21A	120.3
O1^{i}—Na2—O2^{i}	51.64 (4)	C23A—C22A—C17A	118.4 (3)
O5—Na2—O5^{i}	130.41 (3)	C23A—C22A—C21A	121.6 (3)
O1S—Na2—O5^{i}	95.26 (5)	C17A—C22A—C21A	120.0 (3)
O4^{i}—Na2—O5^{i}	51.90 (4)	C24A—C23A—C22A	120.8 (2)
O2S—Na2—O5^{i}	74.12 (4)	C24A—C23A—H23A	119.6
O1^{i}—Na2—O5^{i}	116.29 (5)	C22A—C23A—H23A	119.6
O2^{i}—Na2—O5^{i}	72.89 (4)	C23A—C24A—C15A	121.7 (3)
C12—O1—Na2^{ii}	92.32 (9)	C23A—C24A—H24A	119.1
C12—O2—Na1	168.53 (13)	C15A—C24A—H24A	119.1
C12—O2—Na2^{ii}	92.62 (10)	O6A—C28A—H28A	109.5
Na1—O2—Na2^{ii}	83.11 (5)	O6A—C28A—H28B	109.5
C6—O3—C14	116.94 (15)	H28A—C28A—H28B	109.5
C27—O4—Na1^{ii}	130.88 (11)	O6A—C28A—H28C	109.5
C27—O4—Na2^{ii}	92.75 (9)	H28A—C28A—H28C	109.5
Na1^{ii}—O4—Na2^{ii}	79.35 (4)	H28B—C28A—H28C	109.5
C27—O5—Na2	132.87 (10)	C20A—O6A—C28A	117.2 (2)
C27—O5—Na1	137.71 (10)	C1S—O1S—Na2	132.12 (12)
Na2—O5—Na1	83.49 (4)	C1S—O1S—Na1^{i}	102.53 (14)
C27—O5—Na2^{ii}	86.79 (9)	Na2—O1S—Na1^{i}	74.36 (5)
Na2—O5—Na2^{ii}	130.68 (5)	C1S—O1S—H1S	105.9 (19)
Na1—O5—Na2^{ii}	79.62 (4)	Na2—O1S—H1S	116.5 (19)
C2—C1—C10	118.34 (13)	Na1^{i}—O1S—H1S	69.3 (19)
C2—C1—C11	122.36 (13)	O1S—C1S—H1S1	109.5
C10—C1—C11	119.30 (13)	O1S—C1S—H1S2	109.5
C1—C2—C3	121.66 (13)	H1S1—C1S—H1S2	109.5
C1—C2—H2	119.2	O1S—C1S—H1S3	109.5
C3—C2—H2	119.2	H1S1—C1S—H1S3	109.5
C8—C3—C2	119.54 (14)	H1S2—C1S—H1S3	109.5
C8—C3—C4	118.47 (14)	C2S—O2S—Na1	113.32 (13)

