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Poly[[triaqua[μ_4-*N*-(4-carboxylatophenyl)iminodiacetato]sodium(I)zinc(II)] dihydrate]

Dong-Sheng Ma

College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China
Correspondence e-mail: hgf1000@163.com

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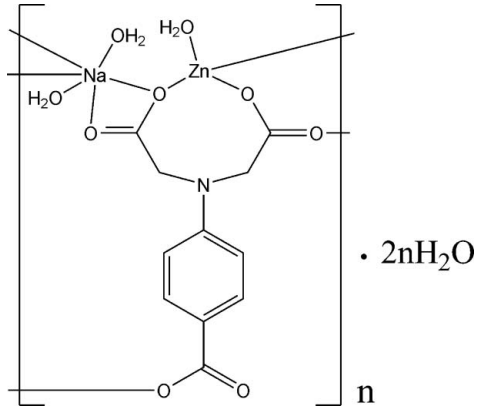
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.065; data-to-parameter ratio = 16.2.

In the title coordination polymer, {[NaZn($C_{11}H_8NO_6$)(H_2O)$_3$]·2H_2O}$_n$, the Zn atom is coordinated in a distorted tetrahedral environment by three carboxylate O atoms from two (4-carboxylatophenylimino)diacetate ligands and one water molecule; the Na atom is in an distorted octahedral coordination environment formed by four carboxylate O atoms from three (4-carboxylatophenylimino)diacetate ligands and two water molecules. The Zn atoms and Na atoms are linked by (4-carboxylatophenylimino)diacetate ligands into a three-dimensional framework; the uncoordinated water molecules fill the voids of the skeleton and stabilize it by O—H···O hydrogen bonds.

Related literature

For the synthesis of 2,2′-(4-carboxyphenylazanediyl)diacetic acid, see: Young & Sweet (1958).



Experimental

Crystal data

[NaZn($C_{11}H_8NO_6$)(H_2O)$_3$]·2H_2O
M_r = 428.62
Triclinic, $P\overline{1}$
a = 7.925 (4) Å
b = 8.989 (6) Å
c = 11.726 (6) Å
α = 96.28 (3)°
β = 98.63 (2)°
γ = 98.97 (2)°
V = 808.1 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.61 mm^{-1}
T = 291 (2) K
0.22 × 0.18 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.718, T_{max} = 0.782
8055 measured reflections
3668 independent reflections
3320 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.065
S = 1.10
3668 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H10···O9^{i}	0.85	1.87	2.716 (3)	174
O7—H9···O5^{ii}	0.85	2.06	2.867 (2)	159
O8—H12···O5^{iii}	0.85	1.90	2.748 (3)	173
O8—H11···O11^{i}	0.85	1.97	2.798 (2)	163
O9—H14···O1^{iv}	0.85	2.07	2.910 (2)	168
O9—H13···O8^{i}	0.85	1.96	2.801 (2)	172
O10—H17···O1^{iv}	0.85	1.92	2.762 (3)	174
O11—H15···O6^{vi}	0.85	2.16	2.949 (3)	154
O11—H16···O10	0.85	1.89	2.721 (3)	165

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

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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The authors thank Heilongjiang University for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2512).

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supporting information

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Poly[[triaqua[μ_4-*N*-(4-carboxylatophenyl)iminodiacetato]sodium(I)zinc(II)] dihydrate]

Dong-Sheng Ma

S1. Comment

2,2′-(4-Carboxyphenylazanediyl)diacetic acid is a multidentate flexible ligand with versatile binding abilities and capability of participating in hydrongen bonds, thus representing an excellent candidate for the construction of supramolecular complexe. In this paper, we report a novel title compound, (I), which is prepared by 2,2′-(4-carboxyphenylazanediyl)diacetic acid ligand and Zinc dinitrate under neutral aqueous conditions, which forms a three-dimensional framework structure.

