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Poly[[(μ_3-5-aminoisophthalato-κ^3O^1:O^3:N)(1*H*-imidazole-κN^3)zinc] 0.25-hydrate]

Hai-Wei Kuai* and Xiao-Chun Cheng

Faculty of Life Science and Chemical Engineering, Huaiyin Institute of Technology, Huaian 223003, People's Republic of China
Correspondence e-mail: hyitshy@126.com

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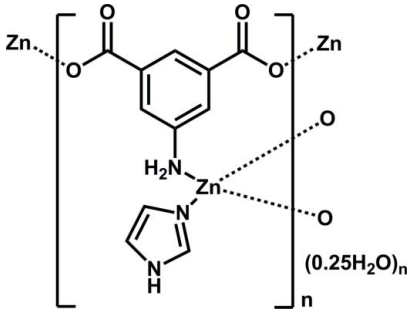
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.048; wR factor = 0.098; data-to-parameter ratio = 13.1.

In the title coordination polymer, $\{[Zn(C_8H_5NO_4)(C_3H_4N_2)]\cdot 0.25H_2O\}_n$, the Zn^{2+} cation has an N_2O_2 donor set involving two carboxylate O atoms from two 5-aminoisophthalate anions, one N atom from a 5-aminoisophthalate anion, and one imidazole N atom displaying a slightly distorted tetrahedral geometry with two additional O-atom neighbours, with Zn-to-ligand distances of 2.711 (2) and 2.717 (2) Å, respectively. Each 5-aminoisophthalate anion acts as a μ_3-bridge linking symmetry-related Zn^{II} ions into a layered polymeric structure parallel to (100). The asymmetric unit also comprises a disordered crystal water molecule located on an inversion centre with 0.25 occupancy. In the crystal, N—H···O hydrogen bonds form a three-dimensional network.

Related literature

For related structures, see: Zhang *et al.* (2007).



Experimental

Crystal data

$[Zn(C_8H_5NO_4)(C_3H_4N_2)]\cdot 0.25H_2O$ M_r = 317.09
Monoclinic, $P2_1/c$
a = 9.6239 (11) Å
b = 10.1916 (11) Å
c = 12.1927 (13) Å
β = 95.146 (2)°
V = 1191.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.08 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.681, T_{max} = 0.706
6327 measured reflections
2340 independent reflections
1542 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.098
S = 1.09
2340 reflections
178 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Table 1
Selected bond lengths (Å).

N2—Zn1	1.983 (3)	Zn1—O4^{i}	1.998 (3)
O2—Zn1	1.989 (2)	Zn1—N1^{ii}	2.082 (3)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O4^{iii}	0.91	2.21	3.018 (4)	147
N1—H1A···O2^{iv}	0.88	2.17	2.943 (4)	146
N3—H3···O3^{v}	0.95	1.88	2.822 (4)	174

Symmetry codes: (iii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (v) $-x+2, y-\frac{1}{2}, -z+\frac{5}{2}$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2000); 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: KP2352).

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supporting information

Acta Cryst. (2011). E**67**, m1835 [https://doi.org/10.1107/S1600536811050045]

Poly[[(μ_3-5-aminoisophthalato-κ^3O^1:O^3:N)(1*H*-imidazole-κN^3)zinc] 0.25-hydrate]

Hai-Wei Kuai and Xiao-Chun Cheng

S1. Comment

5-Aminoisophthalic acid is often used as organic ligand to synthesise complexes with variable coordination modes. Herein, we report the crystal structure of title coordination polymer. The asymmetric unit consists of one zinc ion, one 5-aminoisophthalate anion, one imidazole and partly occupied crystal water. Each Zn ion has a N_2O_2 donor set and is coordinated by two carboxylate O atoms from two 5-aminoisophthalate anions, one N atom from the amino group of 5-aminoisophthalate anion, and one N atom from an imidazole, displaying a slightly distorted tetrahedral geometry (Fig. 1 and Table 1) with the two additional neighbours O1 and O3 with Zn-ligad distances of 2.711 (2) and 2.717 (2) Å, respectively. Each 5-aminoisophthalate anion acts as a μ_3-bridge. So in the structure of title complex, every 5-amino-isophthalate anion links three zinc ions and every zinc ion bridges three 5-aminoisophthalate anions. This kind of connection proceeds infinitely to form a layer (Fig. 2). Whithin the crystal structure, there are N—H···O hydrogen bonds (Table 2).

