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Bis(μ-3-amino-5-carboxybenzoato-$\kappa^2O:O'$)bis[(5-aminoisophthalato)-triaquasodium(I)]

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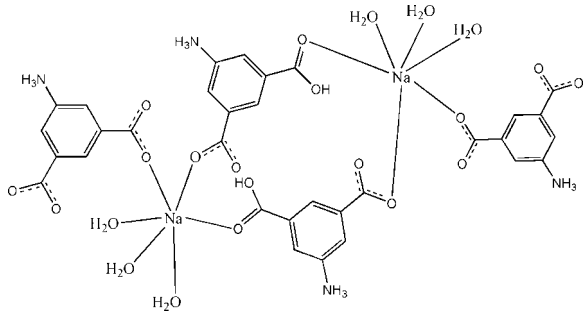
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.110; data-to-parameter ratio = 12.0.

In the title dinuclear complex, $[Na_2(C_8H_6NO_4)_2(C_8H_7NO_4)_2(H_2O)_6]$, which is located on a crystallographic inversion centre, each Na^+ cation is coordinated by three carboxylate O atoms from three isophthalate ligands and by three water molecules, displaying a distorted octahedral geometry. The separation in the centrosymmetric dinuclear complex is 10.251 (3) Å. Intra- and intermolecular N—H···O and O—H···O hydrogen bonds and π–π interactions (interplanar distance of about 3.43 Å) produce a supramolecular network.

Related literature

For related literature, see: Iglesias *et al.* (2003); Kim *et al.* (2003); Moulton & Zaworotko (2001).



Experimental

Crystal data

$[Na_2(C_8H_6NO_4)_2(C_8H_7NO_4)_2(H_2O)_6]$
M_r = 876.64
Triclinic, $P\overline{1}$
a = 8.1889 (3) Å
b = 8.8821 (3) Å
c = 12.6381 (5) Å
α = 95.251 (2)°
β = 98.649 (2)°
γ = 95.200 (2)°
V = 899.86 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 293 (2) K
0.19 × 0.16 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: none
11809 measured reflections
3506 independent reflections
2714 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.110
S = 1.06
3506 reflections
292 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Na1—O5	2.3520 (14)	Na1—O1*W*	2.4011 (16)
Na1—O2*W*	2.3535 (16)	Na1—O3*W*	2.4115 (15)
Na1—O1	2.3922 (14)	Na1—O3^{i}	2.4347 (15)
O5—Na1—O2*W*	110.25 (5)	O1—Na1—O3*W*	83.12 (5)
O5—Na1—O1	82.66 (5)	O1*W*—Na1—O3*W*	85.74 (5)
O2*W*—Na1—O1	166.86 (6)	O5—Na1—O3^{i}	97.80 (5)
O5—Na1—O1*W*	87.51 (5)	O2*W*—Na1—O3^{i}	85.57 (5)
O2*W*—Na1—O1*W*	87.97 (6)	O1—Na1—O3^{i}	90.33 (5)
O1—Na1—O1*W*	95.25 (6)	O1*W*—Na1—O3^{i}	172.76 (6)
O5—Na1—O3*W*	163.62 (6)	O3*W*—Na1—O3^{i}	90.36 (5)
O2*W*—Na1—O3*W*	84.43 (5)		

Symmetry code: (i) $-x, -y, -z+2$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*A*···O3*W*^{ii}	0.89	1.89	2.763 (2)	168
N1—H1*B*···O8^{iii}	0.89	1.93	2.810 (2)	170
N1—H1*C*···O4^{iv}	0.89	1.91	2.7808 (19)	165
N2—H2*A*···O7^{v}	0.89	1.94	2.8221 (18)	169
N2—H2*A*···O8^{v}	0.89	2.58	3.1815 (18)	126
N2—H2*B*···O3^{vi}	0.89	1.93	2.7981 (19)	165
N2—H2*C*···O8^{vii}	0.89	1.86	2.750 (2)	175
O2—H2···O5	0.82	1.73	2.5491 (17)	177
O1*W*—H1*W*···O4^{viii}	0.816 (9)	2.002 (10)	2.8150 (19)	175 (2)
O2*W*—H4*W*···O6^{iv}	0.818 (9)	2.024 (11)	2.8128 (19)	162 (2)
O3*W*—H6*W*···O1*W*^{ix}	0.829 (9)	1.977 (10)	2.778 (2)	162 (2)
O2*W*—H3*W*···O7	0.822 (9)	2.013 (10)	2.8322 (19)	174 (2)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2034).

