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catena-Poly[[[tetra-μ_2-aqua-heptaaqua-(μ_2-benzene-1,3,5-tricarboxylato)-μ_3-hydroxido-trinickel(II)sodium]-μ_4-benzene-1,3,5-tricarboxylato] sesquihydrate]

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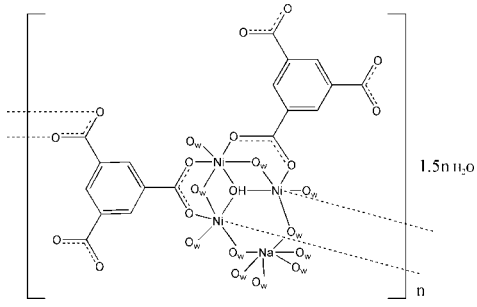
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.010 Å; disorder in solvent or counterion; R factor = 0.057; wR factor = 0.127; data-to-parameter ratio = 15.1.

The title coordination polymer, $\{[Ni_3Na(OH)(C_9H_3O_6)_2(H_2O)_{11}]\cdot 1.5H_2O\}_n$, is built up from three independent Ni^{II} ions and one Na^{I} cation bridged by benzene-2,4,6-tricarboxylate (BTC) ligands and water molecules. Three Ni^{II} ions are bridged by three bidentate carboxylate groups of three BTC ligands, two aqua ligands and one OH^- unit, to form a trinuclear metal cluster. The Na^{I} cation is bonded to the Ni^{II} cluster by two bridging water molecules. One of the three BTC ligands bridges neighbouring clusters into one-dimensional chains, which are further connected through a complex hydrogen-bonding scheme, forming a three-dimensional suprastructure. The title complex is isomorphous with the previously reported Co^{II} complex.

Related literature

For related literature, see: Guo *et al.* (2006) Yaghi *et al.* (1996); Wei & Han (2005); Eddaoudi *et al.* (2001); Cheng *et al.* (2004).



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Experimental

Crystal data

$[Ni_3Na(OH)(C_9H_3O_6)_2(H_2O)_{11}]\cdot 1.5H_2O$
M_r = 855.56
Orthorhombic, *Pbca*
a = 18.842 (5) Å
b = 14.557 (4) Å
c = 21.343 (6) Å
V = 5854 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.03 mm^{-1}
T = 293 (2) K
0.18 × 0.12 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1995)
T_{min} = 0.712, T_{max} = 0.820
43629 measured reflections
6693 independent reflections
2994 reflections with $I > 2\sigma(I)$
R_{int} = 0.133

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.127
S = 0.89
6693 reflections
442 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O8W	0.98	1.83	2.807 (7)	173
O1W—H1WA···O13^{i}	0.97	1.90	2.797 (8)	152
O1W—H1WB···O16^{ii}	0.97	1.70	2.596 (7)	152
O2W—H2WB···O10W^{iii}	0.82	1.99	2.752 (9)	155
O4W—H4B···O15^{iv}	0.82	2.28	3.049 (8)	157
O4W—H4A···O24^{v}	0.72	2.04	2.757 (7)	174
O5W—H5WA···O16^{v}	0.82	2.03	2.818 (8)	160
O5W—H5WB···O13^{iv}	0.97	1.88	2.772 (7)	151
O7W—H7WA···O14^{vi}	0.82	2.10	2.841 (8)	150
O7W—H7WB···O24^{v}	0.82	1.96	2.778 (8)	174
O8W—H8WA···O11^{v}	0.82	2.07	2.821 (8)	153
O9W—H9WA···O16^{v}	0.82	2.12	2.909 (10)	162
O9W—H9WB···O23^{iii}	0.82	2.32	3.062 (9)	150
O10W—H10B···O15^{i}	0.84	2.14	2.981 (10)	177
O11W—H11A···O15^{ii}	0.97	1.71	2.659 (7)	166
O11W—H11B···O24^{vii}	0.97	1.74	2.693 (6)	165
O13W—H13A···O14^{viii}	0.82	1.99	2.79 (2)	168

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, z$; (iv) $-x+\frac{1}{2}, -y+2, z+\frac{1}{2}$; (v) $-x+1, -y+2, -z$; (vi) $-x+\frac{1}{2}, y+\frac{1}{2}, z$; (vii) $x-\frac{1}{2}, -y+\frac{3}{2}, -z$; (viii) $x+\frac{1}{2}, y, -z+\frac{1}{2}$.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994) and *XPREP* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2098).

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supplementary materials

Acta Cryst. (2007). E**63**, m1921-m1922 [**doi:10.1107/S1600536807026359**]

catena-Poly[[[tetra-μ_2-aqua-heptaaqua(μ_2-benzene-1,3,5-tricarboxylato)-μ_3-hydroxido-trinickel(II)sodium]-μ_4-benzene-1,3,5-tricarboxylato] sesquihydrate]

Y. Yan, W.-H. Li and B.-R. Hou

Comment

Benzenetricarboxylate (BTC) ligands are universal bridging ligands in the construction of a number of coordination networks (Yaghi *et al.*, 1996; Wei & Han, 2005; Guo *et al.*, 2006; Eddaoudi *et al.*, 2001). In this paper, we present the synthesis and structural characterization of a new coordination polymer of trinuclear Ni^{II} units bridged by BTC ligands, $\{[Ni_3Na(OH)(C_9H_3O_6)_2(H_2O)_{11}]\cdot 1.5H_2O\}_n$, (I), which was synthesized by the reaction of nickel(II) salt with H_3BTC in basic conditions. The title compound is isomorphous with the Co^{II} complex published by Cheng *et al.* (2004).

