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Diacetatobis[1,3-bis(benzimidazol-2-yl)-benzene]zinc(II) dihydrate

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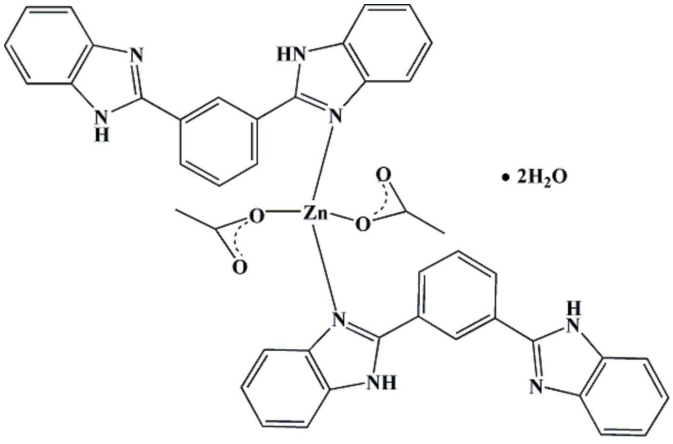
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.027; wR factor = 0.080; data-to-parameter ratio = 15.7.

In the title complex, $[Zn(CH_3COO)_2(C_{20}H_{14}N_4)_2]\cdot 2H_2O$, the Zn^{II} atom, which lies on a crystallographic twofold axis, is coordinated by two O atoms of two acetate ligands and two N atoms from two 1,3-bis(benzimidazol-2-yl)benzene ligands in a distorted tetrahedral geometry. The complex molecules and solvent water molecules are connected *via* O—H···N, O—H···O and N—H···O hydrogen bonds, forming a three-dimensional network.

Related literature

For related literature, see: Meng *et al.* (2007); Chawla *et al.* (1997); Shivakumaraiah *et al.* (2003).



Experimental

Crystal data

$[Zn(C_2H_3O_2)_2(C_{20}H_{14}N_4)_2]\cdot 2H_2O$
M_r = 840.19
Orthorhombic, *Pbcn*
a = 14.1429 (3) Å
b = 16.7005 (4) Å
c = 16.5588 (3) Å
V = 3911.08 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.69 mm^{-1}
T = 153 (2) K
0.42 × 0.29 × 0.26 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer
Absorption correction: multi-scan (Higashi, 1995)
T_{min} = 0.760, T_{max} = 0.841
36097 measured reflections
4483 independent reflections
4032 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.080
S = 1.06
4483 reflections
285 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*N*···O3	0.871 (9)	1.817 (9)	2.6848 (14)	174.0 (17)
N3—H3*N*···O1^{i}	0.858 (9)	2.158 (10)	3.0079 (14)	170.6 (17)
O3—H3*A*O···N4^{ii}	0.839 (9)	1.968 (10)	2.8046 (16)	175 (2)
O3—H3*BO*···O2^{iii}	0.839 (9)	1.991 (10)	2.8295 (15)	179 (2)

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

Data collection: *RAPID-AUTO* (Rigaku 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 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: BG2142).

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supplementary materials

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Diacetatobis[1,3-bis(benzimidazol-2-yl)benzene]zinc(II) dihydrate

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Comment

Benzimidazolyl derivatives and their transition metal complexes have been extensively investigated (Shivakumaraiah *et al.*, 2003). In previous works zinc terephthalate and zinc succinate adducts of 1,3-bis(benzimidazol-2-ylmethyl)benzene have been reported (Meng *et al.*, 2007; Meng *et al.*, 2007). The present work reports the crystal structure of $[Zn(ac)_2(L)_2]\cdot 2H_2O$, (I), where *L* is 1,3-bis(benzimidazol-2-ylmethyl)benzene and *ac* is the acetate ion, which assumes a similar geometry to previously reported complexes in the literature (Meng *et al.*, 2007). (shown in scheme I). The crystal structure of (I) consists of the mononuclear zinc(II) complex and solvato water molecules (Fig. 1). The Zn atom is four-coordinate with two N atoms and two O atoms from the 1,3-bis(benzimidazol-2- ylmethyl)benzene and the acetate ligands, respectively. (Zn—O: 2.0145 (9) Å, Zn—N: 2.0477 (10) Å, coordination angle range: 101.39 (4)- 127.50 (5) °.). The complex and solvent water molecules are connected *via* O—H···N, O—H···O and N—H···O hydrogen bonds to form a three-dimensional network (Table 1).