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supplementary materials

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Bis(μ-3-amino-5-carboxybenzoato-$\kappa^2O:O'$)bis[(5-aminoisophthalato)triaquasodium(I)]

R.-H. Zeng, Z.-Q. Fang, F. Sun, L.-S. Jiang and Y.-W. Tang

Comment

Molecular self-assembly of supramolecular architectures has received much attention during recent decades (Kim *et al.*, 2003; Iglesias *et al.*, 2003; Moulton & Zaworotko, 2001). The structures and properties of such systems depend on the coordination and geometric preferences of both the central metals ions and bridging building blocks as well as the influence of weaker non-covalent interactions, such as hydrogen bonds and π-π stacking interactions.

As illustrated in Fig. 1, in the dinuclear centrosymmetric structure of (I) each Na^I centre is coordinated by three carboxyl O atoms from three 5-aminoisophthalato ligands, and three water molecules. In the distorted octahedral geometry each of the water molecules is located *trans* to a carboxyl O atom (Table 1). The Na···Na separation within the centrosymmetric dinuclear complex is 10.251 (3) Å, and the the two central 5-aminoisophthalato ligands are parallel to each other at a plane to plane distance of about 3.43 Å, thus indicating a π stacking interaction (Fig 1). The structure is further extended to a supramolecular network through intra and intermolecular N—H···O and O—H···O hydrogen bonding interactions (Fig 2., Table 2).

Experimental

The title complex was prepared by the addition of 5-aminoisophthalic acid to a hot aqueous solution. The pH was then adjusted to 7.0 to 8.0 with NaOH (0.1 mol/*L*). The resulting solution was filtered, and colourless crystals were obtained at room temperature on slow evaporation of the solvent over several days.

Refinement

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 Å, N—H = 0.96 Å and with U_{iso}(H) = 1.2 U_{eq}(C) and 1.5 U_{eq}(N). Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O–H = 0.82 Å and H···H = 1.29 Å, each within a standard deviation of 0.01 Å, and U_{iso}(H) = 1.5 U_{eq}(O).

Figures

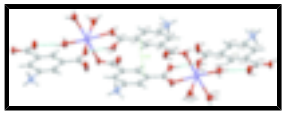


Fig. 1. The structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. Unlabelled atoms are related to the labelled atoms by the symmetry operator (−*x*, −*y*, 2 − *z*). Intramolecular hydrogen bonds are shown as blue dashed lines and the π-stacking interaction between the central 5-aminoisophthalato ligands is indicated as a dashed green line, connecting the centroid of the atoms C1 through C6 and O1 and O2 with that of their counterparts created by the inversion center.

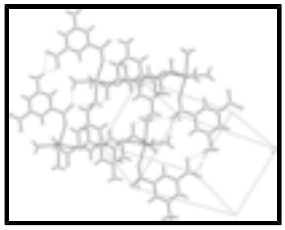


Fig. 2. View of the supramolecular network *via* intra and intermolecular hydrogen bonds. The hydrogen bonds are indicated as dashed lines.

Bis(μ-3-amino-5-carboxybenzoato-κ^2*O*:*O*')bis[(5- aminoisophthalato)triaquasodium(I)]

Crystal data

$[Na_2(C_8H_6NO_4)_2(C_8H_7NO_4)_2(H_2O)_6]$	$Z = 1$
$M_r = 876.64$	$F_{000} = 456$
Triclinic, $P\overline{1}$	$D_x = 1.618$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.1889$ (3) Å	Cell parameters from 3500 reflections
$b = 8.8821$ (3) Å	$\theta = 1.7$–26.0º
$c = 12.6381$ (5) Å	$\mu = 0.16$ mm^{-1}
$\alpha = 95.251$ (2)º	$T = 293$ (2) K
$\beta = 98.649$ (2)º	Block, colourless
$\gamma = 95.200$ (2)º	0.19 × 0.16 × 0.15 mm
$V = 899.86$ (6) Å^3	

