Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[bis(1*H*-imidazole)bis(μ_2-1*H*-imidazolido)bis(μ_2-7-oxabicyclo[2.2.1]-heptane-2,3-dicarboxylato)trizinc(II)]

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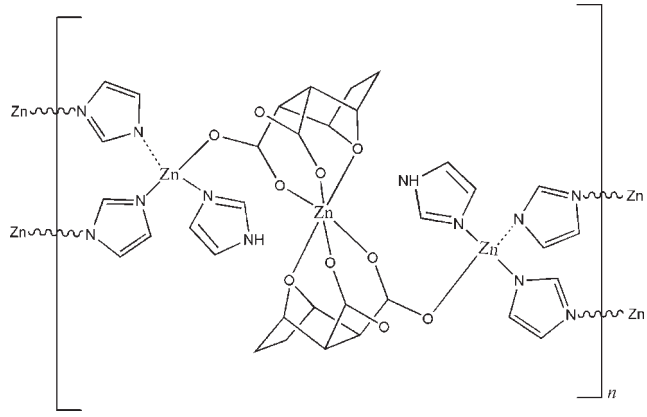
Received 21 April 2010; accepted 14 May 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.024; wR factor = 0.060; data-to-parameter ratio = 16.7.

The title polymer, $[Zn_3(C_8H_8O_5)_2(C_3H_3N_2)_2(C_3H_4N_2)_2]_n$, was formed by the reaction of zinc acetate with imidazole and 7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylic anhydride (norcantharidine). One of the two crystallographically unique Zn^{II} atoms is four-coordinated by three N atoms of three imidazole ligands, two of which are deprotonated, and by one carboxylate O atom of the demethylcantharate anion. The second Zn^{II} atom is situated on an inversion centre and is six-coordinated by the bridging O atoms of two symmetry-related demethylcantharate anions and by four carboxylate O atoms of the corresponding carboxylate groups. The polymeric crystal structure is additionally stabilized by N—H···O hydrogen bonding between the imidazole ligands and carboxylate O atoms.

Related literature

7-Oxabicyclo[2.2.1]heptane-2,3-dicarboxylic anhydride (norcantharidin) is a lower toxicity anticancer drug, see: Shimi *et al.* (1982). For cobalt complexes of norcantharidin, see: Wang *et al.* (1988) and for those including imidazole ligands, see: Furenlid *et al.* (1986); Zhu *et al.* (2003).



Experimental

Crystal data

$[Zn_3(C_8H_8O_5)_2(C_3H_3N_2)_2(C_3H_4N_2)_2]$
M_r = 834.71
Monoclinic, $P2_1/c$
a = 7.9993 (1) Å
b = 22.3923 (2) Å
c = 9.7586 (1) Å
β = 112.633 (1)°
V = 1613.37 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.28 mm^{-1}
T = 296 K
0.28 × 0.17 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.629, T_{max} = 0.822
13439 measured reflections
3714 independent reflections
3197 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.060
S = 1.03
3714 reflections
223 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O2	1.9570 (12)	Zn2—O5	2.0266 (12)
Zn1—N1	1.9686 (14)	Zn2—O4	2.0819 (12)
Zn1—N2^{i}	1.9944 (14)	Zn2—O1	2.1862 (12)
Zn1—N3	1.9968 (16)		

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4B···O5^{ii}	0.86	1.91	2.756 (2)	167

Symmetry code: (ii) $-x+1, -y+1, -z+2$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge financial support from the Natural Science Foundation of Zhejiang Province, China (grant No. Y407301).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2332).

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supplementary materials

Acta Cryst. (2010). E**66**, m705-m706 [**doi:10.1107/S1600536810017915**]

Poly[bis(1*H*-imidazole)bis(μ_2-1*H*-imidazolido)bis(μ_2-7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylato)trizinc(II)]

Q.-Y. Lin, N. Wang and Y.-Z. Wu

Comment

7-oxabicyclo[2,2,1] heptane-2,3-dicarboxylic anhydride (norcantharidin) derived from cantharidin is a lower toxicity anti-cancer drug (Shimi *et al.*, 1982). Imidazole is reputed as biocatalyst and biological ligand. Several cobalt complexes of norcantharidin (Wang *et al.*, 1988) and of imidazole (Furenlid *et al.*, 1986; Zhu *et al.*, 2003) have been reported previously.

