

$[\mu\text{-}10,21\text{-Dimethyl-3,6,14,17-tetraaza-tricyclo[17.3.1.1}^{8,12}\text{]tetracosa-1(23),8,-10,12(24),19,21\text{-hexaene-23,24-diolato-\kappa}^4\text{N}^3,\text{N}^6,\text{O}^{23},\text{O}^{24}:\kappa}^4\text{N}^{14},\text{N}^{17},\text{O}^{23},\text{O}^{24}]\text{-bis(maleato-\kappa O)zinc(II)}$

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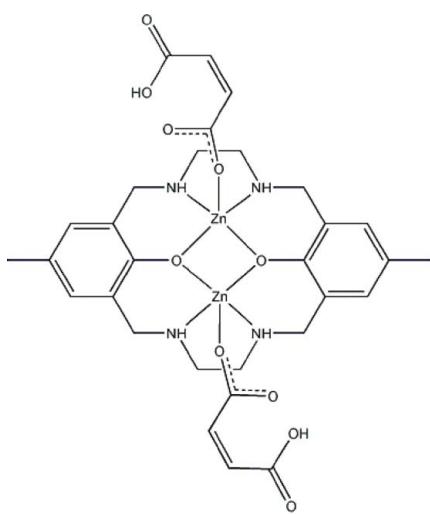
Received 13 November 2007; accepted 18 November 2007

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C-C}) = 0.003$ Å; R factor = 0.029; wR factor = 0.085; data-to-parameter ratio = 16.7.

The centrosymmetric title compound, $[\text{Zn}_2(\text{C}_{22}\text{H}_{22}\text{N}_4\text{O}_2)_2(\text{C}_4\text{H}_7\text{O}_4)_2]$, is a dinuclear zinc(II) complex. Each Zn^{II} atom has a square-pyramidal geometry with N_2O_3 donors, being coordinated by two N atoms and two O atoms from the 10,21-dimethyl-3,6,14,17-tetraazatricyclo[17.3.1.1^{8,12}]tetracosa-1(23),-8,10,12(24),19,21-hexaene-23,24-diolate ligand and one O atom from a maleate anion. The two pentacoordinated Zn^{II} atoms are linked by two phenolate O atoms. This leads to the formation of a four-membered Zn_2O_2 ring. The molecule exhibits a strong intramolecular O–H···O hydrogen bond, with an O···O distance of 2.480 (2) Å.

Related literature

For related literature, see: Dealwis *et al.* (1995); Burley *et al.* (1990); Roderick & Mathews (1993); Dutta *et al.* (2005); Mandal & Nag (1986); Bazzicalupi *et al.* (1997).



Experimental

Crystal data

$[\text{Zn}_2(\text{C}_{22}\text{H}_{22}\text{N}_4\text{O}_2)_2(\text{C}_4\text{H}_7\text{O}_4)_2]$	$V = 1550.0$ (2) \AA^3
$M_r = 743.37$	$Z = 2$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 9.4233$ (7) \AA	$\mu = 1.61 \text{ mm}^{-1}$
$b = 11.2691$ (8) \AA	$T = 293$ (2) K
$c = 14.6870$ (11) \AA	$0.35 \times 0.30 \times 0.25$ mm
$\beta = 96.3816$ (8)°	

Data collection

Bruker APEX CCD area-detector diffractometer	9199 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	3614 independent reflections
$T_{\min} = 0.548$, $T_{\max} = 0.667$	3166 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.015$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.085$	$\Delta\rho_{\text{max}} = 0.86 \text{ e } \text{\AA}^{-3}$
$S = 1.06$	$\Delta\rho_{\text{min}} = -0.30 \text{ e } \text{\AA}^{-3}$
3614 reflections	
217 parameters	

Table 1
Hydrogen-bond geometry (\AA , °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
O4—H2O···O2	0.91 (4)	1.60 (4)	2.480 (2)	161 (4)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

The authors thank the National Natural Science Foundation of China (grant No. 20471014), the Programme for New Century Excellent Talents in Chinese Universities (grant No. NCET-05-0320), the Fok Ying Tung Education Foundation and the Analysis and Testing Foundation of Northeast Normal University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2073).

