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(5,5′-Dicarboxybiphenyl-2,2′-dicarboxylato-$\kappa^2O^2,O^{2'}$)bis(1,10-phenanthroline-κ^2N,N')zinc(II) dihydrate

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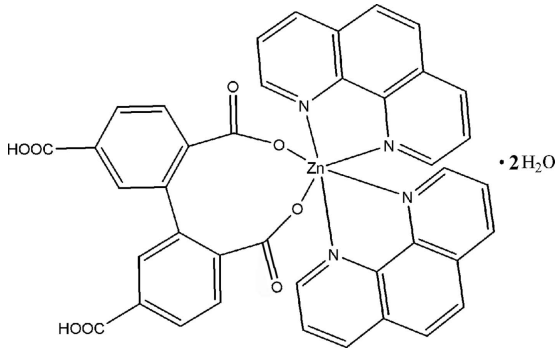
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.058; wR factor = 0.125; data-to-parameter ratio = 13.7.

In the title compound, $[Zn(C_{16}H_8O_8)(C_{12}H_8N_2)_2]\cdot 2H_2O$, the Zn^{II} atom is located on a twofold rotation axis and is six-coordinated by two O atoms from a 5,5′-dicarboxybiphenyl-2,2′-dicarboxylate ligand and four N atoms from two 1,10-phenanthroline molecules in a distorted octahedral geometry. The crystal structure involves O—H···O hydrogen bonds.

Related literature

For related literature, see: Che *et al.* (2006); Chen *et al.* (2008); Lehn (1990); Zang *et al.* (2006).



Experimental

Crystal data

$[Zn(C_{16}H_8O_8)(C_{12}H_8N_2)_2]\cdot 2H_2O$
M_r = 790.03
Monoclinic, $C2/c$
a = 16.901 (5) Å
b = 9.473 (3) Å
c = 22.126 (7) Å
β = 96.429 (5)°
V = 3520.4 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 293 (2) K
0.26 × 0.22 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.817, T_{max} = 0.853
9664 measured reflections
3487 independent reflections
2437 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.124
S = 1.04
3487 reflections
255 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.102 (2)	Zn1—N2	2.199 (3)
Zn1—N1	2.130 (3)		
O1—Zn1—O1^{i}	106.16 (11)	N1—Zn1—N2	76.44 (13)
O1—Zn1—N1^{i}	98.70 (10)	O1—Zn1—N2^{i}	82.94 (10)
O1—Zn1—N1	87.72 (10)	N1—Zn1—N2^{i}	96.08 (12)
N1^{i}—Zn1—N1	169.36 (16)	N2—Zn1—N2^{i}	92.23 (15)
O1—Zn1—N2	162.88 (11)		

Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2^{ii}	0.82	1.74	2.538 (3)	162
O1W—H1B···O4^{iii}	0.86 (3)	2.24 (2)	2.966 (4)	143 (3)
O1W—H1A···O2	0.85 (3)	2.00 (2)	2.808 (4)	159 (4)

Symmetry codes: (ii) $x+\frac{1}{2}, y-\frac{1}{2}, z$; (iii) $-x+1, -y, -z+2$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2133).

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supporting information

Acta Cryst. (2008). E**64**, m855 [doi:10.1107/S1600536808015742]

(5,5′-Dicarboxybiphenyl-2,2′-dicarboxylato-$\kappa^2O^2,O^{2'}$)bis(1,10-phenanthroline-κ^2N,N')zinc(II) dihydrate

Rui-Zhan Chen, Fei-Jun Guo and Fan-Lei Meng

S1. Comment

In the construction of new coordination polymers, multi-carboxylates act as multifunctional organic ligands not only due to their various coordination modes, resulting from fully or partially deprotonated sites, to allow for the large diversity in topologies, but also due to the ability to act as hydrogen-bond acceptors and donors to assemble supramolecular structures (Che *et al.*, 2006; Chen *et al.*, 2008; Lehn, 1990). We chose biphenyl-2,5,2′,5′-tetracarboxylic acid (H_4bptc) as a bridging ligand, 1,10-phenanthroline (phen) as a neutral ligand, and zinc(II) as a metal center, generating the title compound. We report here its crystal structure.