As shown in Fig. 1, the asymmetric unit contains three crystallographically independent Ni^{II} centers, which are all octahedrally coordinated by six O atoms, which are from two BTC carboxylate groups, one OH^- unit and three aqua ligands (Table 2). The three Ni^{II} ions are bridged by three bidentate carboxylates of three BTC ligands, two aqua ligands and one OH^- anion, to form a new trinuclear metal cluster. The Na^I ion is coordinated by six water molecules, and the distorted octahedron is attached to the trinuclear unit though two bridging aqua ligands.

The BTC ligands exhibit two different coordination modes in (I). In the first one, the BTC ligand acts as a bidentate ligand bridging two Ni^{II} centers, while another one acts as a tetradentate ligand linking four Ni^{II} centers of neighboring trinuclear units to form a one-dimensional zigzag chain (Fig. 2). The chains are further connected into a three-dimensional framework through a complex hydrogen bonding scheme involving water molecules and carboxylate groups of BTC (Table 3 and Fig. 3). The hydrogen bonds D···A separations range from 2.597 to 3.437 Å.

Experimental

An aqueous solution (20 ml) of benzene-1,3,5-tricarboxylic acid (H_3BTC) (0.96 g, 0.5 mmol) and NaOH (0.04 g, 1 mmol) was added into an aqueous solution (10 ml) of $Ni(CH_3CO_2)_2\cdot 2H_2O$ (0.12 g, 0.5 mmol) under stirring. The resulting solution was filtered and a solution of 4,4'-bipy (0.05 g, 0.5 mmol in 15 ml e thanol) was added dropwise. After 15 days, green crystals suitable for X-ray single-crystal diffraction studies were collected by filtration and washed with ethanol. Yield: 68%.

Refinement

A lattice water molecule with occupancy 1/2 is disordered over two sites, O13w and O14w, with 1/4 occupancy for each. The C-bonded H atoms were placed geometrically and refined with C—H bond lengths constrained to 0.93 Å and U_{iso}(H) = 1.2U_{eq}(carrier C). H atoms of water molecules and hydroxy group were clearly visible in a difference map, and were included in the refinement as riding atoms after regularizing some bond lengths [O—H in the range 0.82 to 0.97 Å] and with fixed isotropic displacement parameters: U_{iso}(H) = 1.2U_{eq}(carrier O).

Figures

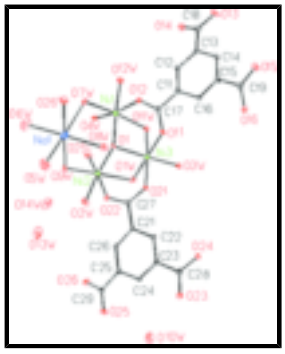

Fig. 1. *ORTEP*like representation of the symmetry expanded local structure for (I) (25% probability ellipsoids).

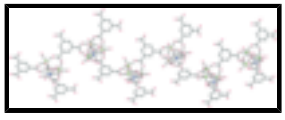

Fig. 2. The one-dimensional zigzag chain of the trinuclear Ni^{II} units bridged by the BTC ligands.

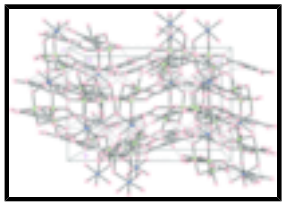

Fig. 3. Crystal packing diagram of (I) viewed down the [100] axis, showing the complex hydrogen bonding.

catena-Poly[[[tetra-μ_2-aqua-heptaaqua(μ_2-benzene-1,3,5-tricarboxylato)- μ_3-hydroxido-trinickel(II)sodium]-μ_4-benzene-1,3,5-tricarboxylato] sesquihydrate]

Crystal data

$[Ni_3Na(OH)(C_9H_3O_6)_2(H_2O)_{11}]\cdot 1.5H_2O$	F_{000} = 3472
M_r = 855.56	D_x = 1.921 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	θ = 3.2–27.5º
a = 18.842 (5) Å	μ = 2.03 mm^{-1}
b = 14.557 (4) Å	*T* = 293 (2) K
c = 21.343 (6) Å	Prism, green
V = 5854 (3) Å^3	0.18 × 0.12 × 0.10 mm
Z = 8	

Data collection

Siemens SMART CCD area-detector diffractometer	6693 independent reflections
Radiation source: fine-focus sealed tube	2994 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.133
T = 293(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 3.2º
Absorption correction: multi-scan	*h* = −24→17

(SADABS; Sheldrick, 1995)

T_{min} = 0.712, T_{max} = 0.820

43629 measured reflections

k = −18→18

l = −27→27

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.057

$wR(F^2)$ = 0.127

S = 0.89

6693 reflections

442 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0069P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.003