The asymmetric unit of (1) consists of one Zn(II) ion, one Na(I) ion, one 4-carboxylatophenylimino)diacetate anion, three coordinated water molecules and two uncoordinated water molecules (Fig. 1). The Zn(II) ion is in a tetrahedral coordination environment, formed by three carboxylate O atoms from two 4-carboxylatophenylimino)diacetate ligands and one water molecules. The Na(I) ion exists in a distorted octahedral configuration with the equatorial plane being defined by the atoms O1, O2, O4^{II} and O8, and with O9 and o4^{III} occupy the axial sites. Each 4-carboxylatophenylimino)-diacetate anion bridged two Zn(II) ions and three Na(I) ions to form a three-dimensional supramolecular framework network in which uncoordinated water molecules filled the space of the skelecton and stabilized by O—H···O hydrogen bonds(Fig. 2, Table 1).

S2. Experimental

2,2′-(4-Carboxyphenylazanediyl)diacetic acid was synthesized by the literature method (Young *et al.*, 1958). The complex (I) was synthesized with znic(II) dinitrate (0.375 g, 2 mmol) and 2,2′-(4-Carboxyphenylazanediyl)diacetic acid (0.253 g, 1 mmol) were dissolved in methanol and the pH was adjusted to about 7 with 0.01*M* sodium hydroxide. Colorless crystals were separated from the filtered solution after several days.

S3. Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å, 0.97 Å for aromatic and methylene H atoms respectively; U_{iso}(H) was set to = 1.2U_{eq} of the carrier atom. Water H atoms were placed in calculated positions, with O—H=0.85 Å, U_{iso}(H) = 1.U_{eq}(O).

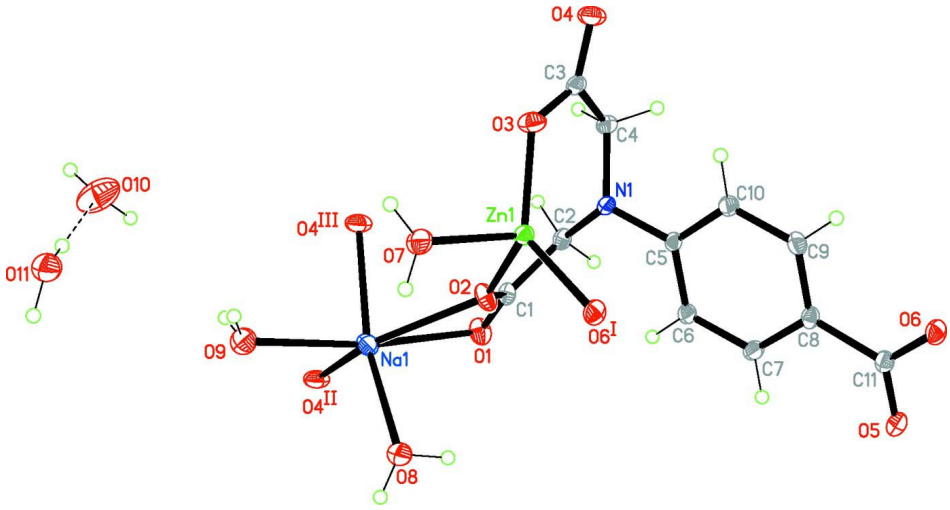

Figure 1

The molecular structure of (I), showing displacement ellipsoids at the 30% probability level for non-H atoms. Dashed lines indicate the hydrogen-bonding interactions [Symmetry code: (I) -*x* + 2, -*y*, -*z* + 2; (II) *x*, *y* + 1, *z*;(III) -*x* + 1, -*y*, *z* + 1].

