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Poly[[μ_2 -aqua- μ_3 -(4-carboxy-2-propyl-1*H*-imidazole-5-carboxylato- $\kappa^4N^3,O^4:O^4:O^5$)-sodium] hemihydrate]

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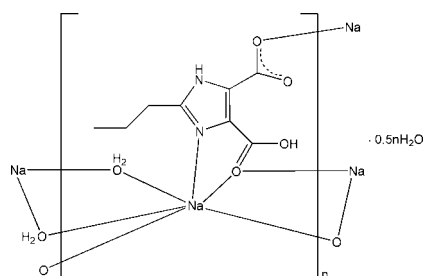
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.034; wR factor = 0.106; data-to-parameter ratio = 13.1.

In the title compound, $\{[Na(C_8H_9N_2O_4)(H_2O)] \cdot 0.5H_2O\}_n$, the Na^+ ion is coordinated by two bridging water molecules, one N atom and three O atoms from three 4-carboxy-2-propyl-1*H*-imidazole-5-carboxylate (H_2pimdc) ligands. Adjacent Na^+ ions are linked alternately by two water O atoms and two carboxy O atoms into a chain along [001]. These chains are connected through the coordination of the carboxylate O atoms to the Na^+ ions, forming a three-dimensional structure. An intramolecular $O-H \cdots O$ hydrogen bond and intermolecular $N-H \cdots O$ and $O-H \cdots O$ hydrogen bonds are present in the crystal structure.

Related literature

For the properties and biological activity of imidazole-4,5-dicarboxylic acid and its derivatives, see: Baures (1999); Bogdanova *et al.* (1992); Borodkin *et al.* (1984); Reichardt *et al.* (1992); Su *et al.* (2001).



Experimental

Crystal data

$[Na(C_8H_9N_2O_4)(H_2O)] \cdot 0.5H_2O$ $b = 15.478$ (4) Å
 $M_r = 247.18$ $c = 10.734$ (3) Å
 Monoclinic, $C2/c$ $\beta = 118.364$ (3)°
 $a = 15.406$ (4) Å $V = 2252.4$ (9) Å³

$Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.15$ mm⁻¹

$T = 296$ K
 $0.52 \times 0.47 \times 0.44$ mm

Data collection

Bruker APEX CCD diffractometer 5971 measured reflections
 Absorption correction: multi-scan 1986 independent reflections
 (SADABS; Sheldrick, 1996) 1669 reflections with $I > 2\sigma(I)$
 $T_{min} = 0.528$, $T_{max} = 0.562$ $R_{int} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$ 152 parameters
 $wR(F^2) = 0.106$ H-atom parameters constrained
 $S = 1.10$ $\Delta\rho_{max} = 0.23$ e Å⁻³
 1986 reflections $\Delta\rho_{min} = -0.21$ e Å⁻³

Table 1

Selected bond lengths (Å).

Na1—O1	2.3658 (15)	Na1—O5	2.4011 (15)
Na1—O1 ⁱ	2.3644 (14)	Na1—O5 ⁱⁱⁱ	2.3818 (16)
Na1—O3 ⁱⁱ	2.5550 (15)	Na1—N1	2.4848 (16)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2—H2A \cdots O3 ^{iv}	0.86	2.00	2.8384 (18)	164
O2—H2 \cdots O4	0.82	1.64	2.4603 (18)	178
O5—H5B \cdots O2 ⁱ	0.91	2.07	2.9493 (18)	164
O5—H5A \cdots O6	0.86	1.97	2.8234 (19)	169
O6—H6C \cdots O4 ⁱⁱ	0.88	2.03	2.8835 (16)	163

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2402).

