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Poly[dimethylammonium [bis(dimethylamine)tri-μ_4-terephthalato-sodium(I)-dizinc(II)]]

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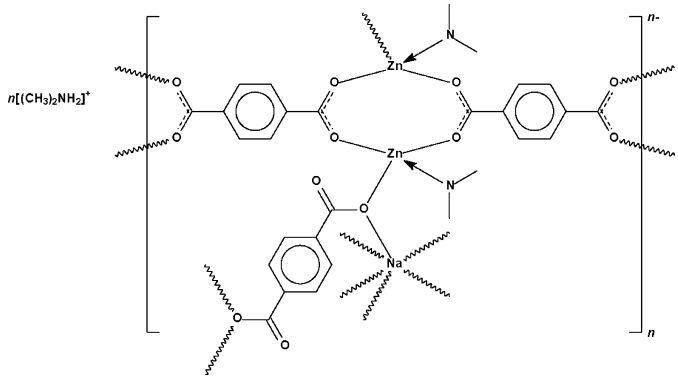
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.044; wR factor = 0.133; data-to-parameter ratio = 17.4.

The three terephthalate groups in the title polymeric coordination compound, $\{(C_2H_8N)[NaZn_2(C_8H_4O_4)_3(C_2H_7N)_2]\}_n$, lie on inversion centers. One functions as a bridge to two Na and two Zn atoms. The O atoms of the other two terephthalate groups bind to only one Zn atom. The Zn atom is additionally coordinated by a dimethylamine molecule; together with bonding from the O atoms of the three terephthalate groups, the geometry is tetrahedral. The manner of bridging of the terephalate groups gives rise to a polyanionic honeycomb sheet motif; the sheets are held into a three-dimensional network through the Na atoms. The cavities in the network are occupied by the dimethylammonium cations. The organic cation is disordered about a centre of inversion.

Related literature

A similar compound, bis(μ_5-terephthalato)(μ_4-terephthalato)bis(dimethyformamide)sodiumzinc, was synthesized by using a conventional preparation; the DMF is incorporated into the crystal structure (see Yang *et al.*, 2002). Under hydrothermal conditions, the DMF is decomposed into dimethylamine, which coordinates to zinc in the title compound.



Experimental

Crystal data

$(C_2H_8N)[NaZn_2(C_8H_4O_4)_3(C_2H_7N)_2]$
M_r = 782.33
Triclinic, $P\overline{1}$
a = 9.7893 (4) Å
b = 10.3641 (4) Å
c = 10.6649 (4) Å
α = 111.801 (1)°
β = 100.498 (1)°
γ = 109.257 (1)°
V = 889.29 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.42 mm^{-1}
T = 295 (2) K
0.32 × 0.26 × 0.20 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.500, T_{max} = 0.764
8744 measured reflections
4032 independent reflections
3743 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.134
S = 1.08
4032 reflections
232 parameters
21 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2587).

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supplementary materials

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Poly[dimethylammonium [bis(dimethylamine)tri-μ_4-terephthalato-sodium(I)dizinc(II)]]

L.-N. Zhu, S. Gao and S. W. Ng

Experimental

Zinc formate (1.55 g, 1 mmol) and terephthalic acid (1.66 g, 1 mmol) in dissolved in DMF (10 ml). The solution was heated in a 25-ml, Teflon-lined stainless-steel Parr bomb at 433 K for five days. The bomb was allowed to cool to room temperature. Several colorless prisms were picked out by hand.

Refinement

Carbon- and nitrogen-bound H atoms were placed in calculated positions [C—H 0.93–0.97 Å and U_{iso}(H) 1.2–1.5U_{eq}(C)], and were included in the refinement in the riding-model approximation.

The dimethylammonium cation is disordered about an inversion site, and was refined as a half-occupancy species, subject to distance restraints of C–N 1.45±01 and C···C 2.37±0.01 Å. Their anisotropic temperature factors were restrained to be nearly isotropic.

