

catena-Poly[[[diaquasodium]-di- μ -aqua] 2-(2-pyridyl)quinoline-4-carboxylate]

Hu-Jun Hao,^{a,b} Cui-Wu Lin,^b Xian-Hong Yin,^{a*} Fei-Long Hu^a and Yue Zhuang^a

^aCollege of Chemistry and Ecological Engineering, Guangxi University for Nationalities, Nanning 530006, People's Republic of China, and ^bSchool of Chemistry & Chemical Engineering, Guangxi University, Nanning 530004, People's Republic of China

Correspondence e-mail: yxhphd@163.com

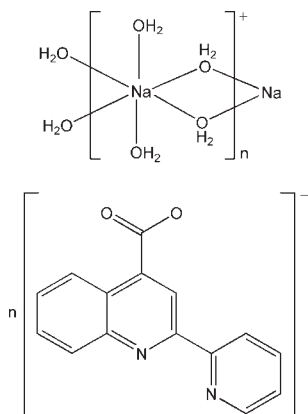
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.035; wR factor = 0.103; data-to-parameter ratio = 16.7.

In the title compound, $[\text{Na}(\text{H}_2\text{O})_4](\text{C}_{15}\text{H}_9\text{N}_2\text{O}_2)$, the Na^+ ion is coordinated by six water molecules in an octahedral geometry. The NaO_6 octahedra are connected by sharing edges, forming a cationic chain along the b -axis direction. $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds link the chains and the 2-(2-pyridyl)quinoline-4-carboxylate anions into a two-dimensional network parallel to (100).

Related literature

For the syntheses of sodium 2-(2-pyridyl)quinoline-4-carboxylate and 2-(2-pyridyl)quinoline-4-carboxylic acid, see: Bass *et al.* (1997); Convers *et al.* (2004). For the structures of 2-(2-pyridyl)-4-methylcarboxyquinoline and its Ru complex, see: Farah *et al.* (2003).



Experimental

Crystal data

$[\text{Na}(\text{H}_2\text{O})_4](\text{C}_{15}\text{H}_9\text{N}_2\text{O}_2)$
 $M_r = 344.30$
 Monoclinic, $P2_1/c$
 $a = 19.0409$ (17) Å
 $b = 5.2987$ (5) Å
 $c = 16.8305$ (16) Å
 $\beta = 103.107$ (5)°

$V = 1653.8$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.13$ mm⁻¹
 $T = 296$ K
 $0.43 \times 0.35 \times 0.30$ mm

Data collection

Siemens SMART 1000 CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.944$, $T_{\max} = 0.962$

14472 measured reflections
 3647 independent reflections
 2902 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.103$
 $S = 1.05$
 3647 reflections

218 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.30$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O3}-\text{H50}\cdots\text{N2}$	0.85	2.02	2.8657 (14)	172
$\text{O3}-\text{H51}\cdots\text{O2}^i$	0.85	1.92	2.7722 (14)	174
$\text{O4}-\text{H4A}\cdots\text{O5}^i$	0.85	1.98	2.8222 (14)	172
$\text{O4}-\text{H4B}\cdots\text{O1}^{ii}$	0.85	1.91	2.7494 (14)	171
$\text{O5}-\text{H5A}\cdots\text{O2}$	0.82	2.04	2.8093 (14)	156
$\text{O5}-\text{H5B}\cdots\text{O2}^{ii}$	0.85	1.97	2.8243 (13)	178
$\text{O6}-\text{H6A}\cdots\text{O1}^{iii}$	0.85	2.10	2.8914 (14)	156
$\text{O6}-\text{H6B}\cdots\text{O3}^{iv}$	0.85	2.00	2.8321 (14)	168

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x, -y+\frac{5}{2}, z+\frac{1}{2}$; (iv) $x, y+1, z$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; 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: HY2255).