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supporting information

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Poly[[μ_2 -aqua- μ_3 -(4-carboxy-2-propyl-1*H*-imidazole-5-carboxylato- $\kappa^4N^3,O^4:O^4:O^5$)-sodium] hemihydrate]

Zhong-Jing Huang, Jin-Niu Tang, Zhi-Rong Luo, Dai-Yin Wang and Huan Wei

S1. Comment

1*H*-Imidazole and its derivatives are a kind of excellent supramolecular synthons. The N atoms of imidazole can coordinate to metal ions in monodentate or bidentate mode (Su *et al.*, 2001). Imidazole-4,5-dicarboxylic acid and derivatives have been studied in terms of their physical properties as well as for their diverse biological activities (Bogdanova *et al.*, 1992; Borodkin *et al.*, 1984; Reichardt *et al.*, 1992), including the use of imidazole-4,5-dicarboxylic acid amides in the development of human immunodeficiency virus (HIV-1) protease inhibitors (Baures, 1999). Here we present the synthesis and structure of the title complex derived from 2-propyl-1*H*-imidazole-4,5-dicarboxylic acid. The distinct binding modes of the ligands as well as the coordination preferences of the metal ion are discussed.

In the title compound, the 2-propyl-4-carboxy-1*H*-imidazole-5-carboxylate (H₂pimdc) ligand is bonded to Na ions in a μ_3 -mode. The coordination of Na ion is achieved by two water molecules, one N atom and three O atoms from three H₂pimdc ligands (Fig. 1, Table 1). Two O1 atoms of the H₂pimdc ligand bridge two Na atoms, forming a parallelogram and two O5 atoms of the water molecules form another parallelogram with two Na atoms, leading to a chain along [0 0 1]. The chains are connected through the coordination of the carboxylate O3 atoms to the Na ions, forming a three-dimensional structure (Fig. 2). The propyl group becomes an ornament in the coordination network. The crystal structure is stabilized by intramolecular O—H \cdots O hydrogen bond and intermolecular N—H \cdots O and O—H \cdots O hydrogen bonds (Table 2).

S2. Experimental

An ethanol solution (5 ml) containing 2-propyl-1*H*-imidazole-4,5-dicarboxylic acid (1 mmol, 0.198 g) was added dropwise to a water solution (10 ml) containing NaOH (0.5 mmol, 0.040 g). After stirring for 6 h, the solution was filtered. The filtered solution were evaporated for several days in air and colorless block-shaped crystals suitable for single-crystal X-ray diffraction were obtained (yield: 80% based on the ligand).

S3. Refinement

H atoms except those of water molecules were positioned geometrically and refined using a riding model, with C—H = 0.97 (CH₂) and 0.96 (CH₃), N—H = 0.86 and O—H = 0.82 Å and with $U_{\text{iso}}(\text{H}) = 1.2(1.5 \text{ for methyl})U_{\text{eq}}(\text{C}, \text{N}, \text{O})$. H atoms of water molecules were located in a difference Fourier map and refined as riding atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

