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Bis(benzimidazole-κ*N*)bis(4-formylbenzoato-κ*O*)zinc(II) monohydrate

Zhao-Peng Deng,[a] Shan Gao[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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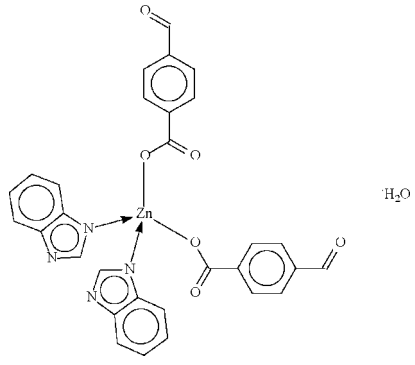
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.057; wR factor = 0.194; data-to-parameter ratio = 14.1.

The zinc center in the title compound, $[Zn(C_8H_5O_3)_2(C_7H_6N_2)_2]\cdot H_2O$, shows tetrahedral coordination. The molecules are linked by N—H···O and O—H···O hydrogen bonds. One of the two formylbenzoate ligands is disordered, approximately equally, over two positions.

Related literature

For the diaqua complex, see Deng *et al.* (2006*a*), and for the aqua phenanthroline adduct, see Deng *et al.* (2006*b*).



Experimental

Crystal data

$[Zn(C_8H_5O_3)_2(C_7H_6N_2)_2].H_2O$
M_r = 617.90
Monoclinic, $C2/c$
a = 13.7968 (8) Å
b = 17.0524 (8) Å
c = 23.848 (1) Å
β = 92.954 (1)°
V = 5603.1 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 295 (2) K
0.35 × 0.26 × 0.19 mm

Data collection

Rigaku RAXIS-RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.558, T_{max} = 0.843
27096 measured reflections
6393 independent reflections
3298 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.194
S = 1.09
6393 reflections
453 parameters
178 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2n···O1w'^{i}	0.86	2.12	2.907 (8)	152
N2—H2n···O1w'^{ii}	0.86	2.17	2.960 (8)	154
N4—H4n···O5^{iii}	0.86	2.11	2.864 (5)	145
O1w—H1w1···O1	0.84	2.064 (7)	2.87 (1)	159
O1w—H1w2···O5	0.86	1.873 (4)	2.69 (1)	157
O1w'—H1w3···O5	0.86	2.353 (4)	3.112 (8)	148

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

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2365).

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supplementary materials

Acta Cryst. (2007). E**63**, m1712 [**doi:10.1107/S1600536807023604**]

Bis(benzimidazole-*κN*)bis(4-formylbenzoato-*κO*)zinc(II) monohydrate

Z.-P. Deng, S. Gao and S. W. Ng

Comment

Bis(4-formylbenzoato)zinc, which exists as a tetrahedral diaqua compound (Deng *et al.*, 2006*a*), form a five-coordinate aqua complex with phenathroline (Deng *et al.*, 2006*b*). The title compound is a 1:2 adduct of Bis(4-formylbenzoato)zinc with benzimidazole, crystallizing with a molecule of water (I). The metal center shows tetrahedral coordination (Fig. 1). Adjacent molecules are linked by hydrogen bonds.

Experimental

Zinc diacetate dihydrate (0.11 g, 0.5 mmol) was added to a 1:1 aqueous-ethanol solution (20 ml) of 4-formylbenzoic acid (0.15 g, 1 mmol) and benzimidazole (0.07 g, 1 mmol). Sodium hydroxide was added to a pH value of about 5. The filtered solution was set aside for the formation of colorless prismatic crystals. CH&N analysis. Calculated for $C_{30}H_{24}N_4O_7Zn$: C 58.31, H 3.91, N 9.07%. Found: C 58.28, H 3.93, N 9.04%.

Refinement

One of the two formylbenzoate anions is disordered over two positions; the occupancy factors refined to 0.535 (5):0.465 (5). For both components, the phenylene ring was refined as a rigid hexagon of 1.39Å sides. The C–C single-bond length was restrained to 1.50±0.01Å and the C=O double-bond distance to 1.25±0.01 Å. The $C_{aliphatic}\cdots C_{ortho}$ distances were restrained to 2.50±0.01 Å and the entire anion was restrained to be planar. As the C8 atom is less than 0.2 Å from C8', the temperature factors were restrained to be identical; those of the O3 and O3' were similarly treated for the same reason. Additionally, the disordered atoms were restrained to be nearly isotropic. A consideration of the hydrogen bonding distances led to pairing the O1w' water molecule with the primed anion.

The carbon- and nitrogen bound H atoms were generated geometrically (C–H 0.93, N–H 0.86 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C). The water H atoms could were placed in chemically sensible positions on the basis of hydrogen bonding interactions but they were not refined.

Figures

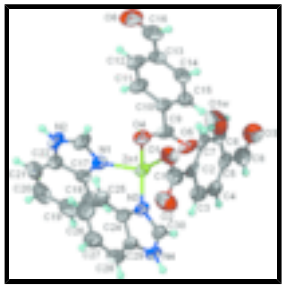


Fig. 1. **Figure 1**. Thermal ellipsoid plot of the molecular structure of (I). Only one of the disorder components is shown. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii.