In the structure of the title compound, the Zn1(II) cation is four-coordinated by three nitrogen atoms of three imidazoles ligands, two of which are deprotonated, and by one carboxylate oxygen atom of the demethylcantharate anion. The deprotonated imidazole rings are responsible for bridging neighbouring Zn1 atoms. The Zn2(II) cation is located on a crystallographic centre of inversion. Two bridge oxygen atoms of two symmetry-related demethylcantharate anions and four carboxylate oxygen atoms give rise to a slightly distorted octahedral ZnO_6 coordination environment. Each demethylcantharate anion adopts simultaneously a bridging coordination mode (O2 towards Zn1, O4 towards Zn2) and a monodentate coordination mode (through O5 towards Zn2).

The crystal lattice is stabilized through N—H···O hydrogen bonds between the uncoordinated nitrogen atom (N4) of the imidazole molecule and one of the carboxylate oxygen atoms (O3) of the demethylcantharate anion.

Experimental

7-oxabicyclo[2,2,1] heptane-2,3-dicarboxylic anhydride, zinc acetate and imidazole were dissolved in 15 mL distilled water. The mixture was sealed in a 25 mL Teflon-lined stainless vessel and heated at 443 K for 3 d, then cooled slowly to room temperature. Crystals suitable for X-ray diffraction were obtained.

Refinement

The H atoms bonded to C and N atoms were positioned geometrically and refined using a riding model [aromatic C—H 0.93 Å, aliphatic C—H = 0.97 (2) Å and N—H = 0.86 Å with $U_{iso}(H) = 1.2U_{eq}(C,N)$].

Figures

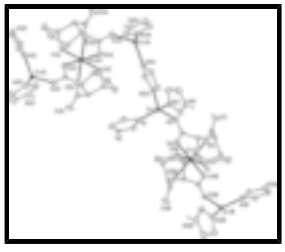


Fig. 1. A view of the molecule of the title compound showing the atom-labelling and connectivity of the Zn^{II} atoms. Displacement ellipsoids drawn at the 30% probability level.

Poly[bis(1*H*-imidazole)bis(μ$_2$-1*H*-imidazolido)bis(μ$_2$- 7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylato)trizinc(II)]

Crystal data

$[Zn_3(C_8H_8O_5)_2(C_3H_3N_2)_2(C_3H_4N_2)_2]$	$F(000) = 848$
$M_r = 834.71$	$D_x = 1.718$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 5397 reflections
$a = 7.9993$ (1) Å	$\theta = 1.8$–$27.6°$
$b = 22.3923$ (2) Å	$\mu = 2.28$ mm^{-1}
$c = 9.7586$ (1) Å	$T = 296$ K
$\beta = 112.633$ (1)°	Block, colourless
$V = 1613.37$ (3) Å^3	0.28 × 0.17 × 0.09 mm
$Z = 2$	

