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Aquabis(*N*-benzoylalaninato-κ*O*)(1,10-phenanthroline-κ^2*N*,*N*′)zinc(II)

Ai-Yun Fu,[a]* Yong-Ling Sun,[b] Da-Qi Wang,[c] Wen-Sheng Zhang[a] and An-Kun Ren[a]

[a]Department of Chemistry, Dezhou University, Shandong Dezhou 253023, People's Republic of China, [b]Department of Biology, Dezhou University, Shandong Dezhou 253023, People's Republic of China, and [c]Department of Chemistry, Liaocheng University, Shandong Liaocheng 252059, People's Republic of China

Correspondence e-mail:
aiyunfu@yahoo.com.cn

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In the title compound, $[Zn(C_{10}H_{10}NO_3)_2(C_{12}H_8N_2)(H_2O)]$, the Zn^{II} atom is five-coordinated by the two N atoms of the 1,10-phenanthroline ligand, two O atoms from two benzoylalanine ligands and one O from a water molecule. The complex exhibits a slightly distorted square-pyramidal geometry. The crystal structure is stabilized by hydrogen bonds of the types N—H···O, O—H···O and C—H···O.

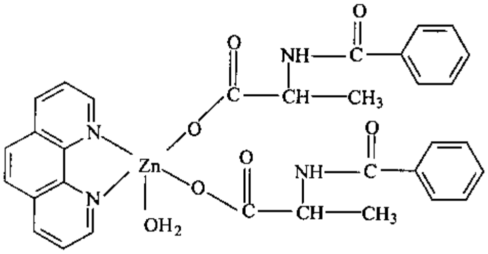
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.093
Data-to-parameter ratio = 12.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The asymmetric unit of the title compound, (I), contains one monomeric five-coordinate zinc complex. The Zn atom is coordinated by one 1,10-phenanthroline (phen) ligand *via* atoms N3 and N4 (Fig. 1) [Zn1—N3 = 2.147 (3) Å and Zn1—N4 = 2.100 (4) Å], two *N*-benzoylalanine anions *via* O1 and O4 [Zn1—O1 = 1.962 (3) Å and Zn1—O4 = 2.020 (3) Å], and one water molecule [Zn1—O7 = 1.979 (3) Å]. Other bond lengths and angles are unexceptional. The complex exhibits a slightly distorted square-pyramidal geometry about the Zn^{II} atom, with the apical position occupied by atom O1 of one *N*-benzoylalanine ligand. The Zn atom is displaced by 0.5055 (3) Å from the basal plane defined by atoms O7, O4, N4 and N3. The distance from atom O1 to the same plane is 2.437 (9) Å. The dihedral angle between the two phenyl rings is 82.6 (2)°. The dihedral angles between the 1,10-phenanthroline plane and the two phenyl rings are 43.7 (1) and 40.3 (1)°.



(I)

The geometry of (I) is different from two other five-coordinate zinc complexes where the coordination is distorted trigonal bipyramidal: aqua-bis[pyridine-5-(carboxylic acid)-2-carboxylato-*N*,*O*]zinc(II) (Liang *et al.*, 2001) and (μ_2-2,6-bis-{bis[(2-benzimidazolyl)methyl]aminomethyl}-4-methylphenolato)(isonicotinato)(isonicotinic acid)dizinc(II) (μ_2-2,6-bis-{bis[(2-benzimidazolyl)methyl]aminomethyl}-4-methylphenolato)aqua(isonicotinato)dizinc(II) tetraperchlorate tetrahydrate (Nie *et al.*, 1998).

The crystal structure is stabilized by intramolecular and intermolecular N—H···O, O—H···O and C—H···O hydrogen bonds (Table 1).

Experimental

DL-*N*-Benzoylalanine (*L*) was prepared by adding benzoyl chloride (15 mmol) and NaOH (15 mmol) dissolved in 20 ml distilled water to 30 ml of an aqueous mixture of DL-alanine (15 mmol) and NaOH (15 mmol). The reaction mixture was stirred for 1 h at 273–278 K and then acidified to pH 4 with hydrochloric acid, yielding a white deposit of *L*. The deposit was isolated, washed and dried (m.p 435.1–437.0 K). For the synthesis of (I), $ZnSO_4$ (1 mmol) and phen (1 mmol) were dissolved in 20 ml anhydrous ethanol. To this solution was added, dropwise at 313 K, 30 ml of an aqueous mixture of *L* (2 mmol) and NaOH (2 mmol). The mixture was stirred for 4 h and about half of the solvent was evaporated in a rotary vacuum evaporator at the same temperature. The temperature was then gradually lowered by 1 K each day. Two weeks later, green blocks of the title complex formed, which were isolated, washed and dried. Analysis found: C 59.10, H 4.55, N 8.46%; calculated for $C_{32}H_{30}N_2O_7Zn$: C 59.31, H 4.67, N 8.65%.