Data collection

Bruker APEXII area-detector diffractometer	2714 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.029$
Monochromator: graphite	$\theta_{max} = 26.0$º
$T = 293(2)$ K	$\theta_{min} = 1.6$º
φ and ω scans	$h = -10\rightarrow10$
Absorption correction: none	$k = -10\rightarrow10$
11809 measured reflections	$l = -15\rightarrow14$
3506 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.110$	$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.2242P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
3506 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}

292 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
9 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.1175 (2)	0.2786 (2)	1.00350 (14)	0.0251 (4)
C2	0.0923 (2)	0.16994 (19)	1.08453 (14)	0.0233 (4)
C3	0.2264 (2)	0.0955 (2)	1.12436 (14)	0.0253 (4)
H3	0.3292	0.1168	1.1031	0.030*
C4	0.2060 (2)	−0.01048 (19)	1.19577 (14)	0.0241 (4)
C5	0.0531 (2)	−0.04674 (19)	1.22571 (14)	0.0242 (4)
H5	0.0403	−0.1214	1.2717	0.029*
C6	−0.0814 (2)	0.02815 (19)	1.18715 (14)	0.0230 (4)
C7	−0.0614 (2)	0.13772 (19)	1.11621 (14)	0.0237 (4)
H7	−0.1507	0.1890	1.0902	0.028*
C8	−0.2484 (2)	−0.0130 (2)	1.22114 (14)	0.0247 (4)
C9	−0.0748 (2)	0.5059 (2)	0.74424 (15)	0.0288 (4)
C10	−0.0515 (2)	0.60556 (19)	0.65623 (14)	0.0237 (4)
C11	−0.1875 (2)	0.6705 (2)	0.60714 (14)	0.0252 (4)
H11	−0.2909	0.6513	0.6279	0.030*
C12	−0.1679 (2)	0.76336 (19)	0.52771 (14)	0.0228 (4)
C13	−0.0155 (2)	0.79463 (19)	0.49608 (14)	0.0242 (4)
H13	−0.0042	0.8585	0.4427	0.029*
C14	0.12133 (19)	0.72997 (19)	0.54466 (14)	0.0234 (4)
C15	0.1019 (2)	0.63570 (19)	0.62487 (14)	0.0246 (4)
H15	0.1930	0.5924	0.6578	0.030*
C16	0.2881 (2)	0.7633 (2)	0.50918 (15)	0.0258 (4)
N1	0.34825 (17)	−0.08917 (17)	1.23537 (13)	0.0293 (4)
H1A	0.3487	−0.1741	1.1922	0.044*
H1B	0.3411	−0.1124	1.3017	0.044*
H1C	0.4417	−0.0291	1.2364	0.044*
N2	−0.31119 (17)	0.83326 (16)	0.47749 (12)	0.0264 (3)
H2A	−0.4044	0.7823	0.4892	0.040*
H2B	−0.3106	0.8305	0.4070	0.040*