Data collection

Bruker APEXII CCD diffractometer	3714 independent reflections
Radiation source: fine-focus sealed tube	3197 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.023$
ω scans	$\theta_{max} = 27.6°$, $\theta_{min} = 1.8°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{min} = 0.629$, $T_{max} = 0.822$	$k = -29 \rightarrow 28$
13439 measured reflections	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.024$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.060$	H-atom parameters constrained
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0306P)^2 + 0.4382P]$ where $P = (F_o^2 + 2F_c^2)/3$
3714 reflections	$(\Delta/\sigma)_{max} = 0.001$
223 parameters	$\Delta\rho_{max} = 0.36$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.28$ 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. 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}
Zn1	0.02705 (3)	0.327653 (8)	0.68480 (2)	0.02488 (7)
Zn2	0.0000	0.5000	1.0000	0.02427 (8)
C1	0.5856 (3)	0.35035 (11)	0.8423 (3)	0.0508 (6)
H1A	0.7015	0.3415	0.8476	0.061*
C2	0.4334 (3)	0.31994 (10)	0.7673 (3)	0.0471 (5)
H2A	0.4259	0.2860	0.7103	0.057*
C3	0.3601 (3)	0.39293 (9)	0.8744 (2)	0.0391 (5)
H3A	0.2943	0.4196	0.9073	0.047*
C4	−0.1719 (3)	0.18968 (8)	0.8571 (2)	0.0333 (4)
H4A	−0.2451	0.1565	0.8488	0.040*
C5	−0.1783 (3)	0.22588 (8)	0.7447 (2)	0.0325 (4)
H5A	−0.2566	0.2218	0.6459	0.039*
C6	0.0280 (3)	0.25794 (8)	0.94487 (19)	0.0293 (4)
H6A	0.1206	0.2810	1.0110	0.035*
C7	−0.1093 (2)	0.44234 (7)	0.70651 (18)	0.0222 (3)
C8	−0.1796 (2)	0.50314 (7)	0.64085 (19)	0.0230 (3)
H8A	−0.2375	0.5001	0.5325	0.028*
C9	−0.3146 (2)	0.52910 (8)	0.70277 (19)	0.0267 (4)
H9A	−0.3937	0.4991	0.7198	0.032*
C10	−0.4169 (3)	0.58168 (8)	0.6063 (2)	0.0364 (4)
H10A	−0.5217	0.5927	0.6277	0.044*
H10B	−0.4555	0.5726	0.5015	0.044*
C11	−0.2716 (3)	0.63123 (8)	0.6539 (2)	0.0395 (5)
H11A	−0.2465	0.6459	0.5702	0.047*
H11B	−0.3078	0.6644	0.7003	0.047*
C12	−0.1090 (3)	0.59822 (8)	0.7649 (2)	0.0296 (4)
H12A	−0.0177	0.6248	0.8336	0.036*
C13	−0.0311 (2)	0.55369 (7)	0.68508 (19)	0.0250 (4)
H13A	−0.0282	0.5722	0.5950	0.030*
C14	0.1603 (2)	0.53377 (8)	0.78551 (19)	0.0265 (4)
N1	−0.0501 (2)	0.26968 (6)	0.80047 (16)	0.0281 (3)
N2	−0.0394 (2)	0.20990 (6)	0.98546 (16)	0.0288 (3)
N3	0.2899 (2)	0.34675 (7)	0.78774 (18)	0.0333 (4)
N4	0.5372 (2)	0.39636 (8)	0.9085 (2)	0.0429 (4)
H4B	0.6087	0.4232	0.9632	0.051*
O1	−0.19478 (17)	0.55896 (5)	0.83772 (13)	0.0271 (3)
O2	−0.09952 (19)	0.40346 (5)	0.61684 (13)	0.0326 (3)
O3	0.2753 (2)	0.52710 (8)	0.73430 (17)	0.0515 (4)