Bis(benzimidazole-κ*N*)bis(4-formylbenzoato-κ*O*)\ zinc(II) monohydrate

Crystal data

$[Zn(C_8H_5O_3)_2(C_7H_6N_2)_2].H_2O$	F_{000} = 2544
M_r = 617.90	D_x = 1.465 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 13980 reflections
a = 13.7968 (8) Å	θ = 3.1–27.5º
b = 17.0524 (8) Å	μ = 0.93 mm^{-1}
c = 23.848 (1) Å	*T* = 295 (2) K
β = 92.954 (1)º	Prism, colourless
V = 5603.1 (5) Å^3	0.35 × 0.26 × 0.19 mm
Z = 8	

Data collection

Rigaku RAXIS-RAPID IP diffractometer	6393 independent reflections
Radiation source: fine-focus sealed tube	3298 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.068
T = 295(2) K	θ_{max} = 27.5º
ω scan	θ_{min} = 3.1º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*h* = −17→17
T_{min} = 0.558, T_{max} = 0.843	*k* = −21→22
27096 measured reflections	*l* = −30→30

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.057	H-atom parameters constrained
$wR(F^2)$ = 0.194	$w = 1/[\sigma^2(F_o^2) + (0.0884P)^2 + 4.8786P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.09	$(\Delta/\sigma)_{max}$ = 0.001
6393 reflections	$\Delta\rho_{max}$ = 0.70 e Å^{-3}
453 parameters	$\Delta\rho_{min}$ = −0.67 e Å^{-3}
178 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: 0.0008 (2)

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.28971 (4)	0.59229 (3)	0.38356 (2)	0.0525 (2)	
N1	0.2248 (3)	0.4871 (2)	0.36616 (14)	0.0554 (9)	
N2	0.1303 (3)	0.4014 (2)	0.32177 (19)	0.0726 (12)	
H2n	0.0868	0.3830	0.2982	0.087*	
N3	0.2451 (3)	0.6254 (2)	0.45870 (14)	0.0522 (9)	
N4	0.2390 (3)	0.6728 (2)	0.54477 (15)	0.0606 (10)	
H4n	0.2587	0.6909	0.5770	0.073*	
O4	0.2136 (3)	0.64849 (19)	0.32459 (13)	0.0658 (9)	
O5	0.2842 (3)	0.7626 (2)	0.34589 (14)	0.0768 (10)	
O6	−0.0635 (3)	0.8200 (3)	0.10574 (17)	0.1046 (15)	
O1	0.4180 (6)	0.5925 (4)	0.3560 (4)	0.079 (2)	0.535 (5)
O2	0.4492 (6)	0.5579 (4)	0.4422 (4)	0.103 (3)	0.535 (5)
O3	0.9173 (18)	0.5162 (7)	0.3088 (8)	0.098 (2)	0.535 (5)
O1w	0.4534 (8)	0.7360 (6)	0.2980 (5)	0.141 (4)	0.535 (5)
H1w1	0.4569	0.6904	0.3115	0.169*	0.535 (5)
H1w2	0.4005	0.7568	0.3089	0.169*	0.535 (5)
C1	0.4754 (5)	0.5692 (3)	0.3940 (4)	0.072 (4)	0.535 (5)
C2	0.5795 (4)	0.5542 (3)	0.3815 (3)	0.061 (3)	0.535 (5)
C7	0.6133 (5)	0.5658 (3)	0.3283 (2)	0.054 (3)	0.535 (5)
H7	0.5712	0.5833	0.2992	0.064*	0.535 (5)
C6	0.7101 (5)	0.5513 (4)	0.3184 (3)	0.051 (2)	0.535 (5)
H6	0.7327	0.5590	0.2827	0.061*	0.535 (5)
C5	0.7731 (4)	0.5251 (5)	0.3618 (4)	0.059 (4)	0.535 (5)
C4	0.7393 (5)	0.5135 (5)	0.4150 (3)	0.065 (3)	0.535 (5)
H4	0.7814	0.4959	0.4441	0.078*	0.535 (5)
C3	0.6425 (6)	0.5280 (4)	0.4249 (2)	0.069 (3)	0.535 (5)
H3	0.6199	0.5202	0.4606	0.083*	0.535 (5)
C8	0.8764 (6)	0.5092 (6)	0.3522 (6)	0.078 (2)	0.535 (5)
H8	0.9143	0.4918	0.3831	0.094*	0.535 (5)
O1'	0.4345 (9)	0.5846 (5)	0.3997 (5)	0.090 (3)	0.465 (5)
O2'	0.4298 (7)	0.6000 (5)	0.3094 (5)	0.116 (4)	0.465 (5)
O3'	0.915 (2)	0.4944 (9)	0.3035 (9)	0.098 (2)	0.465 (3)
O1w'	0.4547 (5)	0.8194 (4)	0.2757 (3)	0.061 (2)	0.465 (5)
H1w3	0.4127	0.8226	0.3009	0.073*	0.465 (5)
H1w4	0.4651	0.7706	0.2692	0.073*	0.465 (5)
C1'	0.4733 (6)	0.5834 (4)	0.3539 (4)	0.077 (4)	0.465 (5)
C2'	0.5783 (5)	0.5604 (3)	0.3534 (4)	0.074 (4)	0.465 (5)
C7'	0.6228 (6)	0.5587 (5)	0.3025 (3)	0.094 (5)	0.465 (5)
H7'	0.5876	0.5717	0.2694	0.113*	0.465 (5)
C6'	0.7200 (6)	0.5377 (5)	0.3009 (4)	0.067 (4)	0.465 (5)
H6'	0.7498	0.5365	0.2668	0.081*	0.465 (5)
C5'	0.7725 (5)	0.5183 (6)	0.3502 (5)	0.058 (4)	0.465 (5)
C4'	0.7280 (7)	0.5200 (6)	0.4011 (4)	0.072 (4)	0.465 (5)
H4'	0.7632	0.5071	0.4342	0.086*	0.465 (5)
C3'	0.6308 (6)	0.5411 (5)	0.4028 (3)	0.072 (4)	0.465 (5)

