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Crystal structure of $[NaZn(BTC)(H_2O)_4]\cdot 1.5H_2O$ (BTC = benzene-1,3,5-tricarboxylate): a heterometallic coordination compound

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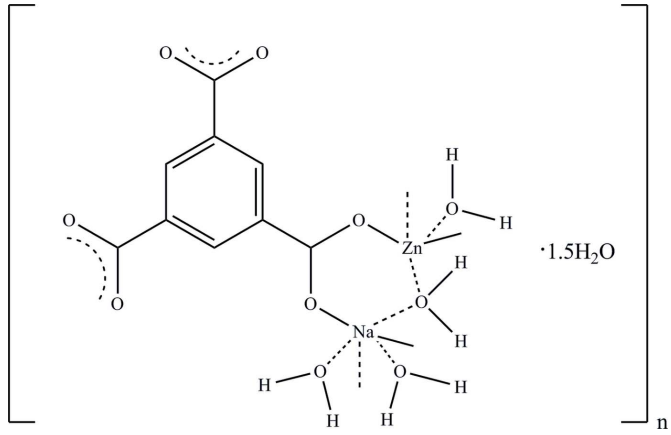
The title coordination polymer, poly[[μ-aqua-triaqua-(μ_3-benzene-1,3,5-tricarboxylato)sodiumzinc] sesquihydrate], $\{[NaZn(C_9H_3O_6)(H_2O)_4]\cdot 1.5H_2O\}_n$, was obtained in ionic liquid microemulsion at room temperture by the reaction of benzene-1,3,5-tricarboxylic acid (H_3BTC) with $Zn(NO_3)_2\cdot 6H_2O$ in the presence of NaOH. The asymmetric unit comprises two Na^+ ions (each located on an inversion centre), one Zn^{2+} ion, one BTC ligand, four coordinating water molecules and two solvent water molecules, one of which is disordered about an inversion centre and shows half-occupation. The Zn^{2+} cation is five-coordinated by two carboxylate O atoms from two different BTC ligands and three coordinating H_2O molecules; the Zn—O bond lengths are in the range 1.975 (2)–2.058 (3) Å. The Na^+ cations are six-coordinated but have different arrangements of the ligands: one is bound to two carboxylate O atoms of two BTC ligands and four O atoms from four coordinating H_2O molecules while the other is bound by four carboxylate O atoms from four BTC linkers and two O atoms of coordinating H_2O molecules. The completely deprotonated BTC ligand acts as a bridging ligand binding the Zn^{2+} atom and Na^+ ions, forming a layered structure extending parallel to (100). An intricate network of O—H···O hydrogen bonds is present within and between the layers.

Keywords: crystal structure; heterometallic coordination compound; benzene-1,3,5-tricarboxylic acid; hydrogen bonding.

CCDC reference: 1055450

1. Related literature

For general background to heterometallic coordination compounds, see: Stock & Biswas (2012); Gao *et al.* (2005); Zhou *et al.* (2012). For details of the synthesis, see: Shang *et al.* (2013); Fu *et al.* (2011). For the potential application of this compound, see: Huang *et al.* (2014).



2. Experimental

2.1. Crystal data

$[NaZn(C_9H_3O_6)(H_2O)_4]\cdot 1.5H_2O$
M_r = 394.56
Triclinic, $P\overline{1}$
a = 7.0980 (11) Å
b = 9.8000 (16) Å
c = 11.2043 (17) Å
α = 66.923 (2)°
β = 73.598 (2)°
γ = 84.720 (3)°
V = 687.68 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.88 mm^{-1}
T = 296 K
0.05 × 0.03 × 0.02 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.912, T_{max} = 0.963
7585 measured reflections
4331 independent reflections
2567 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.113
S = 0.97
4331 reflections
214 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O5^{i}	0.82	1.79	2.587 (4)	162
O7—H7B···O12^{ii}	0.82	1.93	2.740 (4)	172
O8—H8A···O10	0.82	2.40	3.114 (5)	146
O8—H8A···O11	0.82	1.98	2.672 (8)	142
O8—H8B···O6^{ii}	0.82	2.05	2.641 (5)	128
O9—H9A···O12^{iii}	0.82	1.95	2.734 (4)	159
O9—H9B···O2^{iv}	0.82	2.01	2.823 (4)	170
O10—H10A···O5^{v}	0.82	2.06	2.719 (6)	137

