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Betaine (trimethylammonioacetate) binary compound with sodium iodide

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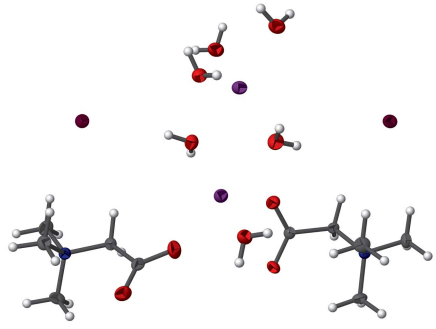
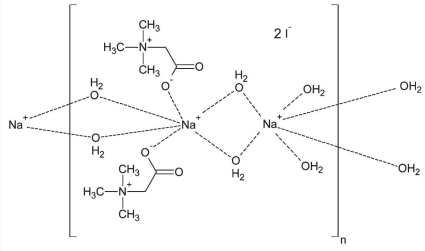
In the title compound, *catena*-poly[[[bis[2-(trimethylazaniumyl)acetato-κO]-sodium]-di-μ-aqua-[diaquasodium]-di-μ-aqua] diiodide], $\{[Na_2(C_5H_{11}NO_2)_2(H_2O)_6]I_2\}_n$, both Na^+ ions have distorted octahedral environments (coordination number 6). The coordination polyhedra of the sodium ions are connected by common edges forming an infinite chain of ions along [100]. The chains and betaine zwitterions are assembled into infinitive layers *via* hydrogen bonds. These layers are connected *via* electrostatic attraction between iodide ions and positive trimethylazanium groups in the crystal.

3D view



Chemical scheme



Structure description

Betaines represent a wide class of zwitterionic compounds with an onium group that bears no hydrogen atoms and that is not adjacent to the anionic atom. The parent compound of the betaine class, trimethylammonioacetate (TMA), has a very rich crystal chemistry: the Cambridge Structural Database (CSD Version 5.39; Groom *et al.*, 2016) contains 217 different structures of its compounds. There are several known crystal structures of TMA binary compounds with potassium iodide (HIPQIG; Andrade *et al.*, 1999), rubidium iodide (NEMKIZ; Andrade *et al.*, 2001), potassium bromide (WIQPUH01; Andrade *et al.*, 2000) and sodium bromide (JAZNEE; Rodrigues *et al.*, 2005). In a continuation of studies (Nazarenko, 2018) of zwitterionic binary compounds, an unreported structure of trimethylammonioacetate with sodium iodide is presented here.

The numbering scheme for the title compound is shown in Fig. 1. Both Na^+ ions have distorted octahedral environments. The coordination sphere of Na1 (Table 1, Fig. 2) contains two pairs of bridging O atoms of water molecules (O1 and O6; O4 and O5) and two terminal water molecules (atoms O2 and O3). The coordination sphere of Na2

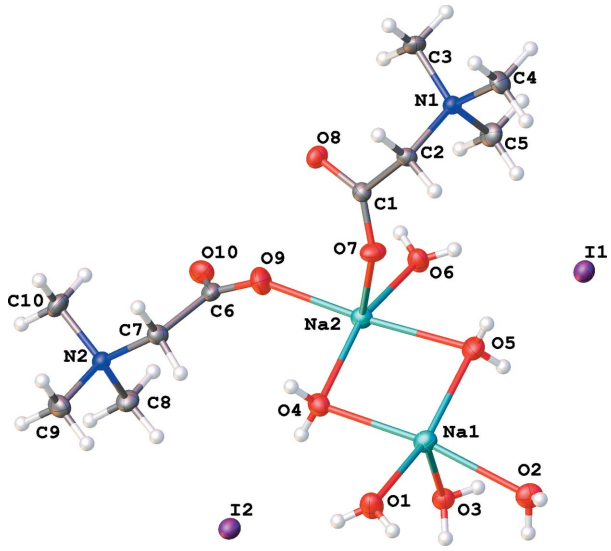


Figure 1
Numbering scheme for the title compound with 50% probability displacement ellipsoids.

contains two anionic oxygen atoms of monodentate carboxylic groups (O7 and O9) and the same four bridging atoms (Table 1, Fig. 2).

The distribution of the Hirshfeld surface electrostatic potential of the zwitterion (Fig. 3) shows that only the area around the carboxyl oxygen atoms is negatively charged. The remaining Hirshfeld surface has positive electrostatic potential, which makes this area attractive for iodide anions.