H3'	0.6010	0.5422	0.4368	0.087*	0.465 (5)
C8'	0.8763 (7)	0.4958 (8)	0.3482 (7)	0.078 (2)	0.465
H8'	0.9117	0.4828	0.3812	0.094*	0.465 (5)
C9	0.2289 (4)	0.7213 (3)	0.31636 (18)	0.0580 (12)	
C10	0.1726 (3)	0.7564 (3)	0.26685 (17)	0.0531 (11)	
C11	0.1190 (4)	0.7085 (3)	0.22931 (19)	0.0687 (14)	
H11	0.1211	0.6544	0.2338	0.082*	
C12	0.0636 (4)	0.7405 (3)	0.1862 (2)	0.0707 (14)	
H12	0.0291	0.7081	0.1610	0.085*	
C13	0.0587 (4)	0.8214 (3)	0.17986 (18)	0.0588 (12)	
C14	0.1134 (4)	0.8688 (3)	0.2157 (2)	0.0605 (12)	
H14	0.1117	0.9229	0.2107	0.073*	
C15	0.1708 (3)	0.8370 (3)	0.25929 (18)	0.0578 (12)	
H15	0.2079	0.8695	0.2833	0.069*	
C16	−0.0066 (4)	0.8548 (4)	0.1356 (2)	0.0796 (16)	
H16	−0.0032	0.9087	0.1303	0.096*	
C17	0.2429 (3)	0.4136 (3)	0.38937 (17)	0.0514 (11)	
C18	0.3076 (4)	0.3910 (3)	0.4323 (2)	0.0693 (14)	
H18	0.3472	0.4272	0.4516	0.083*	
C19	0.3107 (5)	0.3118 (4)	0.4455 (3)	0.094 (2)	
H19	0.3533	0.2945	0.4743	0.113*	
C20	0.2518 (5)	0.2577 (4)	0.4165 (3)	0.096 (2)	
H20	0.2562	0.2050	0.4264	0.115*	
C21	0.1878 (4)	0.2798 (3)	0.3739 (3)	0.0748 (15)	
H21	0.1486	0.2435	0.3546	0.090*	
C22	0.1838 (4)	0.3586 (3)	0.36096 (19)	0.0569 (11)	
C23	0.1566 (4)	0.4757 (3)	0.3263 (2)	0.0722 (15)	
H23	0.1299	0.5156	0.3038	0.087*	
C24	0.1479 (3)	0.6321 (3)	0.47185 (17)	0.0517 (11)	
C25	0.0638 (4)	0.6154 (3)	0.4404 (2)	0.0715 (14)	
H25	0.0656	0.5964	0.4039	0.086*	
C26	−0.0223 (4)	0.6278 (4)	0.4648 (2)	0.0824 (16)	
H26	−0.0801	0.6174	0.4443	0.099*	
C27	−0.0258 (4)	0.6556 (4)	0.5192 (2)	0.0814 (16)	
H27	−0.0858	0.6615	0.5347	0.098*	
C28	0.0567 (4)	0.6746 (3)	0.5511 (2)	0.0720 (15)	
H28	0.0541	0.6948	0.5872	0.086*	
C29	0.1443 (4)	0.6621 (3)	0.52625 (17)	0.0541 (11)	
C30	0.2954 (4)	0.6502 (2)	0.50375 (18)	0.0559 (11)	
H30	0.3628	0.6517	0.5067	0.067*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0559 (4)	0.0557 (3)	0.0447 (3)	0.0063 (2)	−0.0098 (2)	−0.0017 (2)
N1	0.054 (2)	0.061 (2)	0.050 (2)	0.0063 (18)	−0.0054 (17)	−0.0018 (18)
N2	0.072 (3)	0.069 (3)	0.073 (3)	−0.005 (2)	−0.024 (2)	−0.014 (2)
N3	0.053 (2)	0.054 (2)	0.048 (2)	0.0027 (17)	−0.0162 (16)	0.0006 (17)