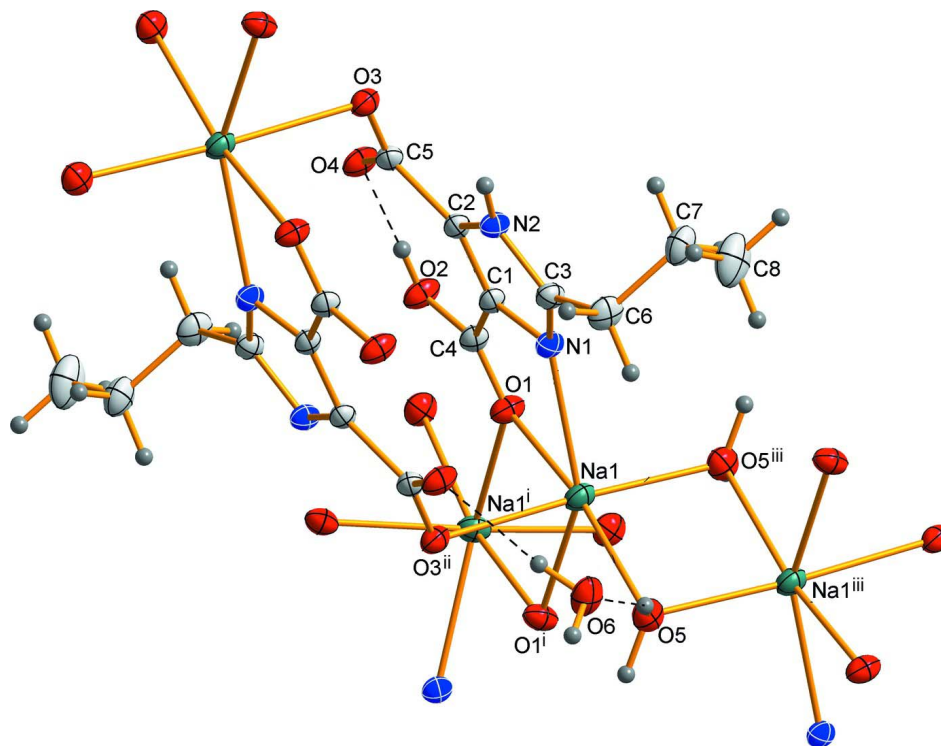
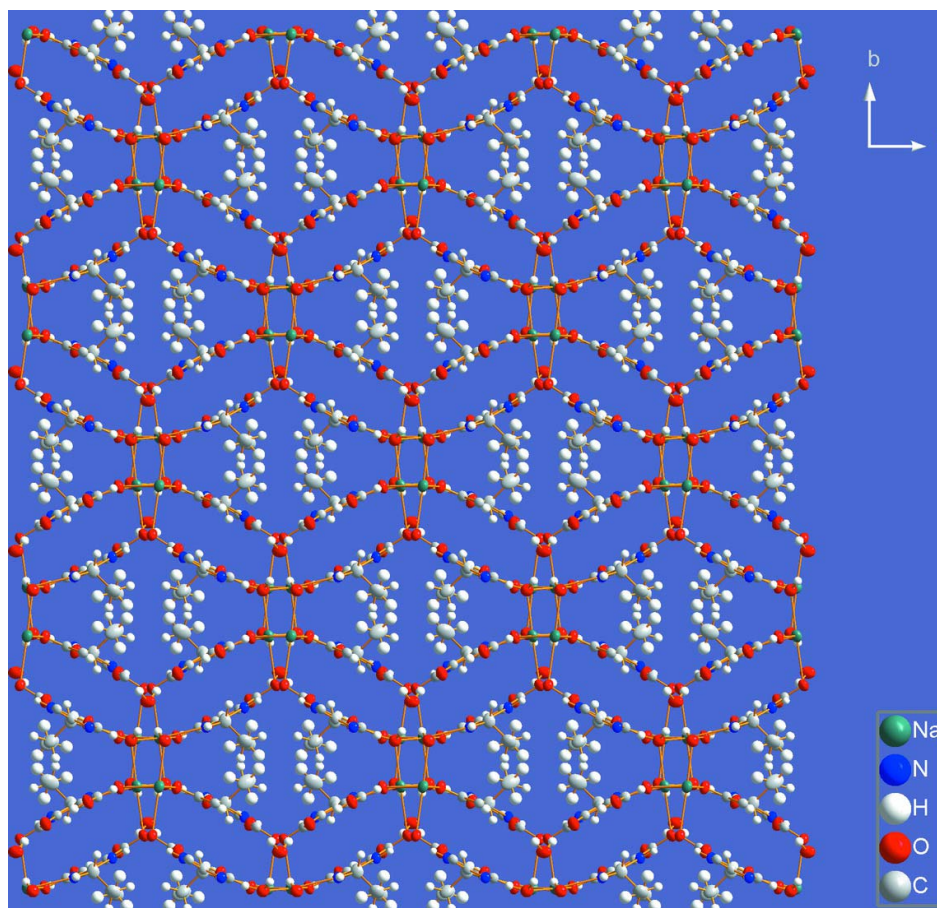


Figure 1

The structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines denote hydrogen bonds. [Symmetry codes: (i) $-x, y, 1/2-z$; (ii) $1/2-x, 1/2-y, 1-z$; (iii) $-x, -y, 1-z$.]

**Figure 2**

Crystal packing of the title compound viewed along the c axis.