The coordination polyhedra of the sodium ions are connected by common edges (two pairs of bridging water molecules, O1 & O6 and O4 & O5), forming an infinite chain of ions along [100] (Fig. 4). In addition to Na—O interactions,

Table 1
Selected bond lengths (Å).

Na1—O1	2.3733 (17)	Na2—O1^{ii}	2.6120 (18)
Na1—O2	2.3842 (17)	Na2—O4	2.3944 (16)
Na1—O3	2.4650 (16)	Na2—O5	2.4697 (17)
Na1—O4	2.3926 (16)	Na2—O6	2.3412 (16)
Na1—O5	2.4926 (17)	Na2—O7	2.3937 (15)
Na1—O6^{i}	2.4943 (17)	Na2—O9	2.3175 (16)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···I2^{i}	0.74 (3)	3.03 (3)	3.7008 (17)	152 (3)
O1—H1B···O3^{i}	0.78 (3)	2.01 (3)	2.781 (2)	172 (3)
O2—H2A···O9^{iii}	0.78 (3)	2.19 (3)	2.915 (2)	154 (3)
O2—H2B···O8^{iii}	0.76 (3)	2.00 (3)	2.7641 (19)	175 (3)
O3—H3A···O10^{iii}	0.80 (3)	1.99 (3)	2.772 (2)	169 (3)
O3—H3B···O8^{iv}	0.76 (3)	2.13 (3)	2.860 (2)	160 (3)
O4—H4A···I2	0.79 (3)	2.85 (3)	3.6300 (14)	172 (2)
O4—H4B···O10^{i}	0.81 (3)	2.04 (3)	2.823 (2)	165 (2)
O5—H5A···O8^{iv}	0.79 (3)	1.97 (3)	2.7484 (19)	167 (3)
O6—H6A···I1^{ii}	0.76 (3)	2.85 (3)	3.5864 (17)	165 (3)
O6—H6B···O7^{ii}	0.79 (3)	2.05 (3)	2.829 (2)	168 (3)
C8—H8A···O10	0.98	2.33	2.976 (2)	122
C3—H3D···O8	0.98	2.39	2.999 (2)	120
C10—H10A···O10	0.98	2.34	2.994 (2)	123

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

this chain is supported by three hydrogen bonds (Table 2, Fig. 4): O1—H1B···O3, O4—H4B···O10, and O6—H6B···O10. The last two of these, connecting the anionic oxygen atom of the carboxylic group, are electrostatically enhanced. The chains are interconnected *via* five hydrogen bonds (O2—H2A···O9, O2—H2B···O8, O3—H3A···O10, O3—H3B···O8, O5—H5A···O8, see Table 2 and Fig. 5). Three more water hydrogen atoms are involved in hydrogen

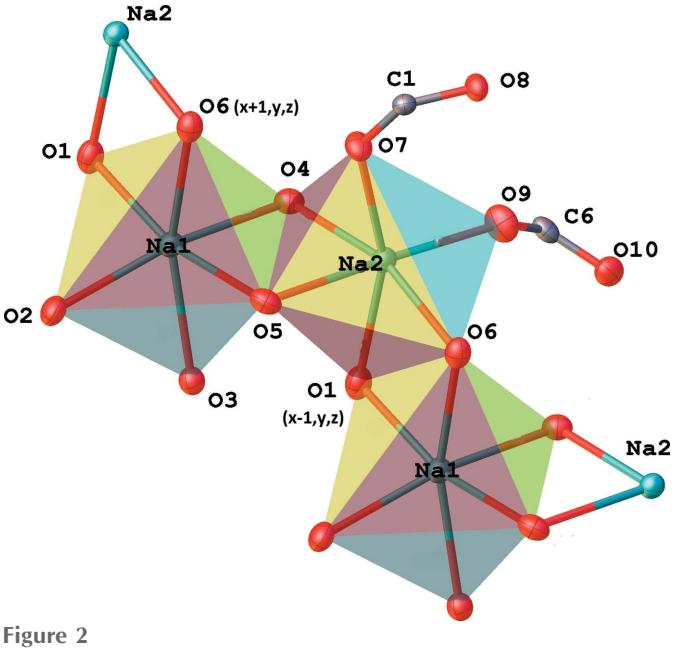


Figure 2
Coordination polyhedra of the sodium ions.

