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Poly[tetraaqua(μ_4-benzene-1,3,5-tricarboxylato)sodium(I)zinc(II)]

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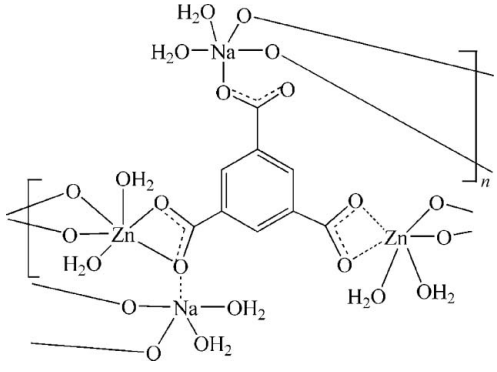
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.065; wR factor = 0.187; data-to-parameter ratio = 15.6.

In the title compound, $[NaZn(C_9H_3O_6)(H_2O)_4]_n$, the Zn^{II} atom is six-coordinated by four O atoms from two different benzene-1,3,5-tricarboxylate anions and two water O atoms in a distorted tetragonal-bipyramidal geometry and the Na^{I} atom is five-coordinated by three O atoms from three different benzene-1,3,5-tricarboxylate anions and two water O atoms in a distorted trigonal-bipyramidal geometry. The benzene-1,3,5-tricarboxylate anion bridges two Zn^{II} atoms and two Na^{I} atoms, resulting in the formation of a two-dimensional layer structure. Intermolecular O—H···O hydrogen-bonding interactions generate a three-dimensional superamolecular structure.

Related literature

For related sructures, see: Chui *et al.* (1999); Majumder *et al.* (2005).



Experimental

Crystal data

$[NaZn(C_9H_3O_6)(H_2O)_4]$
M_r = 367.54
Monoclinic, $C2/c$
a = 23.425 (5) Å
b = 10.146 (2) Å
c = 14.427 (3) Å
β = 126.50 (3)°
V = 2756.3 (15) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.86 mm^{-1}
T = 293 K
0.23 × 0.22 × 0.20 mm

Data collection

Oxford Diffraction Gemini R Ultra diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2007)
T_{min} = 0.765, T_{max} = 0.876
13077 measured reflections
3348 independent reflections
2119 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.187
S = 0.99
3348 reflections
214 parameters
106 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O5^{i}	0.93 (5)	2.35 (8)	3.090 (6)	137 (9)
O2W—H2WA···O2^{ii}	0.93 (5)	2.28 (9)	2.998 (6)	133 (9)
O3W—H3WA···O6	0.85 (5)	2.11 (7)	2.747 (7)	132 (7)
O4W—H4WB···O4^{iii}	1.00 (5)	1.71 (5)	2.686 (8)	166 (8)
O4W—H4WA···O3W^{iv}	0.85 (4)	2.37 (7)	2.948 (8)	126 (9)

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *DIAMOND* (Brandenburg, 1998).

We thank Jilin Agricultural Science and Technology College for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2022).

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supporting information

Acta Cryst. (2010). E**66**, m416 [doi:10.1107/S1600536810009232]

Poly[tetraaqua(μ_4-benzene-1,3,5-tricarboxylato)sodium(I)zinc(II)]

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S1. Comment

In the title compound, (I), each Zn^{II} cation is six-coordinated by five O atoms from two different benzene-1,3,5-tricarboxylate anions and two water molecules. The Zn—O (carboxylate) distance in I is similar to the equivalent value in a related compounds (Majumder *et al.* 2005). Each Na^{I} cation is five coordinated by three oxygen atoms from three different benzene-1,3,5-tricarboxylate anions and two water molecules. The Na—O (carboxylate) distance is similar to the related compounds (Chui *et al.* 1999) (Fig. 1). The Zn^{II} centers and the Na^{I} centers are bridged by benzene-1,3,5-tricarboxylate anions, resulting in a two dimensional layer (Fig. 2). In (I), there are intra and intermolecular O-H···O hydrogen bonds involving the water molecules and the oxygen atoms of the carboxylate groups (Table 1). The adjacent layers are bridged by the hydrogen bonds, and the whole structure displays a three dimensional supramolecular framework (Fig. 3).