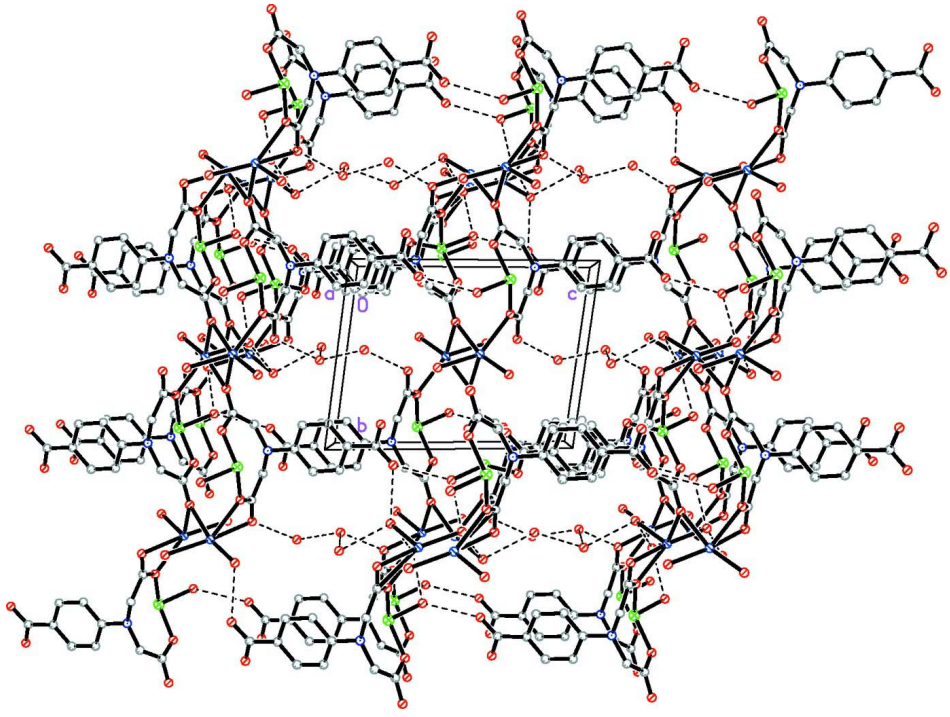

Figure 2

Part of the polymeric structure of (I), showing a three-dimensional framework.Dashed lines indicate the hydrogen-bonding interactions

Poly[[triaqua[μ_4-N-(4-carboxylatophenyl)iminodiacetato]sodium(I)zinc(II)] dihydrate]

Crystal data

$[NaZn(C_{11}H_8NO_6)(H_2O)_3]\cdot 2H_2O$
$M_r = 428.62$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.925$ (4) Å
$b = 8.989$ (6) Å
$c = 11.726$ (6) Å
$\alpha = 96.28$ (3)°
$\beta = 98.63$ (2)°
$\gamma = 98.97$ (2)°
$V = 808.1$ (8) Å^3
$Z = 2$
$F(000) = 440$
$D_x = 1.762$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7215 reflections
$\theta = 3.1$–27.5°
$\mu = 1.61$ mm^{-1}
$T = 291$ K
Block, colorless
0.22 × 0.18 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.718$, $T_{max} = 0.782$
8055 measured reflections
3668 independent reflections
3320 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -10\rightarrow 9$
$k = -11\rightarrow 11$
$l = -14\rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.065$
$S = 1.11$
3668 reflections
226 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
$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 0.3237P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ 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. 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}
C1	0.5758 (2)	0.2908 (2)	0.70951 (15)	0.0234 (4)
C2	0.4639 (2)	0.1504 (2)	0.73561 (15)	0.0228 (4)
H1	0.4196	0.1764	0.8066	0.027*