H2C	−0.3056	0.9294	0.5058	0.040*
Na1	0.32524 (8)	0.39379 (8)	0.81767 (6)	0.0301 (2)
O1	0.25624 (15)	0.31616 (16)	0.98325 (11)	0.0368 (4)
O2	−0.01689 (14)	0.32523 (15)	0.95567 (11)	0.0339 (3)
H2	0.0044	0.3713	0.9052	0.051*
O3	−0.26498 (14)	−0.13253 (14)	1.26574 (11)	0.0322 (3)
O4	−0.36025 (15)	0.07342 (15)	1.20278 (12)	0.0395 (4)
O5	0.05126 (15)	0.45954 (16)	0.79542 (11)	0.0371 (4)
O6	−0.21793 (16)	0.4762 (2)	0.76354 (14)	0.0593 (5)
O7	0.40436 (15)	0.69099 (17)	0.54356 (12)	0.0427 (4)
O8	0.30116 (15)	0.86535 (14)	0.44630 (11)	0.0314 (3)
O1W	0.41376 (17)	0.65365 (16)	0.88767 (13)	0.0410 (4)
O2W	0.44720 (16)	0.44095 (16)	0.66516 (12)	0.0386 (4)
O3W	0.60029 (16)	0.34300 (16)	0.89387 (12)	0.0373 (4)
H1W	0.394 (2)	0.7293 (17)	0.8580 (17)	0.045*
H4W	0.5484 (12)	0.447 (2)	0.6801 (17)	0.045*
H6W	0.618 (2)	0.342 (2)	0.9601 (8)	0.045*
H3W	0.430 (2)	0.5095 (19)	0.6268 (16)	0.045*
H2W	0.5147 (12)	0.662 (2)	0.9063 (17)	0.045*
H5W	0.678 (2)	0.402 (2)	0.8828 (15)	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0227 (9)	0.0293 (9)	0.0253 (10)	0.0025 (7)	0.0064 (7)	0.0093 (8)
C2	0.0221 (8)	0.0267 (9)	0.0227 (9)	0.0019 (7)	0.0060 (7)	0.0081 (7)
C3	0.0188 (8)	0.0320 (10)	0.0272 (10)	0.0012 (7)	0.0080 (7)	0.0094 (8)
C4	0.0196 (8)	0.0292 (9)	0.0256 (10)	0.0062 (7)	0.0046 (7)	0.0088 (7)
C5	0.0244 (9)	0.0277 (9)	0.0232 (10)	0.0035 (7)	0.0064 (7)	0.0110 (7)
C6	0.0202 (8)	0.0265 (9)	0.0234 (10)	0.0012 (7)	0.0062 (7)	0.0064 (7)
C7	0.0198 (8)	0.0289 (9)	0.0250 (10)	0.0045 (7)	0.0057 (7)	0.0100 (7)
C8	0.0197 (8)	0.0336 (10)	0.0225 (10)	0.0017 (7)	0.0059 (7)	0.0096 (8)
C9	0.0228 (9)	0.0380 (11)	0.0288 (10)	0.0034 (7)	0.0068 (7)	0.0164 (8)
C10	0.0209 (8)	0.0285 (9)	0.0235 (10)	0.0023 (7)	0.0045 (7)	0.0114 (7)
C11	0.0165 (8)	0.0320 (9)	0.0298 (10)	0.0020 (7)	0.0081 (7)	0.0114 (8)
C12	0.0179 (8)	0.0266 (9)	0.0252 (10)	0.0052 (6)	0.0034 (7)	0.0080 (7)
C13	0.0226 (8)	0.0281 (9)	0.0251 (10)	0.0041 (7)	0.0071 (7)	0.0126 (7)
C14	0.0191 (8)	0.0293 (9)	0.0243 (10)	0.0037 (7)	0.0073 (7)	0.0093 (7)
C15	0.0188 (8)	0.0305 (9)	0.0270 (10)	0.0061 (7)	0.0040 (7)	0.0121 (8)
C16	0.0192 (8)	0.0327 (10)	0.0287 (10)	0.0041 (7)	0.0087 (7)	0.0104 (8)
N1	0.0208 (7)	0.0370 (9)	0.0346 (9)	0.0085 (6)	0.0090 (6)	0.0155 (7)
N2	0.0203 (7)	0.0315 (8)	0.0309 (9)	0.0071 (6)	0.0074 (6)	0.0131 (7)
Na1	0.0243 (4)	0.0364 (4)	0.0333 (4)	0.0055 (3)	0.0091 (3)	0.0139 (3)
O1	0.0230 (7)	0.0520 (9)	0.0403 (9)	0.0012 (6)	0.0096 (6)	0.0268 (7)
O2	0.0253 (7)	0.0444 (8)	0.0382 (9)	0.0081 (6)	0.0090 (6)	0.0269 (6)
O3	0.0261 (7)	0.0376 (8)	0.0378 (8)	0.0032 (5)	0.0111 (6)	0.0204 (6)
O4	0.0219 (7)	0.0433 (8)	0.0612 (10)	0.0099 (6)	0.0156 (6)	0.0261 (7)
O5	0.0241 (7)	0.0519 (9)	0.0415 (9)	0.0095 (6)	0.0062 (6)	0.0312 (7)

O6	0.0203 (7)	0.1007 (14)	0.0673 (11)	0.0035 (7)	0.0110 (7)	0.0613 (10)
O7	0.0201 (7)	0.0584 (9)	0.0607 (10)	0.0144 (6)	0.0170 (6)	0.0377 (8)
O8	0.0275 (7)	0.0370 (7)	0.0362 (8)	0.0061 (5)	0.0150 (6)	0.0191 (6)
O1W	0.0332 (7)	0.0402 (8)	0.0507 (10)	0.0047 (6)	0.0033 (7)	0.0152 (7)
O2W	0.0291 (7)	0.0446 (9)	0.0455 (9)	0.0031 (6)	0.0092 (6)	0.0189 (7)
O3W	0.0290 (7)	0.0459 (9)	0.0384 (9)	0.0006 (6)	0.0062 (6)	0.0148 (7)