Experimental

The *N*-heterocycle was prepared according to reported procedure (Chawla & Gill,1997). Zinc nitrate hexahydrate (0.074 g, 0.25 mmol), 1,3-bis(benzimidazolyl-2-ylmethyl)benzene (0.15 g, 0.5 mmol), acetic acid (2 ml) and water (15 ml) were placed in a 23 ml Teflon-lined stainless steel Parr bomb. The bomb was heated at 433 K for 5 days and cooled to room temperature at 5 K h^{-1}.Colorless block crystals were obtained in 15% yield.

Refinement

H atoms attached to oxygen and nitrogen were located in the Fourier maps, and refined with restrained N—H = 0.87 Å, O—H = 0.84 Å distances and free isotropic displacement factots. C—H's were placed at geometrically idealized positions with C—H = 0.95 Å (aromatic), 0.98 Å (methyl) and U_{iso}(H) = 1.2(aromatic), 1.5(methyl)U_{eq}(C).

Figures

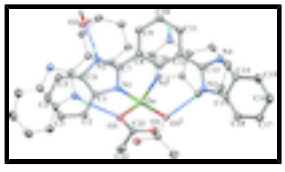


Fig. 1. Molecular unit of (I) showing the coordination geometry of zinc. Displacement ellipsoids drawn at a 50% probability level. The independent part of the molecule drawn with heavy bonds; the (overlapping) symmetry related one, with light bonds. Only H atoms invovled in H-bonding (in dashed lines) have been included.[Symmery code (i): 1 - *x*, *y*, 1/2 - *z*].

Diacetatobis[1,3-bis(benzimidazol-2-yl)benzene]zinc(II) dihydrate

Crystal data

$[Zn(C_2H_3O_2)_2(C_{20}H_{14}N_4)_2]\cdot 2H_2O$	$F(000) = 1744$
$M_r = 840.19$	$D_x = 1.427$ Mg m^{-3}
Orthorhombic, *Pbcn*	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2n 2ab	Cell parameters from 29371 reflections
$a = 14.1429$ (3) Å	$\theta = 3.1$–$27.5°$
$b = 16.7005$ (4) Å	$\mu = 0.69$ mm^{-1}
$c = 16.5588$ (3) Å	$T = 153$ K
$V = 3911.08$ (13) Å^3	Block, colourless
$Z = 4$	0.42 × 0.29 × 0.26 mm