The refinement initially assumed two independent zinc atoms in the asymmetric unit; however, the difference Fourier consistently had a deep hole near that atom on the inversion site. The occupancy of the zinc atom at (1/2, 1/2, 1/2) refined to 0.188, an occupancy consistent with sodium. The refinement with magnesium in place of sodium led to worse convergence. Furthermore, the octahedral environment of oxygen atoms at distances of 2.3 to 2.5 Å is consistent with this assumption. Sodium could have come from the water used to clean the containers, or the terephthalic acid was contaminated with unknown amounts of the sodium salt.

The final difference Fourier map had a large peak at 2.66 Å from H13*a*; this peak could not be refined as an oxygen atom.

Figures

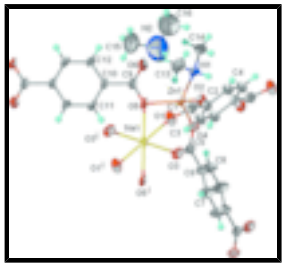

Fig. 1. **Figure 1**. Thermal ellipsoid plot of a portion of the polymeric structure; displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. (Symmetry code is given in Table 1.)

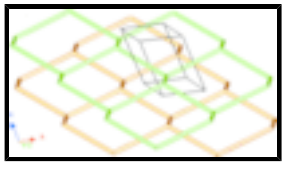

Fig. 2. **Figure 2**. Layer structure of the zinc-terepthalate network as illustrated by *OLEX* (Dolomanov *et al.*, 2003).

Poly[dimethylammonium [bis(dimethylamine)tri-μ4-terephthalato-sodium(I)dizinc(II)]]

Crystal data

$(C_2H_8N)[NaZn_2(C_8H_4O_4)_3(C_2H_7N)_2]$	$Z = 1$
$M_r = 782.33$	$F_{000} = 402$
Triclinic, $P\overline{1}$	$D_x = 1.461$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.7893$ (4) Å	Cell parameters from 8042 reflections
$b = 10.3641$ (4) Å	$\theta = 3.1$–27.5º
$c = 10.6649$ (4) Å	$\mu = 1.42$ mm^{-1}
$\alpha = 111.801$ (1)º	$T = 295$ (2) K
$\beta = 100.498$ (1)º	Prism, colorless
$\gamma = 109.257$ (1)º	0.32 × 0.26 × 0.20 mm
$V = 889.29$ (6) Å^3	