H2	0.3653	0.1200	0.6730	0.027*
C3	0.5765 (2)	−0.1842 (2)	0.59130 (15)	0.0225 (4)
C4	0.4695 (2)	−0.1219 (2)	0.67581 (15)	0.0249 (4)
H8	0.3614	−0.1063	0.6318	0.030*
H7	0.4413	−0.1979	0.7259	0.030*
C5	0.6392 (2)	0.00980 (19)	0.86167 (14)	0.0189 (3)
C6	0.6706 (2)	0.13196 (19)	0.95095 (15)	0.0223 (3)
H3	0.6319	0.2219	0.9372	0.027*
C7	0.7589 (2)	0.1201 (2)	1.05973 (15)	0.0232 (4)
H4	0.7757	0.2014	1.1189	0.028*
C8	0.8230 (2)	−0.0111 (2)	1.08227 (14)	0.0210 (3)
C9	0.7931 (2)	−0.1318 (2)	0.99287 (16)	0.0247 (4)
H5	0.8350	−0.2205	1.0063	0.030*
C10	0.7025 (2)	−0.1227 (2)	0.88446 (15)	0.0237 (4)
H6	0.6834	−0.2053	0.8261	0.028*
C11	0.9258 (2)	−0.0177 (2)	1.19854 (15)	0.0223 (4)
N1	0.5524 (2)	0.02088 (16)	0.74928 (12)	0.0218 (3)
Na1	0.70264 (10)	0.49576 (8)	0.57052 (7)	0.02913 (17)
O1	0.52052 (19)	0.41253 (16)	0.71895 (12)	0.0337 (3)
O2	0.71665 (17)	0.27959 (15)	0.67283 (12)	0.0294 (3)
O3	0.70204 (18)	−0.09667 (16)	0.56440 (12)	0.0310 (3)
O4	0.53062 (19)	−0.31883 (15)	0.54829 (12)	0.0340 (3)
O5	0.9395 (2)	0.08672 (16)	1.28035 (11)	0.0331 (3)
O6	1.00014 (17)	−0.13340 (15)	1.21007 (11)	0.0272 (3)
O7	0.9495 (2)	0.17005 (17)	0.52465 (12)	0.0381 (3)
H9	0.9528	0.1236	0.4581	0.057*
H10	1.0276	0.2489	0.5443	0.057*
O8	0.9626 (2)	0.60310 (17)	0.69752 (13)	0.0380 (3)
H12	0.9924	0.6993	0.7101	0.057*
H11	0.9728	0.5703	0.7630	0.057*
O9	0.81948 (19)	0.56713 (17)	0.40602 (13)	0.0371 (3)
H13	0.8786	0.5073	0.3756	0.056*
H14	0.7250	0.5671	0.3609	0.056*
O10	0.6141 (3)	0.4735 (3)	0.09255 (19)	0.0770 (7)
H15	1.0046	0.6401	0.1287	0.116*
H16	0.8541	0.5354	0.0951	0.116*
O11	0.9641 (2)	0.54605 (19)	0.10841 (14)	0.0459 (4)
H17	0.5653	0.5064	0.1476	0.069*
H18	0.5412	0.4016	0.0505	0.069*
Zn1	0.81967 (3)	0.09629 (2)	0.651229 (17)	0.02072 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0252 (9)	0.0272 (9)	0.0201 (8)	0.0090 (7)	0.0039 (7)	0.0070 (7)
C2	0.0215 (8)	0.0277 (9)	0.0206 (8)	0.0076 (7)	0.0028 (7)	0.0054 (7)
C3	0.0231 (9)	0.0225 (8)	0.0186 (8)	0.0043 (7)	−0.0058 (7)	0.0019 (6)
C4	0.0249 (9)	0.0242 (9)	0.0217 (8)	−0.0020 (7)	0.0002 (7)	0.0000 (7)

C5	0.0194 (8)	0.0215 (8)	0.0163 (7)	0.0018 (6)	0.0045 (6)	0.0046 (6)
C6	0.0267 (9)	0.0198 (8)	0.0210 (8)	0.0070 (7)	0.0020 (7)	0.0037 (6)
C7	0.0248 (9)	0.0239 (9)	0.0198 (8)	0.0040 (7)	0.0018 (7)	0.0005 (7)
C8	0.0181 (8)	0.0269 (9)	0.0189 (8)	0.0032 (7)	0.0043 (7)	0.0070 (7)
C9	0.0289 (9)	0.0217 (8)	0.0260 (9)	0.0080 (7)	0.0058 (8)	0.0077 (7)
C10	0.0319 (9)	0.0209 (8)	0.0193 (8)	0.0073 (7)	0.0054 (7)	0.0013 (6)
C11	0.0172 (8)	0.0266 (9)	0.0226 (8)	−0.0008 (7)	0.0031 (7)	0.0085 (7)
N1	0.0267 (8)	0.0208 (7)	0.0165 (6)	0.0044 (6)	−0.0005 (6)	0.0019 (5)
Na1	0.0296 (4)	0.0250 (4)	0.0319 (4)	0.0013 (3)	0.0037 (3)	0.0070 (3)
O1	0.0411 (8)	0.0296 (7)	0.0385 (8)	0.0181 (6)	0.0157 (7)	0.0107 (6)
O2	0.0273 (7)	0.0265 (7)	0.0412 (8)	0.0108 (5)	0.0144 (6)	0.0143 (6)
O3	0.0303 (7)	0.0297 (7)	0.0298 (7)	−0.0017 (6)	0.0099 (6)	−0.0067 (5)
O4	0.0383 (8)	0.0212 (7)	0.0369 (8)	0.0023 (6)	−0.0018 (6)	−0.0049 (6)
O5	0.0431 (8)	0.0325 (7)	0.0206 (6)	0.0053 (6)	−0.0041 (6)	0.0043 (5)
O6	0.0240 (6)	0.0305 (7)	0.0269 (6)	0.0076 (5)	−0.0019 (5)	0.0081 (5)
O7	0.0432 (9)	0.0404 (8)	0.0272 (7)	−0.0084 (7)	0.0159 (6)	−0.0012 (6)
O8	0.0471 (9)	0.0291 (7)	0.0329 (7)	0.0003 (6)	−0.0020 (7)	0.0049 (6)
O9	0.0320 (8)	0.0427 (9)	0.0359 (8)	0.0032 (6)	0.0076 (6)	0.0048 (6)
O10	0.0630 (13)	0.0963 (18)	0.0657 (13)	0.0182 (12)	0.0178 (11)	−0.0318 (12)
O11	0.0583 (10)	0.0381 (9)	0.0392 (8)	0.0073 (8)	0.0024 (8)	0.0052 (7)
Zn1	0.02166 (11)	0.02060 (11)	0.01927 (10)	0.00437 (7)	0.00116 (8)	0.00223 (7)