Poly[[μ_2 -aqua- μ_3 -(4-carboxy-2-propyl-1*H*-imidazole-5-carboxylato- $\kappa^4N^3,O^4:O^4:O^5$)-sodium] hemihydrate]

Crystal data

$[\text{Na}(\text{C}_8\text{H}_9\text{N}_2\text{O}_4)(\text{H}_2\text{O})] \cdot 0.5\text{H}_2\text{O}$

$M_r = 247.18$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 15.406\ (4)\ \text{\AA}$

$b = 15.478\ (4)\ \text{\AA}$

$c = 10.734\ (3)\ \text{\AA}$

$\beta = 118.364\ (3)^\circ$

$V = 2252.4\ (9)\ \text{\AA}^3$

$Z = 8$

$F(000) = 1032$

$D_x = 1.458\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2142 reflections

$\theta = 2.4\text{--}26.8^\circ$

$\mu = 0.15\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Block, colorless

$0.52 \times 0.47 \times 0.44\ \text{mm}$

Data collection

Bruker APEX CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\text{min}} = 0.528$, $T_{\text{max}} = 0.562$

5971 measured reflections

1986 independent reflections

1669 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$
 $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.0^\circ$
 $h = -18 \rightarrow 17$

$k = -18 \rightarrow 17$
 $l = -11 \rightarrow 12$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.106$
 $S = 1.10$
 1986 reflections
 152 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
 $w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.6897P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.23 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.21 \text{ e } \text{\AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O3	0.48386 (8)	0.25613 (8)	0.57288 (12)	0.0379 (3)
C5	0.41043 (11)	0.21569 (11)	0.48692 (17)	0.0310 (4)
Na1	0.04274 (5)	0.08063 (4)	0.43441 (7)	0.0385 (2)
O1	0.10965 (9)	0.08373 (8)	0.27653 (13)	0.0411 (3)
O2	0.22662 (9)	0.13103 (9)	0.23128 (12)	0.0416 (3)
H2	0.2806	0.1544	0.2746	0.062*
O4	0.38682 (9)	0.20490 (9)	0.35643 (12)	0.0417 (3)
N2	0.36555 (10)	0.18188 (9)	0.67516 (14)	0.0321 (3)
H2A	0.4177	0.2046	0.7425	0.039*
O5	-0.06348 (10)	0.07199 (8)	0.54055 (14)	0.0437 (3)
H5A	-0.0517	0.1150	0.5978	0.052*
H5B	-0.1209	0.0894	0.4662	0.052*
N1	0.22111 (10)	0.11704 (9)	0.56488 (14)	0.0329 (3)
C2	0.34437 (11)	0.17694 (10)	0.53667 (16)	0.0290 (4)
C4	0.19168 (12)	0.11485 (11)	0.31776 (17)	0.0313 (4)
C1	0.25389 (11)	0.13611 (10)	0.46930 (16)	0.0292 (4)
C3	0.29110 (12)	0.14524 (11)	0.68890 (18)	0.0338 (4)
C6	0.29259 (14)	0.13640 (14)	0.82798 (19)	0.0454 (5)
H6A	0.2276	0.1191	0.8121	0.054*
H6B	0.3074	0.1922	0.8748	0.054*
C7	0.36813 (17)	0.07062 (14)	0.9247 (2)	0.0525 (5)
H7A	0.3512	0.0141	0.8804	0.063*
H7B	0.4327	0.0861	0.9367	0.063*
C8	0.3727 (2)	0.06594 (17)	1.0677 (2)	0.0757 (8)
H8A	0.3924	0.1210	1.1138	0.113*
H8B	0.4198	0.0228	1.1242	0.113*
H8C	0.3089	0.0510	1.0564	0.113*
O6	0.0000	0.20200 (12)	0.7500	0.0512 (5)
H6C	0.0310	0.2400	0.7245	0.061*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0294 (6)	0.0443 (7)	0.0345 (7)	-0.0048 (5)	0.0108 (5)	0.0028 (5)
C5	0.0256 (8)	0.0338 (9)	0.0317 (9)	0.0040 (7)	0.0121 (7)	0.0032 (7)
Na1	0.0328 (4)	0.0462 (4)	0.0354 (4)	-0.0046 (3)	0.0154 (3)	0.0024 (3)
O1	0.0309 (7)	0.0564 (8)	0.0319 (7)	-0.0082 (6)	0.0115 (5)	-0.0032 (5)
O2	0.0347 (7)	0.0600 (8)	0.0289 (6)	-0.0111 (6)	0.0142 (5)	-0.0073 (6)
O4	0.0391 (7)	0.0574 (8)	0.0332 (7)	-0.0083 (6)	0.0209 (6)	-0.0025 (5)
N2	0.0269 (7)	0.0400 (8)	0.0254 (7)	-0.0013 (6)	0.0091 (5)	-0.0007 (6)
O5	0.0472 (8)	0.0453 (8)	0.0372 (7)	0.0025 (6)	0.0190 (6)	0.0020 (5)
N1	0.0298 (7)	0.0401 (8)	0.0291 (7)	-0.0001 (6)	0.0142 (6)	0.0024 (6)
C2	0.0288 (8)	0.0305 (8)	0.0266 (8)	0.0032 (7)	0.0122 (7)	0.0004 (6)
C4	0.0299 (9)	0.0346 (9)	0.0280 (9)	0.0012 (7)	0.0126 (7)	0.0000 (7)
C1	0.0270 (8)	0.0319 (9)	0.0282 (9)	0.0030 (6)	0.0127 (7)	0.0017 (6)
C3	0.0299 (9)	0.0408 (10)	0.0294 (9)	0.0031 (7)	0.0131 (7)	0.0034 (7)
C6	0.0457 (11)	0.0611 (12)	0.0319 (10)	-0.0014 (9)	0.0205 (8)	0.0018 (9)
C7	0.0587 (13)	0.0574 (13)	0.0383 (11)	-0.0110 (10)	0.0205 (9)	0.0054 (9)
C8	0.104 (2)	0.0765 (17)	0.0368 (12)	-0.0225 (15)	0.0254 (13)	0.0041 (11)
O6	0.0693 (13)	0.0439 (11)	0.0553 (12)	0.000	0.0417 (11)	0.000

