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Poly[bis(μ_4-acetato-κ^4O:O:O':O')bis(μ_3-acetato-κ^3O:O:O)(μ_2-acetato-κ^2O:O')-(μ_2-acetic acid-κ^2O:O')di-μ-aqua-copper(II)trisodium]

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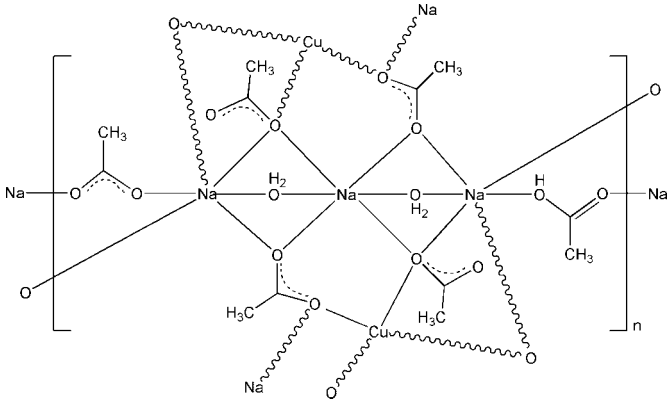
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.068; data-to-parameter ratio = 17.6.

In the title compound, $[CuNa_3(CH_3CO_2)_5(CH_3COOH)(H_2O)_2]_n$, the Cu^{II} atom lies on an inversion center and is coordinated by four O atoms from four acetate ligands, leading to a square-planar geometry. One Na^I atom, lying on an inversion center, is coordinated by four O atoms from four acetate ligands and two bridging water molecules in a distorted octahedral geometry. The other Na^I atom is coordinated by five O atoms from five acetate ligands and a bridging water molecule. A hydroxy H atom lies on a twofold rotation axis and is shared by two acetate ligands. The crystal packing exhibits a polymeric layer parallel to (100), which is further stablized by intralayer O—H···O hydrogen bonds. The layers are linked by interlayer O—H···O hydrogen bonds.

Related literature

For related structures, see: Chiari *et al.* (1988); Vives *et al.* (2003).



Experimental

Crystal data

$[CuNa_3(C_2H_3O_2)_5(C_2H_4O_2)(H_2O)_2]$
M_r = 523.81
Monoclinic, $C2/c$
a = 14.571 (6) Å
b = 6.768 (3) Å
c = 22.653 (10) Å
β = 103.426 (19)°
V = 2173.0 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 290 K
0.27 × 0.25 × 0.23 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.752, T_{max} = 0.777
10214 measured reflections
2493 independent reflections
2192 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.068
S = 1.03
2493 reflections
142 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O1	0.79	2.05	2.835 (2)	172
O7—H7B···O1^{i}	0.80	2.03	2.8104 (19)	168

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2345).

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supporting information

Acta Cryst. (2010). E**66**, m1244 [doi:10.1107/S1600536810035683]

Poly[bis(μ_4-acetato-$\kappa^4O:O:O':O'$)bis(μ_3-acetato-$\kappa^3O:O:O$)(μ_2-acetato-$\kappa^2O:O'$)(μ_2-acetic acid-$\kappa^2O:O'$)di-μ-aquacopper(II)trisodium]

Xiang-Yu Jiang and Xi-Gui Yue

S1. Comment

There has been increasing interest in the study of copper-containing complexes due to their various coordination styles and potential applications. We report here the crystal structure of the title compound, a new copper complex with acetate.

In the title compound, as shown in Fig. 1, the Cu^{II} atom lies on an inversion center and is four-coordinated by four O atoms from four acetate ligands, forming a square-planar coordination geometry. In a comparison with the tiltle compound, the complexes previously reported (Chiari *et al.*, 1988; Vives *et al.*, 2003) show different coordination behaviors of the central Cu^{II} ion. The two Na^{I} ions are each coordinated by six O atoms, forming a distorted octahedral coordination geometry. Na1 atom lies on an inversion center, while Na2 atom is on a general position. In the crystal structure, the metal ions, acetate ligands and water molecules are connected each other, forming a two-dimensional network (Fig. 2). The crystal packing is further stabilized by intermolecular O—H···O hydrogen bonds (Table 1).