S2. Experimental

Reaction mixture of zinc nitrate hexahydrate (29.7 mg, 0.1 mmol), 5-aminoisophthalic acid (18.1 mg, 0.1 mmol), imidazole (6.81 mg, 0.1 mmol), and potassium hydroxide (11.2 mg, 0.2 mmol) in 8 mL H_2O was sealed in a 16 mL Teflon-lined stainless steel container and heated to(1) 453 K for 3 days. After cooling to the room temperature, colourless block crystals of the title complex were obtained.

S3. Refinement

The hydrogen atoms in all C atoms were located in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The hydrogen atoms in N or O atoms can be found at reasonable positions in the difference Fourier maps and located there [U_{iso}(H) = 1.2U_{eq}(N or O)].

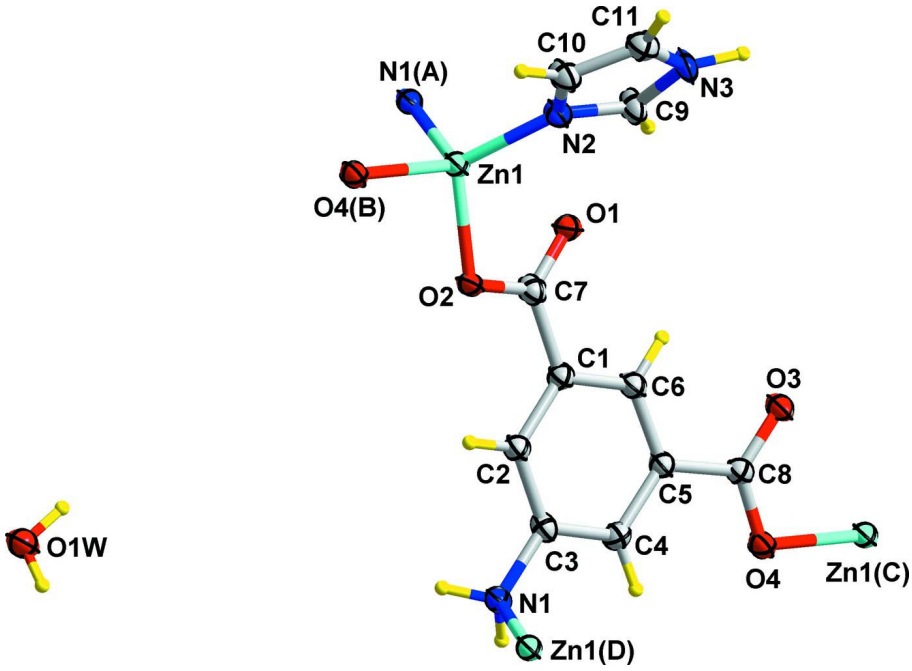

Figure 1

The coordination environment of zinc ion in the title complex with the ellipsoids drawn at the 30% probability level. Symmetry code used: (A) *x*, 1/2 - *y*, 1/2 + *z*; (B) *x*, -1 + *y*, *z*; (C) *x*, 1 + *y*, *z*; (D) *x*, 1/2 - *y*, -1/2 + *z*.

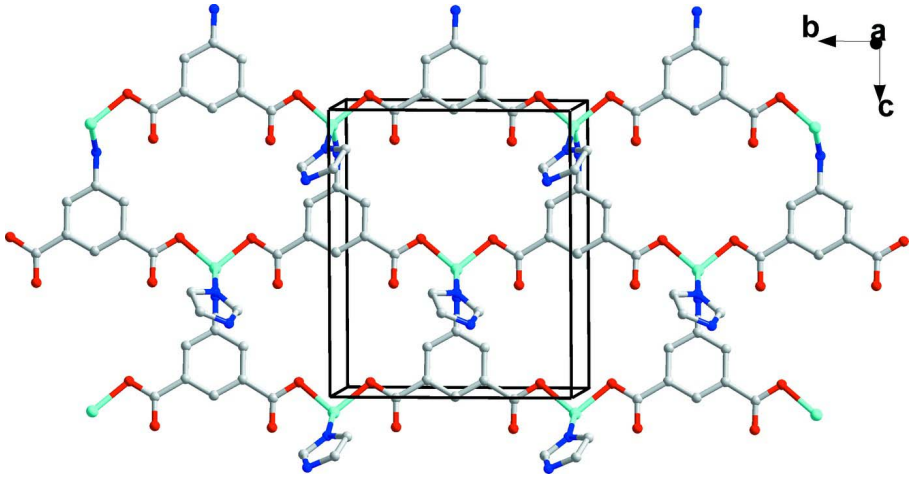

Figure 2

The layer built from infinite connection of zinc ions and 5-aminoisophthalate anions.