O4	−0.06572 (18)	0.43224 (5)	0.84191 (13)	0.0293 (3)
O5	0.19131 (16)	0.52692 (6)	0.92484 (13)	0.0299 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03053 (12)	0.02231 (11)	0.02322 (11)	−0.00257 (8)	0.01193 (9)	−0.00100 (7)
Zn2	0.02831 (15)	0.02813 (15)	0.01822 (14)	−0.00145 (11)	0.01100 (12)	−0.00224 (10)
C1	0.0314 (11)	0.0607 (14)	0.0607 (15)	−0.0008 (10)	0.0180 (11)	−0.0062 (12)
C2	0.0400 (12)	0.0476 (13)	0.0559 (14)	0.0009 (9)	0.0209 (11)	−0.0142 (10)
C3	0.0339 (10)	0.0342 (10)	0.0435 (12)	0.0002 (8)	0.0085 (9)	−0.0071 (9)
C4	0.0360 (10)	0.0285 (9)	0.0353 (11)	−0.0069 (8)	0.0135 (9)	0.0026 (8)
C5	0.0348 (10)	0.0339 (10)	0.0254 (9)	−0.0060 (8)	0.0077 (8)	0.0002 (7)
C6	0.0355 (10)	0.0247 (9)	0.0267 (9)	−0.0021 (7)	0.0107 (8)	0.0007 (7)
C7	0.0217 (8)	0.0222 (8)	0.0228 (9)	−0.0034 (6)	0.0088 (7)	−0.0027 (6)
C8	0.0265 (9)	0.0228 (8)	0.0185 (8)	−0.0016 (6)	0.0075 (7)	−0.0007 (6)
C9	0.0256 (9)	0.0266 (9)	0.0275 (9)	−0.0022 (7)	0.0096 (7)	−0.0005 (7)
C10	0.0303 (10)	0.0353 (10)	0.0400 (11)	0.0077 (8)	0.0095 (9)	0.0041 (8)
C11	0.0435 (12)	0.0266 (10)	0.0465 (12)	0.0070 (8)	0.0154 (10)	0.0055 (8)
C12	0.0342 (10)	0.0217 (8)	0.0334 (10)	−0.0031 (7)	0.0134 (8)	−0.0021 (7)
C13	0.0287 (9)	0.0253 (8)	0.0229 (8)	−0.0028 (7)	0.0121 (7)	0.0023 (6)
C14	0.0271 (9)	0.0272 (9)	0.0270 (9)	−0.0059 (7)	0.0124 (8)	−0.0009 (7)
N1	0.0341 (8)	0.0252 (7)	0.0249 (8)	−0.0016 (6)	0.0114 (7)	0.0028 (6)
N2	0.0376 (9)	0.0254 (8)	0.0256 (8)	0.0013 (6)	0.0148 (7)	0.0035 (6)
N3	0.0301 (8)	0.0309 (8)	0.0371 (9)	−0.0032 (7)	0.0110 (7)	−0.0046 (7)
N4	0.0319 (9)	0.0396 (9)	0.0461 (11)	−0.0091 (7)	0.0028 (8)	−0.0045 (8)
O1	0.0316 (7)	0.0272 (6)	0.0250 (6)	0.0010 (5)	0.0136 (5)	−0.0020 (5)
O2	0.0497 (8)	0.0243 (6)	0.0235 (6)	0.0059 (5)	0.0137 (6)	−0.0031 (5)
O3	0.0368 (8)	0.0864 (12)	0.0406 (9)	0.0114 (8)	0.0249 (7)	0.0152 (8)
O4	0.0439 (8)	0.0233 (6)	0.0203 (6)	0.0005 (5)	0.0120 (6)	−0.0004 (5)
O5	0.0258 (6)	0.0419 (7)	0.0226 (6)	−0.0049 (5)	0.0099 (5)	−0.0012 (5)

Geometric parameters (Å, °)

Zn1—O2	1.9570 (12)	C6—H6A	0.9300
Zn1—N1	1.9686 (14)	C7—O4	1.251 (2)
Zn1—N2^{i}	1.9944 (14)	C7—O2	1.2578 (19)
Zn1—N3	1.9968 (16)	C7—C8	1.518 (2)
Zn2—O5^{ii}	2.0266 (12)	C8—C9	1.540 (2)
Zn2—O5	2.0266 (12)	C8—C13	1.576 (2)
Zn2—O4	2.0819 (12)	C8—H8A	0.9800
Zn2—O4^{ii}	2.0819 (12)	C9—O1	1.459 (2)
Zn2—O1^{ii}	2.1862 (12)	C9—C10	1.533 (2)
Zn2—O1	2.1862 (12)	C9—H9A	0.9800
C1—C2	1.340 (3)	C10—C11	1.543 (3)
C1—N4	1.350 (3)	C10—H10A	0.9700
C1—H1A	0.9300	C10—H10B	0.9700
C2—N3	1.376 (3)	C11—C12	1.525 (3)