S2. Experimental

The mixture of of benzene-1,3,5-tricarboxylate acid (0.063 g, 0.3 mmol), NaOH (0.024 g, 0.25 mmol), $Zn(Ac)_2$ (0.066 g, 0.3 mmol), and 10 ml H_2O was sealed in 18 ml Teflon-lined stainless steel container. The container was heated to 150 °C and held at that temperature for 72 h, then cooled to room temperature at a rate of 10 °C.h^{-1}. And then crystals of the title compound were isolated.

S3. Refinement

C-bound H-atoms were geometrically positioned (C—H = 0.93 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}$ (C). The H atoms of the water molecules were located in a difference map, and were refined with distance restraints of O—H = 0.85 Å.

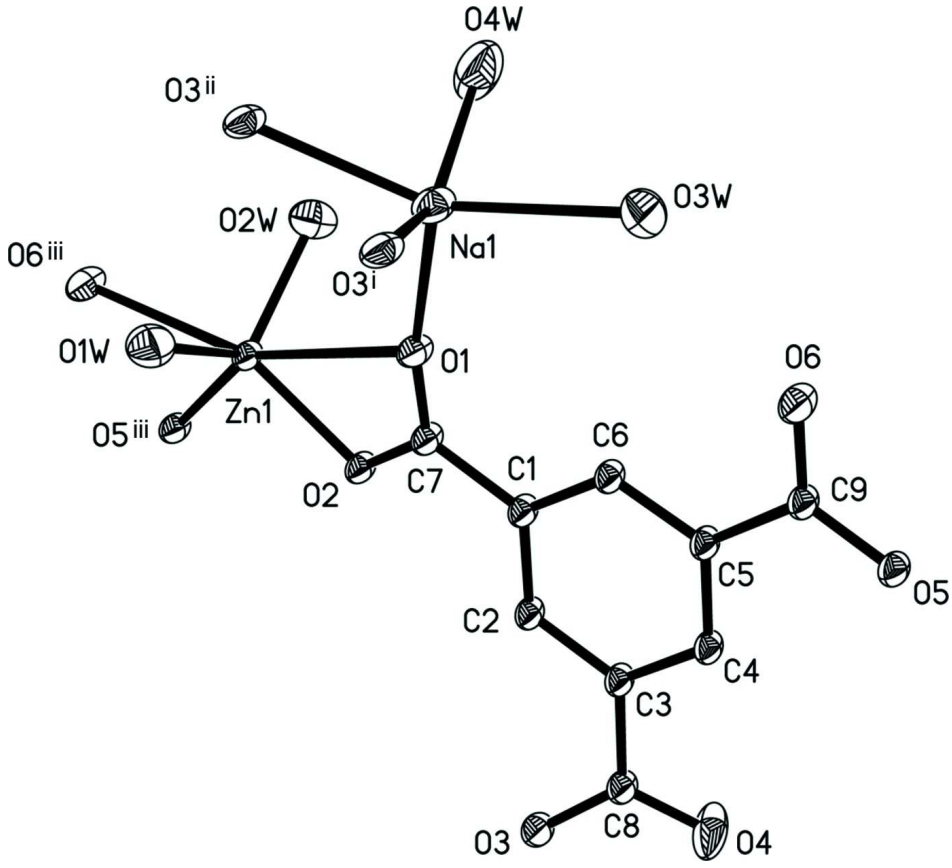

Figure 1

ORTEP diagram of the coordination environments for Zn^{II} atom and Na^{I} atom in (I), showing 30% probability displacement ellipsoids, crystalline water molecules and the atomic numbering scheme [symmetry code: (i) 1-x, y, 1.5-z; (ii) x-0.5, 1.5-y, z-0.5; (iii) x, y-1, z]. H atoms have been omitted for clarity.