S2. Experimental

The title compound was prepared as follows: copper acetate dihydrate (2.18 g, 0.01 mol) was added to a solution of glacial acetic acid (3 ml) in 15 ml water. Then 10 ml NaOH (3 mol/*L*) was added into the mixture. The mixture was heated and stirred for half an hour and then filtered. The filtrate was allowed to stand at room temperature for several days, giving blue block-shaped crystals.

S3. Refinement

C-bound H atoms were placed in calculated positions and refined as riding atoms, with C—H = 0.96 Å and with U_{iso}(H) = 1.5U_{eq}(C). H atoms of water and carboxyl group are located in a difference Fourier map and refined as riding, with U_{iso}(H) = 1.5U_{eq}(O).

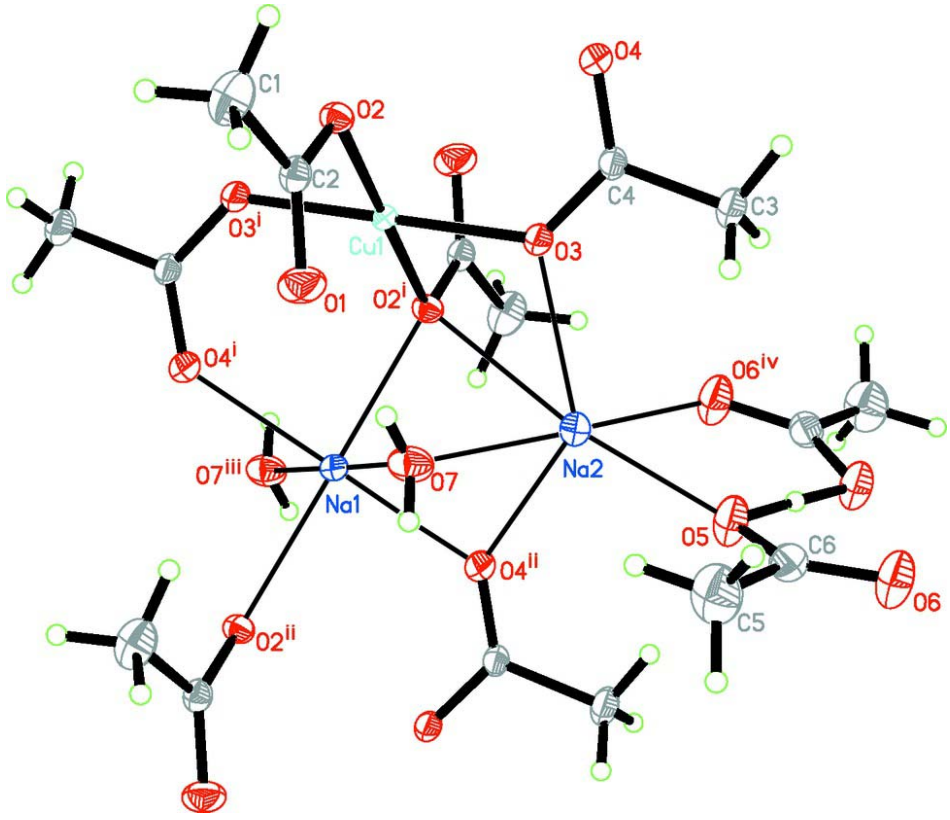

Figure 1

The structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) -*x*+1, -*y*+2, -*z*+1; (ii) *x*, *y*-1, *z*; (iii) -*x*+1, -*y*+1, -*z*+1; (iv) -*x*+1, *y*, -*z*+1/2.]

