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Key indicators

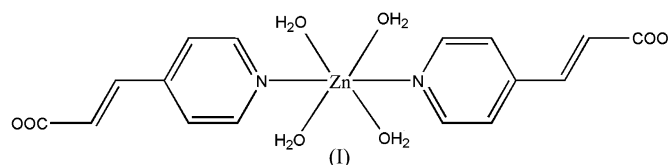
Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.043
 wR factor = 0.096
Data-to-parameter ratio = 16.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*trans*-Tetraaquabis[3-(4-pyridyl)acrylato- κ N]zinc(II)

The title complex, $[\text{Zn}(\text{C}_8\text{H}_6\text{NO}_2)_2(\text{H}_2\text{O})_4]$, consists of a central zinc(II) atom coordinated by two *trans* 3-(4-pyridyl)acrylate ligands *via* their N atoms and by four water ligands. The Zn atom is located on a centre of inversion. Extensive inter-complex hydrogen bonding occurs between the water ligands and the carboxylate groups, resulting in a three-dimensional network.

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Comment

Three Zn^{II} coordination polymers that contain a bridging 3-pyridylacrylate ligand have been reported recently (Li *et al.*, 2005; Qu *et al.*, 2004; Wu *et al.*, 2004). However, if the ligands coordinate only in a monodentate fashion, the possibility of participating in a hydrogen-bonding network arises. We report here the structure of the title compound, (I), in which such a hydrogen-bonded network is found.



In complex (I), the Zn^{II} atom resides on a centre of symmetry and is coordinated by two N atoms from two 3-pyridylacrylate groups and four O atoms from four water molecules in a slightly distorted octahedral geometry. The two 3-pyridylacrylate groups are in *trans* positions (Fig. 1).

The O atom of each coordinated water molecule forms a bifurcated hydrogen bond with the carbonyl O atoms of the 3-pyridylacrylate groups (Table 2 and Fig. 2). The intermolecular hydrogen-bonding interactions link the molecules into a three-dimensional network.

Experimental

The title compound was obtained from an aqueous solution (15 ml) containing $\text{Zn}(\text{NO}_3)_2$, Na_2CO_3 and 3-pyridylacrylic acid (2:1:2 molar ratio).

Crystal data

$[\text{Zn}(\text{C}_8\text{H}_6\text{NO}_2)_2(\text{H}_2\text{O})_4]$
 $M_r = 433.73$
Monoclinic, $P2_1/c$
 $a = 11.243$ (2) Å
 $b = 7.0251$ (8) Å
 $c = 12.930$ (2) Å
 $\beta = 120.687$ (11)°
 $V = 878.2$ (2) Å³

$Z = 2$
 $D_x = 1.640$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 1.45$ mm⁻¹
 $T = 293$ (2) K
Prism, colourless
 $0.15 \times 0.12 \times 0.03$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	6580 measured reflections
φ and ω scans	2014 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1732 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.812$, $T_{\max} = 0.958$	$R_{\text{int}} = 0.036$
	$\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 0.5425P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.096$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.11$	$\Delta\rho_{\text{max}} = 0.36 \text{ e } \text{\AA}^{-3}$
2014 reflections	$\Delta\rho_{\text{min}} = -0.39 \text{ e } \text{\AA}^{-3}$
124 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Zn1—O1W	2.1063 (19)	Zn1—N1	2.181 (2)
Zn1—O2W	2.1090 (19)		
O1W—Zn1—O2W	89.45 (7)	O2W—Zn1—N1	90.27 (8)
O1W—Zn1—N1	87.58 (8)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1 \cdots O2 ⁱ	0.86	1.92	2.756 (3)	163
O1W—H2 \cdots O2 ⁱⁱ	0.85	1.92	2.770 (3)	177
O2W—H3 \cdots O2 ⁱⁱⁱ	0.83	1.99	2.809 (3)	167
O2W—H4 \cdots O1 ⁱⁱ	0.84	1.87	2.686 (3)	164

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

H atoms bonded to C atoms were placed in calculated positions and refined with isotropic displacement parameters using a riding model, with $C-H = 0.93 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. Water H atoms were located in difference maps and refined as riding at the O—H distances given in Table 2, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve

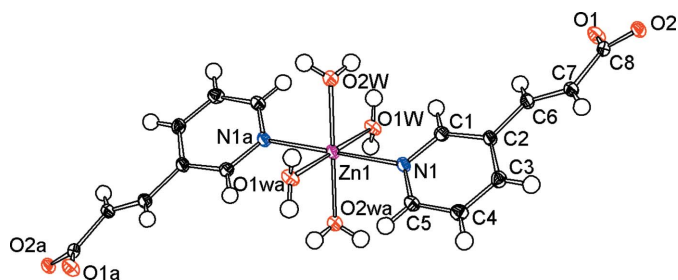


Figure 1

A view of (I), with 30% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii. [Symmetry code: (a) $1 - x, 1 - y, 1 - z$.]

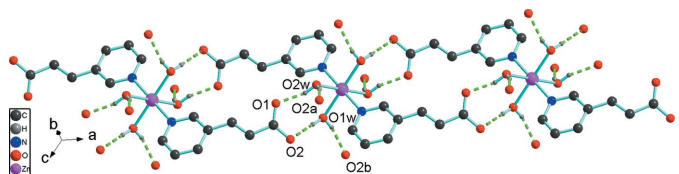


Figure 2

View of the extensive hydrogen bonding between complexes. [Symmetry codes: (a) $1 - x, 1 - y, 1 - z$; (b) $1 - x, -y, 1 - z$.]

structure: SHELXTL (Bruker, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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