Geometric parameters (\AA , $^\circ$)

O3—C5	1.237 (2)	O5—H5A	0.8645
C5—O4	1.280 (2)	O5—H5B	0.9066
C5—C2	1.482 (2)	N1—C3	1.327 (2)
Na1—O1	2.3658 (15)	N1—C1	1.374 (2)
Na1—O1 ⁱ	2.3644 (14)	C2—C1	1.381 (2)
Na1—O3 ⁱⁱ	2.5550 (15)	C4—C1	1.480 (2)
Na1—O5	2.4011 (15)	C3—C6	1.488 (2)
Na1—O5 ⁱⁱⁱ	2.3818 (16)	C6—C7	1.524 (3)
Na1—N1	2.4848 (16)	C6—H6A	0.9700
Na1—Na1 ⁱⁱⁱ	3.4217 (14)	C6—H6B	0.9700
Na1—Na1 ⁱ	3.5291 (16)	C7—C8	1.504 (3)
O1—C4	1.222 (2)	C7—H7A	0.9700
O2—C4	1.300 (2)	C7—H7B	0.9700
O2—H2	0.8200	C8—H8A	0.9600
N2—C3	1.349 (2)	C8—H8B	0.9600
N2—C2	1.364 (2)	C8—H8C	0.9600
N2—H2A	0.8600	O6—H6C	0.8790
C5—O3—Na1 ⁱⁱ	113.64 (10)	Na1 ⁱⁱⁱ —O5—Na1	91.35 (5)
O3—C5—O4	124.46 (15)	Na1 ⁱⁱⁱ —O5—H5A	135.4
O3—C5—C2	118.49 (15)	Na1—O5—H5A	109.5
O4—C5—C2	117.05 (14)	Na1 ⁱⁱⁱ —O5—H5B	114.6
O1 ⁱ —Na1—O1	83.45 (5)	Na1—O5—H5B	99.5
O1 ⁱ —Na1—O5 ⁱⁱⁱ	98.46 (5)	H5A—O5—H5B	100.6
O1—Na1—O5 ⁱⁱⁱ	91.16 (5)	C3—N1—C1	105.47 (14)

