

Bis(4-formylbenzoato- κ O)bis(1*H*-imidazole- κ N³)zinc(II)

Zhao-Peng Deng,^a Shan Gao^a and Seik Weng Ng^{b*}

^aCollege of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and ^bDepartment of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Correspondence e-mail: seikweng@um.edu.my

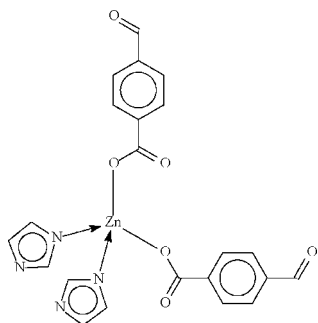
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.012$ Å; R factor = 0.040; wR factor = 0.150; data-to-parameter ratio = 15.0.

The zinc centre in the title complex, $[\text{Zn}(\text{C}_8\text{H}_5\text{O}_3)_2(\text{C}_3\text{H}_4\text{N}_2)_2]$, shows tetrahedral coordination. Adjacent molecules are linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds into a layer structure.

Related literature

For the diaqua complex, see Deng *et al.* (2006*a*), and for the aqua phenanthroline adduct, see Deng *et al.* (2006*b*). The monohydrated bis(benzimidazole) adduct is hydrogen bonded into a chain structure (see Deng *et al.*, 2007).



Experimental

Crystal data

$[\text{Zn}(\text{C}_8\text{H}_5\text{O}_3)_2(\text{C}_3\text{H}_4\text{N}_2)_2]$

$M_r = 499.77$

Monoclinic, $P2_1$

$a = 11.9413$ (9) Å

$b = 7.0455$ (5) Å

$c = 14.2092$ (9) Å

$\beta = 109.904$ (2)°

$V = 1124.1$ (1) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 1.14$ mm⁻¹

$T = 295$ (2) K

$0.36 \times 0.25 \times 0.21$ mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer

Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)

$T_{\text{min}} = 0.662$, $T_{\text{max}} = 0.796$

11106 measured reflections

4493 independent reflections

2901 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.150$

$S = 1.13$

4493 reflections

299 parameters

1 restraint

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 1.17$ e Å⁻³

$\Delta\rho_{\text{min}} = -1.12$ e Å⁻³

Absolute structure: Flack (1983),

1716 Friedel pairs

Flack parameter: 0.01 (2)

Table 1

Selected geometric parameters (Å, °).

Zn1—O1	1.938 (5)	Zn1—N1	2.007 (5)
Zn1—O4	1.966 (5)	Zn1—N3	2.007 (6)
O1—Zn1—O4	118.3 (2)	O4—Zn1—N1	97.4 (2)
O1—Zn1—N1	114.7 (2)	O4—Zn1—N3	111.7 (2)
O1—Zn1—N3	101.9 (2)	N1—Zn1—N3	113.4 (2)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i> ⋯ <i>A</i>
N2—H2N⋯O2 ⁱ	0.86	1.92	2.749 (7)	163
N4—H4N⋯O5 ⁱⁱ	0.86	1.93	2.754 (7)	162

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 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) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *pubCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2375).

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Bis(4-formylbenzoato- κO)bis(1*H*-imidazole- κN^3)zinc(II)

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

Comment

As a part of our ongoing investigation on 4-formylbenzoate complexes (Deng *et al.*, 2006*a*, 2006*b*, 2007), the title Zn^{II} complex has been prepared and its structure is reported here. The molecular structure is shown in Fig. 1. The Zn^{II} ion displays a tetrahedral coordination geometry (Table 1). Adjacent molecules are linked by N—H \cdots O hydrogen bonds into a layer structure (Table 2 and Fig. 2).

Experimental

Zinc sulfate heptahydrate (1.44 g, 5 mmol) was added to an aqueous solution (25 ml) of 4-formylbenzoic acid (1.5 g, 10 mmol) and imidazole (0.68 g, 10 mmol). The pH value of the mixture was about 6. The solution was allowed to evaporate at room temperature; colorless prismatic crystals separated from the filtered solution after several days. CH&N elemental analysis. Calc. for C₂₂H₁₈N₄O₆Zn: C 52.87, H 3.63, N 11.21%. Found: C 52.88, H 3.68, N 11.18%.

Refinement

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 $1.2U_{eq}(C,N)$.

The final difference Fourier map had a large peak /deep hole near Zn1.