D—H···A	D—H	H···A	D···A	D—H···A
O10—H10B···O9^{vi}	0.82	2.31	3.079 (5)	155
O11—H11A···O3^{vii}	0.85	2.03	2.835 (8)	157
O11—H11B···O3^{v}	0.85	2.27	2.866 (7)	127
O11—H11B···O11^{viii}	0.85	1.33	1.973 (9)	128
O12—H12A···O6	0.82	1.86	2.652 (4)	161
O12—H12B···O4^{ix}	0.82	1.97	2.787 (3)	172

Symmetry codes: (i) $x, y+1, z-1$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x+2, -y+2, -z+1$; (iv) $-x+2, -y+2, -z$; (v) $-x+1, -y+1, -z+1$; (vi) $x-1, y, z$; (vii) $x-1, y+1, z$; (viii) $-x, -y+2, -z+1$; (ix) $x, y, z+1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS7* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: ZP2017).

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

Acta Cryst. (2015). E**71**, m143–m144 [doi:10.1107/S2056989015012001]

Crystal structure of $[NaZn(BTC)(H_2O)_4]\cdot 1.5H_2O$ (BTC = benzene-1,3,5-tricarboxylate): a heterometallic coordination compound

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S1. Synthesis and crystallization

In the experiment, the microemulsion of desired composition containing water, $[Bmim]PF_6$, and Triton X-100 was prepared using the method reported previously (Gao *et al.* 2005). H_3BTC (0.210 g, 1.0 mmol), NaOH (0.040 g, 1.0 mmol) and $Zn(NO_3)_2.6H_2O$ (0.298 g, 1.0 mmol) were added one by one into the microemulsion (20 g) which was clear and transparent system including 1.444 g $[Bmim]PF_6$, 10.428 g Triton X-100 and 8.310 g water. The whole system was stirred continuously for 24 h at 25°C. Then, the product crystals were collected by centrifugation at 4500 r/min and washed with alcohol three times (3x20 mL) to remove the surfactant and $[Bmim]PF_6$. Then, the crystals were dried in a vacuum oven at 60°C for 24 h. The resulting colorless crystals of the title compound were obtained.

S2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

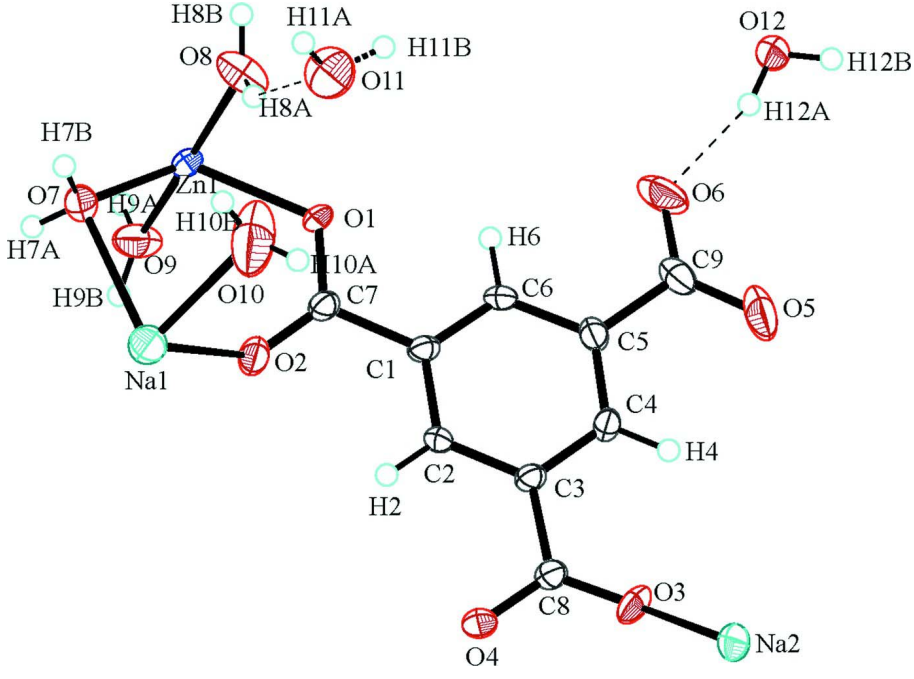

Figure 1

The molecular structure of the title compound with the atom-numbering scheme and 30% probability ellipsoids.