Geometric parameters (Å, º)

C1—O1	1.240 (2)	Na1—O4^{i}	2.3239 (19)
C1—O2	1.269 (2)	Na1—O8	2.353 (2)
C1—C2	1.513 (3)	Na1—O9	2.3687 (19)
C2—N1	1.461 (2)	Na1—O4^{ii}	2.3901 (19)
C2—H1	0.9700	Na1—O2	2.4009 (19)
C2—H2	0.9700	Na1—O1	2.5245 (19)
C3—O4	1.235 (2)	Na1—Na1^{iii}	3.401 (2)
C3—O3	1.270 (2)	Na1—H14	2.6320
C3—C4	1.514 (3)	O2—Zn1	1.9584 (16)
C4—N1	1.465 (2)	O3—Zn1	1.9336 (17)
C4—H8	0.9700	O4—Na1^{iv}	2.3239 (19)
C4—H7	0.9700	O4—Na1^{ii}	2.3901 (19)
C5—C6	1.396 (2)	O6—Zn1^{v}	1.9574 (15)
C5—C10	1.399 (2)	O7—Zn1	2.0400 (16)
C5—N1	1.413 (2)	O7—H9	0.8500
C6—C7	1.383 (2)	O7—H10	0.8500
C6—H3	0.9300	O8—H12	0.8500
C7—C8	1.391 (3)	O8—H11	0.8500
C7—H4	0.9300	O9—H13	0.8500
C8—C9	1.389 (3)	O9—H14	0.8500
C8—C11	1.492 (2)	O10—H17	0.8498
C9—C10	1.380 (3)	O10—H18	0.8504
C9—H5	0.9300	O11—H15	0.8504
C10—H6	0.9300	O11—H16	0.8499