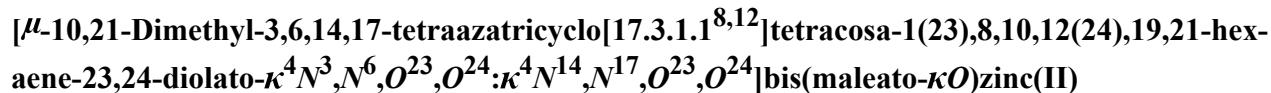
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supplementary materials

Acta Cryst. (2007). E63, m3172-m3173 [doi:10.1107/S1600536807060461]



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Comment

Dinuclear zinc(II) cores have attracted much interest as a result of their significance in biological systems (Dealwis *et al.*, 1995; Burley *et al.*, 1990; Roderick & Mathews, 1993). In addition, some synthetic dinuclear zinc(II) compounds are found to have functions in dephosphorylation (Bazzicalupi *et al.*, 1997). To further widen the scope of application of zinc compounds, there is a need to prepare new series of dinuclear zinc compounds. In this work, a new dinuclear zinc(II) compound has been synthesized and its structure (**I**) is reported here.

As shown in Fig. 1, $[\text{Zn}_2\text{L}(\text{C}_4\text{H}_7\text{O}_4)_2]$ is a centrosymmetric dinuclear zinc compound. The coordination environment around zinc is a square-pyramid with two N atoms and two O atoms from *L* ligand occupying the basal positions and one O atom from maleic acid anion occupying the apical position. In the crystal structure the two O atoms from *L* ligand act as bridging atoms, coordinating two zinc atoms to generate a four-numbered Zn_2O_2 ring. The Zn—O and Zn—N distances and angles are normal (Dutta *et al.*, 2005).

The molecule exhibits a strong intramolecular O4—H20···O2 hydrogen bond with an O4···O2 distance of 2.480 (2) Å.

Experimental

The ligand $\text{C}_{22}\text{H}_{32}\text{N}_4\text{O}_2$ (H_2L) was prepared by the reported procedure (Mandal & Nag, 1986). A mixture of H_2L (0.05 g, 0.13 mmol), $\text{Zn}(\text{OH})_2$ (0.026 g, 0.26 mmol) and maleic acid (0.03 g, 0.26 mmol) in methanol (20 ml) was stirred for 10 min. The resulting solution was filtered. Colorless single crystals were obtained by slow evaporation of the filtrate at room temperature (yield 60%).

Refinement

All H-atoms bound to carbon were refined using a riding model with $d(\text{C—H}) = 0.93\text{--}0.97$ Å, $U_{\text{iso}} = 1.2U_{\text{eq}}$ (C) for aromatic and CH_2 atoms, $U_{\text{iso}} = 1.5U_{\text{eq}}$ (C) for CH_3 atoms. The imino and hydroxy H atoms were located in a difference Fourier map and refined isotropically with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{N, O})$.

supplementary materials

Figures

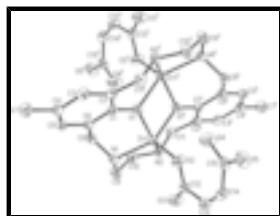
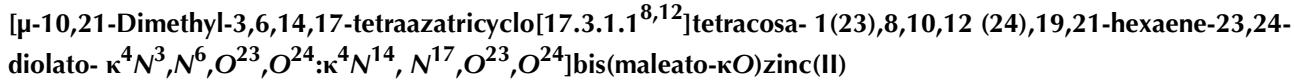


Fig. 1. A view of the molecule of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.



Crystal data

$[Zn_2(C_{22}H_{22}N_4O_2)(C_4H_7O_4)_2]$	$F_{000} = 768$
$M_r = 743.37$	$D_x = 1.593 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
Hall symbol: -P 2yn	$\lambda = 0.71073 \text{ \AA}$
$a = 9.4233 (7) \text{ \AA}$	Cell parameters from 3166 reflections
$b = 11.2691 (8) \text{ \AA}$	$\theta = 2.3\text{--}28.3^\circ$
$c = 14.6870 (11) \text{ \AA}$	$\mu = 1.61 \text{ mm}^{-1}$
$\beta = 96.3816 (8)^\circ$	$T = 293 (2) \text{ K}$
$V = 1550.0 (2) \text{ \AA}^3$	Block, colourless
$Z = 2$	$0.35 \times 0.30 \times 0.25 \text{ mm}$