$\Delta\rho_{max}$ = 0.67 e Å^{-3}

$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni1	0.30004 (5)	0.96049 (7)	0.12261 (4)	0.0209 (2)	
Ni2	0.46166 (5)	0.96371 (7)	0.21056 (4)	0.0221 (2)	
Ni3	0.43621 (5)	0.85216 (7)	0.09272 (4)	0.0203 (2)	
Na1	0.4108 (2)	1.2046 (2)	0.12750 (16)	0.0479 (10)	
O1	0.4066 (2)	0.9715 (3)	0.1299 (2)	0.0177 (11)	
H1A	0.4240	1.0227	0.1043	0.021*	
O1W	0.4691 (3)	0.8171 (3)	0.1864 (2)	0.0231 (12)	
H1WA	0.5168	0.7924	0.1890	0.028*	
H1WB	0.4356	0.7785	0.2088	0.028*	
O2W	0.5213 (3)	0.9412 (4)	0.2905 (2)	0.0386 (16)	
H2WB	0.5444	0.9874	0.2987	0.046*	
H2WA	0.4947	0.9292	0.3198	0.046*	
O3W	0.4550 (3)	0.7222 (3)	0.0684 (2)	0.0298 (13)	
H3WB	0.4190	0.6916	0.0737	0.036*	
H3WA	0.4961	0.7169	0.0563	0.036*	
O4W	0.2878 (3)	1.1036 (3)	0.1260 (2)	0.0302 (14)	
H4B	0.2642	1.1176	0.1568	0.036*	
H4A	0.2685	1.1279	0.1019	0.036*	
O5W	0.4611 (3)	1.1076 (3)	0.2207 (2)	0.0246 (13)	
H5WA	0.5016	1.1258	0.2271	0.030*	
H5WB	0.4339	1.1225	0.2579	0.030*	
O6W	0.3608 (4)	1.2973 (5)	0.2047 (3)	0.072 (2)	
H6WA	0.3423	1.3423	0.1883	0.087*	
H6WB	0.3846	1.2941	0.2368	0.087*	
O7W	0.3552 (3)	1.2859 (4)	0.0450 (2)	0.0418 (16)	
H7WA	0.3798	1.2827	0.0134	0.050*	
H7WB	0.3161	1.2630	0.0383	0.050*	

O8W	0.4635 (3)	1.1087 (4)	0.0522 (2)	0.0359 (15)
H8WB	0.4396	1.1093	0.0201	0.043*
H8WA	0.5037	1.1268	0.0445	0.043*
O9W	0.5163 (4)	1.2981 (5)	0.1248 (3)	0.087 (3)
H9WA	0.5434	1.2818	0.1527	0.105*
H9WB	0.5359	1.2926	0.0907	0.105*
O10W	0.9046 (4)	0.5735 (5)	0.3553 (3)	0.081 (3)
H10A	0.8738	0.5572	0.3800	0.097*
H10B	0.8799	0.6114	0.3355	0.097*
O11	0.4002 (3)	0.8816 (4)	0.0019 (2)	0.0244 (13)
O11W	0.3286 (3)	0.8147 (3)	0.1170 (2)	0.0216 (12)
H11A	0.3248	0.7825	0.1567	0.026*
H11B	0.3040	0.7817	0.0841	0.026*
O12	0.3000 (3)	0.9568 (4)	0.0280 (2)	0.0255 (12)
O12W	0.1917 (3)	0.9377 (4)	0.1137 (2)	0.0382 (15)
H12B	0.1780	0.9051	0.1426	0.046*
H12C	0.1826	0.9074	0.0746	0.046*
O13	0.0850 (3)	0.8013 (4)	−0.1728 (2)	0.0396 (16)
O14	0.0847 (3)	0.8387 (4)	−0.0716 (2)	0.0366 (15)
O15	0.3123 (3)	0.7961 (4)	−0.2849 (2)	0.0501 (19)
O16	0.4126 (3)	0.7897 (4)	−0.2299 (2)	0.0346 (15)
O21	0.5430 (3)	0.8863 (3)	0.0806 (2)	0.0200 (11)
O22	0.5552 (3)	0.9755 (3)	0.1659 (2)	0.0225 (12)
O23	0.8758 (3)	0.8365 (4)	0.0208 (2)	0.0412 (17)
O24	0.7754 (3)	0.7999 (3)	−0.0298 (2)	0.0241 (13)
O25	0.8776 (3)	0.9416 (4)	0.2330 (2)	0.0346 (15)
O26	0.7764 (3)	0.9579 (4)	0.2863 (2)	0.0328 (14)
C11	0.3022 (4)	0.8840 (5)	−0.0699 (3)	0.0214 (17)
C12	0.2288 (4)	0.8807 (5)	−0.0723 (3)	0.0202 (17)
H12A	0.2027	0.9008	−0.0379	0.024*
C13	0.1934 (4)	0.8482 (5)	−0.1249 (3)	0.0220 (17)
C14	0.2331 (4)	0.8259 (5)	−0.1778 (3)	0.0243 (18)
H14A	0.2100	0.8074	−0.2142	0.029*
C15	0.3057 (5)	0.8311 (5)	−0.1770 (3)	0.0244 (18)
C16	0.3418 (4)	0.8565 (5)	−0.1224 (3)	0.0231 (17)
H16A	0.3911	0.8552	−0.1209	0.028*
C17	0.3378 (5)	0.9104 (5)	−0.0088 (3)	0.0238 (18)
C18	0.1150 (5)	0.8302 (6)	−0.1236 (4)	0.030 (2)
C19	0.3468 (5)	0.8048 (5)	−0.2348 (4)	0.032 (2)
C21	0.6585 (4)	0.9124 (4)	0.1226 (3)	0.0140 (15)
C22	0.6952 (4)	0.8773 (5)	0.0710 (3)	0.0198 (17)
H22A	0.6701	0.8592	0.0356	0.024*
C23	0.7686 (4)	0.8689 (5)	0.0717 (3)	0.0173 (16)
C24	0.8055 (4)	0.8929 (4)	0.1251 (3)	0.0170 (16)
H24A	0.8547	0.8884	0.1255	0.020*
C25	0.7701 (4)	0.9238 (5)	0.1788 (3)	0.0188 (17)
C26	0.6972 (4)	0.9336 (5)	0.1762 (3)	0.0182 (16)
H26A	0.6733	0.9550	0.2114	0.022*
C27	0.5799 (4)	0.9255 (5)	0.1228 (3)	0.0183 (16)