C2—H2A	0.9300	C11—H11A	0.9700
C3—N3	1.317 (2)	C11—H11B	0.9700
C3—N4	1.327 (3)	C12—O1	1.457 (2)
C3—H3A	0.9300	C12—C13	1.537 (2)
C4—C5	1.349 (3)	C12—H12A	0.9800
C4—N2	1.369 (2)	C13—C14	1.533 (2)
C4—H4A	0.9300	C13—H13A	0.9800
C5—N1	1.371 (2)	C14—O3	1.213 (2)
C5—H5A	0.9300	C14—O5	1.294 (2)
C6—N1	1.329 (2)	N2—Zn1^{iii}	1.9944 (14)
C6—N2	1.330 (2)	N4—H4B	0.8600
O2—Zn1—N1	122.06 (6)	C10—C9—C8	109.78 (15)
O2—Zn1—N2^{i}	97.25 (6)	O1—C9—H9A	113.8
N1—Zn1—N2^{i}	104.86 (6)	C10—C9—H9A	113.8
O2—Zn1—N3	106.98 (6)	C8—C9—H9A	113.8
N1—Zn1—N3	110.76 (7)	C9—C10—C11	101.84 (15)
N2^{i}—Zn1—N3	114.52 (7)	C9—C10—H10A	111.4
O5^{ii}—Zn2—O5	180.000 (1)	C11—C10—H10A	111.4
O5^{ii}—Zn2—O4	92.34 (5)	C9—C10—H10B	111.4
O5—Zn2—O4	87.66 (5)	C11—C10—H10B	111.4
O5^{ii}—Zn2—O4^{ii}	87.66 (5)	H10A—C10—H10B	109.3
O5—Zn2—O4^{ii}	92.34 (5)	C12—C11—C10	101.71 (15)
O4—Zn2—O4^{ii}	180.0	C12—C11—H11A	111.4
O5^{ii}—Zn2—O1^{ii}	89.15 (5)	C10—C11—H11A	111.4
O5—Zn2—O1^{ii}	90.85 (5)	C12—C11—H11B	111.4
O4—Zn2—O1^{ii}	90.17 (4)	C10—C11—H11B	111.4
O4^{ii}—Zn2—O1^{ii}	89.83 (4)	H11A—C11—H11B	109.3
O5^{ii}—Zn2—O1	90.85 (5)	O1—C12—C11	101.88 (15)
O5—Zn2—O1	89.15 (5)	O1—C12—C13	102.39 (13)
O4—Zn2—O1	89.83 (4)	C11—C12—C13	110.85 (16)
O4^{ii}—Zn2—O1	90.17 (4)	O1—C12—H12A	113.5
O1^{ii}—Zn2—O1	180.0	C11—C12—H12A	113.5
C2—C1—N4	106.4 (2)	C13—C12—H12A	113.5
C2—C1—H1A	126.8	C14—C13—C12	111.41 (14)
N4—C1—H1A	126.8	C14—C13—C8	115.37 (13)
C1—C2—N3	109.4 (2)	C12—C13—C8	101.21 (13)
C1—C2—H2A	125.3	C14—C13—H13A	109.5
N3—C2—H2A	125.3	C12—C13—H13A	109.5
N3—C3—N4	110.88 (18)	C8—C13—H13A	109.5
N3—C3—H3A	124.6	O3—C14—O5	123.32 (17)
N4—C3—H3A	124.6	O3—C14—C13	120.10 (16)
C5—C4—N2	108.61 (16)	O5—C14—C13	116.54 (15)
C5—C4—H4A	125.7	C6—N1—C5	104.69 (15)
N2—C4—H4A	125.7	C6—N1—Zn1	127.96 (13)
C4—C5—N1	108.57 (16)	C5—N1—Zn1	126.56 (12)