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supplementary materials

Acta Cryst. (2010). E66, m113 [doi:10.1107/S1600536809053999]

***catena*-Poly[[[diaquasodium]-di- μ -aqua] 2-(2-pyridyl)quinoline-4-carboxylate]**

H.-J. Hao, C.-W. Lin, X.-H. Yin, F.-L. Hu and Y. Zhuang

Comment

2-(2-pyridyl)quinoline-4-carboxylic acid is a 2,2'-bipyridyl-like ligand containing a carboxylate substituent, which represents a simple route to some important functionalities. The syntheses of sodium 2-(2-pyridyl)quinoline-4-carboxylate and 2-(2-pyridyl)quinoline-4-carboxylic acid have been reported (Bass *et al.*, 1997; Convers *et al.*, 2004). The structures of 2-(2-pyridyl)-4-methylcarboxyquinoline and its Ru complex have been reported by Farah *et al.* (2003). Here we present the structure of a sodium salt of 2-(2-pyridyl)quinoline-4-carboxylate in a tetrahydrate form.

The molecular structure of the title compound is shown in Fig. 1. The Na^I ion is coordinated by six water molecules in an octahedral geometry. Each coordination octahedron is connected with two adjacent ones by sharing edges, forming a cationic [Na(H₂O)₄]_n chain along the *b* direction (Fig. 2).

In the crystal structure, the cationic chains and the organic anions are linked through O—H...O and O—H...N hydrogen bonds into a layer structure (Table 1 and Fig. 3).

Experimental

Sodium 2-(2-pyridyl)quinoline-4-carboxylate was prepared by a literature method (Bass *et al.*, 1997). Colourless crystals were obtained by slow evaporation of an aqueous solution of this compound at room temperature.

Refinement

H atoms bonded C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms of water molecules were found from difference Fourier maps and refined as riding atoms, with O—H = 0.85 Å and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Figures

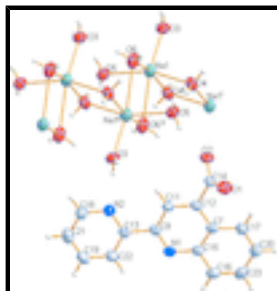


Fig. 1. The structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) 1 - *x*, 1 - *y*, 1 - *z*; (ii) 1 - *x*, 2 - *y*, 1 - *z*.]

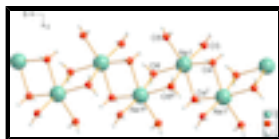


Fig. 2. The chain of NaO₆ octahedra along the *b* axis. [Symmetry codes: (i) 1 - *x*, 1 - *y*, 1 - *z*; (ii) 1 - *x*, 2 - *y*, 1 - *z*.]

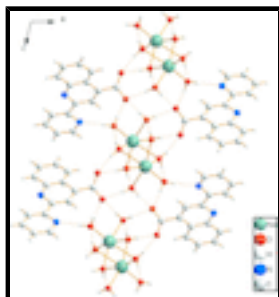


Fig. 3. Crystal packing of the title compound viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

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Crystal data

[Na(H₂O)₄](C₁₅H₉N₂O₂)

$M_r = 344.30$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 19.0409 (17) \text{ \AA}$

$b = 5.2987 (5) \text{ \AA}$

$c = 16.8305 (16) \text{ \AA}$

$\beta = 103.107 (5)^\circ$

$V = 1653.8 (3) \text{ \AA}^3$

$Z = 4$

$F(000) = 720$

$D_x = 1.383 \text{ Mg m}^{-3}$

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

Cell parameters from 1202 reflections

$\theta = 2.2\text{--}27.2^\circ$

$\mu = 0.13 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Block, colourless

$0.43 \times 0.35 \times 0.30 \text{ mm}$

Data collection

Siemens SMART 1000 CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

ϕ and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.944$, $T_{\max} = 0.962$

14472 measured reflections

3647 independent reflections

2902 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\max} = 27.2^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -24 \rightarrow 24$