N4	0.080 (3)	0.059 (2)	0.0417 (19)	−0.002 (2)	−0.0088 (19)	−0.0067 (18)
O4	0.077 (2)	0.061 (2)	0.0581 (19)	0.0088 (17)	−0.0127 (16)	0.0081 (16)
O5	0.095 (3)	0.079 (2)	0.0533 (19)	0.006 (2)	−0.0263 (18)	−0.0135 (18)
O6	0.092 (3)	0.144 (4)	0.075 (3)	0.020 (3)	−0.029 (2)	0.024 (3)
O1	0.071 (5)	0.081 (5)	0.085 (5)	0.008 (4)	0.012 (4)	0.010 (4)
O2	0.102 (6)	0.109 (5)	0.102 (6)	0.021 (4)	0.035 (5)	0.014 (5)
O3	0.077 (3)	0.112 (6)	0.103 (4)	0.014 (5)	0.003 (3)	−0.003 (4)
O1w	0.129 (7)	0.136 (7)	0.161 (7)	−0.003 (6)	0.038 (6)	0.018 (6)
C1	0.090 (8)	0.053 (5)	0.073 (7)	0.003 (5)	0.015 (6)	−0.004 (5)
C2	0.060 (6)	0.062 (5)	0.058 (6)	−0.003 (5)	−0.014 (5)	−0.020 (5)
C7	0.045 (5)	0.044 (4)	0.068 (6)	−0.006 (4)	−0.029 (5)	−0.009 (4)
C6	0.058 (6)	0.047 (5)	0.045 (5)	−0.002 (4)	−0.007 (4)	−0.014 (4)
C5	0.048 (7)	0.054 (6)	0.073 (6)	−0.006 (5)	−0.017 (5)	−0.005 (5)
C4	0.065 (6)	0.067 (6)	0.061 (5)	−0.010 (5)	−0.016 (5)	0.003 (5)
C3	0.073 (7)	0.071 (6)	0.063 (6)	0.002 (5)	−0.002 (5)	−0.002 (5)
C8	0.070 (4)	0.075 (4)	0.089 (4)	0.004 (3)	−0.009 (3)	0.007 (3)
O1'	0.093 (7)	0.091 (6)	0.089 (7)	−0.002 (5)	0.015 (6)	−0.007 (5)
O2'	0.078 (6)	0.163 (8)	0.104 (7)	0.030 (5)	−0.014 (5)	−0.027 (6)
O3'	0.077 (3)	0.112 (6)	0.103 (4)	0.014 (5)	0.003 (3)	−0.003 (4)
O1w'	0.055 (4)	0.058 (4)	0.069 (4)	−0.008 (3)	0.000 (3)	0.000 (3)
C1'	0.075 (8)	0.079 (7)	0.075 (7)	0.028 (6)	−0.003 (6)	−0.014 (6)
C2'	0.065 (7)	0.069 (7)	0.088 (9)	0.011 (6)	0.000 (7)	−0.006 (6)
C7'	0.087 (8)	0.108 (8)	0.086 (8)	0.014 (7)	−0.002 (7)	−0.007 (7)
C6'	0.064 (7)	0.072 (7)	0.065 (7)	0.007 (5)	−0.002 (5)	−0.014 (6)
C5'	0.052 (8)	0.058 (7)	0.063 (6)	−0.003 (6)	−0.011 (5)	−0.001 (6)
C4'	0.068 (8)	0.069 (7)	0.075 (7)	−0.006 (6)	−0.023 (6)	0.009 (6)
C3'	0.069 (8)	0.077 (7)	0.071 (7)	−0.026 (6)	0.012 (6)	−0.003 (6)
C8'	0.070 (4)	0.075 (4)	0.089 (4)	0.004 (3)	−0.009 (3)	0.007 (3)
C9	0.064 (3)	0.065 (3)	0.044 (2)	0.015 (2)	−0.006 (2)	−0.006 (2)
C10	0.060 (3)	0.056 (3)	0.043 (2)	0.013 (2)	−0.003 (2)	0.000 (2)
C11	0.091 (4)	0.056 (3)	0.056 (3)	0.013 (3)	−0.023 (3)	−0.005 (2)
C12	0.082 (4)	0.077 (3)	0.051 (3)	0.010 (3)	−0.023 (2)	−0.005 (3)
C13	0.056 (3)	0.076 (3)	0.045 (2)	0.017 (2)	0.003 (2)	0.012 (2)
C14	0.058 (3)	0.063 (3)	0.061 (3)	0.009 (2)	0.004 (2)	0.014 (2)
C15	0.057 (3)	0.065 (3)	0.050 (2)	0.000 (2)	0.000 (2)	0.004 (2)
C16	0.070 (4)	0.105 (5)	0.063 (3)	0.023 (3)	−0.005 (3)	0.022 (3)
C17	0.055 (3)	0.058 (3)	0.042 (2)	0.012 (2)	0.0107 (19)	0.000 (2)
C18	0.075 (4)	0.076 (3)	0.057 (3)	0.003 (3)	−0.001 (3)	0.008 (3)
C19	0.098 (5)	0.096 (5)	0.089 (4)	0.014 (4)	−0.005 (4)	0.036 (4)
C20	0.099 (5)	0.072 (4)	0.118 (5)	0.004 (4)	0.024 (4)	0.029 (4)
C21	0.075 (4)	0.064 (3)	0.087 (4)	−0.007 (3)	0.023 (3)	−0.005 (3)
C22	0.058 (3)	0.060 (3)	0.053 (3)	−0.002 (2)	0.010 (2)	−0.009 (2)
C23	0.085 (4)	0.062 (3)	0.066 (3)	0.004 (3)	−0.030 (3)	−0.005 (3)
C24	0.053 (3)	0.054 (3)	0.047 (2)	0.003 (2)	−0.009 (2)	0.001 (2)
C25	0.059 (3)	0.092 (4)	0.062 (3)	0.001 (3)	−0.006 (3)	−0.018 (3)
C26	0.058 (4)	0.108 (4)	0.081 (4)	0.000 (3)	−0.006 (3)	−0.012 (3)
C27	0.072 (4)	0.105 (5)	0.068 (3)	0.003 (3)	0.015 (3)	−0.003 (3)
C28	0.086 (4)	0.081 (4)	0.048 (3)	0.011 (3)	0.006 (3)	0.001 (3)
C29	0.064 (3)	0.056 (3)	0.041 (2)	0.000 (2)	−0.004 (2)	−0.001 (2)