C4—C5—H5A	125.7	C6—N2—C4	104.75 (14)
N1—C5—H5A	125.7	C6—N2—Zn1^{iii}	130.16 (12)
N1—C6—N2	113.37 (16)	C4—N2—Zn1^{iii}	125.09 (12)
N1—C6—H6A	123.3	C3—N3—C2	105.22 (17)
N2—C6—H6A	123.3	C3—N3—Zn1	126.68 (14)
O4—C7—O2	122.91 (15)	C2—N3—Zn1	127.52 (14)
O4—C7—C8	121.03 (15)	C3—N4—C1	108.14 (17)
O2—C7—C8	116.06 (15)	C3—N4—H4B	125.9
C7—C8—C9	112.03 (14)	C1—N4—H4B	125.9
C7—C8—C13	114.24 (14)	C12—O1—C9	96.04 (12)
C9—C8—C13	100.96 (13)	C12—O1—Zn2	112.31 (10)
C7—C8—H8A	109.8	C9—O1—Zn2	114.50 (9)
C9—C8—H8A	109.8	C7—O2—Zn1	121.81 (11)
C13—C8—H8A	109.8	C7—O4—Zn2	122.65 (10)
O1—C9—C10	102.25 (14)	C14—O5—Zn2	123.34 (11)
O1—C9—C8	102.16 (13)		
N4—C1—C2—N3	−0.5 (3)	C1—C2—N3—C3	0.3 (3)
N2—C4—C5—N1	−0.1 (2)	C1—C2—N3—Zn1	171.94 (17)
O4—C7—C8—C9	−42.3 (2)	O2—Zn1—N3—C3	38.44 (19)
O2—C7—C8—C9	137.10 (16)	N1—Zn1—N3—C3	−96.74 (18)
O4—C7—C8—C13	71.7 (2)	N2^{i}—Zn1—N3—C3	144.95 (17)
O2—C7—C8—C13	−108.87 (17)	O2—Zn1—N3—C2	−131.53 (18)
C7—C8—C9—O1	86.39 (15)	N1—Zn1—N3—C2	93.29 (19)
C13—C8—C9—O1	−35.59 (15)	N2^{i}—Zn1—N3—C2	−25.0 (2)
C7—C8—C9—C10	−165.65 (14)	N3—C3—N4—C1	−0.4 (3)
C13—C8—C9—C10	72.37 (16)	C2—C1—N4—C3	0.5 (3)
O1—C9—C10—C11	33.06 (18)	C11—C12—O1—C9	57.35 (15)
C8—C9—C10—C11	−74.84 (18)	C13—C12—O1—C9	−57.40 (14)
C9—C10—C11—C12	2.0 (2)	C11—C12—O1—Zn2	176.96 (11)
C10—C11—C12—O1	−36.52 (18)	C13—C12—O1—Zn2	62.21 (13)
C10—C11—C12—C13	71.83 (19)	C10—C9—O1—C12	−55.89 (15)
O1—C12—C13—C14	−88.49 (16)	C8—C9—O1—C12	57.76 (14)
C11—C12—C13—C14	163.49 (15)	C10—C9—O1—Zn2	−173.78 (11)
O1—C12—C13—C8	34.66 (16)	C8—C9—O1—Zn2	−60.13 (13)
C11—C12—C13—C8	−73.36 (17)	O5^{ii}—Zn2—O1—C12	170.75 (10)
C7—C8—C13—C14	0.5 (2)	O5—Zn2—O1—C12	−9.25 (10)
C9—C8—C13—C14	120.96 (15)	O4—Zn2—O1—C12	−96.91 (10)
C7—C8—C13—C12	−119.84 (15)	O4^{ii}—Zn2—O1—C12	83.09 (10)
C9—C8—C13—C12	0.57 (16)	O5^{ii}—Zn2—O1—C9	−81.07 (11)
C12—C13—C14—O3	−140.91 (18)	O5—Zn2—O1—C9	98.93 (11)
C8—C13—C14—O3	104.4 (2)	O4—Zn2—O1—C9	11.27 (11)
C12—C13—C14—O5	36.7 (2)	O4^{ii}—Zn2—O1—C9	−168.73 (11)
C8—C13—C14—O5	−77.90 (19)	O4—C7—O2—Zn1	−11.7 (2)
N2—C6—N1—C5	0.4 (2)	C8—C7—O2—Zn1	168.88 (11)
N2—C6—N1—Zn1	−169.85 (12)	N1—Zn1—O2—C7	61.89 (16)
C4—C5—N1—C6	−0.2 (2)	N2^{i}—Zn1—O2—C7	174.51 (14)
C4—C5—N1—Zn1	170.27 (13)	N3—Zn1—O2—C7	−67.06 (15)