$k = -6 \rightarrow 6$

$l = -21 \rightarrow 21$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

$wR(F^2) = 0.103$

$S = 1.05$

3647 reflections

218 parameters

0 restraints

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.3055P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.30 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Na1	0.46104 (3)	0.74129 (10)	0.43759 (3)	0.03736 (16)
O4	0.53878 (5)	0.39638 (18)	0.42708 (6)	0.0400 (2)
H4A	0.5271	0.2741	0.3940	0.060*
H4B	0.5767	0.4622	0.4175	0.060*
N1	0.12262 (5)	1.0815 (2)	0.20495 (6)	0.0327 (3)
N2	0.21437 (6)	0.6022 (2)	0.34054 (7)	0.0374 (3)
O6	0.40941 (6)	1.10971 (19)	0.47560 (6)	0.0480 (3)
H6A	0.3835	1.1346	0.5099	0.072*
H6B	0.3901	1.2170	0.4397	0.072*
O5	0.49772 (5)	0.96277 (19)	0.33032 (6)	0.0414 (2)
H5A	0.4620	1.0010	0.2950	0.062*
H5B	0.5315	0.8953	0.3123	0.062*
O3	0.36524 (5)	0.5014 (2)	0.36062 (6)	0.0427 (3)
H50	0.3215	0.5470	0.3541	0.064*
H51	0.3705	0.4282	0.3174	0.064*
C7	0.20528 (7)	1.3150 (2)	0.14024 (7)	0.0304 (3)
O2	0.38821 (5)	1.2386 (2)	0.22633 (6)	0.0442 (3)
C9	0.17739 (6)	0.9467 (2)	0.24487 (7)	0.0301 (3)
O1	0.34259 (5)	1.1583 (2)	0.09542 (6)	0.0528 (3)
C11	0.24896 (7)	0.9854 (3)	0.23664 (8)	0.0326 (3)
H11	0.2865	0.8904	0.2675	0.039*
C12	0.26262 (6)	1.1624 (3)	0.18334 (7)	0.0305 (3)
C13	0.15995 (7)	0.7438 (2)	0.29892 (7)	0.0314 (3)
C14	0.33714 (7)	1.1890 (3)	0.16692 (8)	0.0341 (3)
C15	0.13590 (7)	1.2676 (2)	0.15413 (8)	0.0314 (3)
C16	0.07768 (7)	1.4199 (3)	0.11366 (9)	0.0402 (3)
H16	0.0316	1.3888	0.1212	0.048*
C17	0.21427 (8)	1.5153 (3)	0.08769 (8)	0.0389 (3)
H17	0.2596	1.5482	0.0782	0.047*
C18	0.19828 (8)	0.4159 (3)	0.38732 (9)	0.0439 (3)
H18	0.2360	0.3186	0.4167	0.053*
C19	0.07401 (8)	0.5048 (3)	0.35213 (9)	0.0415 (3)
H19	0.0268	0.4718	0.3554	0.050*
C20	0.15707 (8)	1.6597 (3)	0.05106 (9)	0.0449 (4)
H20	0.1637	1.7919	0.0172	0.054*
C21	0.12967 (8)	0.3599 (3)	0.39460 (9)	0.0426 (3)
H21	0.1212	0.2273	0.4274	0.051*