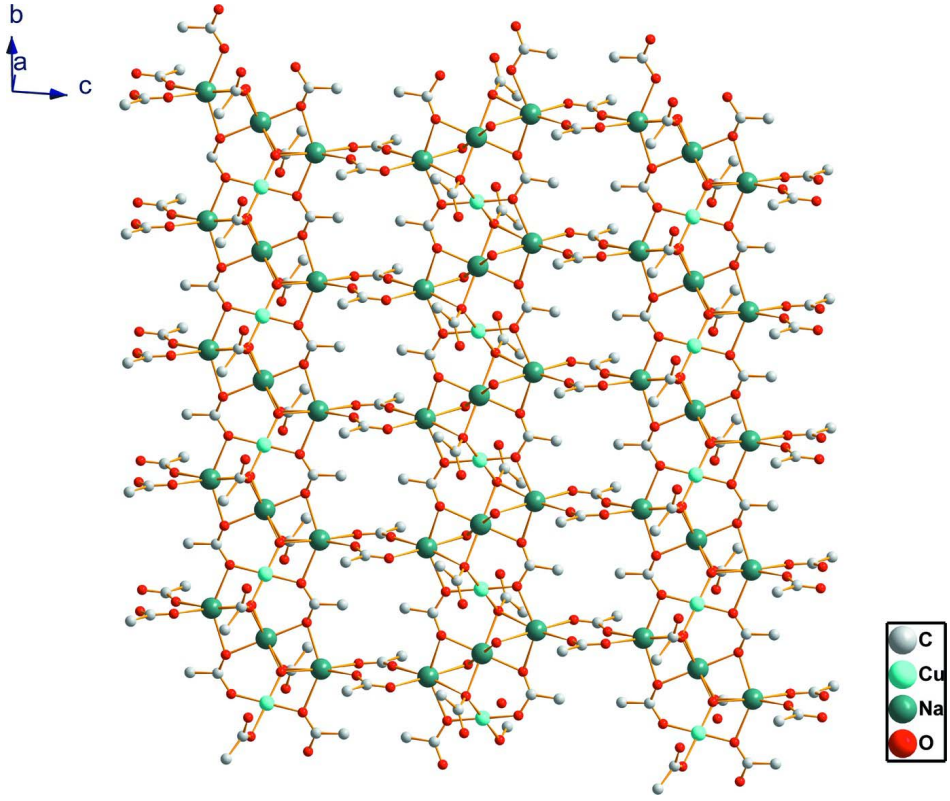

Figure 2

A view of the two-dimensional structure in the title compound.

Poly[bis(μ_4-acetato-κ^4O:O:O':O')bis(μ_3- acetato-κ^3O:O:O)(μ_2-acetato- κ^2O:O')(μ_2-acetic acid-κ^2O:O')di-μ-aquacopper(II)trisodium]

Crystal data

$[CuNa_3(C_2H_3O_2)_5(C_2H_4O_2)(H_2O)_2]$
$M_r = 523.81$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 14.571$ (6) Å
$b = 6.768$ (3) Å
$c = 22.653$ (10) Å
$\beta = 103.426$ (19)°
$V = 2173.0$ (16) Å^3
$Z = 4$
$F(000) = 1076$
$D_x = 1.601$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8924 reflections
$\theta = 3.0$–$27.5°$
$\mu = 1.13$ mm^{-1}
$T = 290$ K
Block, blue
0.27 × 0.25 × 0.23 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotaton anode
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.752$, $T_{max} = 0.777$
10214 measured reflections
2493 independent reflections
2192 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -18 \rightarrow 18$
$k = -8 \rightarrow 8$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.068$
$S = 1.03$
2493 reflections
142 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 1.7139P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.011$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