Data collection

Bruker APEX CCD area-detector diffractometer	3614 independent reflections
Radiation source: fine-focus sealed tube	3166 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.015$
$T = 293(2) \text{ K}$	$\theta_{\max} = 28.3^\circ$
ω scans	$\theta_{\min} = 2.3^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 10$
$T_{\min} = 0.548, T_{\max} = 0.667$	$k = -11 \rightarrow 14$
9199 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.029$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.085$	$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 0.5671P]$

where $P = (F_o^2 + 2F_c^2)/3$
 $S = 1.06$ $(\Delta/\sigma)_{\max} = 0.002$
 3614 reflections $\Delta\rho_{\max} = 0.86 \text{ e } \text{\AA}^{-3}$
 217 parameters $\Delta\rho_{\min} = -0.30 \text{ e } \text{\AA}^{-3}$
 Primary atom site location: structure-invariant direct Extinction correction: none
 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.07989 (2)	1.036471 (19)	0.413650 (13)	0.03090 (9)
C1	0.0822 (2)	0.78759 (17)	0.48550 (13)	0.0347 (4)
C2	0.1329 (2)	0.72414 (18)	0.56441 (14)	0.0367 (4)
C3	0.1730 (2)	0.6061 (2)	0.55428 (16)	0.0441 (5)
H3	0.2051	0.5625	0.6063	0.053*
C4	0.1665 (2)	0.55165 (19)	0.46898 (18)	0.0440 (5)
C5	0.1158 (2)	0.61675 (19)	0.39189 (16)	0.0409 (4)
H5	0.1100	0.5810	0.3345	0.049*
C6	0.07315 (19)	0.73491 (18)	0.39866 (14)	0.0356 (4)
C7	0.2131 (3)	0.4238 (2)	0.4611 (2)	0.0575 (6)
H7A	0.2015	0.4003	0.3979	0.086*
H7B	0.1557	0.3738	0.4952	0.086*
H7C	0.3116	0.4162	0.4852	0.086*
C8	0.0124 (2)	0.80583 (19)	0.31613 (14)	0.0398 (4)
H8A	0.0126	0.7571	0.2617	0.048*
H8B	-0.0859	0.8263	0.3227	0.048*
C9	0.0453 (3)	0.9876 (2)	0.22116 (15)	0.0509 (6)
H9A	0.0122	0.9343	0.1714	0.061*
H9B	0.1250	1.0327	0.2027	0.061*
C10	0.0730 (3)	0.9287 (2)	0.76219 (15)	0.0495 (5)
H10A	0.1564	0.9737	0.7496	0.059*
H10B	0.0988	0.8813	0.8166	0.059*
C11	0.1554 (2)	0.7870 (2)	0.65532 (15)	0.0432 (5)
H11A	0.1874	0.7293	0.7022	0.052*
H11B	0.2314	0.8446	0.6531	0.052*
C12	0.3516 (2)	1.14644 (19)	0.42009 (14)	0.0392 (4)

