metal-organic compounds

Poly[[diaquabis(μ_2-terephthalato-κ^4O:O':O'':O''')dizinc(II)] N,N-dimethyl-acetamide disolvate]

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In the title polymeric compound, $\{[Zn_2(C_8H_4O_4)_2(H_2O)_2]\cdot 2C_4H_9NO\}_n$, each of the terephthalate dianions uses both carboxylate ends to bridge a pair of water-coordinated Zn^{II} atoms [$Zn\cdots Zn$ = 2.9527 (4) Å] into a two-dimensional square-grid motif. One of the dianions lies on a special position of site symmetry $\bar{1}$, whereas the other lies on a general position. Each grid cavity contains two N,N-dimethylacetamide molecules.

Related literature

The Cambridge Structural Database (Version 5.28, November 2006; Allen, 2002) lists several examples of zinc terephthalate systems. Some crystallize with DMF-type solvent molecules. For the DMF solvate, see: Edgar et al. (2001). For the N,N-diethylformamide solvate, see: Grzesiak et al. (2006).
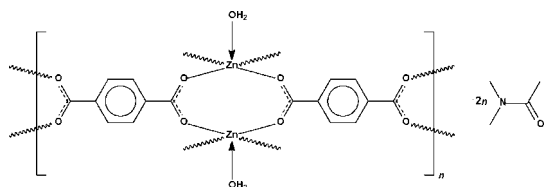
Experimental

Crystal data

$[Zn_2(C_8H_4O_4)_2(H_2O)_2]\cdot 2C_4H_9NO$
$M_r = 669.24$
Triclinic, $P\bar{1}$
$a = 6.9291$ (5) Å
$b = 10.0551$ (7) Å
$c = 20.620$ (2) Å
$\alpha = 78.030$ (1)°
$\beta = 81.044$ (1)°
$\gamma = 77.266$ (1)°
$V = 1361.7$ (2) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.83$ mm^{-1}
$T = 295$ (2) K
$0.33 \times 0.31 \times 0.29$ mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.587$, $T_{max} = 1.000$ (expected range = 0.345–0.589)

7748 measured reflections
5269 independent reflections
4503 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.099$
$S = 1.04$
5269 reflections
383 parameters
4 restraints

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 1.24$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1w—H1w1$\cdots$O9	0.84 (1)	1.76 (1)	2.598 (3)	173 (4)
O1w—H1w2$\cdots$O8^i	0.84 (1)	1.90 (1)	2.734 (3)	173 (4)
O2w—H2w1$\cdots$O10	0.85 (1)	1.76 (1)	2.613 (3)	177 (4)
O2w—H2w2$\cdots$O1^{ii}	0.84 (1)	2.03 (1)	2.869 (3)	176 (4)

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

Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2006); data reduction: SAINT; 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).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2501).

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supplementary materials

Poly[[diaquabis(μ_2-terephthalato-$\kappa^4 O:O':O'':O'''$)dizinc(II)] *N,N*-dimethylacetamide disolvate\]

M. Lv and S. W. Ng

Comment

The Cambridge Structural Database (Version 5.28, November 2006; Allen, 2002) lists several examples of zinc terephthalate systems. Some crystallize with DMF-type of solvent molecules. In the present compound, the terephthalate dianion uses both carboxylate ends to bridge a pair of water-coordinated zinc(II) atoms [Zn···Zn = 2.9527 (4) Å] into a two-dimensional square-grid motif (Fig. 1). Each of the grid cavity (Fig. 2) contains two solvent molecules.

Experimental

A mixture of zinc chloride dihydrate (0.5 mmol), terephthalic acid (0.5 mmol) and *N,N*-dimethylacetamide (12 ml) was heated at 443 K for 3 d. The cooled mixture yielded colourless crystals of the title compound.