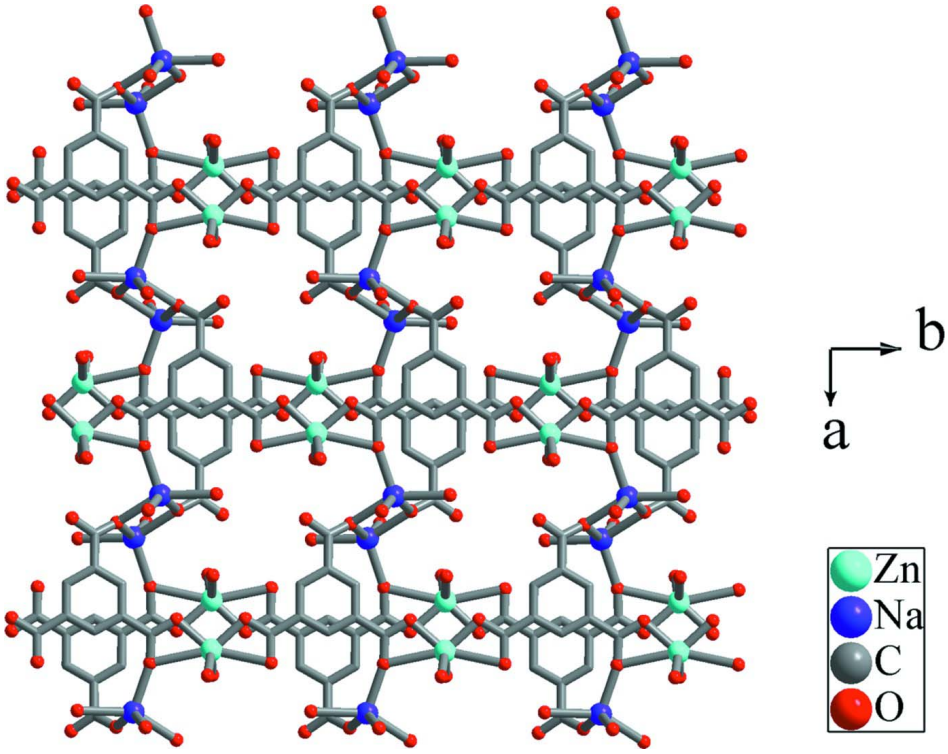

Figure 2

The two dimensional layer of (I). The H atoms have been omitted.