C28	0.8090 (5)	0.8336 (5)	0.0160 (3)	0.0253 (19)	
C29	0.8120 (4)	0.9432 (5)	0.2376 (3)	0.0231 (18)	
O13W	0.5621 (14)	0.9796 (16)	0.4849 (11)	0.071 (7)	0.25
H13A	0.5628	0.9379	0.5108	0.086*	0.25
H13B	0.5850	0.9712	0.4574	0.086*	0.25
O14W	0.4786 (16)	0.975 (2)	0.4410 (12)	0.088 (9)	0.25
H14B	0.4782	0.9293	0.4187	0.105*	0.25
H14C	0.5106	0.9997	0.4106	0.105*	0.25

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0187 (6)	0.0275 (5)	0.0165 (5)	0.0014 (5)	0.0001 (4)	−0.0005 (4)
Ni2	0.0183 (6)	0.0295 (6)	0.0186 (5)	−0.0004 (5)	0.0007 (4)	−0.0014 (4)
Ni3	0.0170 (5)	0.0255 (5)	0.0184 (5)	−0.0001 (5)	−0.0008 (4)	−0.0022 (4)
Na1	0.049 (3)	0.055 (2)	0.040 (2)	0.015 (2)	−0.0016 (19)	−0.0046 (18)
O1	0.015 (3)	0.023 (3)	0.016 (2)	−0.002 (2)	−0.005 (2)	0.000 (2)
O1W	0.018 (3)	0.025 (3)	0.026 (3)	−0.002 (2)	0.000 (2)	0.007 (2)
O2W	0.040 (4)	0.053 (4)	0.022 (3)	−0.008 (3)	−0.006 (3)	0.000 (3)
O3W	0.016 (3)	0.033 (3)	0.041 (3)	−0.004 (3)	−0.002 (3)	−0.008 (2)
O4W	0.038 (4)	0.027 (3)	0.026 (3)	0.016 (3)	0.001 (3)	−0.001 (2)
O5W	0.018 (3)	0.030 (3)	0.026 (3)	−0.004 (3)	0.004 (2)	−0.011 (2)
O6W	0.100 (7)	0.070 (5)	0.047 (4)	0.024 (5)	0.022 (4)	0.013 (4)
O7W	0.035 (4)	0.055 (4)	0.035 (3)	0.002 (3)	0.003 (3)	−0.008 (3)
O8W	0.027 (4)	0.053 (4)	0.027 (3)	−0.008 (3)	0.003 (3)	0.007 (3)
O9W	0.066 (6)	0.111 (7)	0.085 (5)	−0.013 (5)	0.012 (5)	−0.043 (5)
O10W	0.092 (7)	0.067 (5)	0.083 (6)	−0.010 (5)	0.021 (5)	−0.011 (4)
O11	0.017 (3)	0.041 (3)	0.015 (3)	0.001 (3)	−0.004 (2)	−0.003 (2)
O11W	0.025 (3)	0.020 (3)	0.021 (3)	−0.002 (2)	−0.002 (2)	−0.001 (2)
O12	0.027 (3)	0.031 (3)	0.018 (3)	0.009 (3)	−0.003 (2)	−0.003 (2)
O12W	0.025 (4)	0.056 (4)	0.034 (3)	−0.004 (3)	0.001 (3)	−0.009 (3)
O13	0.026 (4)	0.066 (4)	0.027 (3)	−0.011 (3)	−0.008 (3)	0.014 (3)
O14	0.021 (3)	0.050 (4)	0.039 (3)	−0.004 (3)	0.003 (3)	−0.002 (3)
O15	0.048 (5)	0.081 (5)	0.021 (3)	0.018 (4)	−0.012 (3)	−0.014 (3)
O16	0.030 (4)	0.045 (4)	0.029 (3)	0.006 (3)	0.005 (3)	−0.013 (3)
O21	0.012 (3)	0.027 (3)	0.021 (3)	−0.003 (2)	0.000 (2)	−0.004 (2)
O22	0.017 (3)	0.029 (3)	0.021 (3)	−0.002 (2)	0.006 (2)	−0.007 (2)
O23	0.019 (3)	0.068 (5)	0.037 (3)	−0.001 (3)	0.007 (3)	−0.024 (3)
O24	0.027 (3)	0.029 (3)	0.017 (3)	0.003 (3)	−0.002 (2)	−0.007 (2)
O25	0.020 (3)	0.064 (4)	0.020 (3)	0.000 (3)	−0.005 (3)	−0.004 (3)
O26	0.023 (3)	0.059 (4)	0.017 (3)	0.009 (3)	0.002 (2)	−0.003 (3)
C11	0.019 (4)	0.027 (4)	0.018 (4)	−0.007 (4)	0.001 (3)	0.005 (3)
C12	0.020 (5)	0.027 (4)	0.014 (3)	0.000 (3)	0.001 (3)	0.000 (3)
C13	0.019 (4)	0.023 (4)	0.024 (4)	0.005 (4)	0.000 (4)	0.004 (3)
C14	0.025 (5)	0.022 (4)	0.025 (4)	−0.003 (4)	−0.010 (4)	0.001 (3)
C15	0.032 (5)	0.026 (4)	0.015 (4)	−0.004 (4)	−0.002 (4)	−0.004 (3)
C16	0.020 (5)	0.026 (4)	0.023 (4)	0.000 (4)	−0.006 (3)	−0.001 (3)
C17	0.030 (5)	0.021 (4)	0.021 (4)	−0.007 (4)	0.003 (4)	0.001 (3)