In the title compound, the Zn^{II} atom, lying on a twofold rotation axis, is six-coordinated by two O atoms from one H_2bptc ligand and four N atoms from two phen molecules in a distorted octahedral geometry (Fig. 1). The twofold rotation axis passes through the midpoint of the bond connecting two benzene rings of the H_2bptc ligand. The bond lengths are within the normal ranges (Table 1) (Zang *et al.*, 2006). The crystal structure involves O—H···O hydrogen bonds between the carboxylate O atoms and water molecules (Table 2).

S2. Experimental

A mixture of $ZnCl_2.2H_2O$ (0.017 g, 0.1 mmol), H_4bptc (0.066 g, 0.2 mmol), phen (0.040 g, 0.2 mmol) and H_2O(15 ml) in a 25 ml Teflon-lined stainless steel reactor was heated from 298 to 443 K in 2 h and a constant temperature was maintained at 443 K for 72 h. After cooling to 298 K, colorless crystals of the title compound were obtained from the reaction.

S3. Refinement

H atoms bonded to C atoms and carboxylate O atom were positioned geometrically and refined as riding atoms, with C—H = 0.93 and O—H = 0.82 Å and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O). The water H-atoms were located from a difference Fourier map and refined with a distance restraint of O—H = 0.85 (1) Å and U_{iso}(H) = 0.064 Å^2.