Data collection

Rigaku RAXIS-RAPID diffractometer	4032 independent reflections
Radiation source: fine-focus sealed tube	3743 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.019$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 295$(2) K	$\theta_{min} = 3.1$º
ω–scans	$h = -12 \rightarrow 12$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -13 \rightarrow 13$
$T_{min} = 0.500$, $T_{max} = 0.764$	$l = -13 \rightarrow 13$
8744 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.134$	$w = 1/[\sigma^2(F_o^2) + (0.0891P)^2 + 0.691P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
4032 reflections	$\Delta\rho_{max} = 1.52$ e Å^{-3}
232 parameters	$\Delta\rho_{min} = -0.37$ e Å^{-3}
21 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.59102 (3)	0.46809 (3)	0.79701 (3)	0.02569 (13)	
Na1	0.5000	0.5000	0.5000	0.0244 (3)	
O1	0.5534 (4)	0.7060 (3)	0.7200 (3)	0.0504 (6)	
O2	0.5491 (3)	0.6447 (2)	0.8990 (2)	0.0373 (5)	
O3	0.3246 (3)	0.3460 (3)	0.5606 (3)	0.0487 (6)	
O4	0.4059 (2)	0.2685 (3)	0.7140 (3)	0.0442 (5)	
O5	0.6919 (2)	0.4596 (3)	0.6530 (2)	0.0385 (5)	
O6	0.9088 (3)	0.6470 (3)	0.8285 (3)	0.0530 (6)	
N1	0.7009 (3)	0.4443 (3)	0.9649 (3)	0.0379 (6)	
H1	0.6297	0.3985	0.9910	0.045*	
C1	0.5425 (3)	0.7297 (3)	0.8384 (3)	0.0337 (6)	
C2	0.5199 (3)	0.8695 (3)	0.9231 (3)	0.0314 (5)	
C3	0.4778 (4)	0.9489 (3)	0.8546 (3)	0.0368 (6)	
H3	0.4632	0.9147	0.7572	0.044*	
C4	0.5425 (4)	0.9221 (3)	1.0700 (3)	0.0354 (6)	
H4	0.5711	0.8703	1.1168	0.042*	
C5	0.3034 (3)	0.2560 (3)	0.6121 (3)	0.0357 (6)	
C6	0.1461 (4)	0.1213 (4)	0.5529 (4)	0.0409 (7)	
C7	0.0188 (4)	0.1272 (4)	0.4790 (5)	0.0598 (11)	
H7	0.0311	0.2126	0.4640	0.072*	
C8	0.1269 (4)	−0.0070 (5)	0.5731 (5)	0.0597 (11)	
H8	0.2121	−0.0127	0.6218	0.072*	
C9	0.8376 (3)	0.5484 (4)	0.7029 (3)	0.0352 (6)	
C10	0.9209 (3)	0.5225 (3)	0.5965 (3)	0.0307 (5)	
C11	0.8412 (3)	0.4176 (4)	0.4516 (4)	0.0367 (6)	
H11	0.7345	0.3623	0.4187	0.044*	
C12	1.0806 (3)	0.6048 (4)	0.6438 (3)	0.0365 (6)	
H12	1.1350	0.6755	0.7405	0.044*	
C13	0.7748 (5)	0.3415 (5)	0.9174 (5)	0.0580 (10)	
H13A	0.7019	0.2478	0.8332	0.087*	
H13B	0.8092	0.3180	0.9929	0.087*	
H13C	0.8616	0.3917	0.8952	0.087*	
C14	0.8095 (4)	0.5905 (5)	1.0944 (4)	0.0552 (9)	
H14A	0.7582	0.6551	1.1234	0.083*	
H14B	0.8961	0.6424	1.0730	0.083*	
H14C	0.8448	0.5689	1.1711	0.083*	
N2	0.972 (2)	0.971 (5)	0.987 (3)	0.208 (10)	0.50
H2A	0.9050	0.8762	0.9352	0.249*	0.50
H2B	0.9252	1.0288	0.9983	0.249*	0.50
C15	1.083 (2)	1.0104 (17)	0.9171 (17)	0.113 (5)	0.50
H15A	1.0303	1.0028	0.8274	0.170*	0.50
H15B	1.1296	0.9404	0.8991	0.170*	0.50
H15C	1.1609	1.1140	0.9785	0.170*	0.50
C16	1.059 (3)	0.994 (2)	1.1262 (18)	0.156 (8)	0.50
H16A	0.9906	0.9761	1.1783	0.235*	0.50