Data collection

Rigaku R-axis SPIDER diffractometer	4483 independent reflections
Radiation source: Rotating Anode	4032 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.022$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
Absorption correction: multi-scan (Higashi, 1995)	$h = -18\rightarrow18$
$T_{min} = 0.761$, $T_{max} = 0.841$	$k = -21\rightarrow21$
36097 measured reflections	$l = -21\rightarrow20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.027$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.080$	$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 1.3144P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
4483 reflections	$\Delta\rho_{max} = 0.35$ e Å^{-3}
285 parameters	$\Delta\rho_{min} = -0.35$ e Å^{-3}
4 restraints	Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0019 (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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn	0.5000	0.200846 (12)	0.2500	0.02036 (8)
O1	0.43810 (7)	0.14750 (5)	0.15455 (5)	0.0247 (2)
O2	0.38164 (9)	0.08183 (6)	0.25947 (6)	0.0346 (2)
N1	0.59696 (7)	0.27314 (6)	0.19415 (6)	0.0199 (2)
N2	0.65402 (8)	0.38807 (6)	0.14616 (6)	0.0229 (2)
N3	0.58881 (8)	0.23678 (7)	0.50153 (7)	0.0239 (2)
N4	0.62077 (8)	0.34087 (7)	0.58182 (7)	0.0270 (2)
C1	0.62241 (8)	0.26200 (7)	0.11345 (7)	0.0200 (2)
C2	0.62085 (9)	0.19356 (8)	0.06492 (8)	0.0243 (3)
H2	0.5999	0.1434	0.0853	0.029*
C3	0.65122 (10)	0.20211 (8)	−0.01423 (8)	0.0287 (3)
H3	0.6509	0.1567	−0.0488	0.034*
C4	0.68243 (10)	0.27583 (9)	−0.04472 (8)	0.0309 (3)
H4	0.7013	0.2794	−0.0997	0.037*
C5	0.68638 (10)	0.34315 (8)	0.00321 (8)	0.0277 (3)
H5	0.7083	0.3930	−0.0172	0.033*
C6	0.65670 (9)	0.33473 (7)	0.08296 (7)	0.0220 (2)
C7	0.61950 (8)	0.34911 (7)	0.21111 (7)	0.0203 (2)
C8	0.61087 (8)	0.38614 (7)	0.29088 (7)	0.0214 (2)
C9	0.59900 (9)	0.46915 (8)	0.30015 (8)	0.0252 (3)
H9	0.5977	0.5031	0.2541	0.030*
C10	0.58919 (10)	0.50126 (8)	0.37704 (9)	0.0284 (3)
H10	0.5807	0.5573	0.3833	0.034*
C11	0.59159 (9)	0.45248 (8)	0.44476 (8)	0.0264 (3)
H11	0.5852	0.4752	0.4971	0.032*
C12	0.60338 (9)	0.36969 (7)	0.43607 (8)	0.0223 (2)
C13	0.60420 (9)	0.31727 (8)	0.50712 (8)	0.0229 (2)
C14	0.61670 (10)	0.27139 (8)	0.62767 (8)	0.0272 (3)
C15	0.63182 (12)	0.26000 (10)	0.71047 (9)	0.0375 (3)
H15	0.6462	0.3038	0.7450	0.045*
C16	0.62511 (14)	0.18299 (11)	0.74009 (9)	0.0405 (4)
H16	0.6352	0.1738	0.7960	0.049*
C17	0.60381 (11)	0.11817 (9)	0.69005 (9)	0.0359 (3)
H17	0.5993	0.0661	0.7128	0.043*
C18	0.58912 (10)	0.12804 (8)	0.60805 (9)	0.0305 (3)
H18	0.5750	0.0840	0.5738	0.037*
C19	0.59617 (9)	0.20575 (8)	0.57840 (8)	0.0248 (3)
C20	0.61400 (9)	0.33772 (7)	0.35896 (8)	0.0219 (3)

