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Bis[1,3-bis(1*H*-benzimidazol-2-yl)benzene-κN^3](succinato-$\kappa^2 O,O'$)zinc(II), a succinate-chelated monomeric compound

Fa-Yan Meng,[a] Wu-Heng Dong[a] and Seik Weng Ng[b]*

[a]School of Chemistry and Materials Engineering, Huangshi Institute of Technology, Huangshi 435003, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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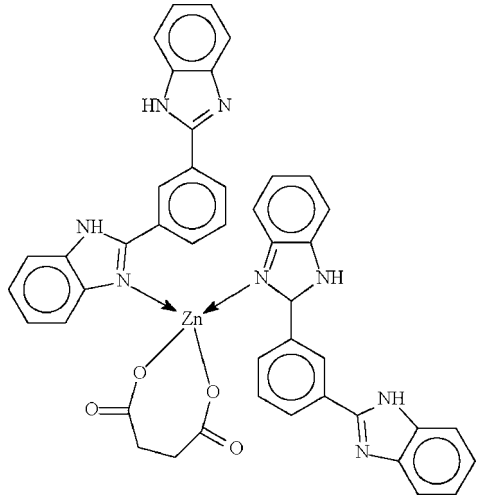
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.103; data-to-parameter ratio = 15.7.

The succinate dianion in the title 1:2 zinc succinate–1,3-bis(benzimidazol-2-yl)benzene adduct, $[Zn(C_4H_4O_4)(C_{20}H_{14}N_4)_2]$, chelates the Zn atom, which is datively bonded to two of the N-heterocycles in a tetrahedral geometry. The Zn atom and the succinate dianion lie on a twofold rotation axis. The amino –NH group of one heterocycle forms a weak intramolecular hydrogen bond to the carbonyl O atom; that of the second heterocycle engages in an intermolecular N—H···N interaction resulting in a linear chain structure.

Related literature

For the structure of the adduct of the N-heterocycle with zinc terephthalate, see: Meng *et al.* (2007). For the rare examples of chelation by a succinate group, see: Forster *et al.* (2004); Gupta & Devi (1978); Zheng, Lin & Sun (2001). For the structure of zinc succinate, see: Bowden *et al.* (2003); Zheng, Peters & von Schnering (2001). For higher-than-four-coordinate amine adducts of zinc succinate, see: Tao *et al.* (2001); Yin *et al.* (2002); Ying *et al.* (2003); Zeng *et al.* (2007); Zheng (2004); Zheng *et al.* (2002); Zhou *et al.* (2005). For the synthesis of the N-heterocycle, see: Chawla & Gill (1997).



Experimental

Crystal data

$[Zn(C_4H_4O_4)(C_{20}H_{14}N_4)_2]$
M_r = 802.15
Monoclinic, $C2/c$
a = 21.453 (2) Å
b = 10.272 (1) Å
c = 17.587 (2) Å
β = 109.411 (1)°
V = 3655.2 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 291 (2) K
0.46 × 0.34 × 0.22 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.687, T_{max} = 0.856
14308 measured reflections
4186 independent reflections
3354 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.103
S = 1.02
4186 reflections
266 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.940 (1)	Zn1—N1	2.019 (2)
O1^{i}—Zn1—O1	110.7 (1)	O1—Zn1—N1^{i}	108.6 (1)
O1—Zn1—N1	113.6 (1)		

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
N2—H2*n*···N4^{ii}	0.85 (1)	1.99 (1)	2.839 (2)	178 (2)
N3—H3*n*···O1	0.85 (1)	2.36 (1)	3.158 (2)	158 (2)

Symmetry code: (ii) $-x+1, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine

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structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG3051).