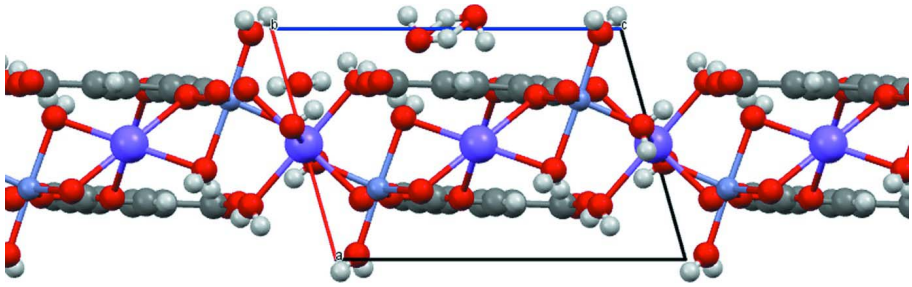

Figure 2

The packing diagram viewed along the *b* axis.

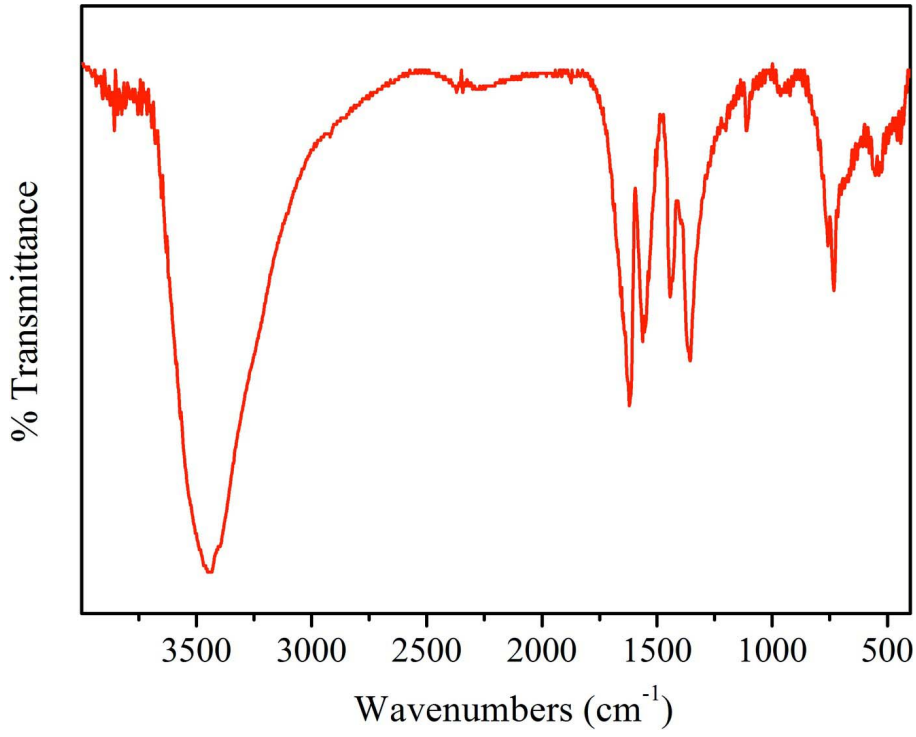

Figure 3

The FT–IR spectrum of the title compound.