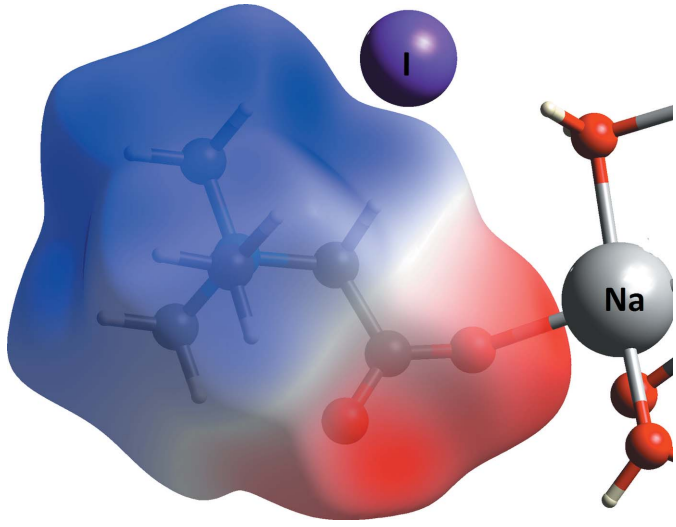


Figure 3
Hirshfeld surface of the zwitterion with electrostatic potential plotted using *CrystalExplorer17* (Turner *et al.*, 2017). Colour key: red – negative, blue – positive.

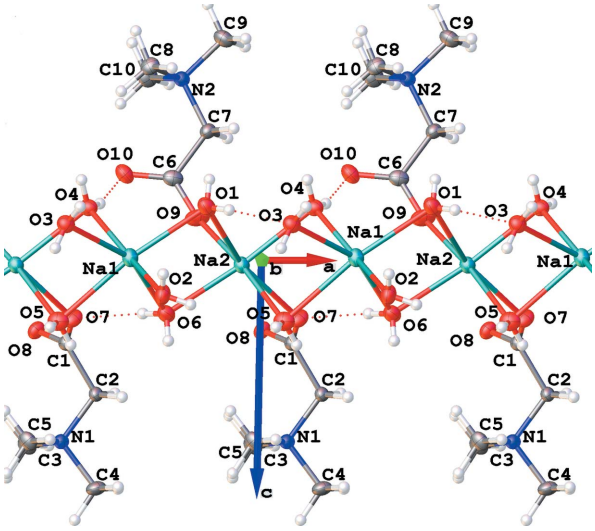


Figure 4
The infinite chain of hydrated sodium ions along [100], viewed along [010].

bonds with iodide ions (Table 2). The resulting network of hydrogen bonds forms layers in the (001) plane with iodide ions and trimethylammonium groups forming each side (Fig. 5). These layers are bound together *via* electrostatic

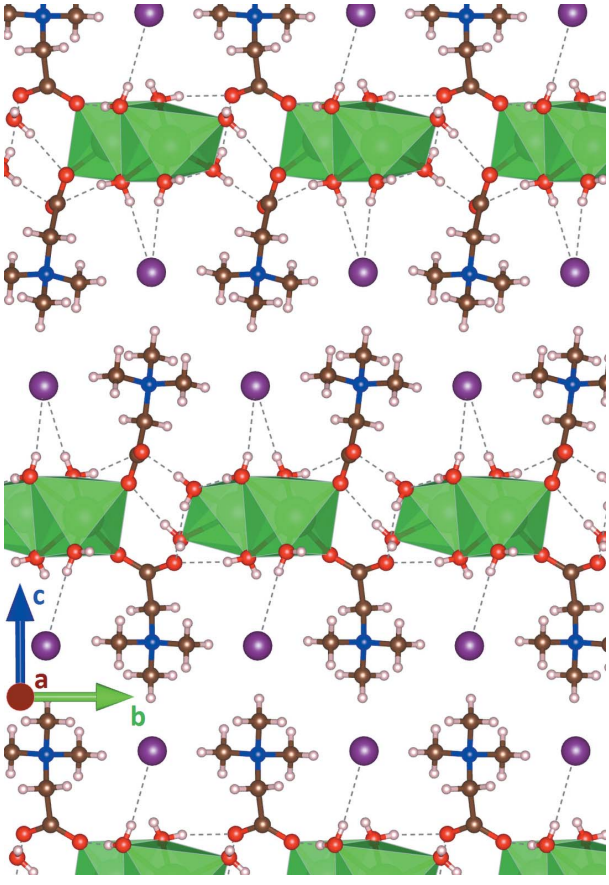


Figure 5
Packing of the title compound, viewed along [100]. Sodium ions are green.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Na_2(C_5H_{11}NO_2)_2(H_2O)_6]I_2$
M_r	642.17
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, b, c (Å)	5.8131 (3), 7.6682 (4), 26.7168 (15)
α, β, γ (°)	90.221 (2), 91.168 (2), 91.440 (3)
V (Å^3)	1190.29 (11)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.72
Crystal size (mm)	0.60 × 0.30 × 0.10
Data collection	
Diffractometer	Bruker PHOTON-100 CMOS
Absorption correction	Numerical (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.076, 0.252
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	49693, 8726, 7237
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.759
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.050, 1.15
No. of reflections	8726
No. of parameters	277
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.79, −0.42