C18	0.024 (5)	0.041 (5)	0.024 (4)	−0.004 (4)	0.002 (4)	0.008 (4)
C19	0.042 (6)	0.026 (5)	0.027 (4)	0.006 (4)	0.006 (4)	−0.003 (4)
C21	0.011 (4)	0.016 (4)	0.015 (3)	0.005 (3)	0.000 (3)	−0.002 (3)
C22	0.016 (4)	0.024 (4)	0.019 (4)	0.003 (3)	−0.002 (3)	−0.003 (3)
C23	0.012 (4)	0.023 (4)	0.017 (3)	−0.004 (3)	0.000 (3)	0.005 (3)
C24	0.015 (4)	0.020 (4)	0.015 (3)	0.003 (3)	−0.005 (3)	−0.004 (3)
C25	0.025 (5)	0.019 (4)	0.012 (3)	0.000 (3)	0.000 (3)	0.000 (3)
C26	0.015 (4)	0.026 (4)	0.013 (3)	−0.004 (3)	0.008 (3)	−0.001 (3)
C27	0.017 (4)	0.025 (4)	0.013 (3)	−0.006 (3)	0.004 (3)	0.004 (3)
C28	0.026 (5)	0.031 (5)	0.019 (4)	−0.001 (4)	0.011 (4)	−0.001 (3)
C29	0.021 (5)	0.022 (4)	0.027 (4)	0.000 (4)	−0.006 (4)	0.001 (3)
O13W	0.127 (19)	0.028 (17)	0.059 (16)	−0.004 (15)	0.020 (15)	0.029 (13)
O14W	0.08 (3)	0.03 (2)	0.16 (2)	−0.005 (19)	0.038 (18)	0.035 (17)

Geometric parameters (Å, °)

Ni1—O26^{i}	1.995 (5)	O11W—H11A	0.9700
Ni1—O12	2.021 (4)	O11W—H11B	0.9700
Ni1—O1	2.021 (5)	O12—C17	1.257 (8)
Ni1—O12W	2.077 (5)	O12W—H12B	0.8200
Ni1—O4W	2.098 (5)	O12W—H12C	0.9595
Ni1—O11W	2.193 (5)	O13—C18	1.265 (9)
Ni2—O22	2.011 (5)	O14—C18	1.253 (8)
Ni2—O1	2.013 (4)	O15—C19	1.260 (9)
Ni2—O25^{i}	2.016 (5)	O16—C19	1.263 (10)
Ni2—O2W	2.069 (5)	O21—C27	1.273 (8)
Ni2—O5W	2.106 (5)	O22—C27	1.262 (8)
Ni2—O1W	2.200 (5)	O23—C28	1.262 (9)
Ni3—O1	1.989 (5)	O24—C28	1.265 (8)
Ni3—O3W	1.993 (5)	O25—C29	1.241 (9)
Ni3—O21	2.088 (5)	O25—Ni2^{ii}	2.016 (5)
Ni3—O11	2.099 (5)	O26—C29	1.255 (8)
Ni3—O1W	2.155 (4)	O26—Ni1^{ii}	1.995 (5)
Ni3—O11W	2.162 (5)	C11—C12	1.385 (10)
Na1—O6W	2.329 (7)	C11—C16	1.403 (10)
Na1—O8W	2.348 (6)	C11—C17	1.516 (10)
Na1—O7W	2.367 (6)	C12—C13	1.388 (9)
Na1—O9W	2.410 (8)	C12—H12A	0.9300
Na1—O5W	2.616 (6)	C13—C14	1.394 (10)
Na1—O4W	2.744 (7)	C13—C18	1.500 (10)
O1—H1A	0.9800	C14—C15	1.370 (11)
O1W—H1WA	0.9700	C14—H14A	0.9300
O1W—H1WB	0.9700	C15—C16	1.401 (9)
O2W—H2WB	0.8200	C15—C19	1.505 (10)
O2W—H2WA	0.8201	C16—H16A	0.9300
O3W—H3WB	0.8200	C21—C26	1.392 (9)
O3W—H3WA	0.8201	C21—C22	1.397 (9)
O4W—H4B	0.8200	C21—C27	1.494 (10)