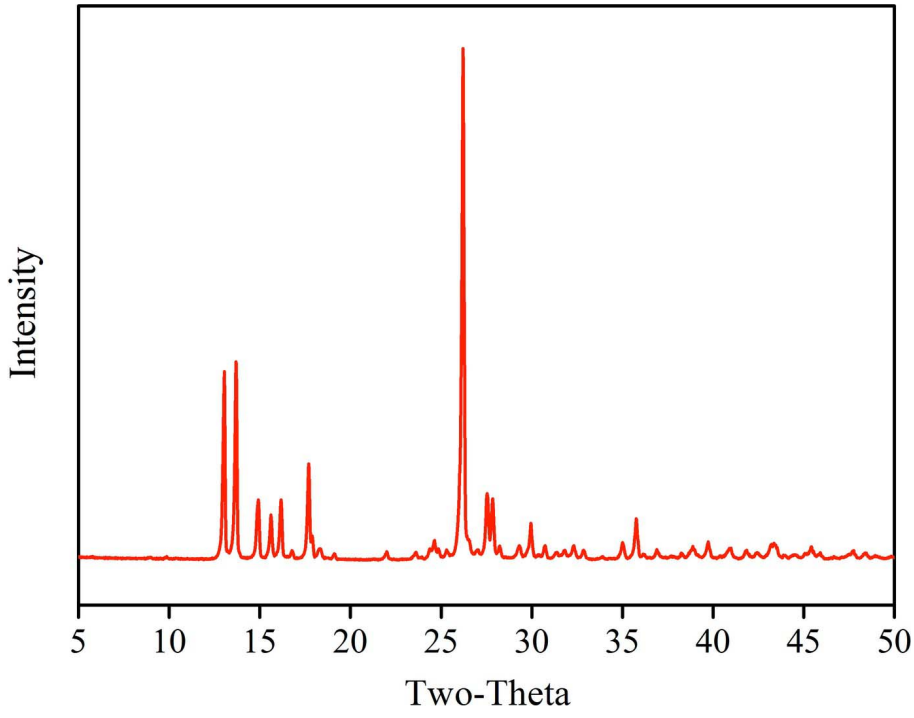

Figure 4

The XRD pattern of the title compound.

Poly[[μ-aqua-triaqua(μ_3-benzene-1,3,5-tricarboxylato)sodiumzinc] sesquihydrate]

Crystal data

$[NaZn(C_9H_3O_6)(H_2O)_4]\cdot 1.5H_2O$
$M_r = 394.56$
Triclinic, $P\overline{1}$
$a = 7.0980$ (11) Å
$b = 9.8000$ (16) Å
$c = 11.2043$ (17) Å
$\alpha = 66.923$ (2)°
$\beta = 73.598$ (2)°
$\gamma = 84.720$ (3)°
$V = 687.68$ (19) Å^3
$Z = 2$
$F(000) = 402$
$D_x = 1.906$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1047 reflections
$\theta = 2.4$–22.5°
$\mu = 1.88$ mm^{-1}
$T = 296$ K
Block, colourless
0.05 × 0.03 × 0.02 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.912$, $T_{max} = 0.963$
7585 measured reflections
4331 independent reflections
2567 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 32.0°$, $\theta_{min} = 2.3°$
$h = -10\rightarrow10$
$k = -14\rightarrow14$
$l = -16\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.113$
$S = 0.97$
4331 reflections
214 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.79$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. olex2_refinement_description 1. Fixed Uiso At 1.2 times of: All C(H) groups At 1.5 times of: All O(H,H) groups 2. Others Fixed Sof: O11(0.5) H11A(0.5) H11B(0.5) 3.a Riding coordinates: O7(H7A,H7B), O8(H8A,H8B), O9(H9A,H9B), O10(H10A,H10B), O12(H12A,H12B) 3.b Free rotating group: O11(H11A,H11B) 3.c Aromatic/amide H refined with riding coordinates: C2(H2), C4(H4), C6(H6)

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.69252 (6)	1.17043 (4)	0.17723 (4)	0.02302 (13)	
Na1	0.5000	1.0000	0.0000	0.0322 (5)	
Na2	0.5000	0.0000	0.5000	0.0319 (5)	
C1	0.7424 (5)	0.7068 (3)	0.3327 (3)	0.0184 (7)	
C2	0.7376 (5)	0.5950 (3)	0.2865 (3)	0.0186 (7)	
H2	0.7312	0.6192	0.1988	0.022*	
C3	0.7423 (5)	0.4476 (3)	0.3710 (3)	0.0188 (7)	
C4	0.7512 (5)	0.4130 (4)	0.5013 (3)	0.0207 (7)	
H4	0.7529	0.3140	0.5581	0.025*	
C5	0.7576 (5)	0.5231 (4)	0.5492 (3)	0.0211 (7)	
C6	0.7566 (5)	0.6703 (4)	0.4623 (3)	0.0204 (7)	
H6	0.7657	0.7455	0.4917	0.024*	
C7	0.7273 (5)	0.8667 (4)	0.2423 (3)	0.0204 (7)	
C8	0.7345 (5)	0.3229 (4)	0.3272 (3)	0.0206 (7)	
C9	0.7632 (5)	0.4837 (5)	0.6923 (4)	0.0291 (8)	
O1	0.7044 (4)	0.9607 (3)	0.2967 (3)	0.0371 (7)	
O2	0.7376 (4)	0.8999 (3)	0.1217 (3)	0.0341 (6)	
O3	0.7335 (4)	0.1931 (3)	0.4071 (3)	0.0325 (6)	
O4	0.7242 (4)	0.3558 (3)	0.2063 (2)	0.0268 (6)	
O5	0.7596 (4)	0.3477 (4)	0.7661 (3)	0.0467 (8)	
O6	0.7682 (4)	0.5863 (4)	0.7316 (3)	0.0479 (8)	
O7	0.5762 (4)	1.2363 (3)	0.0195 (2)	0.0292 (6)	
H7A	0.6483	1.2811	−0.0557	0.044*	
H7B	0.4703	1.2778	0.0249	0.044*	
O8	0.3875 (4)	1.1497 (3)	0.3061 (3)	0.0396 (7)	