C11—O5	1.246 (2)	Zn1—O6^{v}	1.9574 (15)
C11—O6	1.283 (2)		
O1—C1—O2	122.18 (17)	O4^{i}—Na1—O2	138.34 (6)
O1—C1—C2	117.99 (17)	O8—Na1—O2	84.49 (6)
O2—C1—C2	119.71 (16)	O9—Na1—O2	132.16 (6)
N1—C2—C1	114.73 (15)	O4^{ii}—Na1—O2	80.48 (7)
N1—C2—H1	108.6	O4^{i}—Na1—O1	85.66 (6)
C1—C2—H1	108.6	O8—Na1—O1	98.94 (7)
N1—C2—H2	108.6	O9—Na1—O1	168.52 (6)
C1—C2—H2	108.6	O4^{ii}—Na1—O1	78.25 (7)
H1—C2—H2	107.6	O2—Na1—O1	52.90 (5)
O4—C3—O3	123.36 (18)	O4^{i}—Na1—Na1^{iii}	44.60 (5)
O4—C3—C4	116.88 (17)	O8—Na1—Na1^{iii}	153.40 (6)
O3—C3—C4	119.70 (16)	O9—Na1—Na1^{iii}	89.94 (6)
N1—C4—C3	115.30 (15)	O4^{ii}—Na1—Na1^{iii}	43.06 (5)
N1—C4—H8	108.4	O2—Na1—Na1^{iii}	113.22 (5)
C3—C4—H8	108.4	O1—Na1—Na1^{iii}	78.77 (6)
N1—C4—H7	108.4	O4^{i}—Na1—H14	75.5
C3—C4—H7	108.4	O8—Na1—H14	109.2
H8—C4—H7	107.5	O9—Na1—H14	18.6
C6—C5—C10	118.34 (15)	O4^{ii}—Na1—H14	77.8
C6—C5—N1	121.25 (15)	O2—Na1—H14	138.5
C10—C5—N1	120.35 (15)	O1—Na1—H14	149.9
C7—C6—C5	120.44 (16)	Na1^{iii}—Na1—H14	71.4
C7—C6—H3	119.8	C1—O1—Na1	87.44 (12)
C5—C6—H3	119.8	C1—O2—Zn1	127.16 (12)
C6—C7—C8	121.26 (17)	C1—O2—Na1	92.39 (10)
C6—C7—H4	119.4	Zn1—O2—Na1	134.30 (7)
C8—C7—H4	119.4	C3—O3—Zn1	126.24 (12)
C9—C8—C7	118.10 (16)	C3—O4—Na1^{iv}	124.19 (12)
C9—C8—C11	121.76 (16)	C3—O4—Na1^{ii}	143.46 (12)
C7—C8—C11	120.11 (16)	Na1^{iv}—O4—Na1^{ii}	92.34 (7)
C10—C9—C8	121.31 (16)	C11—O6—Zn1^{v}	111.56 (12)
C10—C9—H5	119.3	Zn1—O7—H9	128.8
C8—C9—H5	119.3	Zn1—O7—H10	117.0
C9—C10—C5	120.52 (16)	H9—O7—H10	112.8
C9—C10—H6	119.7	Na1—O8—H12	119.1
C5—C10—H6	119.7	Na1—O8—H11	114.2
O5—C11—O6	121.83 (16)	H12—O8—H11	107.7
O5—C11—C8	120.69 (16)	Na1—O9—H13	116.7
O6—C11—C8	117.47 (16)	Na1—O9—H14	98.5
C5—N1—C2	117.69 (14)	H13—O9—H14	111.0
C5—N1—C4	116.93 (14)	H17—O10—H18	106.8
C2—N1—C4	115.93 (14)	H15—O11—H16	107.9
O4^{i}—Na1—O8	108.97 (7)	O3—Zn1—O6^{v}	128.18 (6)
O4^{i}—Na1—O9	87.74 (7)	O3—Zn1—O2	125.40 (7)
O8—Na1—O9	92.08 (7)	O6^{v}—Zn1—O2	100.31 (7)

O4^{i}—Na1—O4^{ii}	87.66 (7)	O3—Zn1—O7	97.01 (7)
O8—Na1—O4^{ii}	162.99 (6)	O6^{v}—Zn1—O7	103.35 (7)
O9—Na1—O4^{ii}	92.12 (7)	O2—Zn1—O7	93.95 (7)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H10···O9^{vi}	0.85	1.87	2.716 (3)	174
O7—H9···O5^{vii}	0.85	2.06	2.867 (2)	159
O8—H12···O5^{viii}	0.85	1.90	2.748 (3)	173
O8—H11···O11^{vi}	0.85	1.97	2.798 (2)	163
O9—H14···O1^{iii}	0.85	2.07	2.910 (2)	168
O9—H13···O8^{vi}	0.85	1.96	2.801 (2)	172
O10—H17···O1^{iii}	0.85	1.92	2.762 (3)	174
O10—H18···O10^{ix}	0.85	2.41	2.744 (5)	104
O11—H15···O6^{x}	0.85	2.16	2.949 (3)	154
O11—H16···O10	0.85	1.89	2.721 (3)	165

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