O1 ⁱ —Na1—O5	82.24 (5)	C3—N1—Na1	142.55 (12)
O1—Na1—O5	165.50 (5)	C1—N1—Na1	109.17 (10)
O5 ⁱⁱⁱ —Na1—O5	88.65 (5)	N2—C2—C1	104.80 (14)
O1 ⁱ —Na1—N1	149.80 (6)	N2—C2—C5	121.35 (14)
O1—Na1—N1	69.97 (5)	C1—C2—C5	133.75 (15)
O5 ⁱⁱⁱ —Na1—N1	96.21 (5)	O1—C4—O2	121.69 (15)
O5—Na1—N1	124.46 (6)	O1—C4—C1	120.25 (15)
O1 ⁱ —Na1—O3 ⁱⁱ	83.03 (5)	O2—C4—C1	118.06 (14)
O1—Na1—O3 ⁱⁱ	94.36 (5)	N1—C1—C2	110.18 (14)
O5 ⁱⁱⁱ —Na1—O3 ⁱⁱ	174.41 (5)	N1—C1—C4	119.81 (14)
O5—Na1—O3 ⁱⁱ	86.22 (5)	C2—C1—C4	129.97 (15)
N1—Na1—O3 ⁱⁱ	84.91 (5)	N1—C3—N2	110.88 (15)
O1 ⁱ —Na1—Na1 ⁱⁱⁱ	90.44 (4)	N1—C3—C6	126.43 (16)
O1—Na1—Na1 ⁱⁱⁱ	133.90 (5)	N2—C3—C6	122.65 (15)
O5 ⁱⁱⁱ —Na1—Na1 ⁱⁱⁱ	44.55 (4)	C3—C6—C7	112.82 (16)
O5—Na1—Na1 ⁱⁱⁱ	44.10 (4)	C3—C6—H6A	109.0
N1—Na1—Na1 ⁱⁱⁱ	118.18 (5)	C7—C6—H6A	109.0
O3 ⁱⁱ —Na1—Na1 ⁱⁱⁱ	130.28 (5)	C3—C6—H6B	109.0
O1 ⁱ —Na1—Na1 ⁱ	41.76 (4)	C7—C6—H6B	109.0
O1—Na1—Na1 ⁱ	41.73 (3)	H6A—C6—H6B	107.8
O5 ⁱⁱⁱ —Na1—Na1 ⁱ	94.88 (4)	C8—C7—C6	112.2 (2)
O5—Na1—Na1 ⁱ	123.85 (5)	C8—C7—H7A	109.2
N1—Na1—Na1 ⁱ	110.83 (4)	C6—C7—H7A	109.2
O3 ⁱⁱ —Na1—Na1 ⁱ	89.81 (3)	C8—C7—H7B	109.2
Na1 ⁱⁱⁱ —Na1—Na1 ⁱ	116.76 (3)	C6—C7—H7B	109.2
C4—O1—Na1 ⁱ	137.76 (11)	H7A—C7—H7B	107.9
C4—O1—Na1	118.44 (11)	C7—C8—H8A	109.5
Na1 ⁱ —O1—Na1	96.50 (5)	C7—C8—H8B	109.5
C4—O2—H2	109.5	H8A—C8—H8B	109.5
C3—N2—C2	108.66 (14)	C7—C8—H8C	109.5
C3—N2—H2A	125.7	H8A—C8—H8C	109.5
C2—N2—H2A	125.7	H8B—C8—H8C	109.5
Na1 ⁱⁱ —O3—C5—O4	83.19 (17)	Na1 ⁱⁱⁱ —Na1—N1—C1	142.32 (10)
Na1 ⁱⁱ —O3—C5—C2	-96.58 (14)	Na1 ⁱ —Na1—N1—C1	3.70 (11)
O1 ⁱ —Na1—O1—C4	153.03 (11)	C3—N2—C2—C1	0.27 (17)
O5 ⁱⁱⁱ —Na1—O1—C4	-108.59 (13)	C3—N2—C2—C5	177.03 (14)
O5—Na1—O1—C4	162.3 (2)	O3—C5—C2—N2	-3.0 (2)
N1—Na1—O1—C4	-12.40 (12)	O4—C5—C2—N2	177.24 (15)
O3 ⁱⁱ —Na1—O1—C4	70.56 (13)	O3—C5—C2—C1	172.70 (17)
Na1 ⁱⁱⁱ —Na1—O1—C4	-122.69 (12)	O4—C5—C2—C1	-7.1 (3)
Na1 ⁱ —Na1—O1—C4	155.37 (15)	Na1 ⁱ —O1—C4—O2	-27.1 (3)
O1 ⁱ —Na1—O1—Na1 ⁱ	-2.35 (7)	Na1—O1—C4—O2	-169.10 (12)
O5 ⁱⁱⁱ —Na1—O1—Na1 ⁱ	96.04 (5)	Na1 ⁱ —O1—C4—C1	152.23 (13)
O5—Na1—O1—Na1 ⁱ	7.0 (2)	Na1—O1—C4—C1	10.2 (2)
N1—Na1—O1—Na1 ⁱ	-167.77 (6)	C3—N1—C1—C2	-0.50 (19)
O3 ⁱⁱ —Na1—O1—Na1 ⁱ	-84.81 (5)	Na1—N1—C1—C2	165.02 (11)
Na1 ⁱⁱⁱ —Na1—O1—Na1 ⁱ	81.93 (7)	C3—N1—C1—C4	-178.63 (15)