Special details

Experimental. (See detailed section in the paper)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.26112 (13)	1.3050 (3)	0.41200 (9)	0.0451 (5)
H1A	0.2567	1.2814	0.3696	0.068*
H1B	0.2834	1.4370	0.4221	0.068*
H1C	0.2000	1.2893	0.4206	0.068*
C2	0.32852 (10)	1.1606 (2)	0.44894 (7)	0.0252 (3)
C3	0.49416 (15)	1.1930 (3)	0.67768 (7)	0.0400 (4)
H3A	0.4943	1.3232	0.6945	0.060*
H3B	0.5462	1.1188	0.7010	0.060*
H3C	0.4361	1.1277	0.6788	0.060*
C4	0.50335 (11)	1.2077 (2)	0.61301 (6)	0.0237 (3)
C5	0.25974 (15)	0.7130 (4)	0.69424 (11)	0.0614 (6)
H5A	0.2259	0.5966	0.7010	0.092*
H5B	0.2658	0.7151	0.6529	0.092*
H5C	0.2259	0.8282	0.7020	0.092*
C6	0.35605 (13)	0.7116 (3)	0.73620 (8)	0.0352 (4)
Cu1	0.5000	1.0000	0.5000	0.01852 (8)
Na1	0.5000	0.5000	0.5000	0.02776 (19)
Na2	0.50180 (5)	0.70788 (10)	0.62598 (3)	0.03245 (16)
O1	0.30176 (9)	0.99791 (19)	0.46272 (7)	0.0430 (3)
O2	0.41529 (7)	1.21412 (16)	0.46414 (5)	0.0244 (2)
O3	0.49001 (8)	1.04618 (17)	0.58292 (5)	0.0282 (2)
O4	0.52322 (10)	1.36734 (18)	0.59343 (5)	0.0374 (3)
O5	0.42574 (9)	0.6909 (2)	0.71094 (6)	0.0455 (3)
H5	0.5000	0.6936	0.7500	0.068*
O6	0.36605 (10)	0.7272 (3)	0.79096 (6)	0.0517 (4)
O7	0.37443 (8)	0.67127 (19)	0.53741 (6)	0.0382 (3)
H7B	0.3291	0.6111	0.5410	0.057*
H7A	0.3518	0.7657	0.5191	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0326 (9)	0.0591 (13)	0.0409 (10)	0.0154 (9)	0.0033 (7)	0.0106 (9)
C2	0.0234 (7)	0.0315 (8)	0.0213 (7)	0.0002 (6)	0.0061 (5)	0.0000 (6)
C3	0.0630 (12)	0.0376 (10)	0.0218 (8)	−0.0002 (9)	0.0148 (8)	0.0001 (7)
C4	0.0287 (7)	0.0242 (7)	0.0184 (6)	0.0026 (6)	0.0058 (5)	0.0003 (6)
C5	0.0415 (11)	0.0837 (18)	0.0532 (13)	0.0000 (11)	−0.0011 (10)	−0.0001 (12)
C6	0.0386 (9)	0.0332 (9)	0.0328 (8)	−0.0008 (7)	0.0063 (7)	0.0024 (7)
Cu1	0.02176 (13)	0.01720 (13)	0.01633 (12)	−0.00190 (9)	0.00390 (9)	0.00037 (9)
Na1	0.0418 (5)	0.0207 (4)	0.0213 (4)	−0.0071 (4)	0.0084 (4)	−0.0001 (3)
Na2	0.0433 (4)	0.0303 (3)	0.0235 (3)	−0.0038 (3)	0.0071 (3)	−0.0006 (3)
O1	0.0336 (6)	0.0445 (8)	0.0488 (8)	−0.0151 (5)	0.0055 (6)	0.0105 (6)
O2	0.0228 (5)	0.0218 (5)	0.0271 (5)	−0.0013 (4)	0.0026 (4)	0.0006 (4)
O3	0.0426 (6)	0.0230 (5)	0.0205 (5)	−0.0008 (5)	0.0102 (4)	−0.0001 (4)
O4	0.0617 (8)	0.0254 (6)	0.0243 (5)	−0.0066 (6)	0.0084 (5)	0.0017 (5)
O5	0.0401 (7)	0.0691 (10)	0.0281 (6)	−0.0009 (7)	0.0095 (5)	−0.0013 (6)
O6	0.0430 (7)	0.0822 (12)	0.0316 (7)	0.0048 (7)	0.0122 (6)	0.0004 (7)
O7	0.0270 (6)	0.0361 (7)	0.0502 (7)	−0.0062 (5)	0.0060 (5)	0.0030 (6)