H20	0.6236	0.2817	0.3528	0.026*
C21	0.39227 (9)	0.08843 (7)	0.18557 (8)	0.0236 (3)
C22	0.35683 (12)	0.02507 (9)	0.12828 (9)	0.0359 (3)
H22A	0.4009	−0.0202	0.1280	0.043*
H22B	0.3522	0.0475	0.0738	0.043*
H22C	0.2943	0.0067	0.1458	0.043*
H2N	0.6812 (12)	0.4349 (7)	0.1461 (11)	0.043 (5)*
H3N	0.5746 (13)	0.2099 (9)	0.4590 (8)	0.038 (5)*
O3	0.73576 (9)	0.53271 (6)	0.13461 (7)	0.0396 (3)
H3AO	0.7035 (13)	0.5725 (9)	0.1205 (12)	0.055 (6)*
H3BO	0.7795 (12)	0.5466 (12)	0.1658 (11)	0.057 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.02511 (12)	0.01605 (12)	0.01992 (12)	0.000	0.00432 (7)	0.000
O1	0.0304 (5)	0.0176 (4)	0.0262 (5)	−0.0038 (3)	0.0034 (4)	0.0008 (3)
O2	0.0477 (6)	0.0271 (5)	0.0291 (5)	−0.0057 (5)	0.0114 (4)	0.0010 (4)
N1	0.0221 (5)	0.0175 (5)	0.0201 (5)	−0.0003 (4)	0.0027 (4)	−0.0001 (4)
N2	0.0252 (5)	0.0195 (5)	0.0239 (5)	−0.0036 (4)	−0.0017 (4)	0.0035 (4)
N3	0.0279 (6)	0.0229 (5)	0.0208 (5)	−0.0006 (4)	−0.0004 (4)	−0.0012 (4)
N4	0.0323 (6)	0.0267 (6)	0.0219 (5)	−0.0011 (4)	−0.0026 (4)	−0.0012 (4)
C1	0.0184 (5)	0.0218 (6)	0.0196 (6)	0.0018 (4)	0.0014 (4)	0.0022 (5)
C2	0.0241 (6)	0.0228 (6)	0.0260 (6)	0.0022 (5)	0.0035 (5)	−0.0003 (5)
C3	0.0284 (7)	0.0333 (7)	0.0243 (6)	0.0048 (5)	0.0026 (5)	−0.0045 (5)
C4	0.0289 (7)	0.0421 (8)	0.0216 (6)	0.0030 (6)	0.0033 (5)	0.0035 (6)
C5	0.0276 (6)	0.0318 (7)	0.0237 (6)	−0.0022 (5)	0.0004 (5)	0.0090 (5)
C6	0.0205 (6)	0.0229 (6)	0.0226 (6)	−0.0001 (5)	−0.0016 (5)	0.0030 (5)
C7	0.0200 (5)	0.0182 (5)	0.0227 (6)	0.0001 (4)	−0.0008 (5)	0.0020 (5)
C8	0.0205 (6)	0.0202 (6)	0.0236 (6)	−0.0015 (4)	−0.0018 (5)	−0.0015 (5)
C9	0.0278 (6)	0.0191 (6)	0.0287 (6)	−0.0012 (5)	−0.0045 (5)	0.0013 (5)
C10	0.0335 (7)	0.0187 (6)	0.0332 (7)	0.0014 (5)	−0.0055 (6)	−0.0043 (5)
C11	0.0288 (6)	0.0240 (6)	0.0263 (6)	0.0019 (5)	−0.0022 (5)	−0.0063 (5)
C12	0.0211 (6)	0.0219 (6)	0.0239 (6)	−0.0001 (4)	−0.0022 (5)	−0.0009 (5)
C13	0.0219 (6)	0.0233 (6)	0.0233 (6)	0.0009 (5)	−0.0011 (5)	−0.0023 (5)
C14	0.0276 (7)	0.0285 (7)	0.0255 (6)	−0.0005 (5)	−0.0012 (5)	0.0005 (5)
C15	0.0499 (9)	0.0384 (8)	0.0241 (7)	−0.0034 (7)	−0.0054 (6)	−0.0009 (6)
C16	0.0507 (10)	0.0463 (9)	0.0246 (7)	0.0003 (8)	−0.0030 (6)	0.0074 (6)
C17	0.0404 (8)	0.0334 (7)	0.0338 (7)	0.0027 (6)	0.0038 (6)	0.0093 (6)
C18	0.0341 (7)	0.0260 (6)	0.0313 (7)	0.0015 (5)	0.0036 (6)	0.0016 (6)
C19	0.0224 (6)	0.0287 (6)	0.0234 (6)	0.0013 (5)	0.0013 (5)	0.0016 (5)
C20	0.0229 (6)	0.0182 (6)	0.0246 (6)	−0.0002 (4)	−0.0018 (5)	−0.0016 (5)
C21	0.0241 (6)	0.0177 (6)	0.0290 (6)	0.0003 (4)	0.0019 (5)	0.0022 (5)
C22	0.0432 (9)	0.0275 (7)	0.0370 (8)	−0.0092 (6)	−0.0095 (6)	0.0003 (6)
O3	0.0458 (7)	0.0217 (5)	0.0511 (7)	−0.0099 (5)	−0.0215 (5)	0.0115 (5)