Crystal data

$[Zn(C_{10}H_{10}NO_3)_2(C_{12}H_8N_2)(H_2O)]$
$M_r = 647.99$
Monoclinic, $P2_1/c$
$a = 10.005$ (15) Å
$b = 29.38$ (4) Å
$c = 10.323$ (16) Å
$\beta = 111.04$ (2)°
$V = 2832$ (7) Å^3
$Z = 4$
$D_x = 1.520$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4003 reflections
$\theta = 2.5$–22.8°
$\mu = 0.93$ mm^{-1}
$T = 298$ (2) K
Block, green
0.43 × 0.28 × 0.22 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.740$, $T_{max} = 0.816$
11756 measured reflections
5060 independent reflections
3472 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.1°$
$h = -10 \rightarrow 11$
$k = -35 \rightarrow 23$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.093$
$S = 0.99$
5060 reflections
405 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O6^{i}	0.86	2.14	2.968 (6)	162
N2—H2···O3	0.86	2.16	2.938 (5)	151
O7—H3···O5	0.882 (10)	1.809 (15)	2.617 (4)	151 (3)
O7—H4···O2^{ii}	0.892 (10)	1.803 (16)	2.663 (5)	161 (4)
C6—H6···O6^{i}	0.93	2.46	3.378 (6)	170
C17—H17···O2^{iii}	0.93	2.59	3.509 (7)	172
C21—H21···O2^{ii}	0.93	2.59	3.368 (7)	141
C30—H30···O4	0.93	2.53	3.043 (6)	115
C31—H31···O1^{iv}	0.93	2.45	3.293 (7)	152

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

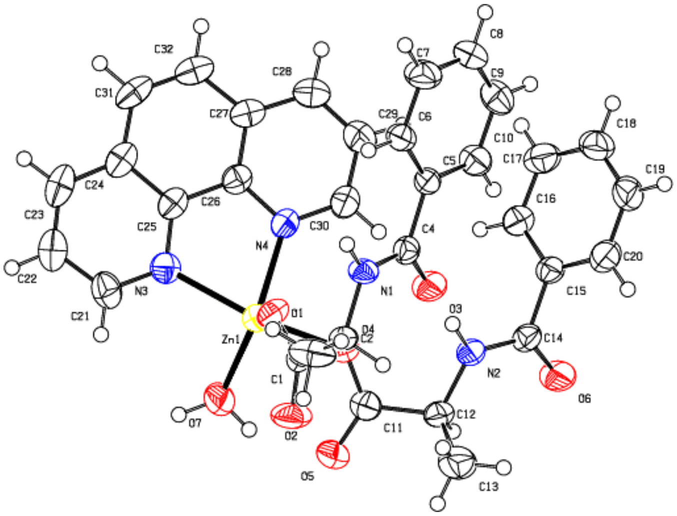


Figure 1
The structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

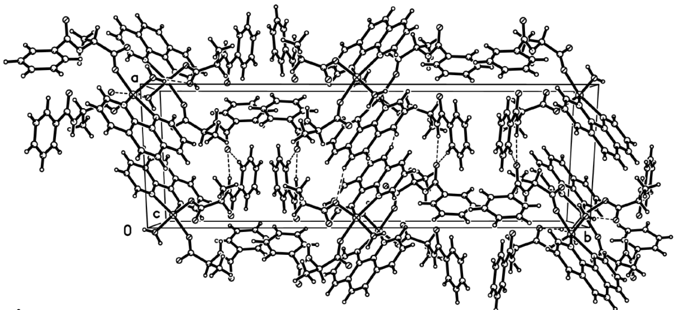


Figure 2
The crystal packing of the title compound, viewed along the *c* axis. Hydrogen bonds are indicated by dashed lines.

The water O—H distances were restrained to 0.90 (1) Å; the U_{iso}(H) values were allowed to refine. All other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with N—H distances of 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(N)$, and C—H distances of 0.93–0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

References

Liang, Y.-C., Hong, M.-C., Cao, R. & Weng, J.-B. (2001). *Jiegou Huaxue* (*Chin. J. Struct. Chem.*), **20**, 455–458.
Nie, F.-M., Wang, R. J., Li, Y.-M., Zhao, Y.-F., Nethaji, M. & Chakravarty, A. R. (1998). *Chin. Chem. Lett.* **9**, 881–884.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

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