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Aquabis[2-(2-pyridyl)-1*H*-benzimidazolato]zinc(II)

Jian-Kui Yang,[a,b] Ming-Hua Zeng[a]* and Seik Weng Ng[c]

[a]Department of Chemistry, Guangxi Normal University, Guilin 541000, Guangxi, People's Republic of China, [b]Department of Applied Chemistry, Hunan Agricultural University, Changsha 410128, Hunan, People's Republic of China, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: zmhzsu@163.com

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Key indicators

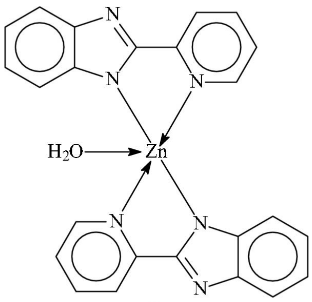
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.048
wR factor = 0.131
Data-to-parameter ratio = 16.2

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

In the title compound, [Zn($C_{12}H_8N_3$)$_2$(H_2O)], the Zn atom is chelated by two heterocycles, and the coordinating N atoms comprise the basal plane of the square-pyramidal environment. The apical position is occupied by an aqua ligand. The complexes are linked by O—H···O hydrogen bonds into a ribbon structure along the *a* axis.

Comment

2-(2-Pyridyl)-1*H*-benzimidazole (Hpybim) is an organic heterocycle that possesses luminescence properties, and the present study was initiated in an investigation of this property in the zinc complex. The crystal structure of [Zn(pybim)$_2$] as well as its electronic structure have been studied (Yue *et al.*, 2002); it is a planar compound. A search through the Cambridge Structural Database (Version 5.26; Allen, 2002) found only two metal complexes containing this ligand, *viz*. a copper(II) isothiocyanate adduct of the neutral Hpybim molecule (Battaglia *et al.*, 1976) and an yttrium(III) complex (Müller-Buschbaum & Quitmann, 2003).



(I)

The Zn atom in the present complex, (I), is chelated by the two pybim$^-$ ligands. The four coordinating N atoms comprise a square plane; the coordinated water molecule occupies the apical position of the square-pyramidal geometry. The aqua ligands link adjacent complexes into a ribbon structure along the *a* axis (Fig. 2).

Experimental

Zinc nitrate hexahydrate (0.149 g, 0.5 mmol) and 2-carboxyphenoxyacetic acid (0.196 g, 1 mmol) were dissolved in ethanol (3 ml) and water (15 ml). The solution was placed in a 23 ml Teflon-lined stainless steel Parr bomb. The bomb was heated at 433 K for 120 h. The cool mixture yielded colourless crystals of (I); these were washed with water and then dried in air (yield *ca* 70%).

Crystal data

$[Zn(C_{12}H_8N_3)_2(H_2O)]$
$M_r = 471.81$
Monoclinic, $P2_1/c$
$a = 12.5448\ (8)$ Å
$b = 13.0525\ (8)$ Å
$c = 13.3493\ (9)$ Å
$\beta = 102.731\ (1)^\circ$
$V = 2132.1\ (2)$ Å^3
$Z = 4$
$D_x = 1.470$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3351 reflections
$\theta = 3.0$–25.4°
$\mu = 1.18$ mm^{-1}
$T = 295\ (2)$ K
Block, colourless
$0.36 \times 0.18 \times 0.11$ mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{\min} = 0.676$, $T_{\max} = 0.881$
12 542 measured reflections
4812 independent reflections
3727 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.025$
$\theta_{\max} = 27.5^\circ$
$h = -16 \rightarrow 16$
$k = -10 \rightarrow 16$
$l = -16 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.131$
$S = 1.01$
4812 reflections
297 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0743P)^2 + 0.521P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.58$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1*w*	2.001 (2)	Zn1—N4	2.002 (2)
Zn1—N1	1.989 (2)	Zn1—N6	2.245 (2)
Zn1—N3	2.239 (2)		
O1*w*—Zn1—N1	117.5 (1)	N1—Zn1—N4	126.9 (1)
O1*w*—Zn1—N3	89.1 (1)	N1—Zn1—N6	108.3 (1)
O1*w*—Zn1—N4	115.5 (1)	N3—Zn1—N4	99.1 (1)
O1*w*—Zn1—N6	85.8 (1)	N3—Zn1—N6	172.7 (1)
N1—Zn1—N3	78.7 (1)	N4—Zn1—N6	78.5 (1)
N1—C7—C8—N3	−3.1 (4)	N4—C19—C20—N6	−3.2 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···N2$^{\text{i}}$	0.85 (1)	1.90 (2)	2.713 (3)	160 (3)
O1*w*—H1*w*2···N5$^{\text{ii}}$	0.84 (1)	1.88 (1)	2.713 (3)	170 (3)