Figures

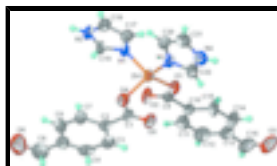


Fig. 1. Thermal ellipsoid plot of the molecular structure. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii.

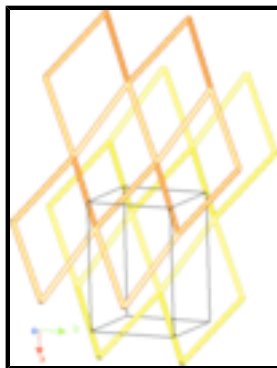


Fig. 2. OLEX (Dolomanov *et al.*, 2003) representation of the hydrogen-bonded layer structure.

Bis(4-formylbenzoato- κ O)bis(1*H*-imidazole- κ N³)zinc(II)

Crystal data

$[\text{Zn}(\text{C}_8\text{H}_5\text{O}_3)_2(\text{C}_3\text{H}_4\text{N}_2)_2]$	$F_{000} = 512$
$M_r = 499.77$	$D_x = 1.477 \text{ Mg m}^{-3}$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
Hall symbol: P 2yb	$\lambda = 0.71073 \text{ \AA}$
$a = 11.9413 (9) \text{ \AA}$	Cell parameters from 8013 reflections
$b = 7.0455 (5) \text{ \AA}$	$\theta = 3.1\text{--}27.5^\circ$
$c = 14.2092 (9) \text{ \AA}$	$\mu = 1.14 \text{ mm}^{-1}$
$\beta = 109.904 (2)^\circ$	$T = 295 (2) \text{ K}$
$V = 1124.1 (1) \text{ \AA}^3$	Prism, colorless
$Z = 2$	$0.36 \times 0.25 \times 0.21 \text{ mm}$

Data collection

Rigaku RAXIS-RAPID IP diffractometer	4493 independent reflections
Radiation source: fine-focus sealed tube	2901 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.042$
$T = 295(2) \text{ K}$	$\theta_{\text{max}} = 27.5^\circ$
ω scan	$\theta_{\text{min}} = 3.1^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -15 \rightarrow 15$
$T_{\text{min}} = 0.662$, $T_{\text{max}} = 0.796$	$k = -9 \rightarrow 8$
11106 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.040$	$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 1.7346P]$
$wR(F^2) = 0.150$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{\text{max}} = 0.001$
4493 reflections	$\Delta\rho_{\text{max}} = 1.17 \text{ e \AA}^{-3}$
299 parameters	$\Delta\rho_{\text{min}} = -1.11 \text{ e \AA}^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983) parameter from 1716 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.01 (2)