C30	0.067 (3)	0.050 (2)	0.050 (2)	−0.002 (2)	−0.014 (2)	0.002 (2)

Geometric parameters (Å, °)

Zn1—O1	1.919 (9)	C7'—H7'	0.9300
Zn1—O4	1.961 (3)	C6'—C5'	1.3900
Zn1—N3	2.006 (4)	C6'—H6'	0.9300
Zn1—O1'	2.020 (13)	C5'—C4'	1.3900
Zn1—N1	2.038 (4)	C5'—C8'	1.485 (6)
N1—C23	1.316 (6)	C4'—C3'	1.3900
N1—C17	1.387 (5)	C4'—H4'	0.9300
N2—C23	1.321 (6)	C3'—H3'	0.9300
N2—C22	1.372 (6)	C8'—H8'	0.9300
N2—H2n	0.8600	C9—C10	1.504 (6)
N3—C30	1.318 (5)	C10—C15	1.386 (6)
N3—C24	1.397 (6)	C10—C11	1.395 (6)
N4—C30	1.338 (6)	C11—C12	1.362 (6)
N4—C29	1.370 (6)	C11—H11	0.9300
N4—H4n	0.8600	C12—C13	1.389 (7)
O4—C9	1.276 (6)	C12—H12	0.9300
O5—C9	1.232 (6)	C13—C14	1.374 (7)
O6—C16	1.190 (7)	C13—C16	1.468 (7)
O1—C1	1.237 (8)	C14—C15	1.385 (6)
O2—C1	1.239 (8)	C14—H14	0.9300
O3—C8	1.209 (8)	C15—H15	0.9300
O1w—H1w1	0.842	C16—H16	0.9300
O1w—H1w2	0.864	C17—C18	1.379 (7)
C1—C2	1.504 (6)	C17—C22	1.396 (6)
C2—C7	1.3900	C18—C19	1.387 (7)
C2—C3	1.3900	C18—H18	0.9300
C7—C6	1.3900	C19—C20	1.389 (9)
C7—H7	0.9300	C19—H19	0.9300
C6—C5	1.3900	C20—C21	1.364 (8)
C6—H6	0.9300	C20—H20	0.9300
C5—C4	1.3900	C21—C22	1.378 (7)
C5—C8	1.481 (6)	C21—H21	0.9300
C4—C3	1.3900	C23—H23	0.9300
C4—H4	0.9300	C24—C25	1.379 (6)
C3—H3	0.9300	C24—C29	1.398 (6)
C8—H8	0.9300	C25—C26	1.366 (8)
O1'—C1'	1.241 (9)	C25—H25	0.9300
O2'—C1'	1.226 (9)	C26—C27	1.384 (7)
O3'—C8'	1.218 (9)	C26—H26	0.9300
O1w'—H1w3	0.86	C27—C28	1.375 (8)
O1w'—H1w4	0.86	C27—H27	0.9300
C1'—C2'	1.500 (6)	C28—C29	1.389 (7)
C2'—C7'	1.3900	C28—H28	0.9300
C2'—C3'	1.3900	C30—H30	0.9300
C7'—C6'	1.3900		