H16B	1.1385	1.0981	1.1802	0.235*	0.50
H16C	1.1050	0.9234	1.1119	0.235*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02318 (18)	0.02679 (19)	0.03174 (19)	0.01195 (14)	0.01341 (13)	0.01542 (14)
Na1	0.0289 (7)	0.0256 (6)	0.0254 (6)	0.0119 (6)	0.0155 (6)	0.0155 (5)
O1	0.0838 (19)	0.0400 (12)	0.0462 (13)	0.0368 (13)	0.0382 (13)	0.0227 (10)
O2	0.0492 (12)	0.0339 (10)	0.0431 (11)	0.0273 (10)	0.0229 (10)	0.0209 (9)
O3	0.0360 (12)	0.0443 (12)	0.0695 (16)	0.0084 (10)	0.0204 (11)	0.0372 (12)
O4	0.0278 (10)	0.0414 (12)	0.0447 (12)	0.0001 (9)	0.0018 (9)	0.0197 (10)
O5	0.0313 (10)	0.0482 (12)	0.0497 (12)	0.0206 (9)	0.0278 (10)	0.0272 (10)
O6	0.0454 (13)	0.0672 (16)	0.0425 (13)	0.0212 (13)	0.0245 (11)	0.0203 (12)
N1	0.0275 (11)	0.0504 (15)	0.0457 (14)	0.0167 (11)	0.0150 (11)	0.0312 (12)
C1	0.0375 (15)	0.0268 (12)	0.0382 (14)	0.0157 (12)	0.0157 (12)	0.0138 (11)
C2	0.0400 (15)	0.0262 (12)	0.0303 (12)	0.0168 (11)	0.0141 (11)	0.0124 (10)
C3	0.0530 (18)	0.0327 (14)	0.0283 (12)	0.0219 (13)	0.0154 (12)	0.0142 (11)
C4	0.0465 (16)	0.0312 (13)	0.0341 (14)	0.0205 (13)	0.0133 (12)	0.0178 (11)
C5	0.0279 (13)	0.0331 (14)	0.0386 (14)	0.0049 (11)	0.0121 (12)	0.0162 (12)
C6	0.0295 (14)	0.0379 (15)	0.0431 (16)	−0.0006 (12)	0.0024 (12)	0.0247 (13)
C7	0.0374 (18)	0.048 (2)	0.088 (3)	0.0028 (16)	0.0022 (18)	0.049 (2)
C8	0.0351 (17)	0.053 (2)	0.079 (3)	0.0040 (16)	−0.0043 (18)	0.043 (2)
C9	0.0346 (14)	0.0458 (16)	0.0438 (15)	0.0244 (13)	0.0245 (13)	0.0279 (14)
C10	0.0281 (13)	0.0396 (14)	0.0397 (14)	0.0192 (12)	0.0204 (11)	0.0254 (12)
C11	0.0251 (12)	0.0440 (16)	0.0494 (16)	0.0160 (12)	0.0203 (12)	0.0257 (14)
C12	0.0286 (14)	0.0452 (16)	0.0389 (14)	0.0165 (13)	0.0169 (12)	0.0200 (13)
C13	0.051 (2)	0.065 (2)	0.086 (3)	0.038 (2)	0.028 (2)	0.049 (2)
C14	0.0416 (18)	0.067 (2)	0.0456 (18)	0.0172 (18)	0.0061 (15)	0.0246 (18)
N2	0.214 (13)	0.208 (15)	0.197 (12)	0.074 (10)	0.097 (10)	0.095 (9)
C15	0.114 (8)	0.088 (7)	0.127 (8)	0.023 (5)	0.066 (7)	0.046 (6)
C16	0.159 (11)	0.128 (10)	0.161 (11)	0.047 (8)	0.053 (9)	0.061 (8)

Geometric parameters (Å, °)

Zn1—O5	1.963 (2)	C6—C8	1.383 (5)
Zn1—O2	1.970 (2)	C7—C8^{iii}	1.386 (5)
Zn1—O4	1.982 (2)	C7—H7	0.9300
Zn1—N1	2.056 (3)	C8—C7^{iii}	1.386 (5)
Na1—O3	2.297 (2)	C8—H8	0.9300
Na1—O3^{i}	2.297 (2)	C9—C10	1.510 (4)
Na1—O1	2.331 (2)	C10—C11	1.390 (4)
Na1—O1^{i}	2.331 (2)	C10—C12	1.393 (4)
Na1—O5	2.505 (2)	C11—C12^{iv}	1.378 (4)
Na1—O5^{i}	2.505 (2)	C11—H11	0.9300
O1—C1	1.226 (4)	C12—C11^{iv}	1.378 (4)
O2—C1	1.282 (4)	C12—H12	0.9300