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.77235 (5)	0.49998 (13)	0.20968 (4)	0.0464 (2)
O1	0.8971 (4)	0.3416 (7)	0.1932 (4)	0.0585 (13)
O2	0.7697 (4)	0.1549 (8)	0.0823 (4)	0.0684 (15)
O3	1.3608 (7)	-0.2711 (12)	0.1953 (5)	0.111 (3)
O4	0.6612 (4)	0.3861 (8)	0.2687 (3)	0.0608 (13)
O5	0.7938 (4)	0.3692 (9)	0.4217 (4)	0.0719 (15)
O6	0.1902 (7)	0.3427 (14)	0.4523 (6)	0.126 (3)
N1	0.6505 (4)	0.5887 (8)	0.0812 (4)	0.0461 (12)
N2	0.4747 (5)	0.6479 (9)	-0.0238 (5)	0.0631 (17)
H2n	0.3998	0.6732	-0.0469	0.076*
N3	0.8663 (4)	0.7125 (8)	0.2943 (4)	0.0473 (13)
N4	1.0097 (5)	0.8557 (10)	0.4062 (4)	0.0622 (16)
H4n	1.0774	0.8759	0.4521	0.075*
C1	0.6901 (5)	0.3684 (10)	0.3637 (5)	0.0498 (16)
C2	0.5873 (6)	0.3511 (9)	0.4011 (4)	0.0462 (15)
C3	0.6076 (7)	0.3316 (11)	0.5034 (5)	0.0585 (18)
H3	0.6847	0.3235	0.5489	0.070*
C4	0.5090 (8)	0.3245 (11)	0.5363 (5)	0.064 (2)
H4	0.5215	0.3125	0.6043	0.077*
C5	0.3954 (7)	0.3348 (11)	0.4702 (6)	0.0616 (19)
C6	0.3780 (7)	0.3571 (12)	0.3701 (6)	0.064 (2)
H6	0.3008	0.3680	0.3249	0.077*
C7	0.4699 (6)	0.3635 (11)	0.3360 (5)	0.0535 (17)
H7	0.4550	0.3765	0.2677	0.064*
C8	0.2937 (10)	0.3301 (16)	0.5073 (8)	0.091 (3)
H8	0.3094	0.3168	0.5757	0.109*
C9	0.8711 (5)	0.1953 (10)	0.1381 (5)	0.0450 (14)
C10	0.9721 (6)	0.0645 (9)	0.1431 (5)	0.0459 (16)
C11	0.9491 (7)	-0.1102 (12)	0.0963 (6)	0.064 (2)
H11	0.8710	-0.1469	0.0618	0.077*
C12	1.0425 (8)	-0.2306 (12)	0.1007 (6)	0.074 (2)
H12	1.0270	-0.3478	0.0688	0.089*
C13	1.1581 (7)	-0.1771 (12)	0.1522 (6)	0.062 (2)
C14	1.1811 (6)	-0.0046 (18)	0.1993 (5)	0.073 (2)
H14	1.2593	0.0317	0.2336	0.087*
C15	1.0887 (5)	0.1152 (11)	0.1958 (6)	0.062 (2)
H15	1.1047	0.2310	0.2292	0.075*
C16	1.2565 (9)	-0.3093 (15)	0.1549 (7)	0.082 (3)
H16	1.2368	-0.4270	0.1241	0.098*
C17	0.6563 (6)	0.5897 (11)	-0.0136 (5)	0.0551 (17)
H17	0.7242	0.5678	-0.0300	0.066*
C18	0.5469 (7)	0.6276 (12)	-0.0788 (5)	0.064 (2)
H18	0.5252	0.6379	-0.1480	0.077*
C19	0.5387 (5)	0.6224 (10)	0.0710 (5)	0.0496 (16)
H19	0.5089	0.6274	0.1235	0.060*