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

The carbon-bound H atoms were positioned geometrically (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with U_{iso}(H) values set at 1.2 times U_{eq}(C). The water H atoms were located in difference Fourier maps and refined isotropically with O—H distances restrained to 0.85 (1) Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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*.

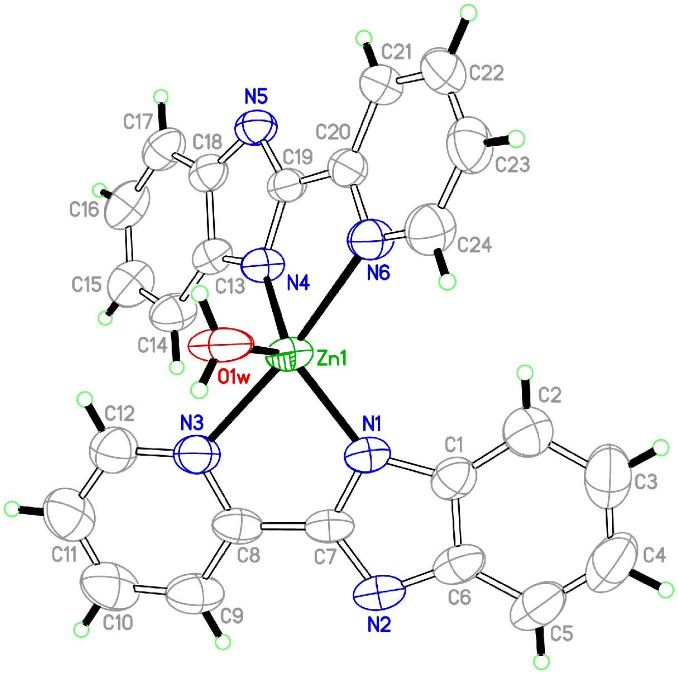


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level.

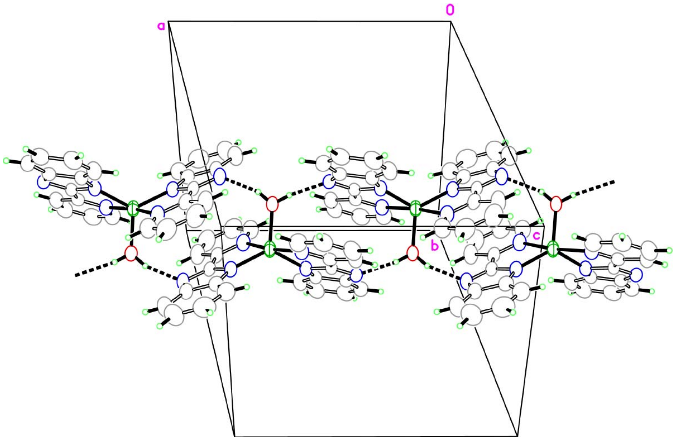


Figure 2
The hydrogen-bonded (dashed lines) chain of (I) in the crystal structure.

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