O3—C5	1.229 (4)	C13—H13A	0.9600
O4—C5	1.271 (4)	C13—H13B	0.9600
O5—C9	1.288 (4)	C13—H13C	0.9600
O6—C9	1.224 (4)	C14—H14A	0.9600
N1—C13	1.468 (5)	C14—H14B	0.9600
N1—C14	1.477 (5)	C14—H14C	0.9600
N1—H1	0.8600	N2—C15	1.455 (10)
C1—C2	1.509 (4)	N2—C16	1.458 (10)
C2—C3	1.393 (4)	N2—H2A	0.8600
C2—C4	1.400 (4)	N2—H2B	0.8600
C3—C4^{ii}	1.382 (4)	C15—H15A	0.9600
C3—H3	0.9300	C15—H15B	0.9600
C4—C3^{ii}	1.382 (4)	C15—H15C	0.9600
C4—H4	0.9300	C16—H16A	0.9600
C5—C6	1.514 (4)	C16—H16B	0.9600
C6—C7	1.381 (5)	C16—H16C	0.9600
O5—Zn1—O2	122.49 (9)	C7—C6—C5	119.5 (3)
O5—Zn1—O4	107.71 (10)	C8—C6—C5	121.3 (3)
O2—Zn1—O4	111.96 (10)	C6—C7—C8^{iii}	120.5 (3)
O5—Zn1—N1	114.27 (10)	C6—C7—H7	119.7
O2—Zn1—N1	101.73 (10)	C8^{iii}—C7—H7	119.7
O4—Zn1—N1	95.35 (10)	C6—C8—C7^{iii}	120.2 (3)
O3—Na1—O3^{i}	180.00 (12)	C6—C8—H8	119.9
O3—Na1—O1	87.36 (10)	C7^{iii}—C8—H8	119.9
O3^{i}—Na1—O1	92.64 (10)	O6—C9—O5	123.9 (3)
O3—Na1—O1^{i}	92.64 (10)	O6—C9—C10	120.2 (3)
O3^{i}—Na1—O1^{i}	87.36 (10)	O5—C9—C10	115.8 (3)
O1—Na1—O1^{i}	180.0	C11—C10—C12	119.0 (3)
O3—Na1—O5	83.95 (8)	C11—C10—C9	121.3 (3)
O3^{i}—Na1—O5	96.05 (8)	C12—C10—C9	119.7 (3)
O1—Na1—O5	82.33 (9)	C12^{iv}—C11—C10	120.4 (3)
O1^{i}—Na1—O5	97.67 (9)	C12^{iv}—C11—H11	119.8
O3—Na1—O5^{i}	96.05 (8)	C10—C11—H11	119.8
O3^{i}—Na1—O5^{i}	83.95 (8)	C11^{iv}—C12—C10	120.5 (3)
O1—Na1—O5^{i}	97.67 (9)	C11^{iv}—C12—H12	119.7
O1^{i}—Na1—O5^{i}	82.33 (9)	C10—C12—H12	119.7
O5—Na1—O5^{i}	180.0	N1—C13—H13A	109.5
C1—O1—Na1	139.5 (2)	N1—C13—H13B	109.5
C1—O2—Zn1	116.88 (18)	H13A—C13—H13B	109.5
C5—O3—Na1	144.9 (2)	N1—C13—H13C	109.5
C5—O4—Zn1	110.7 (2)	H13A—C13—H13C	109.5
C9—O5—Zn1	115.7 (2)	H13B—C13—H13C	109.5
C9—O5—Na1	121.97 (19)	N1—C14—H14A	109.5
Zn1—O5—Na1	94.39 (8)	N1—C14—H14B	109.5
C13—N1—C14	111.2 (3)	H14A—C14—H14B	109.5

