Aquabis(4-formylbenzoato-κO)(1,10-phenanthroline-$\kappa^2 N,N'$)zinc(II)

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The Zn atom in the title complex, $[\mathrm{Zn}(\mathrm{C_8H_5O_3})_2(\mathrm{C_{12}H_8N_2})(\mathrm{H_2O})]$, is coordinated by two O atoms of formylbenzoate carboxylate groups, two N atoms of a 1,10-phenanthroline ligand and one water molecule, giving rise to a square-pyramidal coordination geometry. Adjacent complex molecules are linked into a one-dimensional chain structure *via* π–π stacking interactions, with centroid–centroid distances of 3.531 (3) and 3.664 (3) Å.

Comment

4-Formylbenzoic acid (4-FBAH$_2$), which crystallizes in two forms (Haisa *et al.*, 1976), has been used in the synthesis of metal carboxylates. However, the coordination chemistry of 4-FBAH$_2$ still remains largely unexplored to date. Recently, we have reported some structures containing the 4-FBA$^-$ ligand (Deng *et al.*, 2006*a,b,c,d*), in which the 4-FBA$^-$ ligand shows monodentate coordination modes. Here, we report the crystal structure of the title Zn complex, $[\mathrm{Zn}(4\text{-}\mathrm{FBA})_2(1,10\text{-}\mathrm{phen})(\mathrm{H_2O})]$, (I), which was obtained by the reaction of 4-formylbenzoic acid, zinc diacetate dihydrate and 1,10-phenanthroline in an aqueous ethanol solution.

(I)
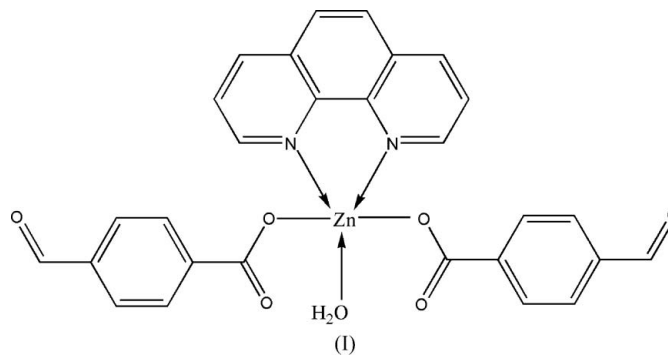
The molecular structure of (I) is shown in Fig. 1, and selected bond distances and angles are given in Table 1. The water molecule forms intramolecular hydrogen bonds with O atoms of the 4-FBA$^-$ ligand (Table 2). The Zn atom displays a square-pyramidal coordination geometry involving two O atoms, two N atoms and one water molecule, in which the apical Zn—O1 distance is somewhat shorter than the basal Zn—O and Zn—N distances.

In addition, there exist π–π stacking interactions between the benzene rings of adjacent 1,10-phen ligands and 4-FBA$^-$ ligands, the centroid–centroid distances being 3.531 (3) ($Cg1\cdots Cg2$) and 3.664 (3) Å ($Cg3\cdots Cg4$) [$Cg1$: C10–C15; $Cg2$: C23^i–C26^i/N2^i/C27^i; $Cg3$: N1^i/C17^i–C20^i/C28^i; $Cg4$: C10^{ii}–

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C15^{ii} (symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $x - 1, y, z$; Fig. 2].

Experimental

Zinc diacetate dihydrate (0.11 g, 0.5 mmol) was added to an aqueous ethanol solution (1:1 v/v) of 4-formylbenzoic acid (0.15 g, 1 mmol) and 1,10-phenanthroline (0.099 g 0.5 mmol). The pH value of the mixture was about 5. The filtered solution was allowed to evaporate at room temperature, and colorless prismatic crystals of (I) were separated from the filtered solution after several days. Analysis calculated for $C_{28}H_{20}N_2O_7Zn$: C 59.86, H 3.59, N 4.99%; found: C 59.88, H 3.54, N 4.96%.