H8A	0.3040	1.0995	0.3031	0.059*	
H8B	0.3305	1.2022	0.3464	0.059*	
O9	0.9800 (4)	1.1943 (3)	0.0630 (3)	0.0382 (7)	
H9A	1.0364	1.2580	0.0713	0.057*	
H9B	1.0536	1.1721	0.0026	0.057*	
O10	0.2322 (5)	0.9423 (4)	0.2021 (4)	0.0790 (13)	
H10A	0.1808	0.8593	0.2402	0.119*	
H10B	0.1445	1.0027	0.1899	0.119*	
O11	0.0497 (9)	0.9938 (8)	0.4107 (6)	0.0482 (16)	0.5
H11A	−0.0558	1.0390	0.3993	0.072*	0.5
H11B	0.0429	0.9553	0.4942	0.072*	0.5
O12	0.7580 (4)	0.6003 (3)	0.9650 (2)	0.0294 (6)	
H12A	0.7717	0.5773	0.9002	0.044*	
H12B	0.7499	0.5234	1.0318	0.044*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0340 (2)	0.01306 (19)	0.0218 (2)	−0.00099 (15)	−0.00540 (16)	−0.00759 (16)
Na1	0.0424 (13)	0.0290 (11)	0.0309 (12)	0.0027 (9)	−0.0169 (10)	−0.0128 (10)
Na2	0.0457 (13)	0.0204 (10)	0.0228 (11)	−0.0072 (9)	−0.0013 (9)	−0.0048 (9)
C1	0.0191 (16)	0.0153 (15)	0.0210 (17)	−0.0019 (12)	−0.0009 (13)	−0.0096 (13)
C2	0.0267 (18)	0.0163 (16)	0.0141 (16)	−0.0003 (13)	−0.0044 (13)	−0.0078 (13)
C3	0.0211 (17)	0.0145 (15)	0.0205 (17)	−0.0018 (12)	−0.0023 (13)	−0.0081 (13)
C4	0.0239 (18)	0.0150 (16)	0.0184 (17)	0.0016 (13)	−0.0045 (13)	−0.0025 (13)
C5	0.0217 (17)	0.0228 (17)	0.0150 (17)	0.0005 (13)	−0.0033 (13)	−0.0045 (14)
C6	0.0259 (18)	0.0190 (16)	0.0194 (17)	0.0014 (13)	−0.0039 (13)	−0.0123 (14)
C7	0.0221 (17)	0.0146 (16)	0.0221 (18)	−0.0014 (13)	−0.0017 (14)	−0.0070 (14)
C8	0.0229 (17)	0.0170 (16)	0.0221 (18)	0.0007 (13)	−0.0047 (14)	−0.0089 (14)
C9	0.0241 (19)	0.044 (2)	0.0187 (19)	0.0110 (16)	−0.0063 (15)	−0.0131 (18)
O1	0.071 (2)	0.0100 (12)	0.0212 (14)	0.0004 (12)	0.0018 (13)	−0.0062 (11)
O2	0.0607 (19)	0.0187 (13)	0.0253 (15)	0.0030 (12)	−0.0202 (13)	−0.0053 (11)
O3	0.0481 (17)	0.0124 (12)	0.0351 (16)	0.0001 (11)	−0.0128 (12)	−0.0058 (11)
O4	0.0411 (15)	0.0191 (12)	0.0235 (14)	−0.0019 (10)	−0.0079 (11)	−0.0117 (11)
O5	0.0529 (19)	0.053 (2)	0.0203 (15)	0.0040 (15)	−0.0114 (13)	0.0006 (14)
O6	0.058 (2)	0.070 (2)	0.0325 (17)	0.0229 (17)	−0.0228 (14)	−0.0346 (17)
O7	0.0337 (15)	0.0261 (14)	0.0213 (14)	0.0047 (11)	−0.0037 (11)	−0.0057 (11)
O8	0.0298 (15)	0.065 (2)	0.0303 (16)	−0.0049 (13)	−0.0034 (12)	−0.0265 (15)
O9	0.0386 (17)	0.0369 (16)	0.0418 (18)	−0.0062 (12)	0.0029 (13)	−0.0260 (14)
O10	0.059 (2)	0.062 (3)	0.068 (3)	0.0028 (18)	−0.0052 (18)	0.016 (2)
O11	0.041 (4)	0.052 (4)	0.052 (4)	0.008 (3)	−0.018 (3)	−0.019 (4)
O12	0.0440 (16)	0.0224 (13)	0.0223 (14)	−0.0001 (11)	−0.0096 (11)	−0.0086 (11)