O4W—H4A	0.7223	C22—C23	1.389 (10)
O5W—H5WA	0.8200	C22—H22A	0.9300
O5W—H5WB	0.9699	C23—C24	1.379 (9)
O6W—H6WA	0.8200	C23—C28	1.502 (9)
O6W—H6WB	0.8194	C24—C25	1.400 (9)
O7W—H7WA	0.8200	C24—H24A	0.9300
O7W—H7WB	0.8199	C25—C26	1.382 (10)
O8W—H8WB	0.8200	C25—C29	1.510 (9)
O8W—H8WA	0.8200	C26—H26A	0.9300
O9W—H9WA	0.8200	O13W—O14W	1.83 (4)
O9W—H9WB	0.8197	O13W—H13A	0.8200
O10W—H10A	0.8200	O13W—H13B	0.7389
O10W—H10B	0.8363	O14W—H14B	0.8200
O11—C17	1.267 (9)	O14W—H14C	0.9557
O26^{i}—Ni1—O12	166.8 (2)	H5WA—O5W—H5WB	106.5
O26^{i}—Ni1—O1	98.6 (2)	Na1—O6W—H6WA	108.9
O12—Ni1—O1	94.5 (2)	Na1—O6W—H6WB	109.6
O26^{i}—Ni1—O12W	82.3 (2)	H6WA—O6W—H6WB	129.8
O12—Ni1—O12W	84.5 (2)	Na1—O7W—H7WA	109.4
O1—Ni1—O12W	175.3 (2)	Na1—O7W—H7WB	108.9
O26^{i}—Ni1—O4W	87.7 (2)	H7WA—O7W—H7WB	109.9
O12—Ni1—O4W	93.5 (2)	Na1—O8W—H8WB	109.5
O1—Ni1—O4W	91.6 (2)	Na1—O8W—H8WA	109.7
O12W—Ni1—O4W	93.1 (2)	H8WB—O8W—H8WA	109.6
O26^{i}—Ni1—O11W	95.1 (2)	Na1—O9W—H9WA	109.5
O12—Ni1—O11W	85.39 (19)	Na1—O9W—H9WB	109.8
O1—Ni1—O11W	80.59 (18)	H9WA—O9W—H9WB	109.7
O12W—Ni1—O11W	94.7 (2)	H10A—O10W—H10B	97.0
O4W—Ni1—O11W	172.0 (2)	C17—O11—Ni3	122.3 (5)
O22—Ni2—O1	92.37 (19)	Ni3—O11W—Ni1	89.96 (17)
O22—Ni2—O25^{i}	170.2 (2)	Ni3—O11W—H11A	113.7
O1—Ni2—O25^{i}	96.6 (2)	Ni1—O11W—H11A	113.7
O22—Ni2—O2W	85.9 (2)	Ni3—O11W—H11B	113.6
O1—Ni2—O2W	173.7 (2)	Ni1—O11W—H11B	113.6
O25^{i}—Ni2—O2W	84.7 (2)	H11A—O11W—H11B	110.9
O22—Ni2—O5W	88.2 (2)	C17—O12—Ni1	129.7 (5)
O1—Ni2—O5W	91.67 (19)	Ni1—O12W—H12B	109.4
O25^{i}—Ni2—O5W	95.4 (2)	Ni1—O12W—H12C	109.2
O2W—Ni2—O5W	94.4 (2)	H12B—O12W—H12C	109.4
O22—Ni2—O1W	85.17 (19)	C27—O21—Ni3	123.1 (4)
O1—Ni2—O1W	83.52 (18)	C27—O22—Ni2	128.3 (5)
O25^{i}—Ni2—O1W	92.0 (2)	C29—O25—Ni2^{ii}	137.1 (5)
O2W—Ni2—O1W	90.26 (19)	C29—O26—Ni1^{ii}	133.7 (5)
O5W—Ni2—O1W	171.62 (18)	C12—C11—C16	119.5 (7)
O1—Ni3—O3W	169.2 (2)	C12—C11—C17	118.8 (7)
O1—Ni3—O21	96.40 (19)	C16—C11—C17	121.5 (7)