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C13	0.4910 (2)	1.1892 (2)	0.46576 (17)	0.0485 (5)
H13	0.5474	1.2276	0.4268	0.058*
C14	0.5497 (2)	1.1825 (2)	0.55234 (17)	0.0505 (6)
H14	0.6399	1.2167	0.5623	0.061*
C15	0.4994 (2)	1.1313 (2)	0.63603 (16)	0.0484 (5)
N1	0.09452 (19)	0.91689 (17)	0.30383 (11)	0.0379 (4)
N2	0.0277 (2)	0.84905 (16)	0.68315 (11)	0.0378 (4)
O1	0.04349 (18)	0.90058 (12)	0.49375 (10)	0.0441 (4)
O2	0.27011 (17)	1.09045 (18)	0.46986 (11)	0.0550 (4)
O3	0.3184 (2)	1.1678 (2)	0.33987 (12)	0.0682 (6)
O4	0.3731 (2)	1.0827 (2)	0.63265 (13)	0.0737 (6)
O5	0.5765 (2)	1.1369 (2)	0.70789 (12)	0.0677 (5)
H2O	0.318 (4)	1.079 (4)	0.578 (3)	0.102*
HN1	0.181 (4)	0.898 (4)	0.296 (3)	0.102*
HN2	-0.035 (4)	0.803 (3)	0.698 (3)	0.102*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03147 (13)	0.03791 (14)	0.02267 (12)	-0.00489 (8)	0.00010 (8)	0.00140 (8)
C1	0.0344 (9)	0.0329 (9)	0.0379 (10)	-0.0010 (7)	0.0089 (8)	0.0004 (8)
C2	0.0323 (9)	0.0385 (10)	0.0392 (10)	-0.0019 (8)	0.0038 (8)	0.0028 (8)
C3	0.0371 (10)	0.0409 (11)	0.0539 (12)	0.0038 (9)	0.0038 (9)	0.0081 (10)
C4	0.0349 (11)	0.0368 (11)	0.0613 (14)	0.0011 (8)	0.0100 (10)	-0.0013 (9)
C5	0.0344 (10)	0.0402 (11)	0.0494 (11)	-0.0014 (8)	0.0104 (9)	-0.0088 (9)
C6	0.0294 (9)	0.0375 (10)	0.0408 (10)	-0.0009 (7)	0.0076 (7)	-0.0019 (8)
C7	0.0555 (14)	0.0392 (12)	0.0793 (18)	0.0096 (11)	0.0141 (13)	0.0002 (12)
C8	0.0355 (10)	0.0463 (11)	0.0367 (10)	0.0021 (8)	-0.0003 (8)	-0.0082 (8)
C9	0.0672 (16)	0.0579 (14)	0.0270 (10)	0.0052 (12)	0.0027 (10)	-0.0011 (9)
C10	0.0617 (14)	0.0528 (12)	0.0307 (10)	0.0034 (11)	-0.0089 (9)	-0.0002 (9)
C11	0.0390 (10)	0.0478 (12)	0.0406 (11)	0.0009 (9)	-0.0055 (8)	0.0026 (9)
C12	0.0336 (10)	0.0443 (11)	0.0394 (11)	0.0002 (8)	0.0031 (8)	-0.0005 (8)
C13	0.0304 (10)	0.0602 (14)	0.0553 (13)	-0.0073 (9)	0.0073 (9)	0.0080 (11)
C14	0.0290 (10)	0.0620 (14)	0.0587 (14)	-0.0079 (10)	-0.0033 (9)	-0.0027 (11)
C15	0.0411 (11)	0.0588 (14)	0.0438 (12)	0.0037 (10)	-0.0021 (9)	-0.0147 (10)
N1	0.0401 (9)	0.0457 (9)	0.0277 (8)	0.0045 (8)	0.0030 (7)	0.0015 (7)
N2	0.0471 (10)	0.0396 (9)	0.0257 (8)	-0.0017 (7)	-0.0010 (7)	-0.0001 (6)
O1	0.0686 (10)	0.0315 (7)	0.0355 (7)	0.0069 (6)	0.0215 (7)	0.0050 (6)
O2	0.0401 (8)	0.0801 (12)	0.0419 (8)	-0.0243 (8)	-0.0085 (7)	0.0132 (8)
O3	0.0540 (10)	0.1097 (16)	0.0403 (9)	-0.0140 (10)	0.0023 (8)	0.0091 (10)
O4	0.0521 (11)	0.1292 (19)	0.0382 (9)	-0.0245 (12)	-0.0023 (8)	0.0104 (11)
O5	0.0567 (11)	0.0953 (15)	0.0468 (10)	0.0056 (10)	-0.0138 (8)	-0.0173 (10)

Geometric parameters (\AA , $^\circ$)

Zn1—O2	1.9838 (15)	C9—C10 ⁱ	1.501 (4)
Zn1—O1	1.9840 (14)	C9—H9A	0.9700
Zn1—O1 ⁱ	2.0140 (14)	C9—H9B	0.9700