Geometric parameters (Å, º)

C1—C2	1.496 (2)	Cu1—O3	1.9426 (13)
C1—H1A	0.9600	Cu1—O2	1.9540 (12)
C1—H1B	0.9600	Cu1—Na1^{i}	3.3842 (14)
C1—H1C	0.9600	Cu1—Na2^{ii}	3.4669 (13)
C2—O1	1.232 (2)	Na1—O4^{iii}	2.2512 (14)
C2—O2	1.2831 (18)	Na1—O2^{iii}	2.3371 (13)
C3—C4	1.505 (2)	Na1—O7	2.4759 (15)
C3—H3A	0.9600	Na1—Na2^{iv}	3.1765 (13)
C3—H3B	0.9600	Na2—O6^{v}	2.3627 (18)
C3—H3C	0.9600	Na2—O7	2.4088 (16)
C4—O4	1.228 (2)	Na2—O5	2.4362 (17)
C4—O3	1.2792 (19)	Na2—O4^{iii}	2.4618 (17)
C5—C6	1.501 (3)	Na2—O3	2.4792 (16)
C5—H5A	0.9600	Na2—O2^{ii}	2.6554 (15)
C5—H5B	0.9600	O5—H5	1.2286
C5—H5C	0.9600	O7—H7B	0.7965
C6—O6	1.220 (2)	O7—H7A	0.7910
C6—O5	1.284 (2)		
C2—C1—H1A	109.5	O2^{ii}—Na1—O7	82.30 (5)
C2—C1—H1B	109.5	O2^{iii}—Na1—O7	97.70 (5)
H1A—C1—H1B	109.5	O7^{iv}—Na1—O7	180.0
C2—C1—H1C	109.5	O4^{ii}—Na1—Na2^{iv}	50.50 (4)
H1A—C1—H1C	109.5	O4^{iii}—Na1—Na2^{iv}	129.50 (4)
H1B—C1—H1C	109.5	O2^{ii}—Na1—Na2^{iv}	124.93 (3)
O1—C2—O2	122.32 (14)	O2^{iii}—Na1—Na2^{iv}	55.07 (3)