O1—Zn1—O4	102.9 (3)	C4'—C3'—C2'	120.0
O1—Zn1—N3	129.5 (3)	C4'—C3'—H3'	120.0
O4—Zn1—N3	108.97 (14)	C2'—C3'—H3'	120.0
O4—Zn1—O1'	131.0 (3)	O3'—C8'—C5'	119.9 (18)
N3—Zn1—O1'	101.2 (3)	O3'—C8'—H8'	120.0
O1—Zn1—N1	109.6 (2)	C5'—C8'—H8'	120.0
O4—Zn1—N1	94.03 (14)	O5—C9—O4	124.7 (4)
N3—Zn1—N1	106.12 (15)	O5—C9—C10	120.1 (4)
O1'—Zn1—N1	113.7 (3)	O4—C9—C10	115.2 (4)
O1—Zn1—C1	26.9 (2)	C15—C10—C11	119.4 (4)
O4—Zn1—C1	129.3 (2)	C15—C10—C9	120.1 (4)
N3—Zn1—C1	107.7 (2)	C11—C10—C9	120.4 (4)
N1—Zn1—C1	107.95 (15)	C12—C11—C10	120.5 (5)
C23—N1—C17	105.1 (4)	C12—C11—H11	119.7
C23—N1—Zn1	124.6 (3)	C10—C11—H11	119.7
C17—N1—Zn1	130.2 (3)	C11—C12—C13	120.1 (5)
C23—N2—C22	108.6 (4)	C11—C12—H12	119.9
C23—N2—H2n	125.7	C13—C12—H12	119.9
C22—N2—H2n	125.7	C14—C13—C12	119.7 (4)
C30—N3—C24	105.2 (4)	C14—C13—C16	121.1 (5)
C30—N3—Zn1	130.2 (3)	C12—C13—C16	119.2 (5)
C24—N3—Zn1	124.5 (3)	C13—C14—C15	120.7 (4)
C30—N4—C29	107.9 (4)	C13—C14—H14	119.6
C30—N4—H4n	126.1	C15—C14—H14	119.6
C29—N4—H4n	126.1	C14—C15—C10	119.5 (4)
C9—O4—Zn1	119.9 (3)	C14—C15—H15	120.3
C1—O1—Zn1	108.4 (7)	C10—C15—H15	120.3
H1w1—O1w—H1w2	107.3	O6—C16—C13	126.8 (6)
O1—C1—O2	121.5 (9)	O6—C16—H16	116.6
O1—C1—C2	119.5 (7)	C13—C16—H16	116.6
O2—C1—C2	118.9 (7)	C18—C17—N1	130.2 (5)
C7—C2—C3	120.0	C18—C17—C22	120.8 (4)
C7—C2—C1	121.6 (4)	N1—C17—C22	109.0 (4)
C3—C2—C1	118.4 (4)	C17—C18—C19	116.9 (5)
C2—C7—C6	120.0	C17—C18—H18	121.6
C2—C7—H7	120.0	C19—C18—H18	121.6
C6—C7—H7	120.0	C18—C19—C20	121.6 (6)
C7—C6—C5	120.0	C18—C19—H19	119.2
C7—C6—H6	120.0	C20—C19—H19	119.2
C5—C6—H6	120.0	C21—C20—C19	121.7 (6)
C6—C5—C4	120.0	C21—C20—H20	119.1
C6—C5—C8	120.9 (5)	C19—C20—H20	119.1
C4—C5—C8	119.1 (5)	C20—C21—C22	117.0 (6)
C3—C4—C5	120.0	C20—C21—H21	121.5
C3—C4—H4	120.0	C22—C21—H21	121.5
C5—C4—H4	120.0	N2—C22—C21	133.3 (5)
C4—C3—C2	120.0	N2—C22—C17	104.6 (4)
C4—C3—H3	120.0	C21—C22—C17	122.1 (5)
C2—C3—H3	120.0	N1—C23—N2	112.6 (4)