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supplementary materials

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Bis[1,3-bis(1*H*-benzimidazol-2-yl)benzene-κN^3](succinato-$\kappa^2 O,O'$)zinc(II), a succinate-chelated monomeric compound

F.-Y. Meng, W.-H. Dong and S. W. Ng

Comment

The reaction between 1,3-bis(benzimidazol-2-ylmethyl)benzene and zinc terephthalate affords the expected 1:1 adduct as a methanol solvate. The compound adopts a layer structure owing to bridging by both the *N*-heterocycle and the terephthalate dianion (Meng *et al.*, 2007). The succinate dianion is not rigid like the terephthalate dianion. It typically lies on a center-of-inversion in most metal succinates (CSD Version 5.28, May 2007) and functions as a bridging dianion; however, the succinate group chelates to the zinc atom in the zinc succinate adduct of this heterocycle. Both the cation and the dianion lie on a twofold rotation axis in the monomeric compound (Scheme I, Fig. 1).

Chelation by a succinate group has been documented in only three cases: the polymeric hexaaquatricobalt(III) (Forster *et al.*, 2004) and monomeric tetraaquanickel(II) (Gupta & Devi, 1978) derivatives, and the salt, diaquabis(phenanthrolinato)manganese(II) bis(phenanthroline)succinatomanganate(II) succinate heptahydrate (Zheng, Lin & Sun, 2001). The title compound has the metal center connected to two *N*-heterocycles; expansion of the coordination number is precluded as the second tertiary *N*-donor site of both ligands is already engaged in hydrogen bonding interactions. This possibly forces the succinate group to bind in the uncommon chelating mode. The amino –NH group of one heterocycle in hydrogen-bonded to the carbonyl oxygen atom [3.158 (2) Å]; that of the second heterocycle engages in an intermolecular N–H···N interaction [2.839 (2) Å] to furnish a linear chain motif.

The zinc-oxygen bond distance is similar to that found in zinc succinate itself; the metal center in this compound shows tetrahedral coordination and the anion behaves as a bridging group to result in the formation of a polymeric network motif (Bowden *et al.*, 2003; Zheng, Peters & von Schnering, 2001). The distance is, however, shorter than those found in other higher-than-four-coordinateamine adducts (Tao *et al.*, 2001; Yin *et al.*, 2002; Ying *et al.*, 2003; Zeng *et al.*, 2007; Zheng, 2004; Zheng *et al.*, 2002; Zhou *et al.*, 2005).

Experimental

The *N*-heterocycle was prepared according to a reported procedure (Chawla & Gill, 1997). Zinc nitrate hexahydrate (0.074 g, 0.25 mmol), succinic acid (0.0148 g, 0.125 mmol),1, 3-bis(benzimidazol-2-ylmethyl)benzene (0.039 g, 0.125 mmol), ethanol (2 ml) and water (15 ml) were placed in a 23 -ml, Teflon-lined, stainless-steel Parr bomb. (Neither sodium hydroxide nor postassium hydroxide was added.) The bomb was heated at 433 K for 5 days and cooled to room temperature at 5 K h^{-1}. Brown block-shaped crystals picked out by hand (in 10% yield).

Refinement

The amino H-atoms were located in a difference Fourier map, and were refined with a distance restraint of 0.85 (1) Å; their temperature factors were freely refined. The carbon-bound H-atoms were generated geometrically (C–H 0.93 to 0.97 Å); they were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C).

Figures

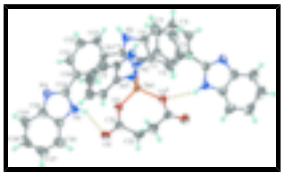


Fig. 1. **Figure 1**. Thermal ellipsoid plot depicting the coordination geometry of zinc; displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. [Symmery code (i): 1 – x, y, 3/2 – z.]