Geometric parameters (Å, °)

C1—O1	1.225 (2)	C13—H13	0.9300
C1—O2	1.295 (2)	C14—C15	1.391 (2)
C1—C2	1.494 (2)	C14—C16	1.513 (2)
C2—C3	1.387 (2)	C15—H15	0.9300
C2—C7	1.391 (2)	C16—O7	1.243 (2)
C3—C4	1.378 (2)	C16—O8	1.267 (2)
C3—H3	0.9300	N1—H1A	0.8900
C4—C5	1.381 (2)	N1—H1B	0.8900
C4—N1	1.460 (2)	N1—H1C	0.8900
C5—C6	1.387 (2)	N2—H2A	0.8900
C5—H5	0.9300	N2—H2B	0.8900
C6—C7	1.397 (2)	N2—H2C	0.8900
C6—C8	1.518 (2)	Na1—O5	2.3520 (14)
C7—H7	0.9300	Na1—O2W	2.3535 (16)
C8—O3	1.253 (2)	Na1—O1	2.3922 (14)
C8—O4	1.256 (2)	Na1—O1W	2.4011 (16)
C9—O6	1.242 (2)	Na1—O3W	2.4115 (15)
C9—O5	1.257 (2)	Na1—O3^{i}	2.4347 (15)
C9—C10	1.507 (2)	O2—H2	0.8200
C10—C15	1.384 (2)	O3—Na1^{i}	2.4347 (15)
C10—C11	1.390 (2)	O1W—H1W	0.816 (9)
C11—C12	1.374 (2)	O1W—H2W	0.819 (9)
C11—H11	0.9300	O2W—H4W	0.818 (9)
C12—C13	1.379 (2)	O2W—H3W	0.822 (9)
C12—N2	1.465 (2)	O3W—H6W	0.829 (9)
C13—C14	1.391 (2)	O3W—H5W	0.824 (9)
O1—C1—O2	123.59 (16)	C14—C15—H15	119.6
O1—C1—C2	121.24 (15)	O7—C16—O8	123.72 (15)
O2—C1—C2	115.14 (14)	O7—C16—C14	118.79 (15)
C3—C2—C7	120.26 (15)	O8—C16—C14	117.48 (15)
C3—C2—C1	117.75 (15)	C4—N1—H1A	109.5
C7—C2—C1	121.93 (15)	C4—N1—H1B	109.5
C4—C3—C2	119.41 (15)	H1A—N1—H1B	109.5
C4—C3—H3	120.3	C4—N1—H1C	109.5
C2—C3—H3	120.3	H1A—N1—H1C	109.5
C3—C4—C5	121.02 (15)	H1B—N1—H1C	109.5
C3—C4—N1	118.45 (14)	C12—N2—H2A	109.5
C5—C4—N1	120.47 (15)	C12—N2—H2B	109.5
C4—C5—C6	119.98 (15)	H2A—N2—H2B	109.5