C2—C3—C4	121.97 (14)	C2S—O2S—Na2	133.15 (13)
C5—C4—C3	120.60 (15)	Na1—O2S—Na2	80.22 (4)
C5—C4—H4	119.7	C2S—O2S—H2S	107 (2)
C3—C4—H4	119.7	Na1—O2S—H2S	108 (2)
C4—C5—C6	120.47 (16)	Na2—O2S—H2S	110 (2)
C4—C5—H5	119.8	O2S—C2S—H2S1	109.5
C6—C5—H5	119.8	O2S—C2S—H2S2	109.5
O3—C6—C7	125.10 (16)	H2S1—C2S—H2S2	109.5
O3—C6—C5	114.18 (15)	O2S—C2S—H2S3	109.5
C7—C6—C5	120.73 (15)	H2S1—C2S—H2S3	109.5
C6—C7—C8	119.44 (15)	H2S2—C2S—H2S3	109.5
C6—C7—H7	120.3	C3S—O3S—Na1	137.38 (12)
C8—C7—H7	120.3	C3S—O3S—H3S	115 (2)
C3—C8—C9	118.21 (13)	Na1—O3S—H3S	108 (2)
C3—C8—C7	120.21 (14)	O3S—C3S—H3S1	109.5
C9—C8—C7	121.56 (14)	O3S—C3S—H3S2	109.5
C10—C9—C8	120.81 (14)	H3S1—C3S—H3S2	109.5
C10—C9—H9	119.6	O3S—C3S—H3S3	109.5
C8—C9—H9	119.6	H3S1—C3S—H3S3	109.5
C9—C10—C1	121.35 (14)	H3S2—C3S—H3S3	109.5
C9—C10—H10	119.3	C28B—O6B—C20B	112.7 (10)
C1—C10—H10	119.3	C16B—C15B—C24B	119.8 (7)
C1—C11—C13	111.54 (13)	C16B—C15B—C25	119.3 (6)
C1—C11—C12	110.58 (12)	C24B—C15B—C25	120.9 (6)
C13—C11—C12	112.24 (13)	C23B—C24B—C15B	120.8 (7)
C1—C11—H11	107.4	C23B—C24B—H24B	119.6
C13—C11—H11	107.4	C15B—C24B—H24B	119.6
C12—C11—H11	107.4	C24B—C23B—C22B	120.2 (7)
O2—C12—O1	123.40 (14)	C24B—C23B—H23B	119.9
O2—C12—C11	118.90 (14)	C22B—C23B—H23B	119.9
O1—C12—C11	117.67 (13)	C23B—C22B—C17B	119.1 (7)
O2—C12—Na2^{ii}	61.83 (9)	C23B—C22B—C21B	122.0 (8)
O1—C12—Na2^{ii}	61.59 (8)	C17B—C22B—C21B	118.9 (8)
C11—C12—Na2^{ii}	179.19 (11)	C20B—C21B—C22B	118.4 (8)
C11—C13—H13A	109.5	C20B—C21B—H21B	120.8
C11—C13—H13B	109.5	C22B—C21B—H21B	120.8
H13A—C13—H13B	109.5	C21B—C20B—C19B	123.1 (7)
C11—C13—H13C	109.5	C21B—C20B—O6B	126.6 (10)
H13A—C13—H13C	109.5	C19B—C20B—O6B	110.4 (9)
H13B—C13—H13C	109.5	C18B—C19B—C20B	119.5 (8)
O3—C14—H14A	109.5	C18B—C19B—H19B	120.3
O3—C14—H14B	109.5	C20B—C19B—H19B	120.3
H14A—C14—H14B	109.5	C19B—C18B—C17B	121.3 (10)
O3—C14—H14C	109.5	C19B—C18B—H18B	119.3
H14A—C14—H14C	109.5	C17B—C18B—H18B	119.3
H14B—C14—H14C	109.5	C15B—C16B—C17B	121.9 (8)
O5—C27—O4	123.49 (14)	C15B—C16B—H16B	119.0
O5—C27—C25	118.22 (14)	C17B—C16B—H16B	119.0

O4—C27—C25	118.26 (14)	C18B—C17B—C16B	123.1 (10)
C25—C26—H26A	109.5	C18B—C17B—C22B	118.8 (9)
C25—C26—H26B	109.5	C16B—C17B—C22B	118.1 (9)
H26A—C26—H26B	109.5	O6B—C28B—H28D	109.5
C25—C26—H26C	109.5	O6B—C28B—H28E	109.5
H26A—C26—H26C	109.5	H28D—C28B—H28E	109.5
H26B—C26—H26C	109.5	O6B—C28B—H28F	109.5
C15A—C25—C26	110.1 (2)	H28D—C28B—H28F	109.5
C15A—C25—C27	113.69 (18)	H28E—C28B—H28F	109.5
C26—C25—C27	108.29 (15)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*S*—H1*S*···O4^{iii}	0.84 (2)	1.90 (2)	2.6756 (18)	153 (3)
O2*S*—H2*S*···O1^{iii}	0.83 (2)	2.06 (2)	2.8331 (18)	156 (3)
O3*S*—H3*S*···O1^{iii}	0.79 (2)	1.94 (2)	2.7226 (19)	172 (3)

Symmetry code: (iii) *x*, *y*−1, *z*.