Bis[1,3-bis(1*H*-benzimidazol-2-yl)benzene-κ*N*^{3}](succinato-\ κ^2*O*,*O*^{i})zinc(II)

Crystal data

$[Zn(C_4H_4O_4)(C_{20}H_{14}N_4)_2]$	F_{000} = 1656
M_r = 802.15	D_x = 1.458 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 4938 reflections
a = 21.453 (2) Å	θ = 2.3–25.0º
b = 10.272 (1) Å	μ = 0.73 mm^{-1}
c = 17.587 (2) Å	*T* = 291 (2) K
β = 109.411 (1)º	Block, brown
V = 3655.2 (6) Å^3	0.46 × 0.34 × 0.22 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	4186 independent reflections
Radiation source: fine-focus sealed tube	3354 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 291(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −27→27
T_{min} = 0.687, T_{max} = 0.856	*k* = −13→13
14308 measured reflections	*l* = −22→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.103$

$S = 1.02$

4186 reflections

266 parameters

2 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 1.7754P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.41$ e Å^{-3}

$\Delta\rho_{min} = -0.24$ e Å^{-3}

Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.19880 (3)	0.7500	0.04623 (12)
O1	0.53016 (8)	0.09147 (13)	0.67838 (9)	0.0592 (4)
O2	0.56800 (11)	−0.08025 (16)	0.63523 (13)	0.0907 (6)
N1	0.42681 (7)	0.32303 (14)	0.69164 (9)	0.0425 (3)
N2	0.38107 (8)	0.50277 (17)	0.62655 (10)	0.0507 (4)
H2n	0.3757 (12)	0.5670 (17)	0.5949 (12)	0.072 (8)*
N3	0.59125 (9)	0.13643 (17)	0.53998 (11)	0.0522 (4)
H3n	0.5727 (11)	0.103 (2)	0.5708 (13)	0.074 (8)*
N4	0.63664 (8)	0.28509 (16)	0.48210 (10)	0.0512 (4)
C1	0.36481 (9)	0.33981 (19)	0.70053 (11)	0.0440 (4)
C2	0.33136 (10)	0.2633 (2)	0.74022 (13)	0.0553 (5)
H2	0.3501	0.1882	0.7680	0.066*
C3	0.26909 (12)	0.3049 (3)	0.73619 (15)	0.0675 (6)
H3	0.2454	0.2565	0.7620	0.081*
C4	0.24068 (11)	0.4171 (3)	0.69462 (15)	0.0727 (7)
H4	0.1986	0.4415	0.6935	0.087*
C5	0.27305 (11)	0.4924 (3)	0.65541 (15)	0.0651 (6)
H5	0.2539	0.5670	0.6274	0.078*
C6	0.33596 (10)	0.4519 (2)	0.65957 (12)	0.0494 (4)
C7	0.43377 (9)	0.42315 (17)	0.64697 (11)	0.0428 (4)
C8	0.49252 (9)	0.44713 (18)	0.62339 (11)	0.0440 (4)
C9	0.51755 (9)	0.34797 (18)	0.58804 (11)	0.0440 (4)
H9	0.4968	0.2672	0.5787	0.053*
C10	0.57367 (9)	0.36922 (19)	0.56657 (11)	0.0453 (4)
C11	0.60443 (10)	0.4902 (2)	0.58136 (13)	0.0530 (5)
H11	0.6423	0.5046	0.5680	0.064*
C12	0.57930 (11)	0.5891 (2)	0.61573 (13)	0.0578 (5)
H12	0.6001	0.6698	0.6251	0.069*
C13	0.52322 (10)	0.56822 (19)	0.63630 (12)	0.0517 (5)
H13	0.5060	0.6353	0.6588	0.062*
C14	0.60041 (9)	0.2648 (2)	0.52894 (11)	0.0464 (4)
C15	0.62476 (10)	0.0671 (2)	0.49841 (12)	0.0523 (5)