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *CrystalExplorer17* (Turner *et al.*, 2017) and *VESTA* (Momma & Izumi, 2008).

interactions between the corresponding positive and negative ions; no short intralayer contacts are visible. A number of short intramolecular C—H···O contacts (Table 2) may play some auxiliary role in the conformation of the zwitterion. There are no suitable acceptor atoms for hydrogen atom H5*B* of a bridging water molecule; its orientation is an interplay between electrostatic attraction by neighboring iodide I1 and repulsion by both sodium ions and trimethylammonium group.

Known TMA binary compounds (Andrade *et al.*, 1999, 2000, 2001; Rodrigues et *al.*, 2005) show features similar to the current structure: an infinite chain of hydrated alkali metal cations and layers of trimethylammonium groups. However, in the current case the bridging in the cation chain is organized *via* water molecules [similar to the sodium iodide co-crystal in Nazarenko (2018)] and not by carboxylic groups. Sodium ions usually form stronger hydrates than rubidium and potassium ions; this observation can serve as a very simplistic explanation.

Synthesis and crystallization

Equimolar amounts of commercial betaine monohydrate were mixed with sodium iodide in aqueous ethanol, similar to the procedure described in Andrade *et al.* (1999, 2000, 2001); subsequent slow evaporation yielded crystals suitable for the single–crystal X-ray experiment.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Funding information

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full crystallographic data

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Betaine (trimethylammonioacetate) binary compound with sodium iodide

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***catena*-Poly[[[bis[2-(trimethylazaniumyl)acetato-*κO*]sodium]-di-*μ*-aqua-[diaquasodium]-di-*μ*-aqua] diiodide]**

Crystal data

$[Na_2(C_5H_{11}NO_2)_2(H_2O)_6]I_2$
M_r = 642.17
Triclinic, $P\overline{1}$
a = 5.8131 (3) Å
b = 7.6682 (4) Å
c = 26.7168 (15) Å
α = 90.221 (2)°
β = 91.168 (2)°
γ = 91.440 (3)°
V = 1190.29 (11) Å^3
Z = 2
$F(000)$ = 632
D_x = 1.792 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9947 reflections
θ = 3.1–32.6°
μ = 2.72 mm^{-1}
T = 173 K
Plate, colourless
0.6 × 0.3 × 0.10 mm

Data collection

Bruker PHOTON-100 CMOS diffractometer
Radiation source: sealedtube
φ and ω scans
Absorption correction: numerical (SADABS; Krause *et al.*, 2015)
T_{min} = 0.076, T_{max} = 0.252
49693 measured reflections
8726 independent reflections
7237 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 32.7°, θ_{min} = 3.1°
h = −8→8
k = −11→11
l = −40→40