O2—Zn1—N1—C6	−105.18 (16)	O2—C7—O4—Zn2	159.29 (13)
N2^{i}—Zn1—N1—C6	146.15 (16)	C8—C7—O4—Zn2	−21.3 (2)
N3—Zn1—N1—C6	22.12 (17)	O5^{ii}—Zn2—O4—C7	124.12 (14)
O2—Zn1—N1—C5	86.57 (16)	O5—Zn2—O4—C7	−55.88 (14)
N2^{i}—Zn1—N1—C5	−22.11 (17)	O1^{ii}—Zn2—O4—C7	−146.73 (14)
N3—Zn1—N1—C5	−146.14 (15)	O1—Zn2—O4—C7	33.27 (14)
N1—C6—N2—C4	−0.5 (2)	O3—C14—O5—Zn2	−150.62 (16)
N1—C6—N2—Zn1^{iii}	179.67 (12)	C13—C14—O5—Zn2	31.8 (2)
C5—C4—N2—C6	0.3 (2)	O4—Zn2—O5—C14	47.74 (14)
C5—C4—N2—Zn1^{iii}	−179.80 (13)	O4^{ii}—Zn2—O5—C14	−132.26 (14)
N4—C3—N3—C2	0.1 (2)	O1^{ii}—Zn2—O5—C14	137.88 (14)
N4—C3—N3—Zn1	−171.69 (14)	O1—Zn2—O5—C14	−42.12 (14)

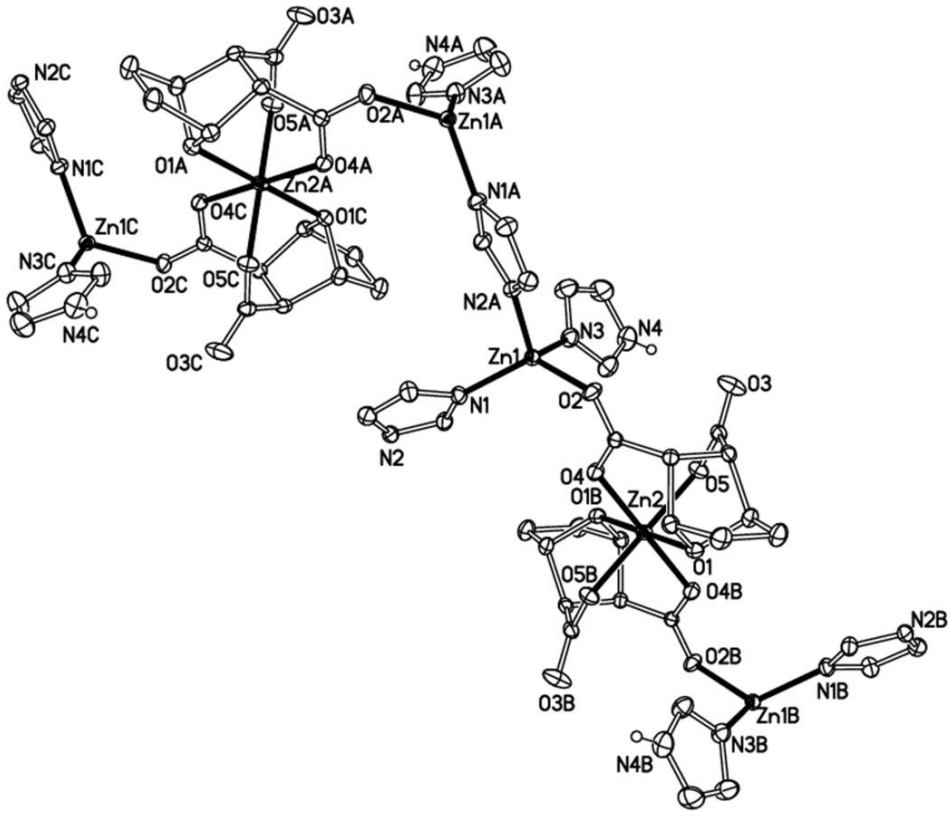
Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*, −*y*+1, −*z*+2; (iii) *x*, −*y*+1/2, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4B···O5^{iv}	0.86	1.91	2.756 (2)	167.

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

Fig. 1


O3A
N4A
N2C
N3A
O5A
O2A
Zn1A
N1C
O1A
O4A
Zn2A
N1A
O4C
O1C
Zn1C
N3C
O2C
O5C
N2A
N3
N4
N4C
Zn1
O3C
O3
N1
O2
N2
O4
O1B
Zn2
O5
O1
O5B
O4B
N2B
O2B
N1B
O3B
Zn1B
N3B
N4B