Refinement

H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding, with $U_{iso}(H) = 1.2$–$1.5 U_{eq}(C)$. The methyl groups were allowed to rotate but not to tip. The water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O—H = 0.85 (1) Å. The four highest peaks in the final difference Fourier map were observed in the vicinity of the DMA molecules. The positions of the peaks indicate that the DMA molecules are probably not disordered.
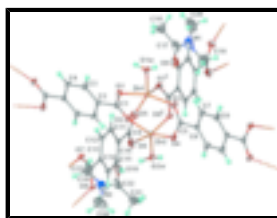
Figures

Fig. 1. Part of a two-dimensional square-grid motif of the title compound. Displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radius. Symmetry code: (i) $x + 1, y - 1, z$.
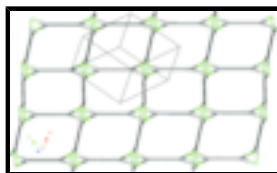

Fig. 2. OLEX (Dolomanov *et al.*, 2003) representation of the square-grid motif.

supplementary materials

Poly[[diaquabis(μ₂-terephthalato- κ⁴O:O':O'':O''')dizinc(II)] N,N-dimethylacetamide disolvate]

Crystal data

[Zn₂(C₈H₄O₄)₂(H₂O)₂]·2C₄H₉NO	$Z = 2$
$M_r = 669.24$	$F_{000} = 688$
Triclinic, $P\bar{1}$	$D_x = 1.632$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.9291$ (5) Å	Cell parameters from 3838 reflections
$b = 10.0551$ (7) Å	$\theta = 2.2–26.0°$
$c = 20.620$ (2) Å	$\mu = 1.83$ mm^{-1}
$\alpha = 78.030$ (1)°	$T = 295$ (2) K
$\beta = 81.044$ (1)°	Block, colourless
$\gamma = 77.266$ (1)°	$0.33 \times 0.31 \times 0.29$ mm
$V = 1361.7$ (2) Å³	

Data collection

Bruker APEXII area-detector diffractometer	5269 independent reflections
Radiation source: fine-focus sealed tube	4503 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.016$
$T = 295(2)$ K	$\theta_{max} = 26.0°$
φ and ω scans	$\theta_{min} = 2.0°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8\rightarrow6$
$T_{min} = 0.587$, $T_{max} = 1.000$	$k = -12\rightarrow12$
7748 measured reflections	$l = -25\rightarrow25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.099$	$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 0.7539P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
5269 reflections	$\Delta\rho_{max} = 1.24$ e Å^{-3}
383 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Zn1	0.63480 (4)	0.67635 (3)	0.719133 (14)	0.01316 (10)
Zn2	0.92767 (4)	0.77920 (3)	0.775812 (14)	0.01324 (10)
O1	0.5123 (3)	0.6234 (2)	0.81850 (9)	0.0236 (5)
O2	0.7888 (3)	0.6531 (2)	0.85183 (9)	0.0245 (5)
O3	0.8096 (3)	0.7535 (2)	0.63769 (9)	0.0250 (5)
O4	0.9806 (3)	0.8735 (2)	0.67983 (9)	0.0246 (5)
O5	0.5119 (3)	0.8748 (2)	0.72861 (11)	0.0299 (5)
O6	0.7024 (3)	0.9401 (2)	0.78959 (11)	0.0309 (5)
O7	−0.1614 (3)	1.49770 (19)	0.73505 (10)	0.0219 (4)
O8	0.0874 (3)	1.59581 (19)	0.74699 (10)	0.0206 (4)
O9	0.4592 (4)	0.6915 (3)	0.54349 (11)	0.0450 (7)
O10	1.0286 (4)	0.8186 (3)	0.95154 (12)	0.0467 (7)
O1W	0.4426 (3)	0.6272 (2)	0.67268 (10)	0.0236 (5)
O2W	1.1323 (3)	0.8078 (2)	0.82510 (10)	0.0217 (4)
N1	0.3480 (6)	0.7018 (5)	0.44740 (18)	0.0657 (11)
N2	1.1224 (6)	0.8029 (4)	1.05090 (18)	0.0602 (10)
C1	0.6258 (4)	0.6158 (3)	0.86252 (13)	0.0178 (6)
C2	0.5584 (4)	0.5557 (3)	0.93373 (13)	0.0181 (6)
C3	0.3839 (4)	0.5026 (3)	0.94995 (14)	0.0226 (6)
H3	0.3063	0.5042	0.9167	0.027*
C4	0.3260 (4)	0.4472 (3)	1.01590 (14)	0.0231 (6)
H4	0.2096	0.4118	1.0266	0.028*
C5	0.9142 (4)	0.8430 (3)	0.63250 (13)	0.0192 (6)
C6	0.9616 (4)	0.9236 (3)	0.56353 (13)	0.0201 (6)
C7	0.8558 (5)	0.9188 (3)	0.51209 (14)	0.0257 (7)
H7	0.7594	0.8641	0.5203	0.031*
C8	0.8933 (5)	0.9948 (3)	0.44886 (14)	0.0256 (7)
H8	0.8218	0.9915	0.4148	0.031*
C9	0.5516 (4)	0.9592 (3)	0.75905 (13)	0.0199 (6)
C10	0.4100 (4)	1.0962 (3)	0.75689 (13)	0.0180 (6)
C11	0.2208 (4)	1.1129 (3)	0.73742 (14)	0.0206 (6)
H11	0.1796	1.0382	0.7274	0.025*
C12	0.0946 (4)	1.2414 (3)	0.73307 (14)	0.0192 (6)
H12	−0.0323	1.2522	0.7208	0.023*
C13	0.1558 (4)	1.3544 (3)	0.74688 (13)	0.0158 (5)
C14	0.3456 (4)	1.3378 (3)	0.76604 (14)	0.0198 (6)
H14	0.3878	1.4128	0.7753	0.024*
C15	0.4704 (4)	1.2094 (3)	0.77112 (14)	0.0200 (6)
H15	0.5963	1.1982	0.7842	0.024*
C16	0.0166 (4)	1.4929 (3)	0.74250 (12)	0.0157 (5)
C17	0.3473 (6)	0.6572 (5)	0.5108 (2)	0.0507 (10)
C18	0.2010 (6)	0.5604 (4)	0.54366 (19)	0.0452 (9)
H18A	0.2192	0.5293	0.5900	0.068*
H18B	0.2261	0.4819	0.5217	0.068*
H18C	0.0668	0.6099	0.5398	0.068*