supplementary materials

C22	0.08920 (7)	0.7007 (3)	0.30439 (8)	0.0387 (3)
H22	0.0522	0.8031	0.2761	0.046*
C23	0.08833 (8)	1.6110 (3)	0.06398 (9)	0.0446 (4)
H23	0.0496	1.7104	0.0383	0.054*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0418 (3)	0.0330 (3)	0.0387 (3)	0.0028 (2)	0.0121 (2)	0.0002 (2)
O4	0.0428 (6)	0.0361 (6)	0.0460 (6)	-0.0033 (4)	0.0199 (4)	-0.0019 (4)
N1	0.0270 (5)	0.0375 (7)	0.0341 (6)	0.0005 (5)	0.0081 (4)	-0.0017 (5)
N2	0.0330 (6)	0.0410 (7)	0.0399 (6)	0.0035 (5)	0.0116 (5)	0.0036 (5)
O6	0.0596 (7)	0.0408 (6)	0.0493 (6)	0.0129 (5)	0.0244 (5)	0.0061 (5)
O5	0.0392 (5)	0.0473 (6)	0.0385 (5)	0.0090 (5)	0.0105 (4)	0.0020 (4)
O3	0.0328 (5)	0.0516 (6)	0.0431 (5)	0.0054 (4)	0.0073 (4)	-0.0010 (5)
C7	0.0299 (6)	0.0330 (7)	0.0283 (6)	-0.0004 (5)	0.0065 (5)	-0.0040 (5)
O2	0.0270 (5)	0.0637 (7)	0.0421 (5)	-0.0008 (4)	0.0082 (4)	0.0001 (5)
C9	0.0277 (6)	0.0346 (7)	0.0286 (6)	0.0009 (5)	0.0081 (5)	-0.0035 (5)
O1	0.0405 (6)	0.0841 (8)	0.0389 (5)	0.0043 (5)	0.0197 (4)	-0.0019 (5)
C11	0.0270 (6)	0.0392 (8)	0.0321 (6)	0.0048 (5)	0.0075 (5)	0.0020 (5)
C12	0.0266 (6)	0.0372 (7)	0.0285 (6)	-0.0002 (5)	0.0078 (5)	-0.0042 (5)
C13	0.0300 (6)	0.0352 (7)	0.0301 (6)	0.0004 (5)	0.0092 (5)	-0.0036 (5)
C14	0.0297 (7)	0.0376 (8)	0.0373 (7)	0.0033 (5)	0.0126 (5)	0.0033 (5)
C15	0.0281 (6)	0.0340 (7)	0.0313 (6)	0.0001 (5)	0.0054 (5)	-0.0053 (5)
C16	0.0304 (7)	0.0451 (9)	0.0428 (8)	0.0047 (6)	0.0035 (6)	0.0002 (6)
C17	0.0395 (7)	0.0412 (8)	0.0368 (7)	-0.0029 (6)	0.0101 (6)	0.0007 (6)
C18	0.0430 (8)	0.0426 (9)	0.0472 (8)	0.0074 (6)	0.0126 (6)	0.0087 (6)
C19	0.0361 (7)	0.0478 (9)	0.0432 (7)	-0.0082 (6)	0.0146 (6)	-0.0019 (6)
C20	0.0521 (9)	0.0400 (8)	0.0407 (8)	0.0014 (7)	0.0068 (6)	0.0063 (6)
C21	0.0513 (9)	0.0369 (8)	0.0430 (8)	-0.0032 (7)	0.0177 (6)	0.0025 (6)
C22	0.0297 (7)	0.0473 (9)	0.0399 (7)	0.0009 (6)	0.0100 (5)	0.0034 (6)
C23	0.0426 (8)	0.0423 (9)	0.0440 (8)	0.0096 (6)	-0.0008 (6)	0.0023 (6)

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

Na1—O6	2.3393 (11)	O2—C14	1.2544 (16)
Na1—O3	2.3559 (11)	C9—C11	1.4157 (17)
Na1—O4	2.3834 (11)	C9—C13	1.4935 (18)
Na1—O5	2.3867 (11)	O1—C14	1.2419 (16)
Na1—O4 ⁱ	2.3909 (11)	C11—C12	1.3632 (18)
Na1—O6 ⁱⁱ	2.6848 (13)	C11—H11	0.9300
Na1—Na1 ⁱ	3.4262 (11)	C12—C14	1.5124 (17)
Na1—Na1 ⁱⁱ	3.5661 (11)	C13—C22	1.3897 (18)
O4—H4A	0.85	C15—C16	1.4148 (18)
O4—H4B	0.85	C16—C23	1.357 (2)
N1—C9	1.3159 (17)	C16—H16	0.9300
N1—C15	1.3660 (17)	C17—C20	1.359 (2)
N2—C18	1.3408 (18)	C17—H17	0.9300