C16	0.63407 (12)	−0.0656 (2)	0.49111 (15)	0.0683 (6)
H16	0.6147	−0.1273	0.5148	0.082*
C17	0.67363 (13)	−0.1007 (3)	0.44680 (16)	0.0766 (7)
H17	0.6812	−0.1886	0.4405	0.092*
C18	0.70266 (12)	−0.0080 (3)	0.41107 (16)	0.0782 (8)
H18	0.7290	−0.0358	0.3816	0.094*
C19	0.69331 (11)	0.1232 (3)	0.41826 (15)	0.0682 (6)
H19	0.7127	0.1844	0.3942	0.082*
C20	0.65334 (10)	0.1610 (2)	0.46324 (12)	0.0520 (5)
C21	0.54524 (11)	−0.02897 (19)	0.68279 (14)	0.0541 (5)
C22	0.53548 (11)	−0.1074 (2)	0.75113 (15)	0.0629 (6)
H22A	0.5632	−0.0715	0.8022	0.075*
H22B	0.5495	−0.1965	0.7479	0.075*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0571 (2)	0.03012 (16)	0.0570 (2)	0.000	0.02633 (15)	0.000
O1	0.0847 (10)	0.0345 (7)	0.0713 (10)	0.0041 (7)	0.0431 (8)	0.0002 (6)
O2	0.1373 (17)	0.0521 (9)	0.1215 (16)	0.0084 (10)	0.0953 (15)	−0.0045 (10)
N1	0.0465 (8)	0.0398 (8)	0.0440 (8)	−0.0014 (6)	0.0189 (7)	−0.0029 (6)
N2	0.0524 (9)	0.0507 (10)	0.0522 (10)	0.0089 (8)	0.0216 (8)	0.0085 (8)
N3	0.0616 (10)	0.0489 (10)	0.0520 (10)	−0.0035 (8)	0.0267 (8)	−0.0015 (8)
N4	0.0473 (9)	0.0584 (10)	0.0526 (10)	0.0051 (7)	0.0229 (7)	0.0056 (8)
C1	0.0455 (10)	0.0478 (10)	0.0410 (10)	−0.0036 (8)	0.0176 (8)	−0.0075 (8)
C2	0.0577 (12)	0.0611 (12)	0.0519 (12)	−0.0071 (10)	0.0247 (10)	−0.0024 (10)
C3	0.0583 (13)	0.0902 (18)	0.0639 (14)	−0.0106 (12)	0.0335 (11)	−0.0048 (12)
C4	0.0502 (12)	0.101 (2)	0.0736 (16)	0.0080 (13)	0.0293 (11)	−0.0012 (14)
C5	0.0545 (12)	0.0783 (16)	0.0647 (14)	0.0146 (11)	0.0227 (11)	0.0048 (12)
C6	0.0501 (10)	0.0562 (11)	0.0440 (11)	0.0029 (9)	0.0183 (8)	−0.0036 (9)
C7	0.0469 (10)	0.0404 (9)	0.0427 (10)	0.0007 (7)	0.0171 (8)	−0.0021 (7)
C8	0.0476 (10)	0.0435 (9)	0.0422 (10)	0.0011 (8)	0.0165 (8)	0.0040 (8)
C9	0.0480 (10)	0.0406 (9)	0.0457 (10)	−0.0011 (8)	0.0187 (8)	0.0020 (8)
C10	0.0460 (10)	0.0477 (10)	0.0435 (10)	0.0017 (8)	0.0168 (8)	0.0050 (8)
C11	0.0501 (11)	0.0536 (11)	0.0595 (13)	−0.0060 (9)	0.0240 (9)	0.0037 (9)
C12	0.0638 (13)	0.0445 (11)	0.0680 (14)	−0.0121 (9)	0.0257 (11)	−0.0024 (10)
C13	0.0600 (12)	0.0428 (10)	0.0554 (12)	0.0005 (9)	0.0234 (9)	−0.0026 (9)
C14	0.0460 (10)	0.0497 (10)	0.0445 (10)	0.0013 (8)	0.0165 (8)	0.0042 (8)
C15	0.0547 (11)	0.0551 (12)	0.0445 (11)	0.0024 (9)	0.0132 (9)	−0.0076 (9)
C16	0.0784 (15)	0.0582 (13)	0.0654 (15)	−0.0043 (11)	0.0200 (12)	−0.0161 (11)
C17	0.0726 (16)	0.0720 (16)	0.0787 (17)	0.0062 (13)	0.0165 (13)	−0.0310 (14)
C18	0.0580 (14)	0.101 (2)	0.0755 (17)	0.0090 (13)	0.0218 (12)	−0.0330 (15)
C19	0.0555 (13)	0.0870 (17)	0.0666 (15)	0.0038 (12)	0.0261 (11)	−0.0113 (13)
C20	0.0434 (10)	0.0651 (12)	0.0458 (11)	0.0061 (9)	0.0128 (8)	−0.0026 (9)
C21	0.0615 (12)	0.0404 (10)	0.0692 (14)	−0.0018 (9)	0.0334 (11)	−0.0061 (9)
C22	0.0720 (14)	0.0428 (11)	0.0751 (15)	0.0132 (10)	0.0261 (12)	0.0016 (10)