Geometric parameters (Å, º)

Zn1—Na1	3.6267 (5)	C3—C8	1.495 (4)
Zn1—Na2^{i}	3.2603 (6)	C4—H4	0.9300
Zn1—O1	1.975 (2)	C4—C5	1.390 (5)

Zn1—O4^{i}	2.009 (2)	C5—C6	1.390 (4)
Zn1—O7	2.013 (2)	C5—C9	1.506 (5)
Zn1—O8	2.214 (3)	C6—H6	0.9300
Zn1—O9	2.058 (3)	C7—O1	1.267 (4)
Na1—Zn1^{ii}	3.6267 (5)	C7—O2	1.242 (4)
Na1—O2	2.369 (3)	C8—O3	1.235 (4)
Na1—O2^{ii}	2.369 (3)	C8—O4	1.286 (4)
Na1—O7	2.529 (3)	C9—O5	1.262 (5)
Na1—O7^{ii}	2.529 (3)	C9—O6	1.252 (5)
Na1—O10	2.413 (3)	O1—Na2^{i}	2.482 (2)
Na1—O10^{ii}	2.413 (3)	O4—Zn1^{iv}	2.009 (2)
Na2—Zn1^{iii}	3.2603 (6)	O7—H7A	0.8201
Na2—Zn1^{iv}	3.2603 (6)	O7—H7B	0.8201
Na2—O1^{iv}	2.482 (2)	O8—Na2^{i}	2.403 (3)
Na2—O1^{iii}	2.482 (2)	O8—H8A	0.8200
Na2—O3	2.339 (3)	O8—H8B	0.8201
Na2—O3^{v}	2.339 (3)	O9—H9A	0.8199
Na2—O8^{iii}	2.403 (3)	O9—H9B	0.8200
Na2—O8^{iv}	2.403 (3)	O10—H10A	0.8200
C1—C2	1.389 (4)	O10—H10B	0.8200
C1—C6	1.384 (4)	O11—H11A	0.8500
C1—C7	1.509 (4)	O11—H11B	0.8500
C2—H2	0.9300	O12—H12A	0.8203
C2—C3	1.386 (4)	O12—H12B	0.8200
C3—C4	1.382 (4)		

Na2^{i}—Zn1—Na1	108.751 (15)	O3^{v}—Na2—O8^{iii}	81.75 (9)
O1—Zn1—Na1	81.47 (8)	O3—Na2—O8^{iii}	98.25 (9)
O1—Zn1—Na2^{i}	49.45 (7)	O3—Na2—O8^{iv}	81.75 (9)
O1—Zn1—O4^{i}	129.50 (11)	O8^{iii}—Na2—Zn1^{iv}	137.24 (6)
O1—Zn1—O7	123.49 (11)	O8^{iv}—Na2—Zn1^{iii}	137.24 (6)
O1—Zn1—O8	83.14 (11)	O8^{iii}—Na2—Zn1^{iii}	42.76 (6)
O1—Zn1—O9	97.22 (11)	O8^{iv}—Na2—Zn1^{iv}	42.76 (6)
O4^{i}—Zn1—Na1	147.26 (7)	O8^{iii}—Na2—O1^{iii}	69.50 (9)
O4^{i}—Zn1—Na2^{i}	89.66 (7)	O8^{iii}—Na2—O1^{iv}	110.50 (9)
O4^{i}—Zn1—O7	105.44 (10)	O8^{iv}—Na2—O1^{iv}	69.50 (9)
O4^{i}—Zn1—O8	88.15 (11)	O8^{iv}—Na2—O1^{iii}	110.50 (9)
O4^{i}—Zn1—O9	89.49 (10)	O8^{iii}—Na2—O8^{iv}	180.0
O7—Zn1—Na1	42.24 (7)	C2—C1—C7	119.8 (3)
O7—Zn1—Na2^{i}	131.91 (7)	C6—C1—C2	119.7 (3)
O7—Zn1—O8	86.91 (10)	C6—C1—C7	120.6 (3)
O7—Zn1—O9	95.17 (11)	C1—C2—H2	119.9
O8—Zn1—Na1	85.30 (7)	C3—C2—C1	120.1 (3)
O8—Zn1—Na2^{i}	47.48 (7)	C3—C2—H2	119.9
O9—Zn1—Na1	97.50 (8)	C2—C3—C8	122.3 (3)
O9—Zn1—Na2^{i}	131.02 (8)	C4—C3—C2	119.4 (3)
O9—Zn1—O8	177.20 (11)	C4—C3—C8	118.2 (3)
Zn1—Na1—Zn1^{ii}	180.0	C3—C4—H4	119.3