O1 ⁱ —Na1—O5—Na1 ⁱⁱⁱ	98.73 (5)	Na1—N1—C1—C4	-13.10 (18)
O1—Na1—O5—Na1 ⁱⁱⁱ	89.4 (2)	N2—C2—C1—N1	0.15 (18)
O5 ⁱⁱⁱ —Na1—O5—Na1 ⁱⁱⁱ	0.0	C5—C2—C1—N1	-176.03 (16)
N1—Na1—O5—Na1 ⁱⁱⁱ	-96.60 (7)	N2—C2—C1—C4	178.02 (16)
O3 ⁱⁱ —Na1—O5—Na1 ⁱⁱⁱ	-177.79 (5)	C5—C2—C1—C4	1.8 (3)
Na1 ⁱ —Na1—O5—Na1 ⁱⁱⁱ	94.97 (4)	O1—C4—C1—N1	3.0 (2)
O1 ⁱ —Na1—N1—C3	139.23 (18)	O2—C4—C1—N1	-177.59 (15)
O1—Na1—N1—C3	169.0 (2)	O1—C4—C1—C2	-174.66 (17)
O5 ⁱⁱⁱ —Na1—N1—C3	-102.0 (2)	O2—C4—C1—C2	4.7 (3)
O5—Na1—N1—C3	-9.4 (2)	C1—N1—C3—N2	0.68 (19)
O3 ⁱⁱ —Na1—N1—C3	72.5 (2)	Na1—N1—C3—N2	-156.48 (14)
Na1 ⁱⁱⁱ —Na1—N1—C3	-61.0 (2)	C1—N1—C3—C6	-177.21 (17)
Na1 ⁱ —Na1—N1—C3	160.36 (18)	Na1—N1—C3—C6	25.6 (3)
O1 ⁱ —Na1—N1—C1	-17.43 (17)	C2—N2—C3—N1	-0.61 (19)
O1—Na1—N1—C1	12.38 (10)	C2—N2—C3—C6	177.38 (16)
O5 ⁱⁱⁱ —Na1—N1—C1	101.34 (11)	N1—C3—C6—C7	107.8 (2)
O5—Na1—N1—C1	-166.03 (10)	N2—C3—C6—C7	-69.8 (2)
O3 ⁱⁱ —Na1—N1—C1	-84.16 (11)	C3—C6—C7—C8	176.85 (18)

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H2A \cdots O3 ^{iv}	0.86	2.00	2.8384 (18)	164
O2—H2 \cdots O4	0.82	1.64	2.4603 (18)	178
O5—H5B \cdots O2 ⁱ	0.91	2.07	2.9493 (18)	164
O5—H5A \cdots O6	0.86	1.97	2.8234 (19)	169
O6—H6C \cdots O4 ⁱⁱ	0.88	2.03	2.8835 (16)	163

Symmetry codes: (i) $-x, y, -z+1/2$; (ii) $-x+1/2, -y+1/2, -z+1$; (iv) $-x+1, y, -z+3/2$.