C19	0.4846 (7)	0.7971 (5)	0.41555 (19)	0.0590 (12)
H19A	0.5368	0.8269	0.4494	0.088*
H19B	0.4133	0.8762	0.3883	0.088*
H19C	0.5923	0.7499	0.3883	0.088*
C20	0.2240 (8)	0.6634 (7)	0.4052 (2)	0.0832 (19)
H20A	0.1502	0.5966	0.4315	0.125*
H20B	0.3077	0.6242	0.3694	0.125*
H20C	0.1330	0.7444	0.3870	0.125*
C21	1.3211 (6)	0.9137 (4)	0.9555 (2)	0.0496 (10)
H21A	1.3178	0.9395	0.9081	0.074*
H21B	1.4445	0.8517	0.9646	0.074*
H21C	1.3099	0.9952	0.9743	0.074*
C22	1.1458 (6)	0.8407 (4)	0.9868 (2)	0.0478 (10)
C23	0.9614 (7)	0.7308 (5)	1.08110 (19)	0.0524 (11)
H23A	0.8818	0.7282	1.0474	0.079*
H23B	0.8800	0.7787	1.1145	0.079*
H23C	1.0160	0.6379	1.1014	0.079*
C24	1.2542 (9)	0.8267 (6)	1.0954 (2)	0.0812 (17)
H24A	1.3640	0.8633	1.0690	0.122*
H24B	1.3037	0.7406	1.1233	0.122*
H24C	1.1806	0.8916	1.1228	0.122*
H1W1	0.438 (6)	0.652 (4)	0.6313 (6)	0.041 (11)*
H1W2	0.329 (3)	0.620 (4)	0.6927 (18)	0.060 (14)*
H2W1	1.095 (6)	0.811 (4)	0.8661 (7)	0.048 (12)*
H2W2	1.246 (3)	0.757 (3)	0.8228 (19)	0.050 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01266 (17)	0.01296 (17)	0.01259 (16)	−0.00214 (12)	−0.00050 (12)	−0.00054 (12)
Zn2	0.01314 (17)	0.01313 (17)	0.01196 (16)	−0.00188 (12)	−0.00091 (12)	−0.00006 (12)
O1	0.0223 (11)	0.0349 (12)	0.0117 (9)	−0.0074 (9)	−0.0020 (8)	0.0016 (8)
O2	0.0229 (11)	0.0334 (12)	0.0158 (10)	−0.0130 (9)	0.0005 (8)	0.0049 (8)
O3	0.0275 (11)	0.0304 (12)	0.0159 (10)	−0.0136 (9)	0.0000 (8)	0.0049 (8)
O4	0.0368 (12)	0.0277 (11)	0.0107 (9)	−0.0144 (10)	−0.0016 (9)	0.0015 (8)
O5	0.0283 (12)	0.0173 (11)	0.0415 (13)	0.0057 (9)	−0.0045 (10)	−0.0099 (9)
O6	0.0290 (12)	0.0245 (11)	0.0347 (12)	0.0101 (9)	−0.0097 (10)	−0.0070 (9)
O7	0.0157 (10)	0.0156 (10)	0.0333 (11)	0.0009 (8)	−0.0069 (9)	−0.0032 (8)
O8	0.0164 (10)	0.0132 (9)	0.0313 (11)	−0.0012 (8)	−0.0006 (8)	−0.0051 (8)
O9	0.0446 (15)	0.0735 (19)	0.0225 (12)	−0.0206 (14)	−0.0096 (11)	−0.0071 (12)
O10	0.0457 (16)	0.073 (2)	0.0252 (12)	−0.0122 (14)	−0.0069 (11)	−0.0158 (12)
O1W	0.0185 (11)	0.0388 (13)	0.0160 (10)	−0.0122 (9)	−0.0023 (9)	−0.0029 (9)
O2W	0.0167 (10)	0.0306 (12)	0.0183 (10)	−0.0030 (9)	−0.0021 (8)	−0.0073 (9)
N1	0.050 (2)	0.104 (3)	0.043 (2)	−0.001 (2)	−0.0125 (17)	−0.023 (2)
N2	0.071 (3)	0.069 (3)	0.044 (2)	−0.006 (2)	−0.0204 (19)	−0.0154 (18)
C1	0.0162 (13)	0.0167 (13)	0.0164 (13)	0.0005 (11)	0.0011 (11)	−0.0003 (11)
C2	0.0203 (14)	0.0187 (14)	0.0131 (12)	−0.0052 (11)	0.0017 (11)	0.0009 (11)
C3	0.0226 (15)	0.0318 (16)	0.0141 (13)	−0.0106 (13)	−0.0022 (11)	0.0002 (12)

