Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

catena-Poly[[[tetraaquazinc(II)]-*μ*-[(2*E*)-*N*,*N*′-bis(pyridin-4-ylmethyl)but-2-enediamide]] dinitrate]

Gareth O. Lloyd

Department of Chemistry, University of Stellenbosch, Private Bag X1, Matieland, South Africa

Correspondence e-mail: gol@sun.ac.za

Received 9 May 2005
Accepted 13 May 2005
Online 28 May 2005

In the title compound, $\{[\mathrm{Zn}(\mathrm{C}_{16}\mathrm{H}_{16}\mathrm{N}_4\mathrm{O}_2)(\mathrm{H}_2\mathrm{O})_4](\mathrm{NO}_3)_2\}_n$, the bidentate ligand (2*E*)-*N*,*N*′-bis(pyridin-4-ylmethyl)but-2-enediamide coordinates in the axial positions of the octahedral zinc centres to form infinite one-dimensional coordination polymeric chains. In the crystal structure, O—H···O and N—H···O hydrogen bonds link these chains into a three-dimensional framework.

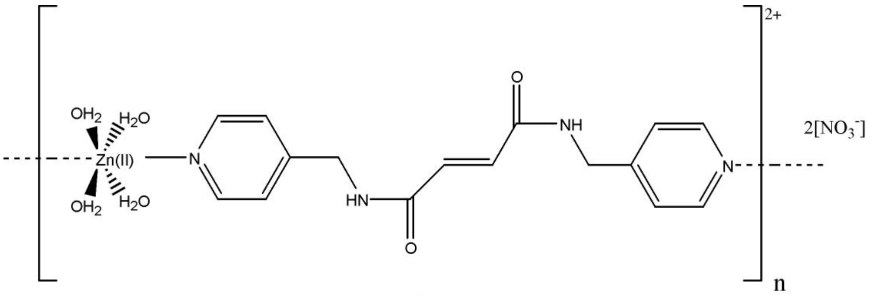
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.081
Data-to-parameter ratio = 15.1

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

Comment

The foremost goal of crystal engineering is to tailor chemical and/or physical properties of crystalline solids, using known motifs or synthons at the molecular level. The hydrogen bond is without doubt the most used non-covalent interaction in crystal engineering. Amide groups and water are extensively used by nature to assemble small molecules into larger aggregates (Atwood *et al.*, 2001; Barbour *et al.*, 1998; Kannan *et al.*, 2003; Lloyd *et al.*, 2005; Orr *et al.*, 1998). In our pursuit of hydrogen-bonded networks that include water, the ligand (2*E*)-*N*,*N*′-bis(pyridin-4-ylmethyl)but-2-enediamide (Lloyd, 2005), which has dipyridyl functionality and amide groups available for hydrogen bonding, has been coordinated to metal centres and the title zinc complex, (I), was prepared.



(I)

In compound (I) (Fig. 1), this results in the formation of a one-dimensional coordination polymer (Fig. 2). The zinc metal

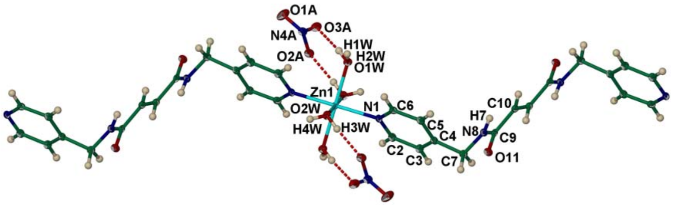


Figure 1
The molecular structure of (I), showing atom labels and 50% probability ellipsoids for non-H atoms. Unlabelled atoms are related by the symmetry codes (−x, 1 − y, −z), (−x, 1 − y, 1 − z) and (x, y, z − 1). The red dashed lines represent hydrogen bonds.

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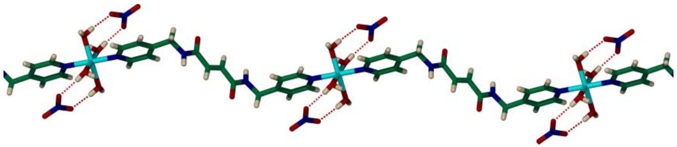

Figure 2
The one-dimensional coordination polymer strand, showing the octahedral zinc metal centres and hydrogen bonding to the nitrate anions. The red dashed lines indicate hydrogen bonds.

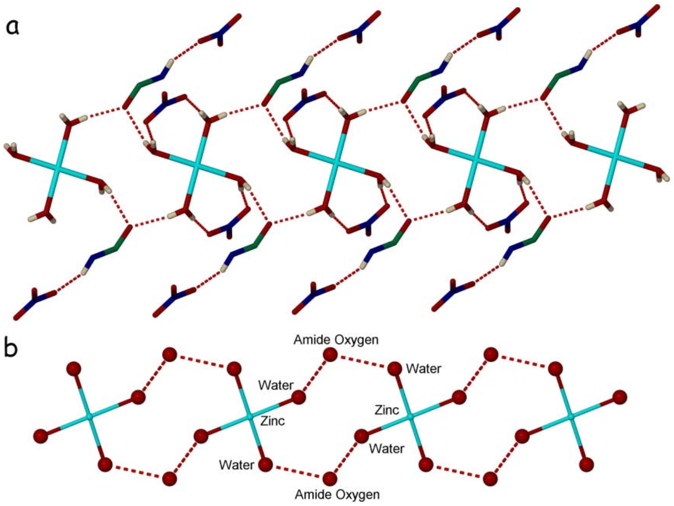

Figure 3
(*a*) All the hydrogen-bonding modes found in compound (I) between the amide groups, coordinated water molecules and nitrate anions. Groups not associated with hydrogen bonding have been removed for clarity. Red dashed lines represent hydrogen bonds. (*b*) Eight-membered hydrogen-bonded rings found in compound (I). Red dashed lines represent O···O contacts of the O—H···O(amide) hydrogen bonds.