O3W—Ni3—O21	91.3 (2)	C11—C12—C13	121.4 (7)
O1—Ni3—O11	95.68 (19)	C11—C12—H12A	119.3
O3W—Ni3—O11	90.6 (2)	C13—C12—H12A	119.3
O21—Ni3—O11	98.54 (19)	C12—C13—C14	118.5 (7)
O1—Ni3—O1W	85.27 (18)	C12—C13—C18	121.2 (7)
O3W—Ni3—O1W	88.06 (18)	C14—C13—C18	120.1 (7)
O21—Ni3—O1W	83.95 (19)	C15—C14—C13	120.8 (7)
O11—Ni3—O1W	177.2 (2)	C15—C14—H14A	119.6
O1—Ni3—O11W	82.07 (18)	C13—C14—H14A	119.6
O3W—Ni3—O11W	89.4 (2)	C14—C15—C16	120.7 (7)
O21—Ni3—O11W	173.16 (18)	C14—C15—C19	119.3 (7)
O11—Ni3—O11W	88.26 (19)	C16—C15—C19	119.9 (8)
O1W—Ni3—O11W	89.27 (18)	C15—C16—C11	118.8 (7)
O6W—Na1—O8W	178.1 (3)	C15—C16—H16A	120.6
O6W—Na1—O7W	93.3 (2)	C11—C16—H16A	120.6
O8W—Na1—O7W	88.6 (2)	O12—C17—O11	126.2 (7)
O6W—Na1—O9W	91.3 (3)	O12—C17—C11	115.0 (7)
O8W—Na1—O9W	88.3 (2)	O11—C17—C11	118.8 (7)
O7W—Na1—O9W	93.7 (3)	O14—C18—O13	124.3 (8)
O6W—Na1—O5W	85.5 (2)	O14—C18—C13	116.6 (7)
O8W—Na1—O5W	92.6 (2)	O13—C18—C13	118.9 (7)
O7W—Na1—O5W	174.8 (3)	O15—C19—O16	124.0 (8)
O9W—Na1—O5W	91.4 (3)	O15—C19—C15	117.1 (8)
O6W—Na1—O4W	88.7 (2)	O16—C19—C15	118.8 (7)
O8W—Na1—O4W	91.7 (2)	C26—C21—C22	118.1 (7)
O7W—Na1—O4W	83.4 (2)	C26—C21—C27	119.3 (6)
O9W—Na1—O4W	177.1 (3)	C22—C21—C27	122.6 (6)
O5W—Na1—O4W	91.47 (19)	C23—C22—C21	121.1 (7)
Ni3—O1—Ni2	98.5 (2)	C23—C22—H22A	119.5
Ni3—O1—Ni1	100.3 (2)	C21—C22—H22A	119.5
Ni2—O1—Ni1	125.0 (2)	C24—C23—C22	119.3 (7)
Ni3—O1—H1A	110.4	C24—C23—C28	119.0 (7)
Ni2—O1—H1A	110.4	C22—C23—C28	121.7 (6)
Ni1—O1—H1A	110.4	C23—C24—C25	121.2 (7)
Ni3—O1W—Ni2	88.23 (17)	C23—C24—H24A	119.4
Ni3—O1W—H1WA	114.0	C25—C24—H24A	119.4
Ni2—O1W—H1WA	114.0	C26—C25—C24	118.3 (6)
Ni3—O1W—H1WB	113.9	C26—C25—C29	122.2 (6)
Ni2—O1W—H1WB	113.9	C24—C25—C29	119.5 (7)
H1WA—O1W—H1WB	111.1	C25—C26—C21	122.0 (6)
Ni2—O2W—H2WB	109.5	C25—C26—H26A	119.0
Ni2—O2W—H2WA	109.3	C21—C26—H26A	119.0
H2WB—O2W—H2WA	109.7	O22—C27—O21	124.9 (7)
Ni3—O3W—H3WB	109.5	O22—C27—C21	116.1 (6)
Ni3—O3W—H3WA	109.8	O21—C27—C21	118.9 (6)
H3WB—O3W—H3WA	140.7	O23—C28—O24	125.0 (7)
Ni1—O4W—Na1	116.1 (2)	O23—C28—C23	115.5 (7)
Ni1—O4W—H4B	109.4	O24—C28—C23	119.4 (7)
Na1—O4W—H4B	108.5	O25—C29—O26	127.0 (7)

Ni1—O4W—H4A	121.1	O25—C29—C25	116.8 (7)
Na1—O4W—H4A	99.9	O26—C29—C25	116.2 (7)
H4B—O4W—H4A	100.2	O14W—O13W—H13A	108.6
Ni2—O5W—Na1	117.4 (2)	O14W—O13W—H13B	95.1
Ni2—O5W—H5WA	109.5	H13A—O13W—H13B	114.0
Na1—O5W—H5WA	106.9	O13W—O14W—H14B	109.5
Ni2—O5W—H5WB	108.0	O13W—O14W—H14C	78.0
Na1—O5W—H5WB	108.0	H14B—O14W—H14C	85.1

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O8W	0.98	1.83	2.807 (7)	173
O1W—H1WA···O13^{iii}	0.97	1.90	2.797 (8)	152
O1W—H1WB···O16^{iv}	0.97	1.70	2.596 (7)	152
O1W—H1WB···O15^{iv}	0.97	2.57	3.438 (8)	149
O2W—H2WB···O10W^{v}	0.82	1.99	2.752 (9)	155
O2W—H2WA···O9W^{vi}	0.82	2.26	2.848 (8)	130
O3W—H3WB···O10W^{i}	0.82	2.31	2.872 (8)	126
O3W—H3WA···O14^{iii}	0.82	1.88	2.601 (8)	145
O4W—H4B···O15^{vii}	0.82	2.28	3.049 (8)	157
O4W—H4A···O24^{viii}	0.72	2.04	2.757 (7)	174
O5W—H5WA···O16^{viii}	0.82	2.03	2.818 (8)	160
O5W—H5WB···O13^{vii}	0.97	1.88	2.772 (7)	151
O6W—H6WB···O13^{vii}	0.82	2.45	3.153 (9)	145
O7W—H7WA···O14^{ix}	0.82	2.10	2.841 (8)	150
O7W—H7WB···O24^{viii}	0.82	1.96	2.778 (8)	174
O8W—H8WB···O21^{viii}	0.82	2.17	2.838 (7)	138
O8W—H8WA···O11^{viii}	0.82	2.07	2.821 (8)	153
O9W—H9WA···O16^{viii}	0.82	2.12	2.909 (10)	162
O9W—H9WB···O23^{v}	0.82	2.32	3.062 (9)	150
O10W—H10A···O12W^{vi}	0.82	2.14	2.764 (9)	133
O10W—H10B···O15^{iii}	0.84	2.14	2.981 (10)	177
O11W—H11A···O15^{iv}	0.97	1.71	2.659 (7)	166
O11W—H11B···O24^{x}	0.97	1.74	2.693 (6)	165
O12W—H12C···O7W^{xi}	0.96	2.01	2.795 (7)	138
O13W—H13A···O14^{ii}	0.82	1.99	2.79 (2)	168

Symmetry codes: (iii) $x+1/2, -y+3/2, -z$; (iv) $x, -y+3/2, z+1/2$; (v) $-x+3/2, y+1/2, z$; (vi) $-x+1, y-1/2, -z+1/2$; (i) $x-1/2, y, -z+1/2$; (vii) $-x+1/2, -y+2, z+1/2$; (viii) $-x+1, -y+2, -z$; (ix) $-x+1/2, y+1/2, z$; (x) $x-1/2, -y+3/2, -z$; (xi) $-x+1/2, y-1/2, z$; (ii) $x+1/2, y, -z+1/2$.