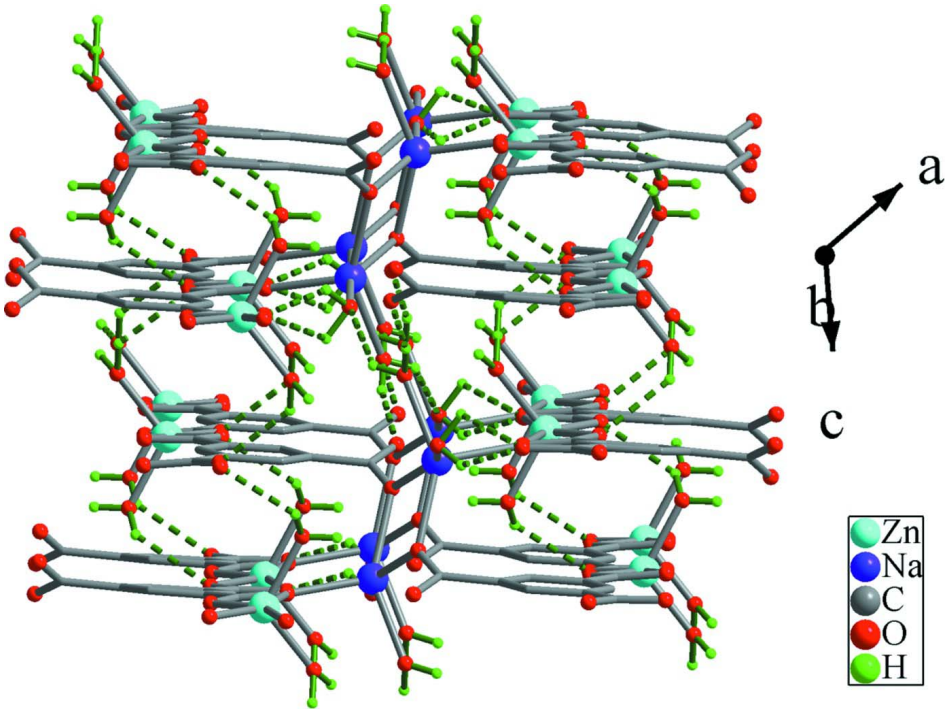

Figure 3

The supramolecular framework of I.

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Crystal data

$[NaZn(C_9H_3O_6)(H_2O)_4]$
$M_r = 367.54$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 23.425$ (5) Å
$b = 10.146$ (2) Å
$c = 14.427$ (3) Å
$\beta = 126.50$ (3)°
$V = 2756.3$ (15) Å^3
$Z = 8$
$F(000) = 1488$
$D_x = 1.771$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3348 reflections
$\theta = 4.7$–$29.2°$
$\mu = 1.86$ mm^{-1}
$T = 293$ K
Block, colorless
0.23 × 0.22 × 0.20 mm

Data collection

Oxford Diffraction Gemini R Ultra diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2007)
$T_{min} = 0.765$, $T_{max} = 0.876$
13077 measured reflections
3348 independent reflections
2119 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 29.2°$, $\theta_{min} = 4.7°$
$h = -31 \rightarrow 29$
$k = -13 \rightarrow 13$
$l = -19 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.187$
$S = 0.99$
3348 reflections
214 parameters
106 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1186P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.68$ e Å^{-3}
$\Delta\rho_{min} = -0.79$ 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
Zn1	0.44260 (3)	0.47289 (5)	0.56752 (5)	0.0277 (2)
Na1	0.29885 (10)	0.8061 (2)	0.4465 (2)	0.0406 (5)
C9	0.4802 (2)	1.2199 (5)	0.5988 (4)	0.0284 (7)