Geometric parameters (Å, °)

Zn—O1	2.0145 (9)	C8—C20	1.3880 (17)

Zn—O1^{i}	2.0145 (9)	C8—C9	1.4047 (17)
Zn—N1	2.0477 (10)	C9—C10	1.3886 (19)
Zn—N1^{i}	2.0477 (10)	C9—H9	0.9500
O1—C21	1.2873 (15)	C10—C11	1.386 (2)
O2—C21	1.2378 (16)	C10—H10	0.9500
N1—C7	1.3380 (16)	C11—C12	1.4001 (17)
N1—C1	1.3964 (15)	C11—H11	0.9500
N2—C7	1.3485 (16)	C12—C20	1.3923 (17)
N2—C6	1.3748 (16)	C12—C13	1.4664 (18)
N2—H2N	0.871 (9)	C14—C19	1.3970 (19)
N3—C13	1.3649 (16)	C14—C15	1.4006 (19)
N3—C19	1.3782 (17)	C15—C16	1.380 (2)
N3—H3N	0.858 (9)	C15—H15	0.9500
N4—C13	1.3193 (17)	C16—C17	1.396 (2)
N4—C14	1.3878 (17)	C16—H16	0.9500
C1—C2	1.3974 (17)	C17—C18	1.384 (2)
C1—C6	1.4020 (17)	C17—H17	0.9500
C2—C3	1.3867 (19)	C18—C19	1.3912 (19)
C2—H2	0.9500	C18—H18	0.9500
C3—C4	1.402 (2)	C20—H20	0.9500
C3—H3	0.9500	C21—C22	1.5069 (18)
C4—C5	1.377 (2)	C22—H22A	0.9800
C4—H4	0.9500	C22—H22B	0.9800
C5—C6	1.3928 (18)	C22—H22C	0.9800
C5—H5	0.9500	O3—H3AO	0.839 (9)
C7—C8	1.4636 (17)	O3—H3BO	0.839 (9)
O1—Zn—O1^{i}	127.50 (5)	C11—C10—C9	120.81 (12)
O1—Zn—N1	101.39 (4)	C11—C10—H10	119.6
O1^{i}—Zn—N1	108.91 (4)	C9—C10—H10	119.6
O1—Zn—N1^{i}	108.91 (4)	C10—C11—C12	120.01 (12)
O1^{i}—Zn—N1^{i}	101.39 (4)	C10—C11—H11	120.0
N1—Zn—N1^{i}	107.74 (6)	C12—C11—H11	120.0
C21—O1—Zn	104.16 (8)	C20—C12—C11	119.07 (12)
C7—N1—C1	105.41 (10)	C20—C12—C13	120.39 (11)
C7—N1—Zn	128.60 (8)	C11—C12—C13	120.54 (12)
C1—N1—Zn	121.75 (8)	N4—C13—N3	112.71 (12)
C7—N2—C6	107.73 (10)	N4—C13—C12	125.12 (12)
C7—N2—H2N	126.4 (12)	N3—C13—C12	122.16 (11)
C6—N2—H2N	124.6 (12)	N4—C14—C19	110.20 (12)
C13—N3—C19	107.19 (11)	N4—C14—C15	130.00 (13)
C13—N3—H3N	127.4 (12)	C19—C14—C15	119.79 (13)
C19—N3—H3N	125.3 (12)	C16—C15—C14	117.66 (14)
C13—N4—C14	104.82 (11)	C16—C15—H15	121.2
N1—C1—C2	130.94 (11)	C14—C15—H15	121.2
N1—C1—C6	108.57 (11)	C15—C16—C17	121.78 (14)
C2—C1—C6	120.46 (11)	C15—C16—H16	119.1
C3—C2—C1	117.04 (12)	C17—C16—H16	119.1