Zn1—N2 ⁱ	2.0960 (17)	C10—N2	1.492 (3)
Zn1—N1	2.1181 (18)	C10—C9 ⁱ	1.501 (4)
C1—O1	1.334 (2)	C10—H10A	0.9700
C1—C2	1.400 (3)	C10—H10B	0.9700
C1—C6	1.401 (3)	C11—N2	1.488 (3)
C2—C3	1.395 (3)	C11—H11A	0.9700
C2—C11	1.505 (3)	C11—H11B	0.9700
C3—C4	1.390 (3)	C12—O3	1.209 (3)
C3—H3	0.9300	C12—O2	1.283 (3)
C4—C5	1.389 (3)	C12—C13	1.488 (3)
C4—C7	1.514 (3)	C13—C14	1.331 (3)
C5—C6	1.397 (3)	C13—H13	0.9300
C5—H5	0.9300	C14—C15	1.482 (4)
C6—C8	1.510 (3)	C14—H14	0.9300
C7—H7A	0.9600	C15—O5	1.214 (3)
C7—H7B	0.9600	C15—O4	1.306 (3)
C7—H7C	0.9600	N1—HN1	0.86 (4)
C8—N1	1.493 (3)	N2—Zn1 ⁱ	2.0960 (17)
C8—H8A	0.9700	N2—HN2	0.83 (4)
C8—H8B	0.9700	O1—Zn1 ⁱ	2.0140 (14)
C9—N1	1.483 (3)	O4—H2O	0.91 (4)
O2—Zn1—O1	101.40 (7)	C10 ⁱ —C9—H9B	109.2
O2—Zn1—O1 ⁱ	100.00 (7)	H9A—C9—H9B	107.9
O1—Zn1—O1 ⁱ	73.78 (6)	N2—C10—C9 ⁱ	110.56 (19)
O2—Zn1—N2 ⁱ	116.11 (7)	N2—C10—H10A	109.5
O1—Zn1—N2 ⁱ	140.78 (7)	C9 ⁱ —C10—H10A	109.5
O1 ⁱ —Zn1—N2 ⁱ	88.23 (6)	N2—C10—H10B	109.5
O2—Zn1—N1	112.32 (8)	C9 ⁱ —C10—H10B	109.5
O1—Zn1—N1	89.46 (6)	H10A—C10—H10B	108.1
O1 ⁱ —Zn1—N1	146.07 (7)	N2—C11—C2	115.23 (16)
N2 ⁱ —Zn1—N1	86.71 (7)	N2—C11—H11A	108.5
O1—C1—C2	118.95 (18)	C2—C11—H11A	108.5
O1—C1—C6	119.84 (18)	N2—C11—H11B	108.5
C2—C1—C6	121.20 (18)	C2—C11—H11B	108.5
C3—C2—C1	118.04 (19)	H11A—C11—H11B	107.5
C3—C2—C11	121.99 (19)	O3—C12—O2	123.2 (2)
C1—C2—C11	119.71 (18)	O3—C12—C13	119.6 (2)
C4—C3—C2	122.1 (2)	O2—C12—C13	117.19 (18)
C4—C3—H3	118.9	C14—C13—C12	131.6 (2)
C2—C3—H3	118.9	C14—C13—H13	114.2
C5—C4—C3	118.56 (19)	C12—C13—H13	114.2
C5—C4—C7	121.1 (2)	C13—C14—C15	132.6 (2)
C3—C4—C7	120.3 (2)	C13—C14—H14	113.7
C4—C5—C6	121.4 (2)	C15—C14—H14	113.7
C4—C5—H5	119.3	O5—C15—O4	120.6 (2)
C6—C5—H5	119.3	O5—C15—C14	119.0 (2)