C13—N1—Zn1	111.3 (2)	N1—C14—H14C	109.5
C14—N1—Zn1	115.2 (2)	H14A—C14—H14C	109.5
C13—N1—H1	106.1	H14B—C14—H14C	109.5
C14—N1—H1	106.2	C15—N2—C16	107.3 (10)
Zn1—N1—H1	106.1	C15—N2—H2A	110.3
O1—C1—O2	125.3 (3)	C16—N2—H2A	110.3
O1—C1—C2	118.9 (3)	C15—N2—H2B	110.3
O2—C1—C2	115.7 (2)	C16—N2—H2B	110.3
C3—C2—C4	119.3 (3)	H2A—N2—H2B	108.5
C3—C2—C1	119.6 (3)	N2—C15—H15A	109.5
C4—C2—C1	121.1 (2)	N2—C15—H15B	109.5
C4^{ii}—C3—C2	120.7 (3)	H15A—C15—H15B	109.5
C4^{ii}—C3—H3	119.7	N2—C15—H15C	109.5
C2—C3—H3	119.7	H15A—C15—H15C	109.5
C3^{ii}—C4—C2	120.0 (3)	H15B—C15—H15C	109.5
C3^{ii}—C4—H4	120.0	N2—C16—H16A	109.5
C2—C4—H4	120.0	N2—C16—H16B	109.5
O3—C5—O4	124.1 (3)	H16A—C16—H16B	109.5
O3—C5—C6	119.0 (3)	N2—C16—H16C	109.5
O4—C5—C6	116.9 (3)	H16A—C16—H16C	109.5
C7—C6—C8	119.3 (3)	H16B—C16—H16C	109.5
O3—Na1—O1—C1	22.2 (4)	Na1—Zn1—N1—C14	92.3 (4)
O3^{i}—Na1—O1—C1	−157.8 (4)	Na1—O1—C1—O2	29.8 (6)
O5—Na1—O1—C1	−62.1 (4)	Na1—O1—C1—C2	−150.5 (3)
O5^{i}—Na1—O1—C1	117.9 (4)	Zn1—O2—C1—O1	3.3 (4)
O5—Zn1—O2—C1	22.2 (3)	Zn1—O2—C1—C2	−176.43 (19)
O4—Zn1—O2—C1	−108.0 (2)	O1—C1—C2—C3	14.2 (5)
N1—Zn1—O2—C1	151.2 (2)	O2—C1—C2—C3	−166.0 (3)
O1—Na1—O3—C5	−96.9 (4)	O1—C1—C2—C4	−165.0 (3)
O1^{i}—Na1—O3—C5	83.1 (4)	O2—C1—C2—C4	14.8 (4)
O5—Na1—O3—C5	−14.4 (4)	C4—C2—C3—C4^{ii}	−0.3 (5)
O5^{i}—Na1—O3—C5	165.6 (4)	C1—C2—C3—C4^{ii}	−179.5 (3)
Zn1—Na1—O3—C5	−40.3 (4)	C3—C2—C4—C3^{ii}	0.3 (5)
Zn1^{i}—Na1—O3—C5	139.7 (4)	C1—C2—C4—C3^{ii}	179.5 (3)
O5—Zn1—O4—C5	−69.6 (2)	Na1—O3—C5—O4	35.7 (6)
O2—Zn1—O4—C5	67.9 (2)	Na1—O3—C5—C6	−144.7 (3)
N1—Zn1—O4—C5	172.8 (2)	Zn1—O4—C5—O3	8.7 (4)
O2—Zn1—O5—C9	73.2 (2)	Zn1—O4—C5—C6	−170.9 (2)
O4—Zn1—O5—C9	−154.8 (2)	O3—C5—C6—C7	−20.8 (5)
N1—Zn1—O5—C9	−50.3 (2)	O4—C5—C6—C7	158.9 (4)
O2—Zn1—O5—Na1	−55.59 (12)	O3—C5—C6—C8	160.1 (4)
O4—Zn1—O5—Na1	76.39 (10)	O4—C5—C6—C8	−20.3 (5)
N1—Zn1—O5—Na1	−179.06 (9)	C8—C6—C7—C8^{iii}	0.8 (8)
O3—Na1—O5—C9	−162.0 (2)	C5—C6—C7—C8^{iii}	−178.4 (4)
O3^{i}—Na1—O5—C9	18.0 (2)	C7—C6—C8—C7^{iii}	−0.8 (8)
O1—Na1—O5—C9	−73.9 (2)	C5—C6—C8—C7^{iii}	178.4 (4)