C3—C2—H2	121.5	C18—C17—C16	121.50 (14)
C1—C2—H2	121.5	C18—C17—H17	119.3
C2—C3—C4	121.89 (13)	C16—C17—H17	119.3
C2—C3—H3	119.1	C17—C18—C19	116.54 (14)
C4—C3—H3	119.1	C17—C18—H18	121.7
C5—C4—C3	121.48 (12)	C19—C18—H18	121.7
C5—C4—H4	119.3	N3—C19—C18	132.16 (13)
C3—C4—H4	119.3	N3—C19—C14	105.07 (11)
C4—C5—C6	116.86 (12)	C18—C19—C14	122.74 (13)
C4—C5—H5	121.6	C8—C20—C12	121.19 (11)
C6—C5—H5	121.6	C8—C20—H20	119.4
N2—C6—C5	131.66 (12)	C12—C20—H20	119.4
N2—C6—C1	106.12 (11)	O2—C21—O1	121.59 (12)
C5—C6—C1	122.22 (12)	O2—C21—C22	121.30 (12)
N1—C7—N2	112.11 (11)	O1—C21—C22	117.02 (12)
N1—C7—C8	124.76 (11)	C21—C22—H22A	109.5
N2—C7—C8	123.11 (11)	C21—C22—H22B	109.5
C20—C8—C9	119.35 (11)	H22A—C22—H22B	109.5
C20—C8—C7	118.95 (11)	C21—C22—H22C	109.5
C9—C8—C7	121.70 (12)	H22A—C22—H22C	109.5
C10—C9—C8	119.55 (12)	H22B—C22—H22C	109.5
C10—C9—H9	120.2	H3AO—O3—H3BO	110.7 (19)
C8—C9—H9	120.2		
$O1^{i}$—Zn—O1—C21	40.82 (7)	C20—C8—C9—C10	−0.95 (19)
N1—Zn—O1—C21	165.66 (8)	C7—C8—C9—C10	178.68 (12)
$N1^{i}$—Zn—O1—C21	−80.92 (8)	C8—C9—C10—C11	0.4 (2)
O1—Zn—N1—C7	137.44 (10)	C9—C10—C11—C12	−0.4 (2)
$O1^{i}$—Zn—N1—C7	−86.05 (11)	C10—C11—C12—C20	0.97 (19)
$N1^{i}$—Zn—N1—C7	23.14 (9)	C10—C11—C12—C13	−178.81 (12)
O1—Zn—N1—C1	−15.92 (10)	C14—N4—C13—N3	0.51 (15)
$O1^{i}$—Zn—N1—C1	120.59 (9)	C14—N4—C13—C12	−178.52 (12)
$N1^{i}$—Zn—N1—C1	−130.22 (10)	C19—N3—C13—N4	−0.16 (15)
C7—N1—C1—C2	175.43 (13)	C19—N3—C13—C12	178.90 (11)
Zn—N1—C1—C2	−25.88 (18)	C20—C12—C13—N4	160.33 (13)
C7—N1—C1—C6	−2.48 (13)	C11—C12—C13—N4	−19.9 (2)
Zn—N1—C1—C6	156.20 (8)	C20—C12—C13—N3	−18.61 (18)
N1—C1—C2—C3	−179.94 (13)	C11—C12—C13—N3	161.17 (12)
C6—C1—C2—C3	−2.24 (19)	C13—N4—C14—C19	−0.68 (15)
C1—C2—C3—C4	0.1 (2)	C13—N4—C14—C15	177.69 (15)
C2—C3—C4—C5	1.5 (2)	N4—C14—C15—C16	−178.56 (15)
C3—C4—C5—C6	−0.9 (2)	C19—C14—C15—C16	−0.3 (2)
C7—N2—C6—C5	−179.54 (13)	C14—C15—C16—C17	−0.2 (3)
C7—N2—C6—C1	−0.20 (13)	C15—C16—C17—C18	0.5 (3)
C4—C5—C6—N2	177.96 (13)	C16—C17—C18—C19	−0.3 (2)
C4—C5—C6—C1	−1.29 (19)	C13—N3—C19—C18	−178.53 (14)
N1—C1—C6—N2	1.67 (13)	C13—N3—C19—C14	−0.26 (14)
C2—C1—C6—N2	−176.50 (11)	C17—C18—C19—N3	177.85 (14)