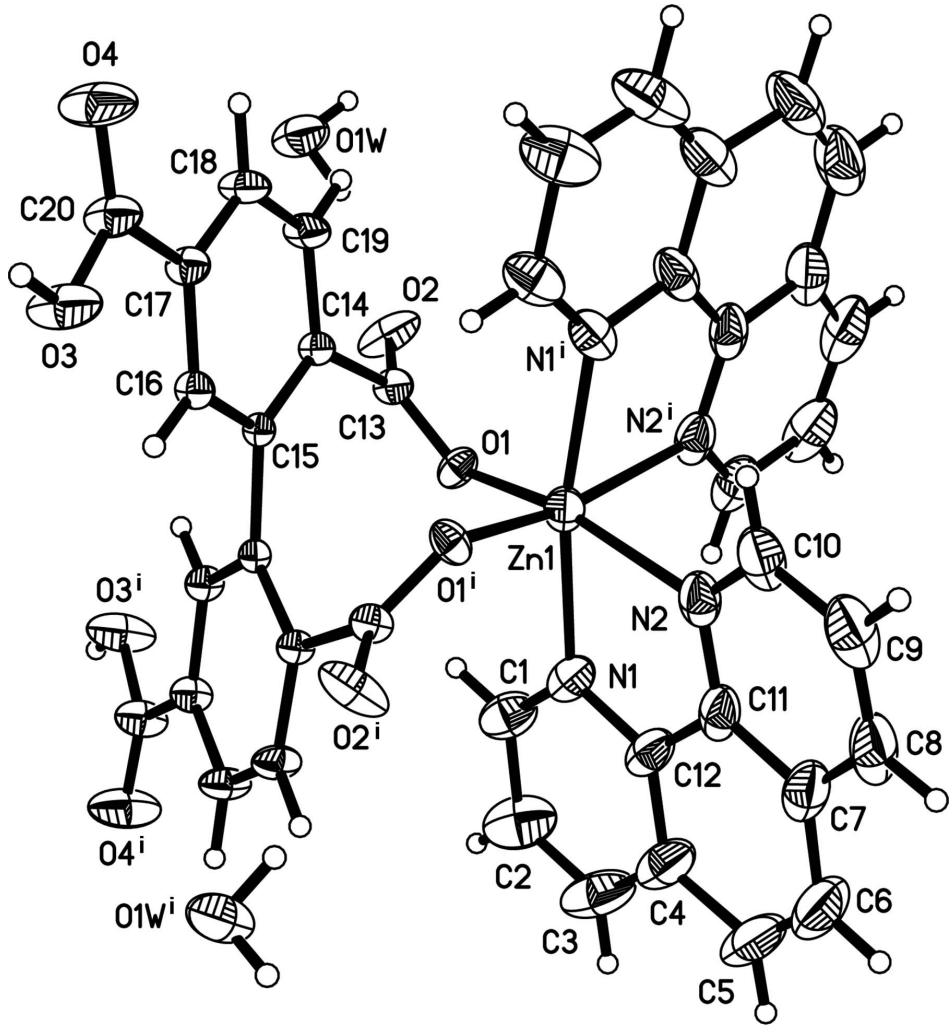

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) 1-x, y, 1.5-z.]

(5,5′-Dicarboxybiphenyl-2,2′-dicarboxylato-$\kappa^2O^2,O^{2'}$)bis(1,10- phenanthroline-κ^2N,N')zinc(II) dihydrate

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$a = 16.901\ (5)$ Å
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$c = 22.126\ (7)$ Å
$\beta = 96.429\ (5)°$
$V = 3520.4\ (19)$ Å^3
$Z = 4$
$F(000) = 1624$
$D_x = 1.491$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3487 reflections
$\theta = 2.0–26.0°$
$\mu = 0.77$ mm^{-1}
$T = 293$ K
Block, colorless
0.26 × 0.22 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.817, T_{max} = 0.853
9664 measured reflections
3487 independent reflections
2437 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 26.2°, θ_{min} = 1.9°
h = −20→18
k = −11→11
l = −21→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.125
S = 1.04
3487 reflections
255 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2 + 0.8309P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3739 (2)	0.3651 (5)	0.63923 (18)	0.0637 (11)
H1	0.3543	0.2958	0.6634	0.076*
C2	0.3354 (3)	0.3873 (6)	0.5804 (2)	0.0880 (16)
H2	0.2913	0.3337	0.5656	0.106*
C3	0.3645 (3)	0.4896 (6)	0.5454 (2)	0.0926 (17)
H3	0.3390	0.5077	0.5067	0.111*
C4	0.4311 (3)	0.5664 (5)	0.5667 (2)	0.0762 (14)
C5	0.4663 (4)	0.6727 (6)	0.5317 (2)	0.0988 (19)
H5	0.4424	0.6948	0.4929	0.119*
C6	0.5326 (4)	0.7401 (6)	0.5538 (3)	0.106 (2)
H6	0.5542	0.8074	0.5298	0.127*
C7	0.5713 (3)	0.7116 (4)	0.6134 (2)	0.0776 (14)
C8	0.6414 (4)	0.7740 (5)	0.6377 (3)	0.098 (2)
H8	0.6659	0.8408	0.6152	0.117*
C9	0.6744 (3)	0.7386 (5)	0.6936 (3)	0.0906 (17)
H9	0.7222	0.7793	0.7098	0.109*
C10	0.6361 (3)	0.6400 (4)	0.7274 (2)	0.0722 (13)
H10	0.6593	0.6164	0.7661	0.087*
C11	0.5368 (3)	0.6116 (4)	0.6493 (2)	0.0600 (11)