C4	0.0196 (14)	0.0309 (16)	0.0185 (14)	−0.0119 (12)	−0.0002 (11)	0.0018 (12)
C5	0.0206 (14)	0.0174 (14)	0.0148 (13)	−0.0017 (11)	0.0016 (11)	0.0026 (11)
C6	0.0244 (15)	0.0210 (14)	0.0131 (13)	−0.0075 (12)	0.0018 (11)	0.0014 (11)
C7	0.0300 (16)	0.0296 (16)	0.0185 (14)	−0.0156 (13)	−0.0019 (12)	0.0034 (12)
C8	0.0318 (17)	0.0323 (17)	0.0150 (14)	−0.0162 (14)	−0.0038 (12)	0.0022 (12)
C9	0.0213 (15)	0.0141 (13)	0.0178 (13)	0.0016 (11)	0.0030 (11)	0.0025 (11)
C10	0.0208 (14)	0.0150 (13)	0.0154 (13)	0.0010 (11)	0.0002 (11)	−0.0026 (10)
C11	0.0226 (15)	0.0137 (13)	0.0254 (15)	−0.0029 (11)	−0.0022 (12)	−0.0041 (11)
C12	0.0156 (13)	0.0188 (14)	0.0229 (14)	−0.0012 (11)	−0.0050 (11)	−0.0032 (11)
C13	0.0155 (13)	0.0137 (13)	0.0156 (13)	0.0000 (11)	0.0001 (10)	−0.0010 (10)
C14	0.0222 (15)	0.0149 (13)	0.0222 (14)	−0.0034 (11)	−0.0032 (12)	−0.0032 (11)
C15	0.0159 (13)	0.0214 (14)	0.0210 (14)	0.0006 (11)	−0.0051 (11)	−0.0023 (11)
C16	0.0181 (14)	0.0133 (13)	0.0124 (12)	−0.0006 (11)	−0.0001 (10)	0.0009 (10)
C17	0.043 (2)	0.064 (3)	0.040 (2)	0.006 (2)	−0.0035 (18)	−0.017 (2)
C18	0.041 (2)	0.054 (2)	0.042 (2)	−0.0116 (18)	0.0001 (17)	−0.0124 (18)
C19	0.059 (3)	0.080 (3)	0.029 (2)	−0.015 (2)	−0.0006 (19)	0.009 (2)
C20	0.061 (3)	0.147 (6)	0.051 (3)	0.001 (3)	−0.024 (2)	−0.048 (3)
C21	0.051 (2)	0.048 (2)	0.052 (2)	−0.013 (2)	−0.005 (2)	−0.0104 (19)
C22	0.055 (3)	0.045 (2)	0.040 (2)	0.0051 (19)	−0.0066 (19)	−0.0160 (18)
C23	0.064 (3)	0.061 (3)	0.030 (2)	−0.019 (2)	0.0014 (19)	−0.0039 (18)
C24	0.102 (4)	0.097 (4)	0.058 (3)	−0.009 (3)	−0.046 (3)	−0.029 (3)