C8	0.7090 (3)	0.9737 (5)	0.8706 (5)	0.0331 (7)
C4	0.5942 (2)	1.0936 (5)	0.7306 (4)	0.0268 (6)
H008	0.6191	1.1727	0.7565	0.032*
C6	0.4854 (3)	0.9745 (4)	0.6091 (4)	0.0264 (6)
H012	0.4365	0.9746	0.5531	0.032*
C5	0.5209 (2)	1.0942 (4)	0.6463 (4)	0.0265 (6)
C3	0.6303 (3)	0.9744 (5)	0.7762 (4)	0.0280 (6)
C2	0.5932 (2)	0.8565 (5)	0.7375 (4)	0.0267 (7)
H017	0.6173	0.7773	0.7687	0.032*
C7	0.4788 (2)	0.7306 (5)	0.6098 (4)	0.0289 (6)
C1	0.5198 (2)	0.8558 (5)	0.6519 (4)	0.0263 (6)
O1	0.41242 (17)	0.7350 (3)	0.5455 (3)	0.0344 (7)
O1W	0.3853 (3)	0.4688 (5)	0.6293 (5)	0.0575 (12)
O2W	0.3838 (2)	0.4876 (6)	0.3961 (4)	0.0546 (12)
O4W	0.2642 (4)	0.7532 (7)	0.2655 (5)	0.094 (2)
O6	0.41411 (19)	1.2178 (4)	0.5267 (4)	0.0448 (10)
O3W	0.3018 (3)	1.0451 (6)	0.4118 (6)	0.087 (2)
O5	0.51477 (17)	1.3279 (3)	0.6362 (3)	0.0316 (7)
O2	0.51282 (16)	0.6223 (3)	0.6419 (3)	0.0292 (6)
O3	0.73536 (18)	0.8792 (4)	0.9374 (3)	0.0376 (7)
O4	0.7451 (2)	1.0708 (6)	0.8821 (6)	0.092 (2)
H1WA	0.392 (5)	0.402 (9)	0.679 (8)	0.138*
H4WA	0.224 (4)	0.730 (11)	0.207 (3)	0.138*
H4WB	0.269 (5)	0.822 (8)	0.221 (4)	0.138*
H3WA	0.331 (5)	1.086 (2)	0.475 (5)	0.138*
H3WB	0.336 (5)	1.053 (3)	0.394 (10)	0.138*
H2WB	0.363 (6)	0.559 (8)	0.345 (8)	0.138*
H1WB	0.340 (3)	0.471 (11)	0.579 (8)	0.138*
H2WA	0.389 (6)	0.440 (10)	0.347 (8)	0.138*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0207 (3)	0.0165 (3)	0.0349 (4)	0.0010 (2)	0.0105 (3)	0.0011 (2)
Na1	0.0259 (10)	0.0345 (12)	0.0480 (13)	0.0002 (9)	0.0148 (10)	−0.0034 (10)
C9	0.0229 (10)	0.0168 (11)	0.0363 (11)	0.0020 (9)	0.0126 (9)	0.0020 (9)
C8	0.0241 (11)	0.0219 (11)	0.0384 (12)	0.0024 (10)	0.0104 (10)	0.0052 (10)
C4	0.0220 (9)	0.0167 (10)	0.0352 (10)	0.0018 (9)	0.0134 (9)	0.0029 (9)
C6	0.0213 (9)	0.0165 (10)	0.0352 (10)	0.0021 (8)	0.0135 (8)	0.0016 (9)
C5	0.0219 (9)	0.0162 (10)	0.0350 (10)	0.0020 (8)	0.0135 (8)	0.0023 (8)
C3	0.0220 (9)	0.0182 (10)	0.0357 (10)	0.0022 (8)	0.0129 (8)	0.0037 (8)
C2	0.0214 (9)	0.0168 (10)	0.0355 (10)	0.0025 (8)	0.0134 (9)	0.0028 (9)
C7	0.0215 (9)	0.0174 (9)	0.0382 (10)	0.0019 (8)	0.0126 (8)	0.0003 (9)
C1	0.0211 (9)	0.0164 (9)	0.0356 (10)	0.0022 (8)	0.0138 (8)	0.0015 (8)
O1	0.0224 (11)	0.0196 (11)	0.0428 (13)	0.0022 (9)	0.0094 (10)	−0.0011 (10)
O1W	0.040 (2)	0.069 (3)	0.054 (3)	0.002 (2)	0.023 (2)	0.007 (2)
O2W	0.045 (2)	0.063 (3)	0.042 (3)	0.005 (2)	0.018 (2)	0.000 (2)
O4W	0.127 (5)	0.088 (4)	0.063 (4)	−0.059 (4)	0.055 (4)	−0.023 (3)

O6	0.0245 (18)	0.0215 (19)	0.060 (3)	0.0045 (15)	0.0098 (18)	0.0032 (18)
O3W	0.054 (3)	0.060 (4)	0.085 (4)	−0.004 (2)	0.007 (3)	0.032 (3)
O5	0.0242 (11)	0.0171 (12)	0.0383 (13)	0.0013 (10)	0.0104 (10)	0.0017 (10)
O2	0.0219 (10)	0.0163 (11)	0.0388 (12)	0.0010 (9)	0.0123 (9)	0.0004 (10)
O3	0.0263 (12)	0.0251 (12)	0.0402 (13)	0.0029 (10)	0.0084 (10)	0.0066 (11)
O4	0.029 (2)	0.058 (3)	0.119 (5)	−0.010 (2)	0.006 (3)	0.044 (3)

Geometric parameters (Å, º)