Geometric parameters (Å, °)

Zn1—O1^{i}	1.940 (1)	C7—C8	1.473 (2)
Zn1—O1	1.940 (1)	C8—C9	1.391 (3)
Zn1—N1^{i}	2.019 (2)	C8—C13	1.390 (3)
Zn1—N1	2.019 (2)	C9—C10	1.394 (3)
O1—C21	1.275 (2)	C9—H9	0.9300
O2—C21	1.219 (2)	C10—C11	1.390 (3)
N1—C7	1.332 (2)	C10—C14	1.473 (3)
N1—C1	1.401 (2)	C11—C12	1.380 (3)
N2—C7	1.344 (2)	C11—H11	0.9300
N2—C6	1.386 (3)	C12—C13	1.383 (3)
N2—H2N	0.846 (10)	C12—H12	0.9300
N3—C14	1.357 (3)	C13—H13	0.9300
N3—C15	1.381 (3)	C15—C16	1.390 (3)
N3—H3N	0.846 (10)	C15—C20	1.393 (3)
N4—C14	1.324 (2)	C16—C17	1.377 (3)
N4—C20	1.394 (3)	C16—H16	0.9300
C1—C6	1.390 (3)	C17—C18	1.396 (4)
C1—C2	1.397 (3)	C17—H17	0.9300
C2—C3	1.382 (3)	C18—C19	1.375 (4)
C2—H2	0.9300	C18—H18	0.9300
C3—C4	1.392 (4)	C19—C20	1.401 (3)
C3—H3	0.9300	C19—H19	0.9300
C4—C5	1.369 (3)	C21—C22	1.518 (3)
C4—H4	0.9300	C22—C22^{i}	1.509 (4)
C5—C6	1.391 (3)	C22—H22A	0.9700
C5—H5	0.9300	C22—H22B	0.9700
O1^{i}—Zn1—O1	110.7 (1)	C10—C9—H9	119.9
O1—Zn1—N1	113.6 (1)	C11—C10—C9	119.24 (18)
O1—Zn1—N1^{i}	108.6 (1)	C11—C10—C14	120.22 (17)
O1^{i}—Zn1—N1	108.6 (1)	C9—C10—C14	120.54 (17)
O1^{i}—Zn1—N1^{i}	113.6 (1)	C12—C11—C10	120.65 (18)
N1^{i}—Zn1—N1	101.6 (1)	C12—C11—H11	119.7
C21—O1—Zn1	130.16 (14)	C10—C11—H11	119.7
C7—N1—C1	105.51 (15)	C13—C12—C11	120.04 (19)
C7—N1—Zn1	124.55 (12)	C13—C12—H12	120.0
C1—N1—Zn1	128.90 (12)	C11—C12—H12	120.0
C7—N2—C6	107.51 (16)	C12—C13—C8	120.13 (18)
C7—N2—H2n	124.7 (17)	C12—C13—H13	119.9
C6—N2—H2n	127.5 (17)	C8—C13—H13	119.9
C14—N3—C15	107.46 (17)	N4—C14—N3	112.65 (18)
C14—N3—H3n	127.5 (18)	N4—C14—C10	124.18 (18)
C15—N3—H3n	124.7 (18)	N3—C14—C10	123.16 (17)
C14—N4—C20	104.75 (17)	N3—C15—C16	132.1 (2)
C6—C1—N1	108.65 (16)	N3—C15—C20	105.13 (17)