Geometric parameters (Å, °)

Zn1—O1	2.100 (2)	C5—C6	1.510 (4)
Zn1—O3	2.032 (2)	C6—C7	1.394 (4)
Zn1—O5	2.026 (2)	C6—C8[iv]	1.395 (4)
Zn1—O7[i]	2.027 (2)	C7—C8	1.386 (4)
Zn1—O1W	1.954 (2)	C7—H7	0.93
Zn1—Zn2	2.9527 (4)	C8—C6[iv]	1.395 (4)
Zn2—O2	2.058 (2)	C8—H8	0.93
Zn2—O4	2.025 (2)	C9—C10	1.501 (4)
Zn2—O6	2.018 (2)	C10—C15	1.394 (4)
Zn2—O8[i]	2.080 (2)	C10—C11	1.395 (4)
Zn2—O2W	1.969 (2)	C11—C12	1.386 (4)
O1—C1	1.271 (3)	C11—H11	0.93
O2—C1	1.241 (3)	C12—C13	1.392 (4)
O3—C5	1.253 (3)	C12—H12	0.93
O4—C5	1.258 (3)	C13—C14	1.397 (4)
O5—C9	1.252 (4)	C13—C16	1.503 (4)
O6—C9	1.262 (4)	C14—C15	1.381 (4)
O7—C16	1.255 (3)	C14—H14	0.93
O7—Zn1[ii]	2.0274 (19)	C15—H15	0.93
O8—C16	1.264 (3)	C17—C18	1.543 (6)
O8—Zn2[ii]	2.0804 (19)	C18—H18A	0.96
O9—C17	1.246 (5)	C18—H18B	0.96
O10—C22	1.252 (5)	C18—H18C	0.96
O1W—H1W1	0.842 (10)	C19—H19A	0.96