C12	0.4662 (3)	0.5378 (4)	0.62567 (18)	0.0588 (11)
C13	0.40756 (18)	0.1983 (3)	0.81456 (14)	0.0328 (7)
C14	0.47901 (16)	0.1060 (3)	0.82887 (12)	0.0264 (7)
C15	0.51756 (16)	0.0460 (3)	0.78249 (12)	0.0240 (6)
C16	0.58975 (17)	−0.0230 (3)	0.79802 (13)	0.0299 (7)
H16	0.6169	−0.0613	0.7676	0.036*
C17	0.62178 (18)	−0.0353 (3)	0.85843 (14)	0.0335 (7)
C18	0.58141 (19)	0.0192 (4)	0.90393 (14)	0.0421 (9)
H18	0.6021	0.0094	0.9445	0.051*
C19	0.51007 (18)	0.0882 (3)	0.88893 (13)	0.0383 (8)
H19	0.4824	0.1235	0.9197	0.046*
C20	0.6999 (2)	−0.1096 (4)	0.87475 (16)	0.0460 (9)
N1	0.43688 (18)	0.4390 (3)	0.66158 (13)	0.0510 (8)
N2	0.5682 (2)	0.5791 (3)	0.70633 (15)	0.0563 (8)
O1	0.40798 (12)	0.2849 (2)	0.77191 (9)	0.0370 (5)
O2	0.35134 (14)	0.1861 (3)	0.84667 (11)	0.0646 (8)
O1W	0.33466 (18)	0.0544 (3)	0.95823 (12)	0.0704 (8)
O3	0.73266 (15)	−0.1494 (3)	0.82746 (11)	0.0707 (9)
H3A	0.7749	−0.1893	0.8384	0.106*
O4	0.72855 (15)	−0.1289 (3)	0.92612 (11)	0.0786 (10)
Zn1	0.5000	0.41820 (6)	0.7500	0.0430 (2)
H1B	0.315 (2)	0.112 (3)	0.9823 (14)	0.064*
H1A	0.333 (2)	0.110 (3)	0.9282 (12)	0.064*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.053 (3)	0.081 (3)	0.058 (3)	0.011 (2)	0.009 (2)	0.017 (2)
C2	0.054 (3)	0.135 (5)	0.074 (3)	0.021 (3)	0.002 (2)	0.021 (3)
C3	0.085 (4)	0.133 (5)	0.061 (3)	0.046 (4)	0.016 (3)	0.038 (3)
C4	0.092 (4)	0.076 (3)	0.065 (3)	0.033 (3)	0.030 (3)	0.029 (3)
C5	0.145 (6)	0.088 (4)	0.072 (4)	0.041 (4)	0.049 (4)	0.042 (3)
C6	0.168 (6)	0.065 (4)	0.097 (5)	0.018 (4)	0.071 (4)	0.030 (3)
C7	0.116 (4)	0.045 (3)	0.084 (4)	0.007 (3)	0.065 (3)	0.006 (2)
C8	0.151 (6)	0.051 (3)	0.109 (5)	−0.032 (3)	0.093 (4)	−0.018 (3)
C9	0.113 (4)	0.068 (3)	0.104 (4)	−0.040 (3)	0.071 (4)	−0.032 (3)
C10	0.093 (4)	0.052 (2)	0.081 (3)	−0.023 (2)	0.047 (3)	−0.020 (2)
C11	0.083 (3)	0.035 (2)	0.070 (3)	0.007 (2)	0.044 (2)	−0.0001 (19)
C12	0.076 (3)	0.051 (2)	0.056 (3)	0.027 (2)	0.033 (2)	0.0180 (19)
C13	0.0281 (18)	0.0396 (18)	0.0312 (18)	0.0106 (14)	0.0054 (14)	0.0015 (15)
C14	0.0225 (16)	0.0314 (17)	0.0255 (16)	0.0040 (12)	0.0037 (12)	−0.0001 (12)
C15	0.0231 (16)	0.0238 (15)	0.0253 (16)	0.0002 (11)	0.0036 (12)	0.0000 (11)
C16	0.0247 (17)	0.0352 (17)	0.0304 (18)	0.0077 (13)	0.0056 (13)	−0.0018 (13)
C17	0.0262 (18)	0.0431 (18)	0.0310 (18)	0.0093 (14)	0.0018 (13)	0.0017 (14)
C18	0.039 (2)	0.063 (2)	0.0236 (18)	0.0165 (17)	0.0000 (14)	−0.0008 (16)
C19	0.0358 (19)	0.054 (2)	0.0266 (17)	0.0185 (16)	0.0097 (14)	−0.0025 (15)
C20	0.033 (2)	0.070 (3)	0.035 (2)	0.0191 (17)	0.0034 (16)	0.0049 (17)
N1	0.051 (2)	0.0519 (19)	0.052 (2)	0.0120 (16)	0.0165 (15)	0.0146 (15)