N2—C13	1.3409 (17)	C18—C21	1.372 (2)
O6—H6A	0.85	C18—H18	0.9300
O6—H6B	0.85	C19—C21	1.371 (2)
O5—H5A	0.82	C19—C22	1.383 (2)
O5—H5B	0.85	C19—H19	0.9300
O3—H50	0.85	C20—C23	1.399 (2)
O3—H51	0.85	C20—H20	0.9300
C7—C15	1.4152 (17)	C21—H21	0.9300
C7—C17	1.4167 (19)	C22—H22	0.9300
C7—C12	1.4187 (18)	C23—H23	0.9300
O6—Na1—O3	106.24 (4)	H50—O3—H51	108.7
O6—Na1—O4	165.19 (4)	C15—C7—C17	119.05 (12)
O3—Na1—O4	87.81 (4)	C15—C7—C12	116.97 (11)
O6—Na1—O5	90.56 (4)	C17—C7—C12	123.93 (12)
O3—Na1—O5	99.92 (4)	N1—C9—C11	122.72 (12)
O4—Na1—O5	91.59 (4)	N1—C9—C13	116.22 (11)
O6—Na1—O4 ⁱ	84.49 (4)	C11—C9—C13	121.04 (11)
O3—Na1—O4 ⁱ	101.12 (4)	C12—C11—C9	119.71 (12)
O4—Na1—O4 ⁱ	88.28 (4)	C12—C11—H11	120.1
O5—Na1—O4 ⁱ	158.94 (4)	C9—C11—H11	120.1
O6—Na1—O6 ⁱⁱ	89.83 (4)	C11—C12—C7	119.27 (11)
O3—Na1—O6 ⁱⁱ	163.58 (4)	C11—C12—C14	120.75 (12)
O4—Na1—O6 ⁱⁱ	75.91 (4)	C7—C12—C14	119.91 (11)
O5—Na1—O6 ⁱⁱ	82.92 (4)	N2—C13—C22	121.29 (12)
O4 ⁱ —Na1—O6 ⁱⁱ	76.62 (4)	N2—C13—C9	117.95 (11)
O6—Na1—Na1 ⁱ	127.27 (4)	C22—C13—C9	120.76 (12)
O3—Na1—Na1 ⁱ	96.20 (3)	O1—C14—O2	125.45 (12)
O4—Na1—Na1 ⁱ	44.23 (3)	O1—C14—C12	116.92 (12)
O5—Na1—Na1 ⁱ	132.11 (4)	O2—C14—C12	117.63 (11)
O4 ⁱ —Na1—Na1 ⁱ	44.05 (3)	N1—C15—C16	118.50 (11)
O6 ⁱⁱ —Na1—Na1 ⁱ	70.68 (3)	N1—C15—C7	122.94 (12)
O6—Na1—Na1 ⁱⁱ	48.84 (3)	C16—C15—C7	118.57 (12)
O3—Na1—Na1 ⁱⁱ	154.91 (4)	C23—C16—C15	120.79 (13)
O4—Na1—Na1 ⁱⁱ	116.80 (3)	C23—C16—H16	119.6
O5—Na1—Na1 ⁱⁱ	85.04 (3)	C15—C16—H16	119.6
O4 ⁱ —Na1—Na1 ⁱⁱ	76.28 (3)	C20—C17—C7	120.47 (13)
O6 ⁱⁱ —Na1—Na1 ⁱⁱ	40.99 (2)	C20—C17—H17	119.8
Na1—O4—Na1 ⁱ	91.72 (4)	C7—C17—H17	119.8
Na1—O4—H4A	123.9	N2—C18—C21	124.12 (14)
Na1 ⁱ —O4—H4A	109.5	N2—C18—H18	117.9
Na1—O4—H4B	105.6	C21—C18—H18	117.9
Na1 ⁱ —O4—H4B	119.2	C21—C19—C22	118.97 (13)
H4A—O4—H4B	107.2	C21—C19—H19	120.5
C9—N1—C15	118.28 (11)	C22—C19—H19	120.5