Poly[[(μ_3-5-aminoisophthalato-$\kappa^3O^1{:}O^3{:}N$)(1*H*-imidazole-κN^3)zinc] 0.25-hydrate]

Crystal data

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Hall symbol: -P 2ybc
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b = 10.1916 (11) Å
c = 12.1927 (13) Å
β = 95.146 (2)°
V = 1191.1 (2) Å^3
Z = 4
F(000) = 642
D_x = 1.768 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2609 reflections
θ = 2.6–28.0°
μ = 2.08 mm^{-1}
T = 293 K
Block, colourless
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.681, T_{max} = 0.706
6327 measured reflections
2340 independent reflections
1542 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.0°, θ_{min} = 2.1°
h = −11→11
k = −12→12
l = −14→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.098
S = 1.09
2340 reflections
178 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 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.

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.6575 (4)	0.3910 (3)	0.9523 (3)	0.0326 (9)	
C2	0.6177 (4)	0.3912 (4)	0.8394 (3)	0.0351 (9)	
H2	0.6037	0.3123	0.8016	0.042*	
C3	0.5989 (4)	0.5098 (3)	0.7836 (3)	0.0320 (8)	
C4	0.6275 (4)	0.6274 (3)	0.8374 (3)	0.0346 (9)	
H4	0.6188	0.7060	0.7987	0.042*	
C5	0.6696 (4)	0.6277 (3)	0.9507 (3)	0.0330 (9)	
C6	0.6827 (4)	0.5094 (4)	1.0076 (3)	0.0361 (9)	
H6	0.7084	0.5093	1.0830	0.043*	
C7	0.6734 (4)	0.2659 (4)	1.0171 (3)	0.0359 (9)	
C8	0.6970 (4)	0.7532 (4)	1.0138 (3)	0.0350 (9)	
C9	0.9582 (5)	0.1183 (4)	1.2027 (4)	0.0439 (11)	