O2—Na1—Zn1	53.49 (6)	C3—C4—C5	121.4 (3)
O2^{ii}—Na1—Zn1^{ii}	53.49 (6)	C5—C4—H4	119.3
O2^{ii}—Na1—Zn1	126.51 (6)	C4—C5—C9	120.8 (3)
O2—Na1—Zn1^{ii}	126.51 (6)	C6—C5—C4	118.3 (3)
O2^{ii}—Na1—O2	180.0	C6—C5—C9	120.8 (3)
O2^{ii}—Na1—O7^{ii}	83.14 (8)	C1—C6—C5	121.0 (3)
O2—Na1—O7	83.14 (8)	C1—C6—H6	119.5
O2^{ii}—Na1—O7	96.86 (8)	C5—C6—H6	119.5
O2—Na1—O7^{ii}	96.86 (8)	O1—C7—C1	116.3 (3)
O2—Na1—O10^{ii}	86.91 (11)	O2—C7—C1	120.1 (3)
O2^{ii}—Na1—O10^{ii}	93.09 (11)	O2—C7—O1	123.6 (3)
O2^{ii}—Na1—O10	86.91 (11)	O3—C8—C3	120.1 (3)
O2—Na1—O10	93.09 (11)	O3—C8—O4	122.0 (3)
O7^{ii}—Na1—Zn1	147.65 (5)	O4—C8—C3	117.9 (3)
O7—Na1—Zn1	32.36 (5)	O5—C9—C5	117.2 (4)
O7^{ii}—Na1—Zn1^{ii}	32.35 (5)	O6—C9—C5	118.8 (4)
O7—Na1—Zn1^{ii}	147.64 (5)	O6—C9—O5	124.0 (4)
O7^{ii}—Na1—O7	180.0	Zn1—O1—Na2^{i}	93.35 (9)
O10^{ii}—Na1—Zn1	99.48 (11)	C7—O1—Zn1	116.3 (2)
O10—Na1—Zn1^{ii}	99.48 (11)	C7—O1—Na2^{i}	140.1 (2)
O10—Na1—Zn1	80.52 (11)	C7—O2—Na1	130.6 (2)
O10^{ii}—Na1—Zn1^{ii}	80.52 (11)	C8—O3—Na2	132.2 (2)
O10—Na1—O7^{ii}	89.62 (12)	C8—O4—Zn1^{iv}	110.2 (2)
O10—Na1—O7	90.38 (12)	Zn1—O7—Na1	105.40 (10)
O10^{ii}—Na1—O7^{ii}	90.38 (12)	Zn1—O7—H7A	117.9
O10^{ii}—Na1—O7	89.62 (12)	Zn1—O7—H7B	118.8
O10^{ii}—Na1—O10	180.0	Na1—O7—H7A	101.6
Zn1^{iii}—Na2—Zn1^{iv}	180.0	Na1—O7—H7B	102.9
O1^{iii}—Na2—Zn1^{iv}	142.80 (5)	H7A—O7—H7B	107.7
O1^{iv}—Na2—Zn1^{iv}	37.20 (5)	Zn1—O8—Na2^{i}	89.76 (9)
O1^{iv}—Na2—Zn1^{iii}	142.80 (5)	Zn1—O8—H8A	121.4
O1^{iii}—Na2—Zn1^{iii}	37.20 (5)	Zn1—O8—H8B	129.0
O1^{iv}—Na2—O1^{iii}	180.0	Na2^{i}—O8—H8A	106.3
O3^{v}—Na2—Zn1^{iv}	123.65 (7)	Na2^{i}—O8—H8B	89.2
O3—Na2—Zn1^{iv}	56.35 (7)	H8A—O8—H8B	107.7
O3^{v}—Na2—Zn1^{iii}	56.35 (7)	Zn1—O9—H9A	109.9
O3—Na2—Zn1^{iii}	123.65 (7)	Zn1—O9—H9B	141.4
O3—Na2—O1^{iii}	102.11 (9)	H9A—O9—H9B	107.7
O3—Na2—O1^{iv}	77.89 (9)	Na1—O10—H10A	120.4
O3^{v}—Na2—O1^{iii}	77.89 (9)	Na1—O10—H10B	110.7
O3^{v}—Na2—O1^{iv}	102.11 (9)	H10A—O10—H10B	107.7
O3—Na2—O3^{v}	180.0	H11A—O11—H11B	109.5
O3^{v}—Na2—O8^{iv}	98.25 (9)	H12A—O12—H12B	107.7