Zn1—O2W	1.996 (5)	C6—C5	1.387 (7)
Zn1—O5^{i}	2.002 (3)	C6—H012	0.9300
Zn1—O1W	2.006 (5)	C3—C2	1.385 (7)
Zn1—O2	2.014 (3)	C2—C1	1.400 (6)
Na1—O1	2.262 (4)	C2—H017	0.9300
Na1—O4W	2.290 (6)	C7—O1	1.251 (6)
Na1—O3^{ii}	2.352 (4)	C7—O2	1.271 (6)
Na1—O3^{iii}	2.365 (5)	C7—C1	1.486 (7)
Na1—O3W	2.486 (5)	O1W—H1WA	0.93 (5)
Na1—Na1^{iv}	3.621 (4)	O1W—H1WB	0.86 (5)
C9—O6	1.250 (6)	O2W—H2WB	0.94 (5)
C9—O5	1.277 (6)	O2W—H2WA	0.93 (5)
C9—C5	1.493 (6)	O4W—H4WA	0.85 (4)
C8—O3	1.233 (6)	O4W—H4WB	1.00 (5)
C8—O4	1.245 (7)	O3W—H3WA	0.85 (5)
C8—C3	1.505 (7)	O3W—H3WB	0.98 (5)
C4—C5	1.394 (7)	O5—Zn1^{v}	2.002 (3)
C4—C3	1.396 (7)	O3—Na1^{vi}	2.352 (4)
C4—H008	0.9300	O3—Na1^{iii}	2.365 (5)
C6—C1	1.374 (6)		

O2W—Zn1—O5^{i}	115.16 (19)	C6—C5—C4	118.5 (4)
O2W—Zn1—O1W	113.7 (2)	C6—C5—C9	119.9 (4)
O5^{i}—Zn1—O1W	110.88 (18)	C4—C5—C9	121.6 (4)
O2W—Zn1—O2	110.30 (19)	C2—C3—C4	119.9 (4)
O5^{i}—Zn1—O2	96.19 (14)	C2—C3—C8	119.8 (4)
O1W—Zn1—O2	109.20 (18)	C4—C3—C8	120.2 (4)
O1—Na1—O4W	97.5 (2)	C3—C2—C1	120.5 (4)
O1—Na1—O3^{ii}	104.33 (15)	C3—C2—H017	119.8
O4W—Na1—O3^{ii}	88.02 (18)	C1—C2—H017	119.8
O1—Na1—O3^{iii}	114.83 (16)	O1—C7—O2	122.3 (4)
O4W—Na1—O3^{iii}	147.3 (2)	O1—C7—C1	119.2 (4)
O3^{ii}—Na1—O3^{iii}	79.70 (15)	O2—C7—C1	118.5 (4)
O1—Na1—O3W	105.94 (18)	C6—C1—C2	118.4 (4)
O4W—Na1—O3W	91.8 (3)	C6—C1—C7	120.2 (4)
O3^{ii}—Na1—O3W	149.48 (19)	C2—C1—C7	121.4 (4)
O3^{iii}—Na1—O3W	84.2 (2)	C7—O1—Na1	162.9 (3)
O1—Na1—Na1^{iv}	115.79 (15)	Zn1—O1W—H1WA	120 (7)
O4W—Na1—Na1^{iv}	121.80 (18)	Zn1—O1W—H1WB	116 (8)