H9	0.9093	0.1936	1.2188	0.053*	
C10	1.0136 (5)	−0.0654 (4)	1.1370 (3)	0.0441 (10)	
H10	1.0093	−0.1433	1.0972	0.053*	
C11	1.1245 (5)	−0.0237 (4)	1.2012 (4)	0.0449 (10)	
H11	1.2095	−0.0667	1.2149	0.054*	
N1	0.5567 (3)	0.5092 (3)	0.6679 (2)	0.0355 (7)	
H1B	0.4983	0.4405	0.6509	0.043*	
H1A	0.5065	0.5794	0.6488	0.043*	
N2	0.9069 (3)	0.0238 (3)	1.1382 (3)	0.0353 (7)	
N3	1.0886 (4)	0.0935 (3)	1.2423 (3)	0.0438 (9)	
H3	1.1418	0.1496	1.2921	0.053*	
O1	0.6978 (3)	0.2682 (2)	1.1177 (2)	0.0401 (7)	
O2	0.6629 (3)	0.1581 (2)	0.9615 (2)	0.0339 (6)	
O3	0.7375 (3)	0.7512 (2)	1.1132 (2)	0.0438 (7)	
O4	0.6761 (3)	0.8610 (2)	0.9600 (2)	0.0384 (7)	
O1W	0.0000	0.0000	0.5000	0.047 (2)	0.50
H1X	0.0422	0.0359	0.4495	0.056*	0.25
H1Y	0.0453	0.0137	0.5620	0.056*	0.25
Zn1	0.71550 (5)	0.01074 (4)	1.06385 (4)	0.03453 (16)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.034 (2)	0.0284 (18)	0.034 (2)	0.0003 (16)	−0.0028 (18)	−0.0004 (15)
C2	0.035 (2)	0.032 (2)	0.036 (2)	−0.0002 (16)	−0.0064 (17)	−0.0001 (16)
C3	0.0285 (19)	0.035 (2)	0.0310 (19)	0.0022 (16)	−0.0039 (15)	−0.0037 (16)
C4	0.040 (2)	0.029 (2)	0.034 (2)	−0.0010 (16)	−0.0003 (18)	0.0027 (15)
C5	0.034 (2)	0.032 (2)	0.031 (2)	0.0018 (15)	−0.0062 (17)	−0.0021 (15)
C6	0.038 (2)	0.036 (2)	0.032 (2)	0.0021 (16)	−0.0083 (16)	0.0001 (15)
C7	0.035 (2)	0.034 (2)	0.037 (2)	0.0038 (16)	−0.0038 (17)	−0.0024 (17)
C8	0.035 (2)	0.032 (2)	0.037 (2)	−0.0009 (15)	−0.0066 (18)	0.0025 (16)
C9	0.048 (3)	0.0297 (19)	0.051 (3)	0.0036 (18)	−0.014 (2)	−0.0107 (18)
C10	0.049 (3)	0.037 (2)	0.044 (3)	0.0067 (19)	−0.0099 (19)	−0.0063 (18)
C11	0.044 (2)	0.043 (2)	0.046 (3)	0.002 (2)	−0.0061 (19)	0.003 (2)
N1	0.0411 (18)	0.0330 (17)	0.0302 (17)	−0.0026 (14)	−0.0086 (13)	0.0019 (13)
N2	0.0377 (18)	0.0316 (16)	0.0345 (18)	0.0041 (14)	−0.0080 (14)	−0.0050 (14)
N3	0.041 (2)	0.0408 (19)	0.045 (2)	−0.0043 (16)	−0.0191 (17)	−0.0124 (15)
O1	0.0579 (19)	0.0300 (14)	0.0304 (16)	−0.0015 (12)	−0.0078 (13)	0.0032 (11)
O2	0.0494 (17)	0.0292 (13)	0.0213 (12)	0.0004 (12)	−0.0069 (12)	0.0014 (10)
O3	0.0579 (19)	0.0308 (14)	0.0385 (17)	0.0036 (13)	−0.0185 (14)	−0.0028 (12)
O4	0.0510 (18)	0.0314 (15)	0.0303 (14)	0.0001 (12)	−0.0095 (13)	−0.0026 (11)
O1W	0.050 (5)	0.056 (5)	0.034 (4)	0.001 (4)	−0.004 (4)	0.004 (4)
Zn1	0.0402 (3)	0.0300 (3)	0.0312 (3)	0.0001 (2)	−0.00893 (17)	0.0000 (2)

Geometric parameters (Å, º)

C1—C6	1.394 (5)	C9—H9	0.9300
C1—C2	1.396 (5)	C10—C11	1.335 (6)

C1—C7	1.500 (5)	C10—N2	1.372 (5)
C2—C3	1.391 (5)	C10—H10	0.9300
C2—H2	0.9300	C11—N3	1.352 (5)
C3—C4	1.382 (5)	C11—H11	0.9300
C3—N1	1.432 (4)	N1—Zn1^{i}	2.082 (3)
C4—C5	1.405 (5)	N1—H1B	0.9104
C4—H4	0.9300	N1—H1A	0.8832
C5—C6	1.391 (5)	N2—Zn1	1.983 (3)
C5—C8	1.503 (5)	N3—H3	0.9504
C6—H6	0.9300	O2—Zn1	1.989 (2)
C7—O1	1.229 (5)	O4—Zn1^{ii}	1.998 (3)
C7—O2	1.290 (4)	O1W—H1X	0.8500
C8—O3	1.239 (5)	O1W—H1Y	0.8501
C8—O4	1.287 (4)	Zn1—O4^{iii}	1.998 (3)
C9—N2	1.312 (5)	Zn1—N1^{iv}	2.082 (3)
C9—N3	1.327 (5)		

