Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[diaquazinc(II)]-μ_2-4,4′-bipyridine-κ^2N:N'-μ_2-*p*-phenylenebis(oxyacetato)-κ^2O:O']

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Received 13 May 2006
Accepted 22 June 2006

The title compound, $[Zn^{II}(C_8H_8O_6)(C_8H_8N_2)(H_2O)_2]_n$, contains a Zn atom coordinated by 4,4′-bipyridine, benzene-1,4-dioxydiacetate and two water molecules. The Zn atom lies on an inversion centre and the benzene-1,4-dioxydiacetate and 4,4-bipyridine ligands lie about other inversion centres.

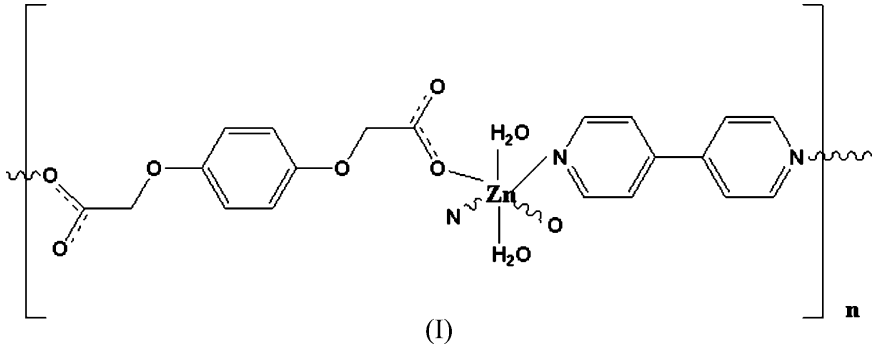
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.024
wR factor = 0.064
Data-to-parameter ratio = 41.8

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

Comment

The title compound, (I), contains a Zn atom coordinated by 4,4′-bipyridine, benzene-1,4-dioxydiacetate and two water molecules. The Zn atom lies on an inversion centre and the benzene-1,4-dioxydiacetate and 4,4-bipyridine ligands lie about other inversion centres. The benzene-1,4-dioxydiacetate ligands bridge the octahedral Zn^{II} coordination centres to form a one-dimensional zigzag chain. The chains are further bridged *via* 4,4-bipyridine, forming a two-dimensional architecture.



(I)

Hydrogen-bonding interactions between the coordinated water molecules and the carboxylate O atoms lead to the formation of a three-dimensional network structure (Table 1). Compound (I) is isostructural with its cobalt analogue (Dai *et al.*, 2005).

Experimental

$Zn(OAc)_2{\cdot}H_2O$ (0.5 mmol, 0.10 g), 4,4′-bpy (0.5 mmol, 0.078 g), benzene-1,4-dioxydiacetic acid (0.5 mmol, 0.113 g) and NaOH (0.04 g, 1 mmol) were mixed in H_2O (15 ml) and heated at 433 K for 3 d in a sealed 25 ml Teflon-lined stainless-steel vessel under autogenous pressure. After cooling to room temperature at 50 K h^{-1}, yellow block crystals of (I) were isolated, and were washed with ethanol and dried in air.

Crystal data

$[Zn(C_8H_8O_6)(C_8H_8N_2)(H_2O)_2]$
M_r = 481.77
Triclinic, $P\overline{1}$
a = 5.7279 (17) Å
b = 8.076 (3) Å
c = 10.668 (3) Å
α = 105.924 (4)°
β = 96.726 (2)°
γ = 97.816 (4)°
V = 463.9 (3) Å^3
Z = 1
D_x = 1.724 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.38 mm^{-1}
T = 293 (2) K
Prism, yellow
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.725, T_{max} = 0.871
2644 measured reflections
2131 independent reflections
1953 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.065
S = 1.02
2131 reflections
51 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*WA*···O3^{i}	0.81 (2)	2.16 (2)	2.9090 (17)	153 (2)
O1*W*—H1*WB*···O2^{ii}	0.83 (2)	1.81 (2)	2.6084 (17)	163 (3)

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

The organic H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 and 0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C). The water H atoms were located in difference maps and refined isotropically, with the O—H distances restrained to 0.82 (2) Å and U_{iso}(H) = 1.5U_{eq}(O).

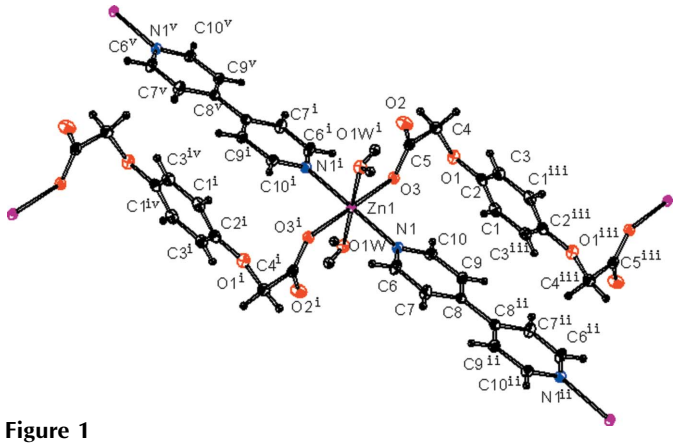


Figure 1
A view of the title compound, showing the atomic labelling scheme and 50% probability displacement ellipsoids. [Symmetry codes: (i) $1-x, -y, 1-z$; (ii) $1-x, -1-y, -z$; (iii) $-x, -y, -z$; (iv) $1+x, y, 1+z$; (v) $x, 1+y, 1+z$].

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was financially supported by the Foundation of the Ministry of Education of Fujian Province (grant No. JB03131).

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