O1—C2—C1	121.35 (15)	O7^{iv}—Na1—Na2^{iv}	48.52 (3)
O2—C2—C1	116.31 (15)	O7—Na1—Na2^{iv}	131.48 (4)
C4—C3—H3A	109.5	O4^{ii}—Na1—Cu1^{iii}	113.51 (3)
C4—C3—H3B	109.5	O4^{iii}—Na1—Cu1^{iii}	66.49 (3)
H3A—C3—H3B	109.5	O2^{ii}—Na1—Cu1^{iii}	145.89 (3)
C4—C3—H3C	109.5	O2^{iii}—Na1—Cu1^{iii}	34.11 (3)
H3A—C3—H3C	109.5	O7^{iv}—Na1—Cu1^{iii}	62.08 (3)
H3B—C3—H3C	109.5	O7—Na1—Cu1^{iii}	117.92 (3)
O4—C4—O3	125.37 (14)	Na2^{iv}—Na1—Cu1^{iii}	63.708 (19)
O4—C4—C3	119.44 (15)	O6^{v}—Na2—O7	175.43 (6)
O3—C4—C3	115.18 (14)	O6^{v}—Na2—O5	79.03 (6)
C6—C5—H5A	109.5	O7—Na2—O5	104.44 (6)
C6—C5—H5B	109.5	O6^{v}—Na2—O4^{iii}	98.84 (6)
H5A—C5—H5B	109.5	O7—Na2—O4^{iii}	77.35 (5)
C6—C5—H5C	109.5	O5—Na2—O4^{iii}	107.75 (5)
H5A—C5—H5C	109.5	O6^{v}—Na2—O3	103.39 (6)
H5B—C5—H5C	109.5	O7—Na2—O3	78.33 (5)
O6—C6—O5	122.86 (17)	O5—Na2—O3	110.60 (5)
O6—C6—C5	121.13 (18)	O4^{iii}—Na2—O3	138.49 (5)
O5—C6—C5	116.00 (17)	O6^{v}—Na2—O2^{ii}	99.73 (6)
O3^{ii}—Cu1—O3	180.0	O7—Na2—O2^{ii}	77.30 (5)
O3^{ii}—Cu1—O2^{ii}	95.78 (5)	O5—Na2—O2^{ii}	171.22 (5)
O3—Cu1—O2^{ii}	84.22 (5)	O4^{iii}—Na2—O2^{ii}	81.02 (5)
O3^{ii}—Cu1—O2	84.22 (5)	O3—Na2—O2^{ii}	61.06 (4)
O3—Cu1—O2	95.78 (5)	C2—O2—Cu1	112.95 (10)
O2^{ii}—Cu1—O2	180.00 (6)	C2—O2—Na1^{i}	137.32 (10)
O3^{ii}—Cu1—Na1^{i}	99.26 (3)	Cu1—O2—Na1^{i}	103.76 (5)
O3—Cu1—Na1^{i}	80.74 (3)	C2—O2—Na2^{ii}	116.47 (9)
O2^{ii}—Cu1—Na1^{i}	137.87 (3)	Cu1—O2—Na2^{ii}	96.36 (5)
O2—Cu1—Na1^{i}	42.13 (3)	Na1^{i}—O2—Na2^{ii}	78.74 (4)
O3^{ii}—Cu1—Na2^{ii}	44.26 (4)	C4—O3—Cu1	128.07 (10)
O3—Cu1—Na2^{ii}	135.74 (4)	C4—O3—Na2	126.27 (10)
O2^{ii}—Cu1—Na2^{ii}	130.43 (4)	Cu1—O3—Na2	102.59 (5)
O2—Cu1—Na2^{ii}	49.57 (4)	C4—O4—Na1^{i}	133.95 (10)
Na1^{i}—Cu1—Na2^{ii}	55.23 (2)	C4—O4—Na2^{i}	131.20 (11)
O4^{ii}—Na1—O4^{iii}	180.0	Na1^{i}—O4—Na2^{i}	84.62 (5)
O4^{ii}—Na1—O2^{ii}	87.05 (5)	C6—O5—Na2	154.01 (12)
O4^{iii}—Na1—O2^{ii}	92.95 (5)	C6—O5—H5	109.4
O4^{ii}—Na1—O2^{iii}	92.95 (5)	Na2—O5—H5	94.7
O4^{iii}—Na1—O2^{iii}	87.05 (5)	C6—O6—Na2^{v}	133.48 (13)
O2^{ii}—Na1—O2^{iii}	180.0	Na2—O7—Na1	81.12 (5)
O4^{ii}—Na1—O7^{iv}	80.02 (5)	Na2—O7—H7B	117.7
O4^{iii}—Na1—O7^{iv}	99.98 (5)	Na1—O7—H7B	119.5
O2^{ii}—Na1—O7^{iv}	97.70 (5)	Na2—O7—H7A	120.0
O2^{iii}—Na1—O7^{iv}	82.30 (5)	Na1—O7—H7A	116.7

O4^{ii}—Na1—O7	99.98 (5)	H7B—O7—H7A	102.2
O4^{iii}—Na1—O7	80.02 (5)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*A*···O1	0.79	2.05	2.835 (2)	172
O7—H7*B*···O1^{vi}	0.80	2.03	2.8104 (19)	168

Symmetry code: (vi) −*x*+1/2, −*y*+3/2, −*z*+1.