O1^{i}—Na1—O5—C9	106.1 (2)	Zn1—O5—C9—O6	−8.9 (4)
O3—Na1—O5—Zn1	−37.89 (10)	Na1—O5—C9—O6	104.7 (3)
O3^{i}—Na1—O5—Zn1	142.11 (10)	Zn1—O5—C9—C10	169.76 (18)
O1—Na1—O5—Zn1	50.25 (9)	Na1—O5—C9—C10	−76.6 (3)
O1^{i}—Na1—O5—Zn1	−129.75 (9)	O6—C9—C10—C11	−176.2 (3)
O5—Zn1—N1—C13	−33.0 (3)	O5—C9—C10—C11	5.1 (4)
O2—Zn1—N1—C13	−167.0 (2)	O6—C9—C10—C12	3.8 (4)
O4—Zn1—N1—C13	79.2 (2)	O5—C9—C10—C12	−174.9 (3)
Na1—Zn1—N1—C13	−35.5 (4)	C12—C10—C11—C12^{iv}	0.2 (5)
O5—Zn1—N1—C14	94.8 (3)	C9—C10—C11—C12^{iv}	−179.8 (3)
O2—Zn1—N1—C14	−39.2 (3)	C11—C10—C12—C11^{iv}	−0.2 (5)
O4—Zn1—N1—C14	−153.0 (2)	C9—C10—C12—C11^{iv}	179.8 (3)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+2, −*z*+2; (iii) −*x*, −*y*, −*z*+1; (iv) −*x*+2, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{v}	0.86	2.29	3.122 (3)	162

Symmetry codes: (v) −*x*+1, −*y*+1, −*z*+2.

Fig. 1

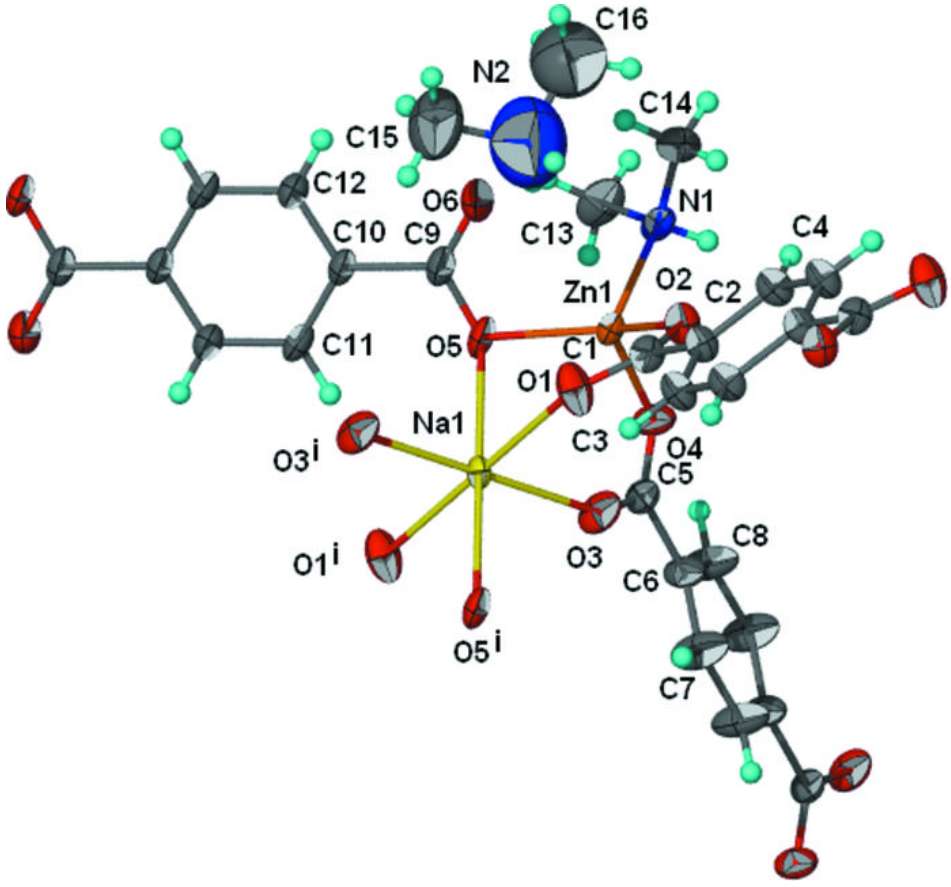
C16
N2
C14
C15
C12
O6
N1
C10
C9
C13
C4
Zn1
O2
C2
C11
O5
C1
O1
Na1
C3
O3i
O4
C5
O1i
O3
C8
C6
O5i
C7

Fig. 2