O1W—H1W2	0.842 (10)	C19—H19B	0.96
O2W—H2W1	0.849 (10)	C19—H19C	0.96
O2W—H2W2	0.841 (10)	C20—H20A	0.96
N1—C17	1.290 (5)	C20—H20B	0.96
N1—C19	1.479 (6)	C20—H20C	0.96
N1—C20	1.472 (6)	C21—C22	1.544 (6)
N2—C22	1.292 (5)	C21—H21A	0.96
N2—C23	1.453 (6)	C21—H21B	0.96
N2—C24	1.477 (5)	C21—H21C	0.96
C1—C2	1.511 (4)	C23—H23A	0.96
C2—C3	1.394 (4)	C23—H23B	0.96
C2—C4^{iii}	1.399 (4)	C23—H23C	0.96
C3—C4	1.391 (4)	C24—H24A	0.96
C3—H3	0.93	C24—H24B	0.96
C4—C2^{iii}	1.399 (4)	C24—H24C	0.96
C4—H4	0.93		
O1W—Zn1—O5	102.58 (9)	C6—C7—H7	119.7
O1W—Zn1—O7^i	102.98 (9)	C7—C8—C6^{iv}	119.8 (3)
O5—Zn1—O7^i	154.30 (9)	C7—C8—H8	120.1
O1W—Zn1—O3	98.14 (8)	C6^{iv}—C8—H8	120.1
O5—Zn1—O3	87.61 (9)	O5—C9—O6	125.5 (3)
O7^i—Zn1—O3	91.40 (8)	O5—C9—C10	116.7 (3)
O1W—Zn1—O1	100.14 (8)	O6—C9—C10	117.8 (3)
O5—Zn1—O1	85.75 (9)	C15—C10—C11	119.5 (3)
O7^i—Zn1—O1	87.20 (8)	C15—C10—C9	120.1 (3)
O3—Zn1—O1	161.51 (8)	C11—C10—C9	120.3 (3)
O1W—Zn1—Zn2	173.06 (6)	C12—C11—C10	119.6 (3)
O5—Zn1—Zn2	73.54 (6)	C12—C11—H11	120.2
O7^i—Zn1—Zn2	81.29 (6)	C10—C11—H11	120.2
O3—Zn1—Zn2	76.13 (6)	C11—C12—C13	120.7 (3)
O1—Zn1—Zn2	85.44 (6)	C11—C12—H12	119.6
O2W—Zn2—O6	102.78 (9)	C13—C12—H12	119.6
O2W—Zn2—O4	107.47 (9)	C12—C13—C14	119.6 (2)
O6—Zn2—O4	88.71 (9)	C12—C13—C16	120.1 (2)
O2W—Zn2—O2	98.12 (8)	C14—C13—C16	120.3 (2)
O6—Zn2—O2	89.76 (9)	C15—C14—C13	119.6 (3)
O4—Zn2—O2	154.05 (8)	C15—C14—H14	120.2
O2W—Zn2—O8^i	96.33 (8)	C13—C14—H14	120.2
O6—Zn2—O8^i	160.78 (9)	C14—C15—C10	120.9 (3)
O4—Zn2—O8^i	87.53 (8)	C14—C15—H15	119.6
O2—Zn2—O8^i	85.46 (8)	C10—C15—H15	119.6
O2W—Zn2—Zn1	167.77 (6)	O7—C16—O8	124.9 (2)
O6—Zn2—Zn1	84.84 (7)	O7—C16—C13	117.7 (2)
O4—Zn2—Zn1	81.98 (6)	O8—C16—C13	117.5 (2)
O2—Zn2—Zn1	72.09 (6)	O9—C17—N1	121.2 (4)
O8^i—Zn2—Zn1	75.97 (6)	O9—C17—C18	122.0 (4)