Fig. 1

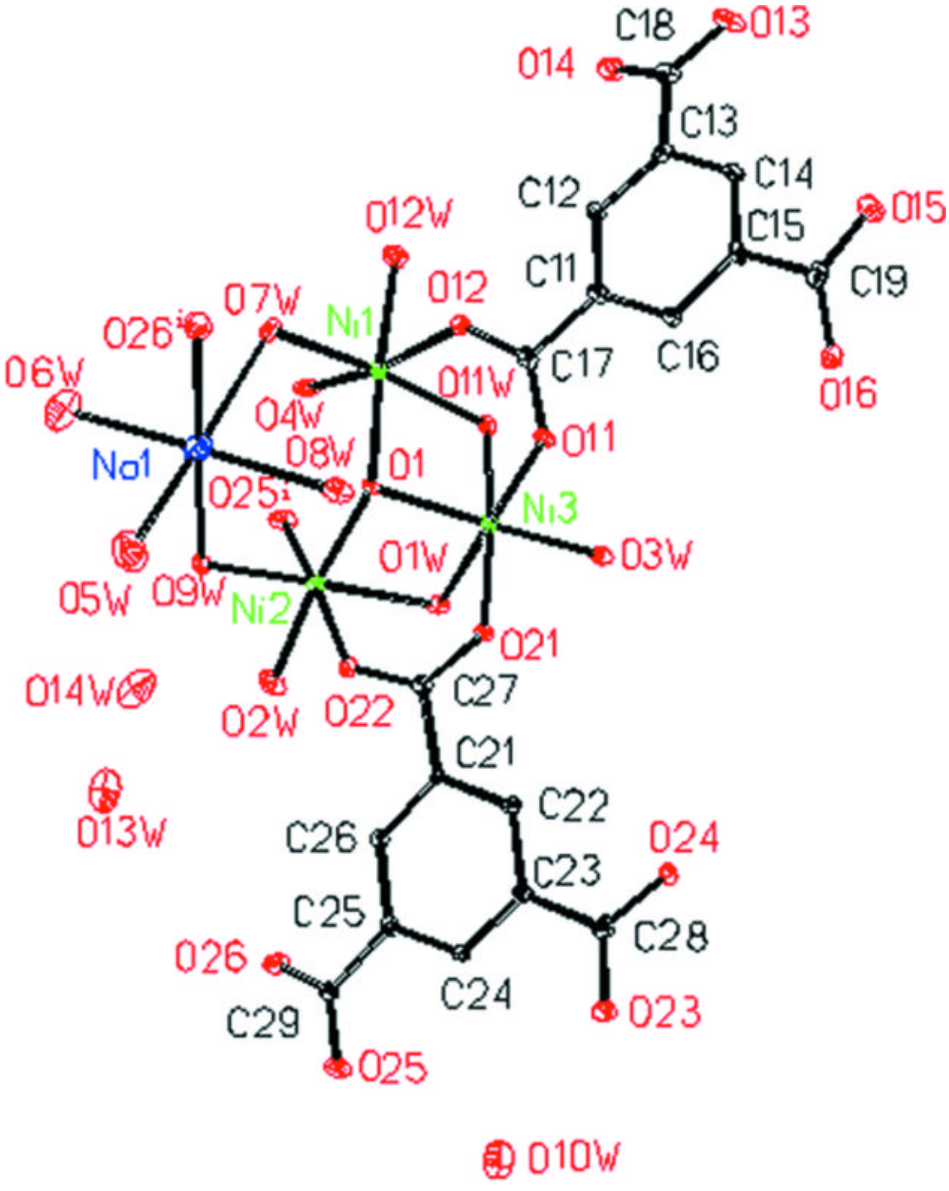
C18
O13
O14
C13
C14
C12
O15
C15
O12W
C11
C19
O12
O7W
Ni1
O26i
C17
C16
O6W
O11W
O16
O4W
O11
Na1
O8W
O1
O25i
Ni3
O3W
O1W
O5W
O9W
Ni2
O21
O14W
C27
O2W
O22
C21
O13W
C22
C26
O24
C23
C25
C28
O26
C24
O23
C29
O25
O10W

Fig. 2

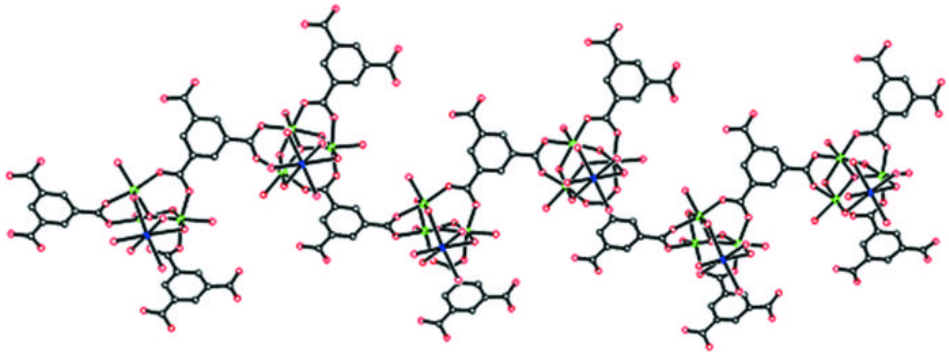

Fig. 3