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.050
S = 1.15
8726 reflections
277 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0152P)^2 + 0.5637P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 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. Hydrogen atoms of water molecules are refined in isotropic approximation with U_{iso} (H) = 1.5U_{iso} (O). Methylene hydrogen atoms are refined with riding coordinates and with U_{iso} (H) = 1.2 U_{iso} (C); methyl hydrogen atoms are refined as rotating idealized methyl groups and with U_{iso} (H) = 1.5U_{iso} (C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.87928 (2)	0.75005 (2)	0.42881 (2)	0.02174 (3)
I2	0.38268 (2)	0.75565 (2)	0.07695 (2)	0.02165 (3)
Na1	0.77571 (13)	0.84390 (10)	0.24815 (3)	0.02154 (15)
Na2	0.27301 (12)	0.57053 (9)	0.25452 (3)	0.01983 (15)
O1	1.1105 (3)	0.8215 (2)	0.19938 (6)	0.0281 (3)
H1A	1.120 (5)	0.793 (4)	0.1729 (11)	0.042*
H1B	1.209 (5)	0.891 (4)	0.2024 (10)	0.042*
O2	0.9199 (3)	1.1102 (2)	0.28457 (6)	0.0260 (3)
H2A	0.919 (5)	1.185 (4)	0.2648 (10)	0.039*
H2B	1.044 (5)	1.114 (3)	0.2941 (10)	0.039*
O3	0.4860 (2)	1.04739 (18)	0.21635 (6)	0.0224 (3)
H3A	0.546 (4)	1.121 (3)	0.1998 (10)	0.034*
H3B	0.440 (4)	1.092 (3)	0.2396 (10)	0.034*
O4	0.5880 (2)	0.61769 (19)	0.19940 (5)	0.0225 (3)
H4A	0.555 (4)	0.655 (3)	0.1729 (10)	0.034*
H4B	0.640 (4)	0.522 (3)	0.1953 (9)	0.034*
O5	0.4634 (3)	0.79289 (19)	0.30936 (6)	0.0255 (3)
H5A	0.426 (5)	0.889 (4)	0.3152 (10)	0.038*
H5B	0.521 (5)	0.755 (4)	0.3320 (10)	0.038*
O6	−0.0568 (3)	0.6113 (2)	0.30161 (6)	0.0237 (3)
H6A	−0.046 (5)	0.649 (3)	0.3278 (10)	0.036*
H6B	−0.160 (5)	0.542 (3)	0.3013 (10)	0.036*
O7	0.5321 (2)	0.40694 (17)	0.30561 (5)	0.0241 (3)
O8	0.3744 (2)	0.14234 (16)	0.31642 (5)	0.0208 (3)
O9	0.0750 (3)	0.3559 (2)	0.20861 (5)	0.0327 (3)
O10	−0.2503 (2)	0.29400 (18)	0.16613 (5)	0.0260 (3)
N1	0.4939 (3)	0.24831 (19)	0.42389 (5)	0.0161 (3)
N2	−0.0051 (3)	0.25810 (18)	0.07475 (6)	0.0162 (3)
C1	0.5049 (3)	0.2687 (2)	0.32903 (6)	0.0157 (3)
C2	0.6431 (3)	0.2491 (2)	0.37817 (6)	0.0164 (3)
H2C	0.727987	0.138840	0.377039	0.020*
H2D	0.757875	0.346356	0.381182	0.020*
C3	0.3445 (3)	0.0862 (2)	0.42715 (7)	0.0226 (4)
H3C	0.441301	−0.016571	0.427063	0.034*
H3D	0.237339	0.080643	0.398366	0.034*
H3E	0.257447	0.088892	0.458162	0.034*
C4	0.6520 (3)	0.2557 (3)	0.46896 (7)	0.0236 (4)
H4C	0.750297	0.153754	0.469022	0.035*
H4D	0.560676	0.255836	0.499392	0.035*
H4E	0.748196	0.362354	0.467905	0.035*
C5	0.3436 (3)	0.4046 (2)	0.42398 (8)	0.0235 (4)
H5C	0.254092	0.405303	0.454664	0.035*
H5D	0.238739	0.399377	0.394805	0.035*
H5E	0.439974	0.511094	0.422547	0.035*
C6	−0.0360 (3)	0.3125 (2)	0.17028 (7)	0.0205 (4)