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C20	0.8343 (6)	0.8961 (11)	0.3001 (5)	0.0549 (17)
H20	0.7622	0.9505	0.2619	0.066*
C21	0.9231 (6)	0.9861 (16)	0.3696 (5)	0.0631 (17)
H21	0.9248	1.1126	0.3887	0.076*
C22	0.9740 (6)	0.6922 (12)	0.3605 (5)	0.0578 (18)
H22	1.0180	0.5803	0.3731	0.069*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0356 (3)	0.0558 (4)	0.0432 (3)	0.0037 (4)	0.0074 (2)	-0.0028 (5)
O1	0.041 (2)	0.057 (3)	0.070 (3)	0.004 (2)	0.009 (2)	-0.011 (3)
O2	0.035 (2)	0.080 (4)	0.074 (3)	0.004 (2)	-0.002 (2)	-0.016 (3)
O3	0.096 (5)	0.148 (7)	0.102 (5)	0.067 (5)	0.051 (4)	0.033 (5)
O4	0.054 (3)	0.076 (4)	0.044 (2)	-0.005 (2)	0.006 (2)	0.003 (2)
O5	0.049 (3)	0.101 (4)	0.055 (3)	0.007 (3)	0.005 (2)	0.016 (3)
O6	0.090 (5)	0.172 (8)	0.134 (6)	0.009 (6)	0.061 (5)	0.006 (6)
N1	0.032 (2)	0.061 (3)	0.043 (3)	0.005 (2)	0.010 (2)	-0.004 (2)
N2	0.034 (3)	0.072 (4)	0.072 (4)	0.007 (3)	0.003 (3)	0.008 (3)
N3	0.037 (3)	0.056 (4)	0.044 (3)	0.004 (2)	0.007 (2)	0.001 (3)
N4	0.058 (4)	0.071 (4)	0.048 (3)	-0.015 (3)	0.006 (3)	-0.015 (3)
C1	0.040 (3)	0.052 (4)	0.051 (4)	0.007 (3)	0.007 (3)	0.002 (3)
C2	0.055 (4)	0.042 (4)	0.042 (3)	0.005 (3)	0.018 (3)	-0.001 (3)
C3	0.062 (4)	0.061 (5)	0.053 (4)	0.010 (3)	0.019 (3)	0.003 (4)
C4	0.096 (6)	0.054 (5)	0.048 (4)	0.006 (4)	0.032 (4)	0.009 (3)
C5	0.061 (5)	0.057 (5)	0.074 (5)	0.007 (4)	0.031 (4)	0.004 (4)
C6	0.050 (4)	0.075 (5)	0.070 (5)	-0.006 (4)	0.025 (4)	-0.004 (4)
C7	0.049 (4)	0.062 (5)	0.047 (3)	0.003 (3)	0.013 (3)	-0.006 (3)
C8	0.099 (8)	0.095 (8)	0.099 (7)	0.014 (6)	0.060 (6)	0.003 (6)
C9	0.040 (3)	0.048 (4)	0.046 (3)	0.005 (3)	0.012 (3)	0.001 (3)
C10	0.040 (3)	0.046 (4)	0.054 (4)	0.008 (2)	0.019 (3)	0.003 (3)
C11	0.059 (5)	0.060 (5)	0.073 (5)	-0.003 (4)	0.023 (4)	-0.013 (4)
C12	0.096 (7)	0.055 (5)	0.077 (5)	0.016 (4)	0.037 (5)	-0.010 (4)
C13	0.067 (5)	0.069 (5)	0.058 (4)	0.019 (4)	0.032 (4)	0.008 (4)
C14	0.046 (3)	0.090 (6)	0.079 (4)	0.027 (6)	0.017 (3)	-0.012 (7)
C15	0.033 (3)	0.067 (5)	0.083 (5)	0.003 (3)	0.013 (3)	-0.021 (4)
C16	0.093 (7)	0.091 (7)	0.073 (5)	0.042 (6)	0.042 (5)	0.018 (5)
C17	0.053 (4)	0.066 (5)	0.043 (3)	0.002 (3)	0.012 (3)	0.003 (3)
C18	0.058 (4)	0.076 (6)	0.046 (4)	0.001 (4)	0.003 (3)	0.008 (4)
C19	0.031 (3)	0.062 (4)	0.049 (3)	0.004 (3)	0.005 (3)	-0.003 (3)
C20	0.049 (4)	0.065 (5)	0.051 (4)	0.011 (3)	0.017 (3)	0.003 (3)
C21	0.077 (4)	0.054 (4)	0.061 (4)	-0.004 (5)	0.027 (3)	-0.010 (5)
C22	0.045 (4)	0.064 (5)	0.052 (4)	-0.003 (3)	0.000 (3)	-0.010 (4)

Geometric parameters (\AA , $^\circ$)

Zn1—O1	1.938 (5)	C5—C6	1.375 (10)
Zn1—O4	1.966 (5)	C5—C8	1.480 (12)
Zn1—N1	2.007 (5)	C6—C7	1.342 (9)