C6—C1—C2	120.71 (18)	C16—C15—C20	122.7 (2)
N1—C1—C2	130.62 (18)	C15—C16—C17	116.3 (2)
C3—C2—C1	116.7 (2)	C15—C16—H16	121.8
C3—C2—H2	121.7	C17—C16—H16	121.8
C1—C2—H2	121.7	C16—C17—C18	121.8 (2)
C2—C3—C4	122.0 (2)	C16—C17—H17	119.1
C2—C3—H3	119.0	C18—C17—H17	119.1
C4—C3—H3	119.0	C19—C18—C17	121.8 (2)
C5—C4—C3	121.7 (2)	C19—C18—H18	119.1
C5—C4—H4	119.1	C17—C18—H18	119.1
C3—C4—H4	119.1	C18—C19—C20	117.3 (3)
C4—C5—C6	116.8 (2)	C18—C19—H19	121.3
C4—C5—H5	121.6	C20—C19—H19	121.3
C6—C5—H5	121.6	N4—C20—C19	129.9 (2)
N2—C6—C1	106.09 (16)	N4—C20—C15	109.99 (17)
N2—C6—C5	131.7 (2)	C19—C20—C15	120.1 (2)
C1—C6—C5	122.2 (2)	O2—C21—O1	121.9 (2)
N1—C7—N2	112.23 (16)	O2—C21—C22	120.37 (19)
N1—C7—C8	124.70 (16)	O1—C21—C22	117.68 (17)
N2—C7—C8	123.06 (17)	C21—C22—C22^{i}	112.5 (2)
C9—C8—C13	119.72 (17)	C21—C22—H22A	109.1
C9—C8—C7	119.80 (16)	C22^{i}—C22—H22A	109.1
C13—C8—C7	120.47 (17)	C21—C22—H22B	109.1
C8—C9—C10	120.20 (17)	C22^{i}—C22—H22B	109.1
C8—C9—H9	119.9	H22A—C22—H22B	107.8
O1^{i}—Zn1—O1—C21	−16.11 (17)	C7—C8—C9—C10	−179.10 (17)
N1^{i}—Zn1—O1—C21	109.22 (19)	C8—C9—C10—C11	0.4 (3)
N1—Zn1—O1—C21	−138.57 (19)	C8—C9—C10—C14	−179.86 (17)
O1^{i}—Zn1—N1—C7	169.60 (14)	C9—C10—C11—C12	−1.0 (3)
O1—Zn1—N1—C7	−66.76 (15)	C14—C10—C11—C12	179.24 (19)
N1^{i}—Zn1—N1—C7	49.62 (13)	C10—C11—C12—C13	0.4 (3)
O1^{i}—Zn1—N1—C1	2.97 (17)	C11—C12—C13—C8	0.8 (3)
O1—Zn1—N1—C1	126.61 (15)	C9—C8—C13—C12	−1.5 (3)
N1^{i}—Zn1—N1—C1	−117.01 (16)	C7—C8—C13—C12	178.48 (19)
C7—N1—C1—C6	0.3 (2)	C20—N4—C14—N3	−1.5 (2)
Zn1—N1—C1—C6	168.86 (13)	C20—N4—C14—C10	177.43 (17)
C7—N1—C1—C2	178.8 (2)	C15—N3—C14—N4	1.0 (2)
Zn1—N1—C1—C2	−12.6 (3)	C15—N3—C14—C10	−177.96 (17)
C6—C1—C2—C3	0.1 (3)	C11—C10—C14—N4	−25.1 (3)
N1—C1—C2—C3	−178.3 (2)	C9—C10—C14—N4	155.19 (19)
C1—C2—C3—C4	0.1 (3)	C11—C10—C14—N3	153.8 (2)
C2—C3—C4—C5	0.0 (4)	C9—C10—C14—N3	−26.0 (3)
C3—C4—C5—C6	−0.4 (4)	C14—N3—C15—C16	177.5 (2)
C7—N2—C6—C1	0.4 (2)	C14—N3—C15—C20	0.0 (2)
C7—N2—C6—C5	−177.9 (2)	N3—C15—C16—C17	−177.0 (2)
N1—C1—C6—N2	−0.4 (2)	C20—C15—C16—C17	0.1 (3)
C2—C1—C6—N2	−179.12 (18)	C15—C16—C17—C18	−0.1 (4)