C7	0.1150 (3)	0.2796 (2)	0.12491 (7)	0.0187 (3)
H7A	0.227645	0.378078	0.122540	0.022*
H7B	0.203265	0.173111	0.131526	0.022*
C8	−0.1491 (3)	0.4124 (2)	0.06276 (7)	0.0219 (4)
H8A	−0.273710	0.419352	0.086793	0.033*
H8B	−0.214731	0.399708	0.028827	0.033*
H8C	−0.053026	0.519188	0.064825	0.033*
C9	0.1769 (4)	0.2449 (3)	0.03578 (7)	0.0249 (4)
H9A	0.103387	0.229314	0.002686	0.037*
H9B	0.273443	0.144916	0.043190	0.037*
H9C	0.272600	0.352033	0.036096	0.037*
C10	−0.1531 (3)	0.0948 (2)	0.07263 (8)	0.0242 (4)
H10A	−0.271890	0.100911	0.098044	0.036*
H10B	−0.057606	−0.006544	0.079092	0.036*
H10C	−0.226413	0.083386	0.039385	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02324 (6)	0.01967 (6)	0.02222 (6)	−0.00166 (4)	0.00118 (5)	−0.00155 (4)
I2	0.02442 (6)	0.01912 (6)	0.02132 (6)	−0.00068 (4)	−0.00071 (5)	0.00098 (4)
Na1	0.0185 (4)	0.0206 (4)	0.0256 (4)	0.0002 (3)	0.0017 (3)	0.0009 (3)
Na2	0.0182 (3)	0.0209 (4)	0.0205 (4)	0.0006 (3)	0.0018 (3)	0.0004 (3)
O1	0.0240 (7)	0.0324 (8)	0.0276 (8)	−0.0055 (6)	0.0063 (6)	−0.0052 (6)
O2	0.0176 (7)	0.0291 (8)	0.0311 (8)	−0.0014 (6)	−0.0019 (6)	0.0021 (6)
O3	0.0230 (7)	0.0215 (7)	0.0225 (7)	−0.0015 (5)	0.0021 (6)	0.0002 (5)
O4	0.0249 (7)	0.0227 (7)	0.0201 (7)	0.0042 (5)	0.0013 (6)	0.0001 (5)
O5	0.0321 (8)	0.0183 (7)	0.0262 (8)	0.0041 (6)	0.0009 (6)	−0.0001 (6)
O6	0.0227 (7)	0.0271 (7)	0.0212 (7)	−0.0035 (5)	0.0035 (6)	−0.0035 (6)
O7	0.0266 (7)	0.0209 (6)	0.0244 (7)	−0.0018 (5)	−0.0044 (6)	0.0074 (5)
O8	0.0201 (6)	0.0193 (6)	0.0227 (7)	−0.0027 (5)	−0.0045 (5)	−0.0011 (5)
O9	0.0439 (9)	0.0337 (8)	0.0200 (7)	−0.0037 (7)	−0.0030 (6)	−0.0054 (6)
O10	0.0245 (7)	0.0270 (7)	0.0267 (7)	−0.0002 (6)	0.0083 (6)	0.0000 (6)
N1	0.0171 (7)	0.0152 (7)	0.0159 (7)	−0.0008 (5)	0.0003 (6)	0.0001 (5)
N2	0.0180 (7)	0.0139 (6)	0.0168 (7)	0.0009 (5)	0.0010 (6)	0.0000 (5)
C1	0.0153 (8)	0.0160 (7)	0.0159 (8)	0.0026 (6)	0.0005 (6)	−0.0001 (6)
C2	0.0144 (8)	0.0188 (8)	0.0160 (8)	−0.0011 (6)	0.0010 (6)	0.0018 (6)
C3	0.0251 (10)	0.0193 (8)	0.0234 (9)	−0.0072 (7)	0.0066 (8)	0.0014 (7)
C4	0.0284 (10)	0.0273 (10)	0.0148 (8)	−0.0008 (8)	−0.0036 (7)	−0.0001 (7)
C5	0.0239 (9)	0.0197 (9)	0.0273 (10)	0.0055 (7)	0.0059 (8)	−0.0019 (7)
C6	0.0298 (10)	0.0129 (8)	0.0188 (9)	−0.0009 (7)	0.0022 (7)	0.0007 (6)
C7	0.0185 (8)	0.0204 (8)	0.0171 (8)	−0.0006 (6)	−0.0017 (7)	0.0017 (7)
C8	0.0254 (9)	0.0174 (8)	0.0229 (9)	0.0041 (7)	−0.0029 (7)	0.0025 (7)
C9	0.0288 (10)	0.0249 (9)	0.0215 (9)	0.0040 (8)	0.0076 (8)	−0.0003 (7)
C10	0.0270 (10)	0.0163 (8)	0.0291 (10)	−0.0049 (7)	0.0003 (8)	−0.0035 (7)

Geometric parameters (Å, º)