N2	0.072 (2)	0.0382 (17)	0.066 (2)	−0.0056 (17)	0.0362 (18)	−0.0067 (16)
O1	0.0319 (13)	0.0374 (12)	0.0422 (13)	0.0101 (10)	0.0063 (10)	0.0116 (10)
O2	0.0449 (16)	0.098 (2)	0.0564 (17)	0.0427 (15)	0.0294 (12)	0.0411 (15)
O1W	0.079 (2)	0.088 (2)	0.0457 (19)	0.0195 (17)	0.0126 (15)	0.0143 (15)
O3	0.0530 (17)	0.121 (2)	0.0388 (15)	0.0559 (17)	0.0072 (12)	0.0098 (15)
O4	0.0610 (19)	0.133 (3)	0.0394 (16)	0.0561 (18)	−0.0040 (13)	0.0029 (16)
Zn1	0.0470 (4)	0.0373 (3)	0.0467 (4)	0.000	0.0144 (3)	0.000

Geometric parameters (Å, º)

C1—N1	1.323 (5)	C13—O2	1.254 (4)
C1—C2	1.405 (6)	C13—C14	1.496 (4)
C1—H1	0.9300	C14—C19	1.383 (4)
C2—C3	1.366 (7)	C14—C15	1.396 (4)
C2—H2	0.9300	C15—C16	1.393 (4)
C3—C4	1.378 (7)	C15—C15^{i}	1.493 (5)
C3—H3	0.9300	C16—C17	1.390 (4)
C4—C12	1.399 (6)	C16—H16	0.9300
C4—C5	1.439 (7)	C17—C18	1.378 (4)
C5—C6	1.334 (7)	C17—C20	1.504 (4)
C5—H5	0.9300	C18—C19	1.379 (4)
C6—C7	1.431 (7)	C18—H18	0.9300
C6—H6	0.9300	C19—H19	0.9300
C7—C8	1.378 (7)	C20—O4	1.198 (4)
C7—C11	1.404 (5)	C20—O3	1.294 (4)
C8—C9	1.341 (7)	N1—Zn1	2.130 (3)
C8—H8	0.9300	N2—Zn1	2.199 (3)
C9—C10	1.399 (6)	O1—Zn1	2.102 (2)
C9—H9	0.9300	O1W—H1B	0.86 (3)
C10—N2	1.321 (5)	O1W—H1A	0.85 (3)
C10—H10	0.9300	O3—H3A	0.8200
C11—N2	1.348 (5)	Zn1—O1	2.102 (2)
C11—C12	1.431 (6)	Zn1—N1	2.130 (3)
C12—N1	1.357 (4)	Zn1—N2	2.199 (3)
C13—O1	1.251 (3)		

N1—C1—C2	122.5 (4)	C16—C15—C14	118.5 (3)
N1—C1—H1	118.8	C16—C15—C15^{i}	118.7 (3)
C2—C1—H1	118.8	C14—C15—C15^{i}	122.7 (3)
C3—C2—C1	118.2 (5)	C17—C16—C15	120.9 (3)
C3—C2—H2	120.9	C17—C16—H16	119.6
C1—C2—H2	120.9	C15—C16—H16	119.6
C2—C3—C4	120.8 (5)	C18—C17—C16	120.0 (3)
C2—C3—H3	119.6	C18—C17—C20	119.5 (3)
C4—C3—H3	119.6	C16—C17—C20	120.5 (3)
C3—C4—C12	117.5 (4)	C17—C18—C19	119.5 (3)
C3—C4—C5	123.8 (5)	C17—C18—H18	120.2
C12—C4—C5	118.7 (5)	C19—C18—H18	120.2