supplementary materials

C18—N2—C13	117.78 (12)	C17—C20—C23	120.49 (14)
Na1—O6—Na1 ⁱⁱ	90.17 (4)	C17—C20—H20	119.8
Na1—O6—H6A	131.3	C23—C20—H20	119.8
Na1 ⁱⁱ —O6—H6A	100.8	C19—C21—C18	118.11 (14)
Na1—O6—H6B	120.3	C19—C21—H21	120.9
Na1 ⁱⁱ —O6—H6B	112.7	C18—C21—H21	120.9
H6A—O6—H6B	98.9	C19—C22—C13	119.71 (13)
Na1—O5—H5A	109.5	C19—C22—H22	120.1
Na1—O5—H5B	116.0	C13—C22—H22	120.1
H5A—O5—H5B	114.6	C16—C23—C20	120.62 (13)
Na1—O3—H50	122.1	C16—C23—H23	119.7
Na1—O3—H51	119.3	C20—C23—H23	119.7
O6—Na1—O4—Na1 ⁱ	60.71 (16)	N1—C9—C13—C22	1.18 (18)
O3—Na1—O4—Na1 ⁱ	-101.20 (4)	C11—C9—C13—C22	-177.58 (12)
O5—Na1—O4—Na1 ⁱ	158.93 (4)	C11—C12—C14—O1	120.27 (15)
O4 ⁱ —Na1—O4—Na1 ⁱ	0.0	C7—C12—C14—O1	-56.85 (18)
O6 ⁱⁱ —Na1—O4—Na1 ⁱ	76.64 (4)	C11—C12—C14—O2	-59.32 (18)
Na1 ⁱⁱ —Na1—O4—Na1 ⁱ	73.68 (4)	C7—C12—C14—O2	123.56 (14)
O3—Na1—O6—Na1 ⁱⁱ	176.58 (4)	C9—N1—C15—C16	-177.42 (12)
O4—Na1—O6—Na1 ⁱⁱ	15.43 (16)	C9—N1—C15—C7	2.51 (18)
O5—Na1—O6—Na1 ⁱⁱ	-82.92 (4)	C17—C7—C15—N1	-178.81 (12)
O4 ⁱ —Na1—O6—Na1 ⁱⁱ	76.58 (3)	C12—C7—C15—N1	-1.38 (18)
O6 ⁱⁱ —Na1—O6—Na1 ⁱⁱ	0.0	C17—C7—C15—C16	1.13 (18)
Na1 ⁱ —Na1—O6—Na1 ⁱⁱ	65.29 (5)	C12—C7—C15—C16	178.56 (12)
C15—N1—C9—C11	-0.61 (19)	N1—C15—C16—C23	178.51 (12)
C15—N1—C9—C13	-179.35 (10)	C7—C15—C16—C23	-1.4 (2)
N1—C9—C11—C12	-2.4 (2)	C15—C7—C17—C20	-0.1 (2)
C13—C9—C11—C12	176.26 (12)	C12—C7—C17—C20	-177.32 (13)
C9—C11—C12—C7	3.49 (19)	C13—N2—C18—C21	0.6 (2)
C9—C11—C12—C14	-173.65 (12)	C7—C17—C20—C23	-0.7 (2)
C15—C7—C12—C11	-1.68 (18)	C22—C19—C21—C18	-0.3 (2)
C17—C7—C12—C11	175.61 (12)	N2—C18—C21—C19	-0.7 (2)
C15—C7—C12—C14	175.49 (11)	C21—C19—C22—C13	1.3 (2)
C17—C7—C12—C14	-7.22 (19)	N2—C13—C22—C19	-1.5 (2)
C18—N2—C13—C22	0.5 (2)	C9—C13—C22—C19	177.24 (12)
C18—N2—C13—C9	-178.27 (12)	C15—C16—C23—C20	0.7 (2)
N1—C9—C13—N2	179.93 (11)	C17—C20—C23—C16	0.4 (2)
C11—C9—C13—N2	1.16 (18)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H50 \cdots N2	0.85	2.02	2.8657 (14)	172
O3—H51 \cdots O2 ⁱⁱⁱ	0.85	1.92	2.7722 (14)	174

O4—H4A···O5 ⁱⁱⁱ	0.85	1.98	2.8222 (14)	172
O4—H4B···O1 ^{iv}	0.85	1.91	2.7494 (14)	171
O5—H5A···O2	0.82	2.04	2.8093 (14)	156
O5—H5B···O2 ^{iv}	0.85	1.97	2.8243 (13)	178
O6—H6A···O1 ^v	0.85	2.10	2.8914 (14)	156
O6—H6B···O3 ^{vi}	0.85	2.00	2.8321 (14)	168

Symmetry codes: (iii) $x, y-1, z$; (iv) $-x+1, y-1/2, -z+1/2$; (v) $x, -y+5/2, z+1/2$; (vi) $x, y+1, z$.