Na1—Na2	3.5607 (10)	N1—C3	1.502 (2)
Na1—Na2^{i}	3.6149 (10)	N1—C4	1.500 (2)
Na1—O1	2.3733 (17)	N1—C5	1.500 (2)
Na1—O2	2.3842 (17)	N2—C7	1.505 (2)
Na1—O3	2.4650 (16)	N2—C8	1.499 (2)
Na1—O4	2.3926 (16)	N2—C9	1.504 (2)
Na1—O5	2.4926 (17)	N2—C10	1.502 (2)
Na1—O6^{i}	2.4943 (17)	C1—C2	1.535 (2)
Na2—O1^{ii}	2.6120 (18)	C2—H2C	0.9900
Na2—O4	2.3944 (16)	C2—H2D	0.9900
Na2—O5	2.4697 (17)	C3—H3C	0.9800
Na2—O6	2.3412 (16)	C3—H3D	0.9800
Na2—O7	2.3937 (15)	C3—H3E	0.9800
Na2—O9	2.3175 (16)	C4—H4C	0.9800
O1—H1A	0.74 (3)	C4—H4D	0.9800
O1—H1B	0.78 (3)	C4—H4E	0.9800
O2—H2A	0.78 (3)	C5—H5C	0.9800
O2—H2B	0.76 (3)	C5—H5D	0.9800
O3—H3A	0.80 (3)	C5—H5E	0.9800
O3—H3B	0.76 (3)	C6—C7	1.535 (3)
O4—H4A	0.79 (3)	C7—H7A	0.9900
O4—H4B	0.81 (3)	C7—H7B	0.9900
O5—H5A	0.79 (3)	C8—H8A	0.9800
O5—H5B	0.75 (3)	C8—H8B	0.9800
O6—H6A	0.76 (3)	C8—H8C	0.9800
O6—H6B	0.79 (3)	C9—H9A	0.9800
O7—C1	1.242 (2)	C9—H9B	0.9800
O8—C1	1.256 (2)	C9—H9C	0.9800
O9—C6	1.239 (2)	C10—H10A	0.9800
O10—C6	1.253 (2)	C10—H10B	0.9800
N1—C2	1.513 (2)	C10—H10C	0.9800
O1—Na1—O2	90.91 (6)	C4—N1—C3	108.32 (14)
O1—Na1—O3	115.58 (6)	C4—N1—C5	109.26 (14)
O1—Na1—O4	90.36 (6)	C5—N1—C2	110.53 (14)
O1—Na1—O5	164.44 (6)	C5—N1—C3	108.92 (14)
O1—Na1—O6^{i}	86.19 (6)	C8—N2—C7	111.16 (14)
O2—Na1—O3	79.70 (5)	C8—N2—C9	108.40 (14)
O2—Na1—O4	167.56 (6)	C8—N2—C10	109.53 (14)
O2—Na1—O5	96.09 (6)	C9—N2—C7	107.71 (14)
O2—Na1—O6^{i}	104.58 (6)	C10—N2—C7	111.46 (14)
O3—Na1—O5	79.44 (5)	C10—N2—C9	108.49 (14)
O3—Na1—O6^{i}	157.96 (6)	O7—C1—O8	126.22 (17)
O4—Na1—O3	88.60 (5)	O7—C1—C2	117.31 (15)
O4—Na1—O5	85.80 (5)	O8—C1—C2	116.47 (15)
O4—Na1—O6^{i}	87.85 (6)	N1—C2—C1	113.03 (14)