C6—C5—C4	121.3 (5)	C18—C19—C14	121.1 (3)
C6—C5—H5	119.4	C18—C19—H19	119.5
C4—C5—H5	119.4	C14—C19—H19	119.5
C5—C6—C7	121.7 (5)	O4—C20—O3	124.0 (3)
C5—C6—H6	119.1	O4—C20—C17	123.3 (3)
C7—C6—H6	119.1	O3—C20—C17	112.7 (3)
C8—C7—C11	117.4 (5)	C1—N1—C12	118.5 (4)
C8—C7—C6	124.2 (5)	C1—N1—Zn1	126.4 (3)
C11—C7—C6	118.3 (5)	C12—N1—Zn1	115.1 (3)
C9—C8—C7	120.2 (5)	C10—N2—C11	117.7 (4)
C9—C8—H8	119.9	C10—N2—Zn1	128.7 (3)
C7—C8—H8	119.9	C11—N2—Zn1	113.5 (3)
C8—C9—C10	119.3 (5)	C13—O1—Zn1	129.41 (19)
C8—C9—H9	120.3	H1B—O1W—H1A	96 (4)
C10—C9—H9	120.3	C20—O3—H3A	109.5
N2—C10—C9	122.6 (5)	O1—Zn1—O1^{i}	106.16 (11)
N2—C10—H10	118.7	O1—Zn1—N1^{i}	98.70 (10)
C9—C10—H10	118.7	O1^{i}—Zn1—N1^{i}	87.72 (10)
N2—C11—C7	122.7 (5)	O1—Zn1—N1	87.72 (10)
N2—C11—C12	117.1 (3)	O1^{i}—Zn1—N1	98.70 (10)
C7—C11—C12	120.2 (5)	N1^{i}—Zn1—N1	169.36 (16)
N1—C12—C4	122.4 (4)	O1—Zn1—N2	162.88 (11)
N1—C12—C11	117.8 (4)	O1^{i}—Zn1—N2	82.94 (10)
C4—C12—C11	119.7 (4)	N1^{i}—Zn1—N2	96.08 (12)
O1—C13—O2	123.8 (3)	N1—Zn1—N2	76.44 (13)
O1—C13—C14	118.1 (3)	O1—Zn1—N2^{i}	82.94 (10)
O2—C13—C14	118.1 (3)	O1^{i}—Zn1—N2^{i}	162.88 (11)
C19—C14—C15	119.9 (3)	N1^{i}—Zn1—N2^{i}	76.44 (13)
C19—C14—C13	119.0 (3)	N1—Zn1—N2^{i}	96.08 (12)
C15—C14—C13	121.0 (2)	N2—Zn1—N2^{i}	92.23 (15)

N1—C1—C2—C3	−0.2 (7)	C16—C17—C20—O4	−176.6 (4)
C1—C2—C3—C4	1.7 (8)	C18—C17—C20—O3	−177.0 (3)
C2—C3—C4—C12	−1.5 (7)	C16—C17—C20—O3	3.8 (5)
C2—C3—C4—C5	178.1 (4)	C2—C1—N1—C12	−1.4 (6)
C3—C4—C5—C6	−177.5 (5)	C2—C1—N1—Zn1	179.3 (3)
C12—C4—C5—C6	2.2 (8)	C4—C12—N1—C1	1.6 (5)
C4—C5—C6—C7	−0.8 (9)	C11—C12—N1—C1	−176.8 (3)
C5—C6—C7—C8	177.4 (5)	C4—C12—N1—Zn1	−179.0 (3)
C5—C6—C7—C11	−1.3 (8)	C11—C12—N1—Zn1	2.6 (4)
C11—C7—C8—C9	0.1 (7)	C9—C10—N2—C11	2.0 (6)
C6—C7—C8—C9	−178.6 (5)	C9—C10—N2—Zn1	178.0 (3)
C7—C8—C9—C10	−1.2 (7)	C7—C11—N2—C10	−3.2 (5)
C8—C9—C10—N2	0.2 (7)	C12—C11—N2—C10	175.9 (3)
C8—C7—C11—N2	2.2 (6)	C7—C11—N2—Zn1	−179.8 (3)
C6—C7—C11—N2	−179.1 (4)	C12—C11—N2—Zn1	−0.8 (4)
C8—C7—C11—C12	−176.9 (4)	O2—C13—O1—Zn1	135.8 (3)
C6—C7—C11—C12	1.9 (6)	C14—C13—O1—Zn1	−42.9 (4)