C6—C1—C2	119.8 (3)	C11—C10—N2	110.1 (4)
C6—C1—C7	118.4 (3)	C11—C10—H10	125.0
C2—C1—C7	121.8 (3)	N2—C10—H10	125.0
C3—C2—C1	119.7 (3)	C10—C11—N3	106.3 (4)
C3—C2—H2	120.1	C10—C11—H11	126.9
C1—C2—H2	120.1	N3—C11—H11	126.9
C4—C3—C2	120.6 (3)	C3—N1—Zn1^{i}	116.3 (2)
C4—C3—N1	119.9 (3)	C3—N1—H1B	110.0
C2—C3—N1	119.4 (3)	Zn1^{i}—N1—H1B	105.0
C3—C4—C5	119.8 (3)	C3—N1—H1A	110.9
C3—C4—H4	120.1	Zn1^{i}—N1—H1A	109.4
C5—C4—H4	120.1	H1B—N1—H1A	104.5
C6—C5—C4	119.6 (3)	C9—N2—C10	104.5 (3)
C6—C5—C8	118.6 (3)	C9—N2—Zn1	127.4 (3)
C4—C5—C8	121.8 (3)	C10—N2—Zn1	128.0 (3)
C5—C6—C1	120.3 (3)	C9—N3—C11	107.4 (3)
C5—C6—H6	119.8	C9—N3—H3	123.7
C1—C6—H6	119.8	C11—N3—H3	128.8
O1—C7—O2	122.7 (3)	C7—O2—Zn1	108.0 (2)
O1—C7—C1	120.7 (3)	C8—O4—Zn1^{ii}	108.5 (2)
O2—C7—C1	116.6 (3)	H1X—O1W—H1Y	109.5
O3—C8—O4	122.3 (3)	N2—Zn1—O2	114.21 (12)
O3—C8—C5	120.8 (3)	N2—Zn1—O4^{iii}	117.19 (12)
O4—C8—C5	117.0 (3)	O2—Zn1—O4^{iii}	98.96 (10)
N2—C9—N3	111.7 (3)	N2—Zn1—N1^{iv}	115.47 (13)
N2—C9—H9	124.1	O2—Zn1—N1^{iv}	107.26 (12)
N3—C9—H9	124.1	O4^{iii}—Zn1—N1^{iv}	101.77 (12)

C6—C1—C2—C3	−2.2 (6)	C4—C3—N1—Zn1^{i}	92.1 (4)
C7—C1—C2—C3	177.4 (4)	C2—C3—N1—Zn1^{i}	−84.6 (4)
C1—C2—C3—C4	4.0 (6)	N3—C9—N2—C10	−0.6 (5)

C1—C2—C3—N1	−179.4 (4)	N3—C9—N2—Zn1	177.5 (3)
C2—C3—C4—C5	−3.0 (6)	C11—C10—N2—C9	0.9 (5)
N1—C3—C4—C5	−179.6 (4)	C11—C10—N2—Zn1	−177.2 (3)
C3—C4—C5—C6	0.3 (6)	N2—C9—N3—C11	0.1 (5)
C3—C4—C5—C8	−177.8 (4)	C10—C11—N3—C9	0.5 (5)
C4—C5—C6—C1	1.5 (6)	O1—C7—O2—Zn1	−6.9 (5)
C8—C5—C6—C1	179.6 (4)	C1—C7—O2—Zn1	171.8 (3)
C2—C1—C6—C5	−0.6 (6)	O3—C8—O4—Zn1^{ii}	−1.3 (5)
C7—C1—C6—C5	179.8 (4)	C5—C8—O4—Zn1^{ii}	178.6 (3)
C6—C1—C7—O1	5.4 (6)	C9—N2—Zn1—O2	59.6 (4)
C2—C1—C7—O1	−174.2 (4)	C10—N2—Zn1—O2	−122.8 (3)
C6—C1—C7—O2	−173.3 (3)	C9—N2—Zn1—O4^{iii}	174.6 (3)
C2—C1—C7—O2	7.1 (6)	C10—N2—Zn1—O4^{iii}	−7.7 (4)
C6—C5—C8—O3	3.8 (6)	C9—N2—Zn1—N1^{iv}	−65.5 (4)
C4—C5—C8—O3	−178.1 (4)	C10—N2—Zn1—N1^{iv}	112.2 (3)
C6—C5—C8—O4	−176.1 (4)	C7—O2—Zn1—N2	−58.7 (3)
C4—C5—C8—O4	2.0 (6)	C7—O2—Zn1—O4^{iii}	176.0 (3)
N2—C10—C11—N3	−0.8 (5)	C7—O2—Zn1—N1^{iv}	70.6 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O4^{v}	0.91	2.21	3.018 (4)	147
N1—H1*A*···O2^{vi}	0.88	2.17	2.943 (4)	146
N3—H3···O3^{vii}	0.95	1.88	2.822 (4)	174

Symmetry codes: (v) $-x+1$, $y-1/2$, $-z+3/2$; (vi) $-x+1$, $y+1/2$, $-z+3/2$; (vii) $-x+2$, $y-1/2$, $-z+5/2$.