Fig. 1

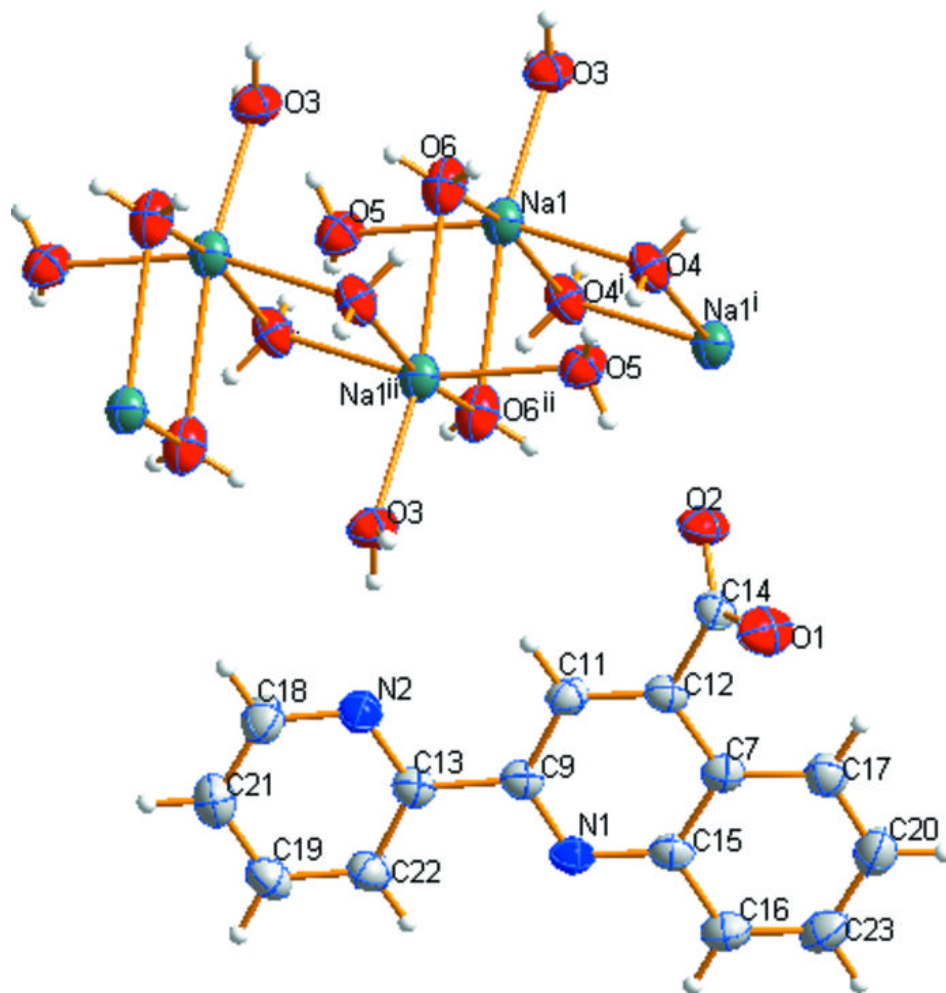


Fig. 2

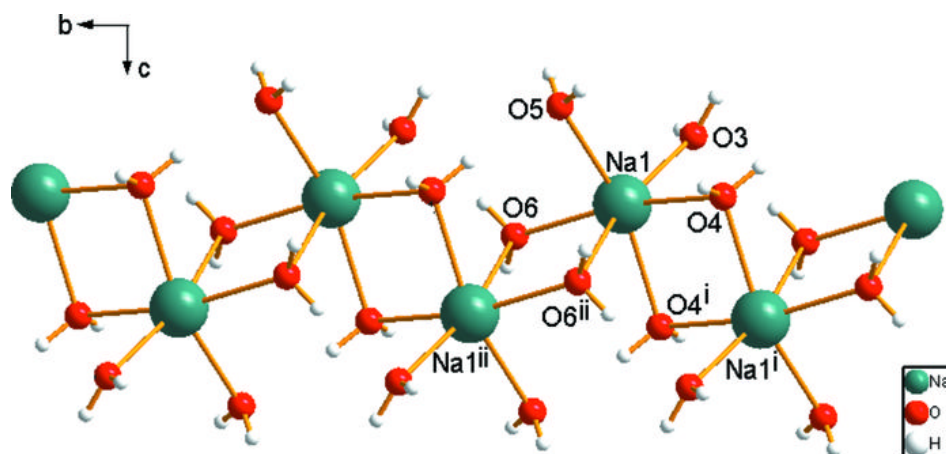


Fig. 3