Crystal data

$[Zn(C_8H_5O_3)_2(C_{12}H_8N_2)(H_2O)]$	$V = 1192.4 (5)$ Å^3
$M_r = 561.83$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.565$ Mg m^{-3}
$a = 7.7953 (16)$ Å	Mo $K\alpha$ radiation
$b = 10.517 (2)$ Å	$\mu = 1.08$ mm^{-1}
$c = 15.323 (3)$ Å	$T = 295 (2)$ K
$\alpha = 106.87 (3)°$	Prism, colorless
$\beta = 93.24 (3)°$	$0.37 \times 0.29 \times 0.15$ mm
$\gamma = 95.32 (3)°$	

Data collection

Rigaku R-AXIS RAPID diffractometer	11625 measured reflections
ω scans	5350 independent reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	4346 reflections with $I > 2\sigma(I)$
$T_{min} = 0.690, T_{max} = 0.854$	$R_{int} = 0.021$
	$\theta_{max} = 27.5°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.033$	$+ 0.354P]$
$wR(F^2) = 0.088$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
5350 reflections	$\Delta\rho_{max} = 0.30$ e Å^{-3}
349 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.0076 (15)	Zn1—N1	2.1049 (17)
Zn1—O4	2.0250 (17)	Zn1—N2	2.170 (2)
Zn1—O1W	2.0859 (18)		
O1—Zn1—O4	102.08 (7)	O4—Zn1—N1	87.83 (7)
O1—Zn1—O1W	101.35 (7)	O4—Zn1—N2	159.61 (7)
O1—Zn1—N1	115.45 (7)	O1W—Zn1—N1	142.49 (7)
O1—Zn1—N2	97.13 (7)	O1W—Zn1—N2	91.39 (7)
O4—Zn1—O1W	91.48 (7)	N1—Zn1—N2	77.70 (7)

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

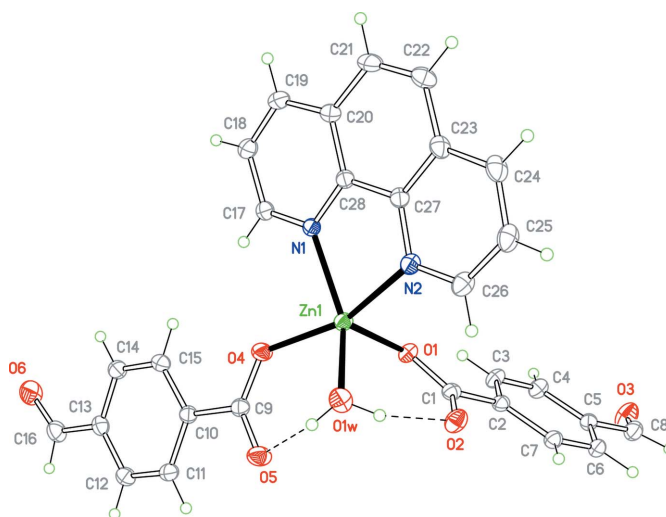| D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D$$\cdots$$A$	D—H$\cdots$$A$
O1W—H1W1$\cdots$O5	0.854 (10)	1.873 (15)	2.691 (3)	160 (3)
O1W—H1W2$\cdots$O2	0.856 (10)	1.878 (16)	2.681 (2)	156 (3)

Figure 1
The molecular structure of the title complex, with displacement ellipsoids drawn at the 30% probability level. The hydrogen bonds are denoted by dashed lines.
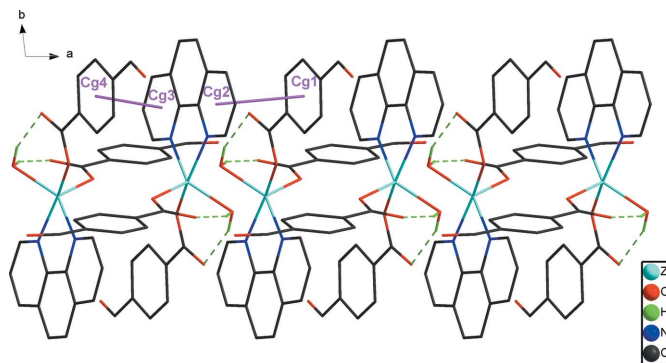

Figure 2
One-dimensional-chain structure of the title complex along the a axis formed by π-π stacking interactions, with the O—H$\cdots$O hydrogen bonds denoted by dashed lines. H atoms not involved in hydrogen bonding have been omitted. $Cg1$, $Cg2$, $Cg3$ and $Cg4$ represent the centroids of adjacent benzene rings of phen ligand 4-FBA$^-$ ligands, as defined in the Comment.

Carbon-bound H atoms were placed in calculated positions, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, and were refined in the riding-model approximation. The H atoms of the water molecule were located in a difference Fourier map and refined with O—H and H$\cdots$H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and with $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: RAPID-AUTO (Rigaku, 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: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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