O3—C8—C5	127.5 (16)	N1—C23—H23	123.7
O3—C8—H8	116.2	N2—C23—H23	123.7
C5—C8—H8	116.2	C25—C24—N3	130.7 (4)
C1'—O1'—Zn1	107.5 (9)	C25—C24—C29	120.7 (5)
H1w3—O1w'—H1w4	108.2	N3—C24—C29	108.6 (4)
O2'—C1'—O1'	123.0 (11)	C26—C25—C24	117.6 (5)
O2'—C1'—C2'	118.9 (8)	C26—C25—H25	121.2
O1'—C1'—C2'	118.2 (9)	C24—C25—H25	121.2
C7'—C2'—C3'	120.0	C25—C26—C27	121.7 (6)
C7'—C2'—C1'	118.9 (5)	C25—C26—H26	119.2
C3'—C2'—C1'	121.1 (5)	C27—C26—H26	119.2
C6'—C7'—C2'	120.0	C28—C27—C26	122.1 (5)
C6'—C7'—H7'	120.0	C28—C27—H27	118.9
C2'—C7'—H7'	120.0	C26—C27—H27	118.9
C7'—C6'—C5'	120.0	C27—C28—C29	116.2 (5)
C7'—C6'—H6'	120.0	C27—C28—H28	121.9
C5'—C6'—H6'	120.0	C29—C28—H28	121.9
C6'—C5'—C4'	120.0	N4—C29—C28	132.7 (4)
C6'—C5'—C8'	119.8 (5)	N4—C29—C24	105.6 (4)
C4'—C5'—C8'	120.2 (5)	C28—C29—C24	121.7 (5)
C3'—C4'—C5'	120.0	N3—C30—N4	112.7 (4)
C3'—C4'—H4'	120.0	N3—C30—H30	123.6
C5'—C4'—H4'	120.0	N4—C30—H30	123.6
O1—Zn1—N1—C23	−104.9 (5)	O4—C9—C10—C15	169.3 (4)
O4—Zn1—N1—C23	0.3 (4)	O5—C9—C10—C11	172.2 (5)
N3—Zn1—N1—C23	111.4 (4)	O4—C9—C10—C11	−8.4 (7)
O1'—Zn1—N1—C23	−138.3 (5)	C15—C10—C11—C12	−1.4 (8)
C1—Zn1—N1—C23	−133.3 (4)	C9—C10—C11—C12	176.3 (5)
O1—Zn1—N1—C17	71.5 (5)	C10—C11—C12—C13	−1.1 (8)
O4—Zn1—N1—C17	176.7 (4)	C11—C12—C13—C14	2.9 (8)
N3—Zn1—N1—C17	−72.2 (4)	C11—C12—C13—C16	−175.7 (5)
O1'—Zn1—N1—C17	38.1 (5)	C12—C13—C14—C15	−2.2 (7)
C1—Zn1—N1—C17	43.1 (4)	C16—C13—C14—C15	176.5 (4)
O1—Zn1—N3—C30	−3.3 (5)	C13—C14—C15—C10	−0.4 (7)
O4—Zn1—N3—C30	−129.4 (4)	C11—C10—C15—C14	2.1 (7)
O1'—Zn1—N3—C30	11.5 (5)	C9—C10—C15—C14	−175.6 (4)
N1—Zn1—N3—C30	130.5 (4)	C14—C13—C16—O6	−172.6 (6)
C1—Zn1—N3—C30	15.0 (4)	C12—C13—C16—O6	6.1 (9)
O1—Zn1—N3—C24	171.5 (4)	C23—N1—C17—C18	179.7 (5)
O4—Zn1—N3—C24	45.4 (4)	Zn1—N1—C17—C18	2.7 (7)
O1'—Zn1—N3—C24	−173.7 (4)	C23—N1—C17—C22	1.0 (5)
N1—Zn1—N3—C24	−54.8 (3)	Zn1—N1—C17—C22	−176.0 (3)
C1—Zn1—N3—C24	−170.2 (3)	N1—C17—C18—C19	−178.5 (5)
O1—Zn1—O4—C9	−67.1 (4)	C22—C17—C18—C19	0.1 (7)
N3—Zn1—O4—C9	73.1 (4)	C17—C18—C19—C20	0.3 (9)
O1'—Zn1—O4—C9	−51.7 (5)	C18—C19—C20—C21	−0.2 (10)
N1—Zn1—O4—C9	−178.3 (3)	C19—C20—C21—C22	−0.2 (9)
C1—Zn1—O4—C9	−61.1 (4)	C23—N2—C22—C21	−178.5 (5)
O4—Zn1—O1—C1	169.7 (3)	C23—N2—C22—C17	0.7 (5)