C1—O1—Zn1	115.60 (17)	N1—C17—C18	116.7 (4)
C1—O2—Zn2	135.28 (18)	C17—C18—H18A	109.5
C5—O3—Zn1	128.33 (19)	C17—C18—H18B	109.5
C5—O4—Zn2	122.57 (18)	H18A—C18—H18B	109.5
C9—O5—Zn1	134.0 (2)	C17—C18—H18C	109.5
C9—O6—Zn2	118.93 (19)	H18A—C18—H18C	109.5
C16—O7—Zn1^{ii}	123.68 (17)	H18B—C18—H18C	109.5
C16—O8—Zn2^{ii}	126.38 (17)	N1—C19—H19A	109.5
Zn1—O1W—H1W1	123 (3)	N1—C19—H19B	109.5
Zn1—O1W—H1W2	119 (3)	H19A—C19—H19B	109.5
H1W1—O1W—H1W2	111 (4)	N1—C19—H19C	109.5
Zn2—O2W—H2W1	114 (3)	H19A—C19—H19C	109.5
Zn2—O2W—H2W2	120 (3)	H19B—C19—H19C	109.5
H2W1—O2W—H2W2	107 (4)	N1—C20—H20A	109.5
C17—N1—C19	117.3 (4)	N1—C20—H20B	109.5
C17—N1—C20	124.4 (5)	H20A—C20—H20B	109.5
C19—N1—C20	118.4 (4)	N1—C20—H20C	109.5
C22—N2—C23	118.8 (4)	H20A—C20—H20C	109.5
C22—N2—C24	123.3 (5)	H20B—C20—H20C	109.5
C23—N2—C24	117.9 (4)	C22—C21—H21A	109.5
O2—C1—O1	125.4 (3)	C22—C21—H21B	109.5
O2—C1—C2	117.0 (2)	H21A—C21—H21B	109.5
O1—C1—C2	117.6 (2)	C22—C21—H21C	109.5
C3—C2—C4^{iii}	119.6 (3)	H21A—C21—H21C	109.5
C3—C2—C1	121.2 (2)	H21B—C21—H21C	109.5
C4^{iii}—C2—C1	119.3 (2)	O10—C22—N2	120.5 (4)
C4—C3—C2	119.9 (3)	O10—C22—C21	121.4 (4)
C4—C3—H3	120.0	N2—C22—C21	118.1 (4)
C2—C3—H3	120.0	N2—C23—H23A	109.5
C3—C4—C2^{iii}	120.5 (3)	N2—C23—H23B	109.5
C3—C4—H4	119.7	H23A—C23—H23B	109.5
C2^{iii}—C4—H4	119.7	N2—C23—H23C	109.5
O3—C5—O4	125.8 (2)	H23A—C23—H23C	109.5
O3—C5—C6	117.2 (2)	H23B—C23—H23C	109.5
O4—C5—C6	117.0 (2)	N2—C24—H24A	109.5
C7—C6—C8^{iv}	119.7 (3)	N2—C24—H24B	109.5
C7—C6—C5	119.6 (3)	H24A—C24—H24B	109.5
C8^{iv}—C6—C5	120.7 (3)	N2—C24—H24C	109.5
C8—C7—C6	120.5 (3)	H24A—C24—H24C	109.5
C8—C7—H7	119.7	H24B—C24—H24C	109.5
O1W—Zn1—O1—C1	165.7 (2)	O3—C5—C6—C7	13.9 (4)
O5—Zn1—O1—C1	−92.2 (2)	O4—C5—C6—C7	−165.0 (3)
O7^{i}—Zn1—O1—C1	63.1 (2)	O3—C5—C6—C8^{iv}	−167.6 (3)
O3—Zn1—O1—C1	−23.0 (4)	O4—C5—C6—C8^{iv}	13.6 (4)
O2W—Zn2—O2—C1	162.7 (3)	C8^{iv}—C6—C7—C8	−0.3 (5)
O6—Zn2—O2—C1	59.8 (3)	C5—C6—C7—C8	178.3 (3)