N1—C1—C6—C5	−178.92 (12)	C17—C18—C19—C14	−0.2 (2)
C2—C1—C6—C5	2.91 (19)	N4—C14—C19—N3	0.59 (15)
C1—N1—C7—N2	2.43 (14)	C15—C14—C19—N3	−177.97 (13)
Zn—N1—C7—N2	−154.27 (9)	N4—C14—C19—C18	179.06 (13)
C1—N1—C7—C8	−175.89 (11)	C15—C14—C19—C18	0.5 (2)
Zn—N1—C7—C8	27.41 (17)	C9—C8—C20—C12	1.52 (18)
C6—N2—C7—N1	−1.44 (14)	C7—C8—C20—C12	−178.12 (11)
C6—N2—C7—C8	176.92 (11)	C11—C12—C20—C8	−1.53 (19)
N1—C7—C8—C20	25.18 (18)	C13—C12—C20—C8	178.26 (12)
N2—C7—C8—C20	−152.96 (12)	Zn—O1—C21—O2	10.67 (15)
N1—C7—C8—C9	−154.45 (12)	Zn—O1—C21—C22	−165.93 (10)
N2—C7—C8—C9	27.41 (18)		

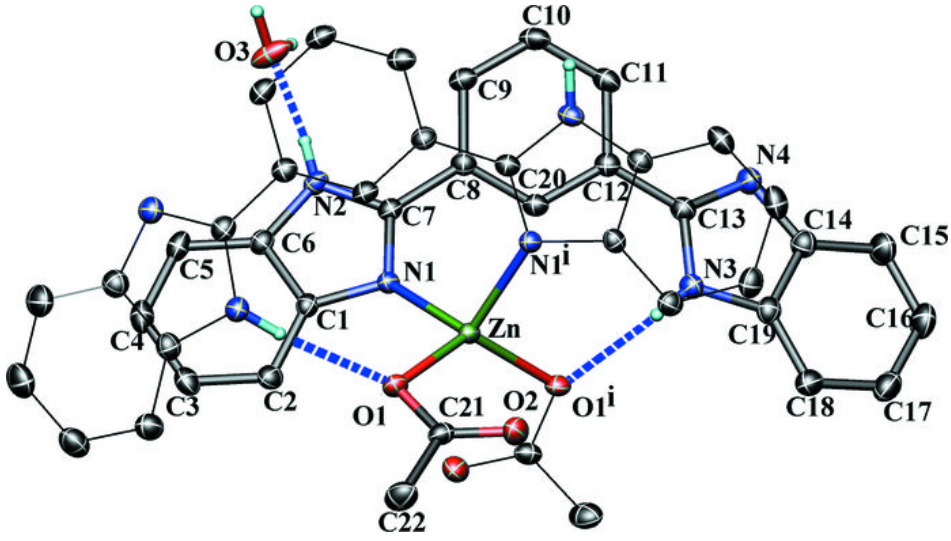
Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2N···O3	0.87 (1)	1.82 (1)	2.6848 (14)	174.(2)
N3—H3N···O1^{i}	0.86 (1)	2.16 (1)	3.0079 (14)	171.(2)
O3—H3AO···N4^{ii}	0.84 (1)	1.97 (1)	2.8046 (16)	175 (2)
O3—H3BO···O2^{iii}	0.84 (1)	1.99 (1)	2.8295 (15)	179 (2)

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

Fig. 1


O3
C10
C11
C9
N4
C8
C20
C12
N2
C7
C13
C14
C15
C6
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N1i
N3
C1
Zn
C19
C16
C4
C3
C2
O1
C21
O2
O1i
C18
C17
C22