Zn1—N3	2.007 (6)	C6—H6	0.9300
O1—C9	1.267 (8)	C7—H7	0.9300
O2—C9	1.235 (7)	C8—H8	0.9300
O3—C16	1.212 (11)	C9—C10	1.500 (9)
O4—C1	1.281 (7)	C10—C11	1.382 (10)
O5—C1	1.232 (7)	C10—C15	1.384 (9)
O6—C8	1.220 (11)	C11—C12	1.385 (11)
N1—C19	1.315 (7)	C11—H11	0.9300
N1—C17	1.373 (8)	C12—C13	1.377 (12)
N2—C19	1.315 (8)	C12—H12	0.9300
N2—C18	1.354 (10)	C13—C14	1.369 (14)
N2—H2n	0.8600	C13—C16	1.489 (11)
N3—C22	1.318 (8)	C14—C15	1.377 (10)
N3—C20	1.360 (9)	C14—H14	0.9300
N4—C22	1.320 (10)	C15—H15	0.9300
N4—C21	1.348 (11)	C16—H16	0.9300
N4—H4n	0.8600	C17—C18	1.346 (10)
C1—C2	1.499 (9)	C17—H17	0.9300
C2—C7	1.395 (9)	C18—H18	0.9300
C2—C3	1.397 (9)	C19—H19	0.9300
C3—C4	1.408 (11)	C20—C21	1.337 (10)
C3—H3	0.9300	C20—H20	0.9300
C4—C5	1.364 (11)	C21—H21	0.9300
C4—H4	0.9300	C22—H22	0.9300
O1—Zn1—O4	118.3 (2)	C5—C8—H8	118.5
O1—Zn1—N1	114.7 (2)	O2—C9—O1	124.4 (6)
O1—Zn1—N3	101.9 (2)	O2—C9—C10	119.1 (6)
O4—Zn1—N1	97.4 (2)	O1—C9—C10	116.5 (5)
O4—Zn1—N3	111.7 (2)	C11—C10—C15	119.3 (6)
N1—Zn1—N3	113.4 (2)	C11—C10—C9	120.0 (7)
C9—O1—Zn1	120.4 (4)	C15—C10—C9	120.7 (6)
C1—O4—Zn1	120.7 (4)	C10—C11—C12	119.9 (8)
C19—N1—C17	106.2 (5)	C10—C11—H11	120.1
C19—N1—Zn1	123.5 (4)	C12—C11—H11	120.1
C17—N1—Zn1	129.1 (4)	C13—C12—C11	120.2 (8)
C19—N2—C18	108.4 (5)	C13—C12—H12	119.9
C19—N2—H2n	125.8	C11—C12—H12	119.9
C18—N2—H2n	125.8	C14—C13—C12	120.1 (7)
C22—N3—C20	106.6 (6)	C14—C13—C16	121.1 (8)
C22—N3—Zn1	123.9 (5)	C12—C13—C16	118.8 (9)
C20—N3—Zn1	129.5 (4)	C13—C14—C15	120.1 (7)
C22—N4—C21	109.2 (6)	C13—C14—H14	120.0
C22—N4—H4n	125.4	C15—C14—H14	120.0
C21—N4—H4n	125.4	C14—C15—C10	120.5 (8)
O5—C1—O4	123.6 (6)	C14—C15—H15	119.8
O5—C1—C2	121.4 (6)	C10—C15—H15	119.8
O4—C1—C2	115.0 (5)	O3—C16—C13	123.3 (10)
C7—C2—C3	118.4 (6)	O3—C16—H16	118.4
C7—C2—C1	121.3 (6)	C13—C16—H16	118.4

supplementary materials

C3—C2—C1	120.3 (6)	C18—C17—N1	108.4 (7)
C2—C3—C4	118.7 (7)	C18—C17—H17	125.8
C2—C3—H3	120.6	N1—C17—H17	125.8
C4—C3—H3	120.6	C17—C18—N2	106.4 (6)
C5—C4—C3	121.1 (7)	C17—C18—H18	126.8
C5—C4—H4	119.4	N2—C18—H18	126.8
C3—C4—H4	119.4	N1—C19—N2	110.6 (6)
C4—C5—C6	118.9 (7)	N1—C19—H19	124.7
C4—C5—C8	119.8 (8)	N2—C19—H19	124.7
C6—C5—C8	121.2 (8)	C21—C20—N3	109.1 (7)
C7—C6—C5	121.5 (7)	C21—C20—H20	125.4
C7—C6—H6	119.2	N3—C20—H20	125.4
C5—C6—H6	119.2	C20—C21—N4	105.9 (8)
C6—C7—C2	121.3 (7)	C20—C21—H21	127.1
C6—C7—H7	119.4	N4—C21—H21	127.1
C2—C7—H7	119.4	N3—C22—N4	109.2 (7)
O6—C8—C5	123.0 (10)	N3—C22—H22	125.4
O6—C8—H8	118.5	N4—C22—H22	125.4
O4—Zn1—O1—C9	61.0 (5)	C4—C5—C8—O6	178.4 (10)
N3—Zn1—O1—C9	-176.1 (5)	C6—C5—C8—O6	1.1 (15)
N1—Zn1—O1—C9	-53.2 (6)	Zn1—O1—C9—O2	9.4 (9)
O1—Zn1—O4—C1	81.4 (6)	Zn1—O1—C9—C10	-170.2 (4)
N3—Zn1—O4—C1	-36.4 (6)	O2—C9—C10—C11	-8.5 (10)
N1—Zn1—O4—C1	-155.2 (5)	O1—C9—C10—C11	171.1 (6)
O1—Zn1—N1—C19	149.5 (5)	O2—C9—C10—C15	172.6 (7)
O4—Zn1—N1—C19	23.6 (6)	O1—C9—C10—C15	-7.7 (10)
N3—Zn1—N1—C19	-94.0 (5)	C15—C10—C11—C12	-1.4 (11)
O1—Zn1—N1—C17	-16.0 (7)	C9—C10—C11—C12	179.8 (7)
O4—Zn1—N1—C17	-141.9 (6)	C10—C11—C12—C13	0.4 (13)
N3—Zn1—N1—C17	100.5 (6)	C11—C12—C13—C14	0.1 (13)
O1—Zn1—N3—C22	-31.2 (6)	C11—C12—C13—C16	-179.6 (8)
O4—Zn1—N3—C22	96.1 (6)	C12—C13—C14—C15	0.4 (13)
N1—Zn1—N3—C22	-155.0 (5)	C16—C13—C14—C15	-179.9 (8)
O1—Zn1—N3—C20	152.0 (6)	C13—C14—C15—C10	-1.4 (13)
O4—Zn1—N3—C20	-80.7 (6)	C11—C10—C15—C14	1.9 (12)
N1—Zn1—N3—C20	28.2 (6)	C9—C10—C15—C14	-179.3 (7)
Zn1—O4—C1—O5	-20.8 (10)	C14—C13—C16—O3	-2.4 (14)
Zn1—O4—C1—C2	157.8 (5)	C12—C13—C16—O3	177.2 (8)
O5—C1—C2—C7	175.5 (7)	C19—N1—C17—C18	1.1 (8)
O4—C1—C2—C7	-3.1 (10)	Zn1—N1—C17—C18	168.6 (5)
O5—C1—C2—C3	-1.3 (11)	N1—C17—C18—N2	-0.6 (9)
O4—C1—C2—C3	-179.8 (6)	C19—N2—C18—C17	-0.2 (9)
C7—C2—C3—C4	0.3 (11)	C17—N1—C19—N2	-1.2 (8)
C1—C2—C3—C4	177.1 (7)	Zn1—N1—C19—N2	-169.6 (5)
C2—C3—C4—C5	0.5 (11)	C18—N2—C19—N1	0.9 (9)
C3—C4—C5—C6	-1.6 (12)	C22—N3—C20—C21	0.3 (8)
C3—C4—C5—C8	-179.0 (8)	Zn1—N3—C20—C21	177.4 (5)
C4—C5—C6—C7	1.9 (13)	N3—C20—C21—N4	0.0 (8)
C8—C5—C6—C7	179.3 (9)	C22—N4—C21—C20	-0.2 (8)