O4—Zn2—O2—C1	−26.7 (4)	C6—C7—C8—C6^{iv}	0.3 (5)
O8^i—Zn2—O2—C1	−101.5 (3)	Zn1—O5—C9—O6	6.5 (5)
O1W—Zn1—O3—C5	152.7 (2)	Zn1—O5—C9—C10	−175.55 (19)
O5—Zn1—O3—C5	50.3 (2)	Zn2—O6—C9—O5	12.3 (4)
O7^i—Zn1—O3—C5	−104.0 (2)	Zn2—O6—C9—C10	−165.71 (18)
O1—Zn1—O3—C5	−18.7 (4)	O5—C9—C10—C15	−160.6 (3)
Zn2—Zn1—O3—C5	−23.3 (2)	O6—C9—C10—C15	17.5 (4)
O2W—Zn2—O4—C5	159.7 (2)	O5—C9—C10—C11	16.2 (4)
O6—Zn2—O4—C5	−97.3 (2)	O6—C9—C10—C11	−165.7 (3)
O2—Zn2—O4—C5	−10.5 (4)	C15—C10—C11—C12	−0.6 (4)
O8^i—Zn2—O4—C5	63.8 (2)	C9—C10—C11—C12	−177.4 (3)
Zn1—Zn2—O4—C5	−12.3 (2)	C10—C11—C12—C13	1.0 (4)
O1W—Zn1—O5—C9	171.8 (3)	C11—C12—C13—C14	−0.7 (4)
O7^i—Zn1—O5—C9	−2.1 (4)	C11—C12—C13—C16	−179.5 (2)
O3—Zn1—O5—C9	−90.4 (3)	C12—C13—C14—C15	−0.1 (4)
O1—Zn1—O5—C9	72.4 (3)	C16—C13—C14—C15	178.7 (2)
O2W—Zn2—O6—C9	173.9 (2)	C13—C14—C15—C10	0.5 (4)
O4—Zn2—O6—C9	66.3 (2)	C11—C10—C15—C14	−0.2 (4)
O2—Zn2—O6—C9	−87.8 (2)	C9—C10—C15—C14	176.7 (3)
O8^i—Zn2—O6—C9	−12.4 (4)	Zn1^{ii}—O7—C16—O8	6.6 (4)
Zn2—O2—C1—O1	18.1 (5)	Zn1^{ii}—O7—C16—C13	−173.87 (16)
Zn2—O2—C1—C2	−162.33 (19)	Zn2^{ii}—O8—C16—O7	22.5 (4)
Zn1—O1—C1—O2	9.3 (4)	Zn2^{ii}—O8—C16—C13	−157.04 (17)
Zn1—O1—C1—C2	−170.23 (18)	C12—C13—C16—O7	9.4 (4)
O2—C1—C2—C3	−175.7 (3)	C14—C13—C16—O7	−169.4 (2)
O1—C1—C2—C3	3.9 (4)	C12—C13—C16—O8	−171.0 (2)
O2—C1—C2—C4^{iii}	3.9 (4)	C14—C13—C16—O8	10.1 (4)
O1—C1—C2—C4^{iii}	−176.5 (3)	C19—N1—C17—O9	−0.9 (6)
C4^{iii}—C2—C3—C4	0.0 (5)	C20—N1—C17—O9	178.5 (4)
C1—C2—C3—C4	179.6 (3)	C19—N1—C17—C18	178.7 (4)
C2—C3—C4—C2^{iii}	0.0 (5)	C20—N1—C17—C18	−1.8 (7)
Zn1—O3—C5—O4	23.0 (4)	C23—N2—C22—O10	1.8 (6)
Zn1—O3—C5—C6	−155.74 (19)	C24—N2—C22—O10	−179.5 (4)
Zn2—O4—C5—O3	0.0 (4)	C23—N2—C22—C21	−178.4 (4)
Zn2—O4—C5—C6	178.80 (18)	C24—N2—C22—C21	0.3 (6)

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

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w1···O9	0.84 (1)	1.76 (1)	2.598 (3)	173 (4)
O1w—H1w2···O8^v	0.84 (1)	1.90 (1)	2.734 (3)	173 (4)
O2w—H2w1···O10	0.85 (1)	1.76 (1)	2.613 (3)	177 (4)
O2w—H2w2···O1^{vi}	0.84 (1)	2.03 (1)	2.869 (3)	176 (4)

Symmetry codes: (v) x, $y-1$, z; (vi) $x+1$, y, z.

Fig. 1

Fig. 2