N1—C1—C6—C5	178.12 (19)	C16—C17—C18—C19	0.0 (4)
C2—C1—C6—C5	−0.6 (3)	C17—C18—C19—C20	0.1 (4)
C4—C5—C6—N2	178.8 (2)	C14—N4—C20—C19	−177.1 (2)
C4—C5—C6—C1	0.7 (3)	C14—N4—C20—C15	1.5 (2)
C1—N1—C7—N2	0.0 (2)	C18—C19—C20—N4	178.3 (2)
Zn1—N1—C7—N2	−169.24 (13)	C18—C19—C20—C15	−0.1 (3)
C1—N1—C7—C8	178.83 (17)	N3—C15—C20—N4	−0.9 (2)
Zn1—N1—C7—C8	9.6 (3)	C16—C15—C20—N4	−178.69 (19)
C6—N2—C7—N1	−0.3 (2)	N3—C15—C20—C19	177.84 (19)
C6—N2—C7—C8	−179.10 (17)	C16—C15—C20—C19	0.0 (3)
N1—C7—C8—C9	51.0 (3)	Zn1—O1—C21—O2	−174.73 (18)
N2—C7—C8—C9	−130.3 (2)	Zn1—O1—C21—C22	3.8 (3)
N1—C7—C8—C13	−129.0 (2)	O2—C21—C22—C22^{i}	−121.7 (2)
N2—C7—C8—C13	49.7 (3)	O1—C21—C22—C22^{i}	59.7 (3)
C13—C8—C9—C10	0.8 (3)		

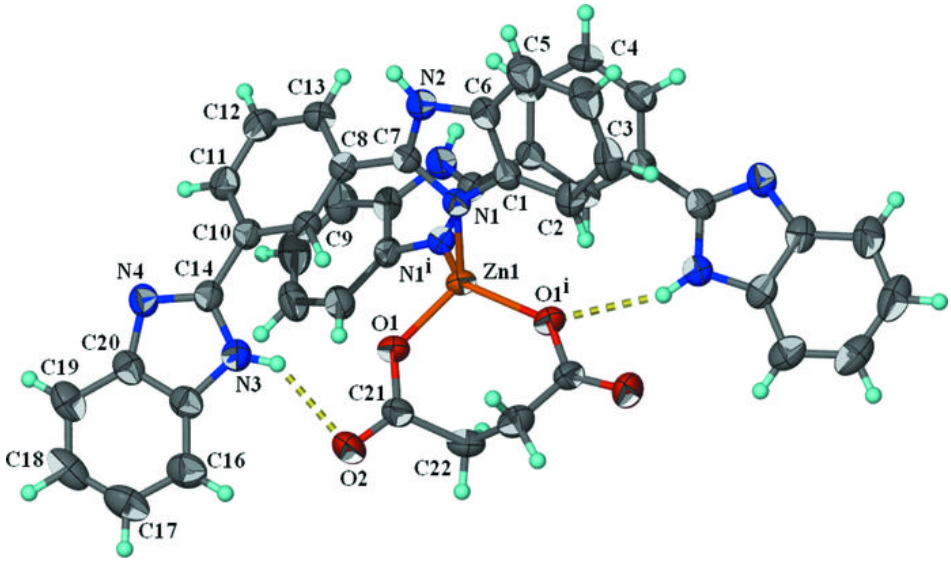
Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2n···N4^{ii}	0.85 (1)	1.99 (1)	2.839 (2)	178 (2)
N3—H3n···O1	0.85 (1)	2.36 (1)	3.158 (2)	158 (2)

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*+1.

Fig. 1


C5
C4
C13
N2
C6
C12
C8
C7
C3
C11
N1
C1
C10
C9
C2
N4
C14
N1i
Zn1
O1i
O1
C20
C19
N3
C21
C18
C16
O2
C22
C17