C1—C2—C3—C4	0.2 (5)	C4—C5—C6—C1	2.3 (5)
C1—C2—C3—C8	179.1 (3)	C4—C5—C9—O5	−0.8 (5)
C1—C7—O1—Zn1	178.2 (2)	C4—C5—C9—O6	−179.8 (3)
C1—C7—O1—Na2^{i}	−48.0 (5)	C6—C1—C2—C3	1.5 (5)

C1—C7—O2—Na1	114.6 (3)	C6—C1—C7—O1	−8.3 (5)
C2—C1—C6—C5	−2.8 (5)	C6—C1—C7—O2	171.6 (3)
C2—C1—C7—O1	170.3 (3)	C6—C5—C9—O5	178.5 (3)
C2—C1—C7—O2	−9.9 (5)	C6—C5—C9—O6	−0.4 (5)
C2—C3—C4—C5	−0.7 (5)	C7—C1—C2—C3	−177.0 (3)
C2—C3—C8—O3	−178.0 (3)	C7—C1—C6—C5	175.7 (3)
C2—C3—C8—O4	0.4 (5)	C8—C3—C4—C5	−179.6 (3)
C3—C4—C5—C6	−0.6 (5)	C9—C5—C6—C1	−177.1 (3)
C3—C4—C5—C9	178.8 (3)	O1—C7—O2—Na1	−65.6 (4)
C3—C8—O3—Na2	116.2 (3)	O2—C7—O1—Zn1	−1.6 (5)
C3—C8—O4—Zn1^{iv}	−175.2 (2)	O2—C7—O1—Na2^{i}	132.1 (3)
C4—C3—C8—O3	0.9 (5)	O3—C8—O4—Zn1^{iv}	3.1 (4)
C4—C3—C8—O4	179.3 (3)	O4—C8—O3—Na2	−62.1 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*A*···O5^{vi}	0.82	1.79	2.587 (4)	162
O7—H7*B*···O12^{vii}	0.82	1.93	2.740 (4)	172
O8—H8*A*···O10	0.82	2.40	3.114 (5)	146
O8—H8*A*···O11	0.82	1.98	2.672 (8)	142
O8—H8*B*···O6^{vii}	0.82	2.05	2.641 (5)	128
O9—H9*A*···O12^{viii}	0.82	1.95	2.734 (4)	159
O9—H9*B*···O2^{ix}	0.82	2.01	2.823 (4)	170
O10—H10*A*···O5^{iii}	0.82	2.06	2.719 (6)	137
O10—H10*B*···O9^{x}	0.82	2.31	3.079 (5)	155
O11—H11*A*···O3^{xi}	0.85	2.03	2.835 (8)	157
O11—H11*B*···O3^{iii}	0.85	2.27	2.866 (7)	127
O11—H11*B*···O11^{xii}	0.85	1.33	1.973 (9)	128
O12—H12*A*···O6	0.82	1.86	2.652 (4)	161
O12—H12*B*···O4^{xiii}	0.82	1.97	2.787 (3)	172

Symmetry codes: (iii) −*x*+1, −*y*+1, −*z*+1; (vi) *x*, *y*+1, *z*−1; (vii) −*x*+1, −*y*+2, −*z*+1; (viii) −*x*+2, −*y*+2, −*z*+1; (ix) −*x*+2, −*y*+2, −*z*; (x) *x*−1, *y*, *z*; (xi) *x*−1, *y*+1, *z*; (xii) −*x*, −*y*+2, −*z*+1; (xiii) *x*, *y*, *z*+1.