centres are in a very slightly distorted octahedral environment, with two ligands coordinated *via* pyridyl groups in the two axial positions and the equatorial positions occupied by four water molecules. The two nitrate ions are each hydrogen bonded by a pair of coordinated water molecules (Figs. 2 and 3*a*). The amide groups of the ligand are also hydrogen bonded to the nitrate ions *via* the NH group (Fig. 3*a*). The last set of hydrogen bonds binds the metal centres to one another. This is accomplished by two coordinated water molecules hydrogen bonding to the C═O groups of the ligand (Fig. 3*a*) to form eight-membered rings. Fig. 3(*b*) shows how the eight-membered rings consist of two zinc ions, four coordinated water molecules and two amide groups. Adjacent strands of coordination polymer are bonded together *via* amide hydrogen bonding links and all these hydrogen bonds link the one-dimensional coordination polymer strands together to form the three-dimensional framework (Fig. 4).

Experimental

(2*E*)-*N*,*N*′-Bis(pyridin-4-ylmethyl)but-2-enediamide dihydrate was synthesized by the reaction of 4-aminomethylpyridine with fumaryl dichloride in a 2:1 molar ratio. Crystals suitable for single-crystal X-ray diffraction analysis were grown from an equimolar solution of (2*E*)-*N*,*N*′-bis(pyridin-4-ylmethyl)but-2-enediamide dihydrate and zinc nitrate hexahydrate in dimethylformamide–water (5:1).

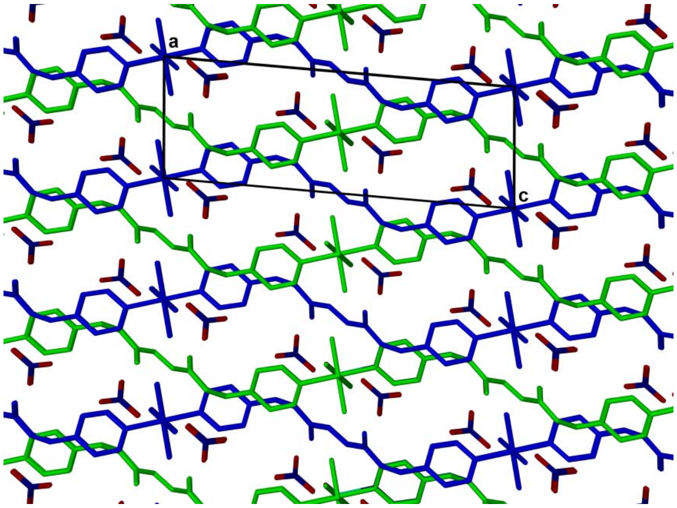

Figure 4
Packing of the one-dimensional coordination polymer chains. The alternating chains are shown in green and blue.

Crystal data

$[Zn(C_{16}H_{16}N_4O_2)(H_2O)_4](NO_3)_2$
$M_r = 557.80$
Monoclinic, $P2_1/n$
$a = 6.506$ (3) Å
$b = 9.294$ (4) Å
$c = 18.822$ (8) Å
$\beta = 94.781$ (6)°
$V = 1134.2$ (9) Å^3
$Z = 2$
$D_x = 1.633$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4749 reflections
$\theta = 2.4$–28.0°
$\mu = 1.16$ mm^{-1}
$T = 100$ (2) K
Plate, colourless
0.19 × 0.17 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
$T_{\min} = 0.810$, $T_{\max} = 0.913$
12176 measured reflections
2656 independent reflections
2273 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\max} = 28.2°$
$h = -8 \rightarrow 8$
$k = -12 \rightarrow 12$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.081$
$S = 1.03$
2656 reflections
176 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 0.3941P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.53$ e Å^{-3}
$\Delta\rho_{\min} = -0.31$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O3A	0.85 (3)	1.93 (3)	2.787 (1)	176 (3)
O1W—H2W···O11$^{\rm i}$	0.79 (3)	1.93 (3)	2.719 (1)	171 (3)
N8—H7···O3$A^{\rm ii}$	0.88	2.12	2.921 (1)	151
O2W—H3W···O2$A^{\rm iii}$	0.81 (3)	1.91 (3)	2.719 (1)	172 (3)
O2W—H4W···O11$^{\rm iv}$	0.81 (3)	2.09 (3)	2.853 (1)	154 (3)

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

All non-water H atoms were positioned geometrically (C—H = 0.95 and 0.99 Å, and N—H = 0.88 Å) and constrained to ride on their parent atoms; $U_{\rm iso}$(H) values were set at 1.2 times $U_{\rm eq}$(C,N). Water H atoms were refined independently.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001; Atwood & Barbour, 2003); software used to prepare material for publication: *X-SEED*.

The author thanks the National Research Foundation of South Africa for financial support.

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