C5—C6—C7—C2	-1.1 (13)	C20—N3—C22—N4	-0.4 (8)
C3—C2—C7—C6	0.0 (11)	Zn1—N3—C22—N4	-177.7 (5)
C1—C2—C7—C6	-176.8 (7)	C21—N4—C22—N3	0.4 (8)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H2 n \cdots O2 ⁱ	0.86	1.92	2.749 (7)	163
N4—H4 n \cdots O5 ⁱⁱ	0.86	1.93	2.754 (7)	162

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

Fig. 1

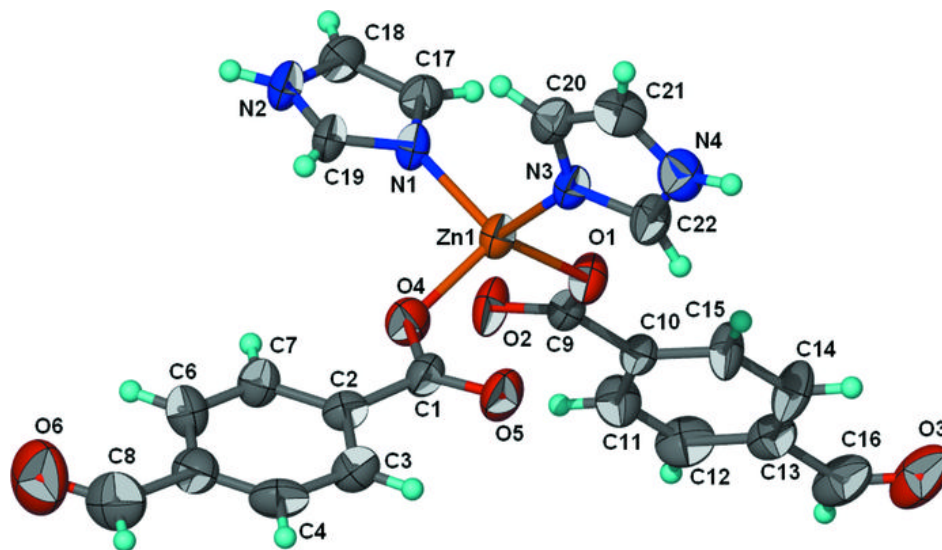


Fig. 2