O3^{ii}—Na1—Na1^{iv}	39.98 (10)	H1WA—O1W—H1WB	104 (7)
O3^{iii}—Na1—Na1^{iv}	39.72 (10)	Zn1—O2W—H2WB	134 (7)
O3W—Na1—Na1^{iv}	119.6 (2)	Zn1—O2W—H2WA	127 (7)
O6—C9—O5	121.8 (4)	H2WB—O2W—H2WA	92 (6)
O6—C9—C5	120.3 (4)	Na1—O4W—H4WA	129 (4)
O5—C9—C5	117.9 (4)	Na1—O4W—H4WB	118 (3)
O3—C8—O4	121.8 (5)	H4WA—O4W—H4WB	92 (5)
O3—C8—C3	119.1 (4)	Na1—O3W—H3WA	111 (3)
O4—C8—C3	119.1 (5)	Na1—O3W—H3WB	105 (2)
C5—C4—C3	120.1 (4)	H3WA—O3W—H3WB	89 (6)
C5—C4—H008	119.9	C9—O5—Zn1^{v}	106.5 (3)
C3—C4—H008	119.9	C7—O2—Zn1	108.7 (3)
C1—C6—C5	122.5 (4)	C8—O3—Na1^{vi}	132.2 (4)
C1—C6—H012	118.7	C8—O3—Na1^{iii}	125.0 (4)
C5—C6—H012	118.7	Na1^{vi}—O3—Na1^{iii}	100.30 (15)
C1—C6—C5—C4	−0.2 (8)	O2—C7—C1—C6	172.8 (5)
C1—C6—C5—C9	−178.2 (5)	O1—C7—C1—C2	170.0 (5)
C3—C4—C5—C6	−0.3 (7)	O2—C7—C1—C2	−9.0 (8)
C3—C4—C5—C9	177.6 (5)	O2—C7—O1—Na1	166.7 (9)
O6—C9—C5—C6	0.8 (8)	C1—C7—O1—Na1	−12.3 (16)
O5—C9—C5—C6	179.3 (5)	O4W—Na1—O1—C7	121.7 (13)
O6—C9—C5—C4	−177.1 (5)	O3^{ii}—Na1—O1—C7	−148.4 (13)
O5—C9—C5—C4	1.3 (7)	O3^{iii}—Na1—O1—C7	−63.3 (13)
C5—C4—C3—C2	0.1 (8)	O3W—Na1—O1—C7	27.6 (13)
C5—C4—C3—C8	−177.5 (5)	Na1^{iv}—Na1—O1—C7	−107.5 (13)
O3—C8—C3—C2	−23.6 (8)	O6—C9—O5—Zn1^{v}	4.6 (6)
O4—C8—C3—C2	159.3 (6)	C5—C9—O5—Zn1^{v}	−173.8 (4)
O3—C8—C3—C4	154.0 (5)	O1—C7—O2—Zn1	2.3 (6)
O4—C8—C3—C4	−23.1 (9)	C1—C7—O2—Zn1	−178.7 (4)
C4—C3—C2—C1	0.8 (8)	O2W—Zn1—O2—C7	59.7 (4)
C8—C3—C2—C1	178.3 (5)	O5^{i}—Zn1—O2—C7	179.4 (3)
C5—C6—C1—C2	1.0 (8)	O1W—Zn1—O2—C7	−65.9 (4)
C5—C6—C1—C7	179.3 (5)	O4—C8—O3—Na1^{vi}	−82.2 (8)
C3—C2—C1—C6	−1.3 (8)	C3—C8—O3—Na1^{vi}	100.7 (5)
C3—C2—C1—C7	−179.5 (5)	O4—C8—O3—Na1^{iii}	119.5 (6)
O1—C7—C1—C6	−8.2 (8)	C3—C8—O3—Na1^{iii}	−57.5 (6)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O5^{vii}	0.93 (5)	2.35 (8)	3.090 (6)	137 (9)
O2*W*—H2*WA*···O2^{viii}	0.93 (5)	2.28 (9)	2.998 (6)	133 (9)
O3*W*—H3*WA*···O6	0.85 (5)	2.11 (7)	2.747 (7)	132 (7)

O4*W*—H4*WB*···O4^{ix}	1.00 (5)	1.71 (5)	2.686 (8)	166 (8)
O4*W*—H4*WA*···O3*W*^{x}	0.85 (4)	2.37 (7)	2.948 (8)	126 (9)

Symmetry codes: (vii) −*x*+1, *y*−1, −*z*+3/2; (viii) −*x*+1, −*y*+1, −*z*+1; (ix) −*x*+1, −*y*+2, −*z*+1; (x) −*x*+1/2, *y*−1/2, −*z*+1/2.