C4—C5—H5	120.0	C12—N2—H2C	109.5
C6—C5—H5	120.0	H2A—N2—H2C	109.5
C5—C6—C7	119.47 (15)	H2B—N2—H2C	109.5
C5—C6—C8	119.25 (15)	O5—Na1—O2W	110.25 (5)
C7—C6—C8	121.27 (15)	O5—Na1—O1	82.66 (5)
C2—C7—C6	119.81 (16)	O2W—Na1—O1	166.86 (6)
C2—C7—H7	120.1	O5—Na1—O1W	87.51 (5)
C6—C7—H7	120.1	O2W—Na1—O1W	87.97 (6)
O3—C8—O4	124.40 (16)	O1—Na1—O1W	95.25 (6)
O3—C8—C6	117.05 (15)	O5—Na1—O3W	163.62 (6)
O4—C8—C6	118.55 (15)	O2W—Na1—O3W	84.43 (5)
O6—C9—O5	123.50 (16)	O1—Na1—O3W	83.12 (5)
O6—C9—C10	118.04 (15)	O1W—Na1—O3W	85.74 (5)
O5—C9—C10	118.45 (15)	O5—Na1—O3^{i}	97.80 (5)
C15—C10—C11	119.60 (15)	O2W—Na1—O3^{i}	85.57 (5)
C15—C10—C9	121.63 (15)	O1—Na1—O3^{i}	90.33 (5)
C11—C10—C9	118.76 (15)	O1W—Na1—O3^{i}	172.76 (6)
C12—C11—C10	119.53 (15)	O3W—Na1—O3^{i}	90.36 (5)
C12—C11—H11	120.2	C1—O1—Na1	127.35 (12)
C10—C11—H11	120.2	C1—O2—H2	109.5
C11—C12—C13	121.37 (15)	C8—O3—Na1^{i}	128.48 (12)
C11—C12—N2	119.21 (14)	C9—O5—Na1	154.20 (12)
C13—C12—N2	119.40 (15)	Na1—O1W—H1W	127.1 (16)
C12—C13—C14	119.52 (15)	Na1—O1W—H2W	108.1 (14)
C12—C13—H13	120.2	H1W—O1W—H2W	105.5 (13)
C14—C13—H13	120.2	Na1—O2W—H4W	110.2 (15)
C15—C14—C13	119.26 (15)	Na1—O2W—H3W	126.7 (15)
C15—C14—C16	121.28 (15)	H4W—O2W—H3W	104.3 (13)
C13—C14—C16	119.45 (15)	Na1—O3W—H6W	115.8 (15)
C10—C15—C14	120.72 (15)	Na1—O3W—H5W	116.8 (15)
C10—C15—H15	119.6	H6W—O3W—H5W	102.8 (13)

Symmetry codes: (i) −*x*, −*y*, −*z*+2.

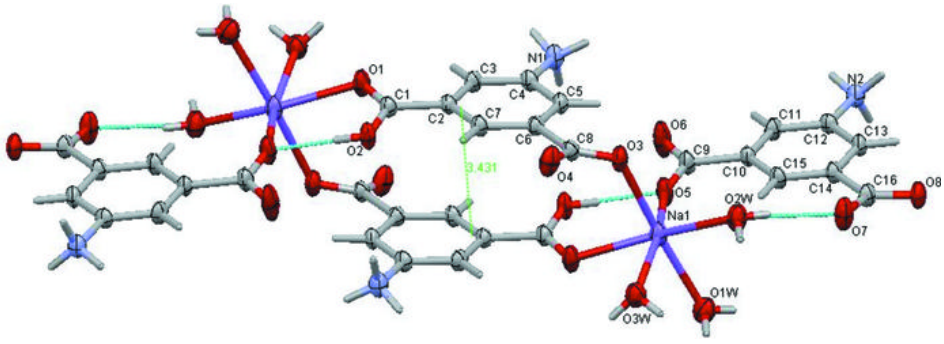
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O3W^{ii}	0.89	1.89	2.763 (2)	168
N1—H1B···O8^{iii}	0.89	1.93	2.810 (2)	170
N1—H1C···O4^{iv}	0.89	1.91	2.7808 (19)	165
N2—H2A···O7^{v}	0.89	1.94	2.8221 (18)	169
N2—H2A···O8^{v}	0.89	2.58	3.1815 (18)	126
N2—H2B···O3^{vi}	0.89	1.93	2.7981 (19)	165
N2—H2C···O8^{vii}	0.89	1.86	2.750 (2)	175
O2—H2···O5	0.82	1.73	2.5491 (17)	177
O1W—H1W···O4^{viii}	0.816 (9)	2.002 (10)	2.8150 (19)	175 (2)
O2W—H4W···O6^{iv}	0.818 (9)	2.024 (11)	2.8128 (19)	162 (2)

O3W—H6W···O1W^{ix}	0.829 (9)	1.977 (10)	2.778 (2)	162 (2)
O2W—H3W···O7	0.822 (9)	2.013 (10)	2.8322 (19)	174 (2)

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

Fig. 1


O1
C1
C2
C3
N1
C4
C5
C7
C6
C8
O2
O4
O3
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C9
C10
C11
C12
C13
N2
C15
C14
C16
O8
O5
Na1
O2W
O7
O1W
O3W

Fig. 2