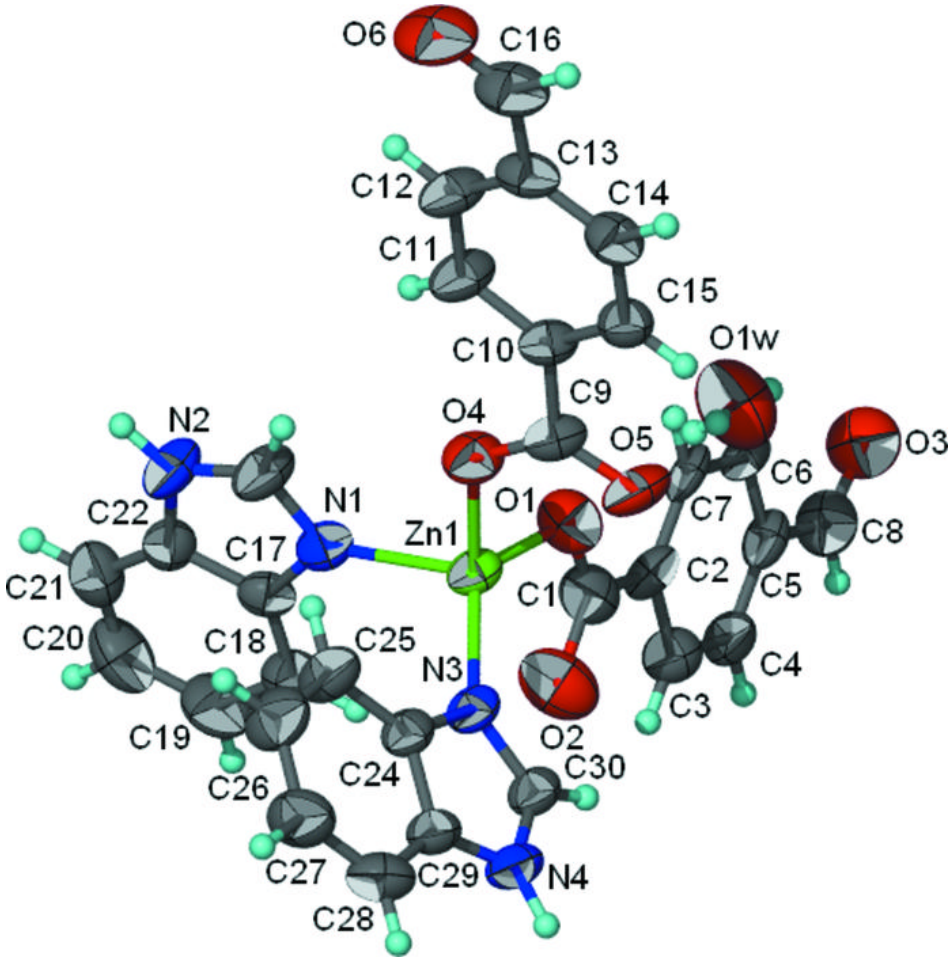
N3—Zn1—O1—C1	41.4 (4)	C20—C21—C22—N2	179.7 (5)
O1'—Zn1—O1—C1	12.5 (6)	C20—C21—C22—C17	0.6 (8)
N1—Zn1—O1—C1	−91.2 (3)	C18—C17—C22—N2	−179.9 (4)
Zn1—O1—C1—O2	−7.5 (3)	N1—C17—C22—N2	−1.0 (5)
Zn1—O1—C1—C2	172.5 (3)	C18—C17—C22—C21	−0.6 (7)
O1—C1—C2—C7	−0.03 (7)	N1—C17—C22—C21	178.3 (4)
O2—C1—C2—C7	−179.99 (4)	C17—N1—C23—N2	−0.5 (6)
Zn1—C1—C2—C7	18.3 (8)	Zn1—N1—C23—N2	176.6 (3)
O1—C1—C2—C3	180.00 (4)	C22—N2—C23—N1	−0.1 (6)
O2—C1—C2—C3	0.04 (7)	C30—N3—C24—C25	179.3 (5)
Zn1—C1—C2—C3	−161.7 (8)	Zn1—N3—C24—C25	3.4 (7)
C6—C5—C8—O3	0.04 (9)	C30—N3—C24—C29	0.3 (5)
C4—C5—C8—O3	−179.97 (5)	Zn1—N3—C24—C29	−175.6 (3)
O1—Zn1—O1'—C1'	−6.3 (5)	N3—C24—C25—C26	179.9 (5)
O4—Zn1—O1'—C1'	−36.2 (5)	C29—C24—C25—C26	−1.2 (8)
N3—Zn1—O1'—C1'	−163.9 (3)	C24—C25—C26—C27	−0.5 (9)
N1—Zn1—O1'—C1'	82.7 (4)	C25—C26—C27—C28	2.2 (10)
C1—Zn1—O1'—C1'	43 (3)	C26—C27—C28—C29	−2.0 (9)
Zn1—O1'—C1'—O2'	13.1 (3)	C30—N4—C29—C28	179.2 (5)
Zn1—O1'—C1'—C2'	−166.9 (3)	C30—N4—C29—C24	−0.2 (5)
O2'—C1'—C2'—C7'	−0.03 (7)	C27—C28—C29—N4	−179.1 (5)
O1'—C1'—C2'—C7'	−179.99 (4)	C27—C28—C29—C24	0.3 (7)
O2'—C1'—C2'—C3'	180.00 (4)	C25—C24—C29—N4	−179.1 (4)
O1'—C1'—C2'—C3'	0.04 (7)	N3—C24—C29—N4	0.0 (5)
C1'—C2'—C3'—C4'	179.97 (5)	C25—C24—C29—C28	1.4 (7)
C6'—C5'—C8'—O3'	0.03 (8)	N3—C24—C29—C28	−179.5 (4)
C4'—C5'—C8'—O3'	−179.98 (4)	C24—N3—C30—N4	−0.5 (5)
Zn1—O4—C9—O5	−5.9 (7)	Zn1—N3—C30—N4	175.1 (3)
Zn1—O4—C9—C10	174.8 (3)	C29—N4—C30—N3	0.5 (5)
O5—C9—C10—C15	−10.1 (7)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2n···O1w^{i}	0.86	2.12	2.907 (8)	152
N2—H2n···O1w^{ii}	0.86	2.17	2.960 (8)	154
N4—H4n···O5^{iii}	0.86	2.11	2.864 (5)	145
O1w—H1w1···O1	0.84	2.064 (7)	2.87 (1)	159
O1w—H1w2···O5	0.86	1.873 (4)	2.69 (1)	157
O1w'—H1w3···O5	0.86	2.353 (4)	3.112 (8)	148

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

Fig. 1


O6
C16
C13
C12
C14
C11
C15
C10
O1w
C9
O4
O5
O3
N2
C6
N1
O1
C7
C8
C22
Zn1
C17
C2
C21
C1
C5
C20
C18
C25
N3
C4
C3
C19
O2
C30
C24
C26
C27
C29
N4
C28