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C5—C6—C1	118.66 (19)	O4—C15—C14	120.4 (2)
C5—C6—C8	122.23 (19)	C9—N1—C8	115.51 (18)
C1—C6—C8	119.06 (18)	C9—N1—Zn1	103.92 (13)
C4—C7—H7A	109.5	C8—N1—Zn1	111.27 (12)
C4—C7—H7B	109.5	C9—N1—HN1	104 (3)
H7A—C7—H7B	109.5	C8—N1—HN1	109 (3)
C4—C7—H7C	109.5	Zn1—N1—HN1	114 (3)
H7A—C7—H7C	109.5	C11—N2—C10	109.06 (17)
H7B—C7—H7C	109.5	C11—N2—Zn1 ⁱ	116.63 (13)
N1—C8—C6	112.68 (16)	C10—N2—Zn1 ⁱ	103.46 (13)
N1—C8—H8A	109.1	C11—N2—HN2	114 (3)
C6—C8—H8A	109.1	C10—N2—HN2	109 (3)
N1—C8—H8B	109.1	Zn1 ⁱ —N2—HN2	105 (3)
C6—C8—H8B	109.1	C1—O1—Zn1	128.02 (12)
H8A—C8—H8B	107.8	C1—O1—Zn1 ⁱ	125.58 (12)
N1—C9—C10 ⁱ	112.01 (18)	Zn1—O1—Zn1 ⁱ	106.22 (6)
N1—C9—H9A	109.2	C12—O2—Zn1	118.93 (13)
C10 ⁱ —C9—H9A	109.2	C15—O4—H2O	119 (3)
N1—C9—H9B	109.2		
O1—C1—C2—C3	−179.92 (18)	O1—Zn1—N1—C9	150.36 (15)
C6—C1—C2—C3	−0.6 (3)	O1 ⁱ —Zn1—N1—C9	91.32 (17)
O1—C1—C2—C11	−5.6 (3)	N2 ⁱ —Zn1—N1—C9	9.41 (15)
C6—C1—C2—C11	173.73 (18)	O2—Zn1—N1—C8	127.55 (13)
C1—C2—C3—C4	1.2 (3)	O1—Zn1—N1—C8	25.43 (13)
C11—C2—C3—C4	−173.0 (2)	O1 ⁱ —Zn1—N1—C8	−33.61 (19)
C2—C3—C4—C5	−1.3 (3)	N2 ⁱ —Zn1—N1—C8	−115.52 (14)
C2—C3—C4—C7	179.1 (2)	C2—C11—N2—C10	−167.27 (18)
C3—C4—C5—C6	0.7 (3)	C2—C11—N2—Zn1 ⁱ	−50.6 (2)
C7—C4—C5—C6	−179.7 (2)	C9 ⁱ —C10—N2—C11	167.38 (19)
C4—C5—C6—C1	−0.1 (3)	C9 ⁱ —C10—N2—Zn1 ⁱ	42.6 (2)
C4—C5—C6—C8	−177.62 (19)	C2—C1—O1—Zn1	139.17 (16)
O1—C1—C6—C5	179.37 (18)	C6—C1—O1—Zn1	−40.2 (3)
C2—C1—C6—C5	0.1 (3)	C2—C1—O1—Zn1 ⁱ	−46.3 (2)
O1—C1—C6—C8	−3.0 (3)	C6—C1—O1—Zn1 ⁱ	134.36 (16)
C2—C1—C6—C8	177.67 (18)	O2—Zn1—O1—C1	−87.41 (18)
C5—C6—C8—N1	−123.2 (2)	O1 ⁱ —Zn1—O1—C1	175.4 (2)
C1—C6—C8—N1	59.3 (2)	N2 ⁱ —Zn1—O1—C1	109.40 (18)
C3—C2—C11—N2	−129.6 (2)	N1—Zn1—O1—C1	25.27 (18)
C1—C2—C11—N2	56.3 (3)	O2—Zn1—O1—Zn1 ⁱ	97.23 (9)
O3—C12—C13—C14	176.7 (3)	O1 ⁱ —Zn1—O1—Zn1 ⁱ	0.0
O2—C12—C13—C14	−1.5 (4)	N2 ⁱ —Zn1—O1—Zn1 ⁱ	−65.96 (12)
C12—C13—C14—C15	−0.5 (5)	N1—Zn1—O1—Zn1 ⁱ	−150.10 (8)
C13—C14—C15—O5	179.6 (3)	O3—C12—O2—Zn1	−0.3 (3)
C13—C14—C15—O4	−1.5 (5)	C13—C12—O2—Zn1	177.79 (16)

C10 ⁱ —C9—N1—C8	86.0 (2)	O1—Zn1—O2—C12	154.68 (18)
C10 ⁱ —C9—N1—Zn1	−36.2 (2)	O1 ⁱ —Zn1—O2—C12	−130.03 (18)
C6—C8—N1—C9	176.86 (17)	N2 ⁱ —Zn1—O2—C12	−37.1 (2)
C6—C8—N1—Zn1	−65.00 (18)	N1—Zn1—O2—C12	60.5 (2)
O2—Zn1—N1—C9	−107.52 (15)		

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

Hydrogen-bond geometry (\AA , °)

$D\text{—H}\cdots A$	$D\text{—H}$	$\text{H}\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
O4—H2O···O2	0.91 (4)	1.60 (4)	2.480 (2)	161 (4)

supplementary materials

Fig. 1