O5—Na1—O6^{i}	78.61 (5)	N1—C2—H2C	109.0
O4—Na2—O1^{ii}	79.92 (5)	N1—C2—H2D	109.0
O4—Na2—O5	86.28 (6)	C1—C2—H2C	109.0
O5—Na2—O1^{ii}	88.89 (6)	C1—C2—H2D	109.0
O6—Na2—O1^{ii}	84.20 (5)	H2C—C2—H2D	107.8
O6—Na2—O4	162.69 (6)	N1—C3—H3C	109.5
O6—Na2—O5	86.57 (6)	N1—C3—H3D	109.5
O6—Na2—O7	106.74 (6)	N1—C3—H3E	109.5
O7—Na2—O1^{ii}	160.57 (6)	H3C—C3—H3D	109.5
O7—Na2—O4	86.76 (5)	H3C—C3—H3E	109.5
O7—Na2—O5	76.09 (5)	H3D—C3—H3E	109.5
O9—Na2—O1^{ii}	92.99 (6)	N1—C4—H4C	109.5
O9—Na2—O4	98.37 (6)	N1—C4—H4D	109.5
O9—Na2—O5	175.22 (6)	N1—C4—H4E	109.5
O9—Na2—O6	89.26 (6)	H4C—C4—H4D	109.5
O9—Na2—O7	102.97 (6)	H4C—C4—H4E	109.5
Na1—O1—Na2^{i}	92.83 (6)	H4D—C4—H4E	109.5
Na1—O1—H1A	129 (2)	N1—C5—H5C	109.5
Na1—O1—H1B	119 (2)	N1—C5—H5D	109.5
Na2^{i}—O1—H1A	107 (2)	N1—C5—H5E	109.5
Na2^{i}—O1—H1B	101 (2)	H5C—C5—H5D	109.5
H1A—O1—H1B	103 (3)	H5C—C5—H5E	109.5
Na1—O2—H2A	111 (2)	H5D—C5—H5E	109.5
Na1—O2—H2B	118 (2)	O9—C6—O10	126.50 (18)
H2A—O2—H2B	102 (3)	O9—C6—C7	113.64 (17)
Na1—O3—H3A	110.1 (18)	O10—C6—C7	119.86 (16)
Na1—O3—H3B	105.0 (19)	N2—C7—C6	117.25 (15)
H3A—O3—H3B	108 (3)	N2—C7—H7A	108.0
Na1—O4—Na2	96.12 (6)	N2—C7—H7B	108.0
Na1—O4—H4A	109.2 (19)	C6—C7—H7A	108.0
Na1—O4—H4B	123.9 (18)	C6—C7—H7B	108.0
Na2—O4—H4A	115.4 (19)	H7A—C7—H7B	107.2
Na2—O4—H4B	104.7 (18)	N2—C8—H8A	109.5
H4A—O4—H4B	107 (3)	N2—C8—H8B	109.5
Na1—O5—H5A	101.7 (19)	N2—C8—H8C	109.5
Na1—O5—H5B	106 (2)	H8A—C8—H8B	109.5
Na2—O5—Na1	91.70 (6)	H8A—C8—H8C	109.5
Na2—O5—H5A	129.2 (19)	H8B—C8—H8C	109.5
Na2—O5—H5B	113 (2)	N2—C9—H9A	109.5
H5A—O5—H5B	110 (3)	N2—C9—H9B	109.5
Na1^{ii}—O6—H6A	106 (2)	N2—C9—H9C	109.5
Na1^{ii}—O6—H6B	100.2 (19)	H9A—C9—H9B	109.5
Na2—O6—Na1^{ii}	96.71 (6)	H9A—C9—H9C	109.5
Na2—O6—H6A	120 (2)	H9B—C9—H9C	109.5
Na2—O6—H6B	121.7 (19)	N2—C10—H10A	109.5
H6A—O6—H6B	108 (3)	N2—C10—H10B	109.5
C1—O7—Na2	131.66 (12)	N2—C10—H10C	109.5
C6—O9—Na2	148.99 (14)	H10A—C10—H10B	109.5

C3—N1—C2	112.49 (14)	H10A—C10—H10C	109.5
C4—N1—C2	107.25 (14)	H10B—C10—H10C	109.5
Na2—O7—C1—O8	32.9 (3)	O10—C6—C7—N2	10.9 (2)
Na2—O7—C1—C2	−147.00 (13)	C3—N1—C2—C1	69.35 (18)
Na2—O9—C6—O10	−101.2 (3)	C4—N1—C2—C1	−171.66 (14)
Na2—O9—C6—C7	79.1 (3)	C5—N1—C2—C1	−52.64 (19)
O7—C1—C2—N1	111.67 (18)	C8—N2—C7—C6	56.0 (2)
O8—C1—C2—N1	−68.3 (2)	C9—N2—C7—C6	174.62 (15)
O9—C6—C7—N2	−169.32 (15)	C10—N2—C7—C6	−66.49 (19)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···I2^{i}	0.74 (3)	3.03 (3)	3.7008 (17)	152 (3)
O1—H1*B*···O3^{i}	0.78 (3)	2.01 (3)	2.781 (2)	172 (3)
O2—H2*A*···O9^{iii}	0.78 (3)	2.19 (3)	2.915 (2)	154 (3)
O2—H2*B*···O8^{iii}	0.76 (3)	2.00 (3)	2.7641 (19)	175 (3)
O3—H3*A*···O10^{iii}	0.80 (3)	1.99 (3)	2.772 (2)	169 (3)
O3—H3*B*···O8^{iv}	0.76 (3)	2.13 (3)	2.860 (2)	160 (3)
O4—H4*A*···I2	0.79 (3)	2.85 (3)	3.6300 (14)	172 (2)
O4—H4*B*···O10^{i}	0.81 (3)	2.04 (3)	2.823 (2)	165 (2)
O5—H5*A*···O8^{iv}	0.79 (3)	1.97 (3)	2.7484 (19)	167 (3)
O6—H6*A*···I1^{ii}	0.76 (3)	2.85 (3)	3.5864 (17)	165 (3)
O6—H6*B*···O7^{ii}	0.79 (3)	2.05 (3)	2.829 (2)	168 (3)
C8—H8*A*···O10	0.98	2.33	2.976 (2)	122
C3—H3*D*···O8	0.98	2.39	2.999 (2)	120
C10—H10*A*···O10	0.98	2.34	2.994 (2)	123

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