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Aquaoxalato(2,4,6-tri-2-pyridyl-1,3,5-triazine)-zinc(II) tetrahydrate

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Key indicators

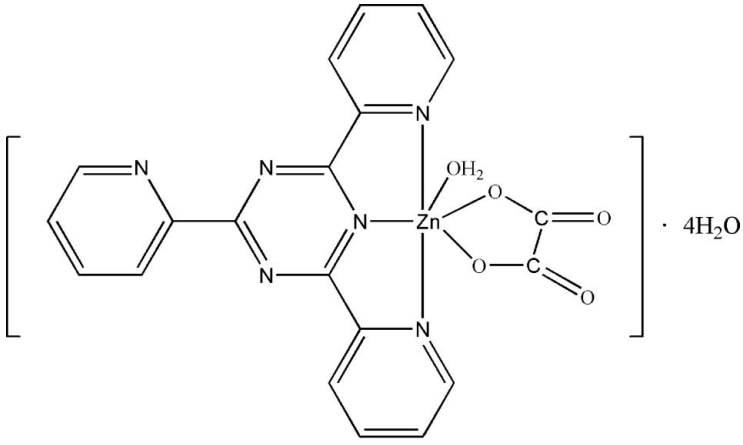
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.088
Data-to-parameter ratio = 14.4

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

The title compound, $[Zn(C_2O_4)(C_{18}H_{12}N_6)(H_2O)]\cdot 4H_2O$, crystallizes isostructurally with the Co [Cheng, Xu & Zheng (2006), *Acta Cryst.* E**62**, m2561–m2563] and Cu [Zheng, Xu, Lin & Fang (2006), *J. Coord. Chem.* **59**, 1825–1834] analogues, with distorted octahedral coordination geometry. O—H···O hydrogen bonds form a chain along the *a* axis.

Comment

Non-covalent interactions, such as hydrogen-bonding and π–π stacking interactions, play important roles in the crystallization process (Stang & Olenyuk, 1997). For a long time, multidentate *O*- or *N*-donor ligands have been widely used to construct complexes (Ghumaan *et al.*, 2006; Zhou *et al.*, 2007). We present here the crystal structure of the title compound, (I).



(I)

Compound (I) crystallizes isostructurally with the the Co (Cheng *et al.*, 2006) and Cu (Zheng *et al.*, 2006) analogues. As illustrated in Fig. 1, the Zn atom shows a distorted octahedral coordination by three N atoms of the tridentate chelating ligand, two O atoms of the oxalate ligand and a water molecule. The plane defined by atoms N1, N2 and N3 is almost perpendicular to that composed of atoms O1, O3 and O5, making a dihedral angle of 89.50 (6)°. Compared with the reported values of 2.073 (4) Å for $Zn—N_{central}$, and 2.193 (4) and 2.271 (4) Å for $Zn—N_{lateral}$ (Harvey *et al.*, 2004), the bond lengths are slightly longer in (I) (Table 1). The $Zn—O_{acid}$ lengths in (I) are slightly shorter than the corresponding bonds in the similar bis-monodentate structure [2.070 and 2.155 Å; Fu *et al.*, 2003).

In the crystal structure of (I), O—H···O hydrogen bonds (Table 2) lead to the formation of a chain along the *a* axis.

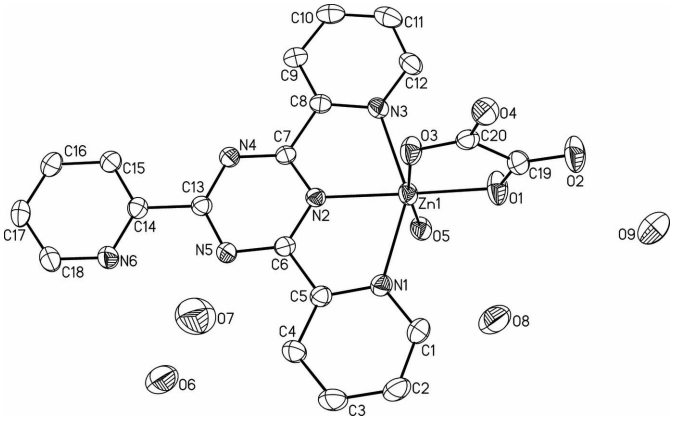


Figure 1
The asymmetric unit of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 45% probability level. H atoms have been omitted for clarity.

Experimental

Dropwise addition of Na_2CO_3 (2.0 ml, 1.0 *M*) to a stirred solution of $ZnCl_2$ (0.136 g, 1.00 mmol) in H_2O (5.0 ml) produced a white precipitate, which was then centrifuged and washed with water until no Cl^- anions were detectable. The collected precipitate and tptz (tptz is 2,4,6-tri-2-pyridyl-1,3,5-triazine) (0.312 g, 1.00 mmol) were added to a stirred solution of oxalic acid (0.126 g, 1.00 mmol) in CH_3OH–H_2O (30.0 ml; 1:1 *v*/*v*). The resulting mixture was stirred for a further 15 min. After filtration, the yellow filtrate (pH = 2.58) was evaporated slowly at room temperature and afforded yellow crystals of (I) over a period of a month (yield 20.1%, based on initial $ZnCl_2$ input).

Crystal data

$[Zn(C_2O_4)(C_{18}H_{12}N_6)(H_2O)]\cdot 4H_2O$
M_r = 555.81
Triclinic, $P\overline{1}$
a = 7.8711 (16) Å
b = 11.766 (2) Å
c = 13.982 (3) Å
α = 97.88 (3)°
β = 102.84 (3)°
γ = 107.74 (4)°
V = 1172.9 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 298 (2) K
0.33 × 0.33 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: empirical (using intensity measurements) (*ABSCOR*; Higashi, 1995)
T_{min} = 0.695, T_{max} = 0.840
11532 measured reflections
5273 independent reflections
4399 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.088
S = 1.11
5273 reflections
365 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn—O1	1.9972 (16)	Zn—N1	2.236 (2)
Zn—O3	2.0853 (15)	Zn—N2	2.0834 (16)
Zn—O5	2.0843 (16)	Zn—N3	2.3017 (18)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H19···O4^{i}	0.75 (3)	2.00 (3)	2.738 (2)	166 (4)
O5—H20···O8	0.82 (3)	1.92 (3)	2.738 (3)	177 (3)
O6—H21···O7^{i}	0.90 (5)	1.93 (5)	2.822 (4)	174 (4)
O6—H22···N6	0.84 (4)	2.25 (4)	3.056 (3)	160 (4)
O7—H23···O9^{ii}	0.77 (4)	2.07 (4)	2.786 (4)	154 (4)
O7—H24···O9^{iii}	1.03 (4)	1.81 (4)	2.830 (3)	168 (4)
O8—H25···O6^{iv}	0.81 (4)	2.03 (4)	2.834 (4)	171 (4)
O8—H26···O7^{v}	0.76 (5)	2.11 (5)	2.861 (5)	174 (4)
O9—H27···N6^{vi}	0.88 (4)	2.21 (4)	3.060 (3)	160 (4)
O9—H28···O2	0.81 (3)	1.92 (3)	2.720 (3)	171 (3)

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

All H atoms bound to C were positioned geometrically and refined as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). H atoms attached to O were located in a difference Fourier map and refined freely refined O—H distances are in Table 2.

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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