C3—C4—C12—N1	−0.2 (6)	C13—O1—Zn1—O1^{i}	63.6 (2)
C5—C4—C12—N1	−179.8 (4)	C13—O1—Zn1—N1^{i}	−26.5 (3)
C3—C4—C12—C11	178.2 (4)	C13—O1—Zn1—N1	162.0 (3)
C5—C4—C12—C11	−1.5 (6)	C13—O1—Zn1—N2	−176.0 (3)
N2—C11—C12—N1	−1.2 (5)	C13—O1—Zn1—N2^{i}	−101.6 (3)
C7—C11—C12—N1	177.9 (3)	C1—N1—Zn1—O1	−9.4 (3)
N2—C11—C12—C4	−179.6 (3)	C12—N1—Zn1—O1	171.3 (2)
C7—C11—C12—C4	−0.5 (6)	C1—N1—Zn1—O1^{i}	96.6 (3)
O1—C13—C14—C19	134.7 (3)	C12—N1—Zn1—O1^{i}	−82.7 (2)
O2—C13—C14—C19	−44.2 (4)	C1—N1—Zn1—N1^{i}	−136.8 (3)
O1—C13—C14—C15	−40.9 (4)	C12—N1—Zn1—N1^{i}	43.9 (2)
O2—C13—C14—C15	140.3 (3)	C1—N1—Zn1—N2	177.1 (3)
C19—C14—C15—C16	−4.1 (4)	C12—N1—Zn1—N2	−2.2 (2)
C13—C14—C15—C16	171.4 (3)	C1—N1—Zn1—N2^{i}	−92.1 (3)
C19—C14—C15—C15^{i}	172.4 (2)	C12—N1—Zn1—N2^{i}	88.6 (2)
C13—C14—C15—C15^{i}	−12.1 (4)	C10—N2—Zn1—O1	162.7 (3)
C14—C15—C16—C17	1.7 (4)	C11—N2—Zn1—O1	−21.1 (5)
C15^{i}—C15—C16—C17	−175.0 (2)	C10—N2—Zn1—O1^{i}	−73.9 (3)
C15—C16—C17—C18	1.1 (5)	C11—N2—Zn1—O1^{i}	102.3 (2)
C15—C16—C17—C20	−179.8 (3)	C10—N2—Zn1—N1^{i}	13.1 (3)
C16—C17—C18—C19	−1.3 (5)	C11—N2—Zn1—N1^{i}	−170.7 (2)
C20—C17—C18—C19	179.5 (3)	C10—N2—Zn1—N1	−174.6 (3)
C17—C18—C19—C14	−1.1 (5)	C11—N2—Zn1—N1	1.6 (2)
C15—C14—C19—C18	3.9 (5)	C10—N2—Zn1—N2^{i}	89.7 (3)
C13—C14—C19—C18	−171.7 (3)	C11—N2—Zn1—N2^{i}	−94.1 (3)
C18—C17—C20—O4	2.6 (6)		

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O2^{ii}	0.82	1.74	2.538 (3)	162
O1*W*—H1*B*···O4^{iii}	0.86 (3)	2.24 (2)	2.966 (4)	143 (3)
O1*W*—H1*A*···O2	0.85 (3)	2.00 (2)	2.808 (4)	159 (4)

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