Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[(2,2′-bipyridine-κ^2N,N')zinc(II)]-μ-imidazole-4,5-dicarboxylato-$\kappa^4N^1,O^5:N^3,O^4$]

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.074
Data-to-parameter ratio = 13.0

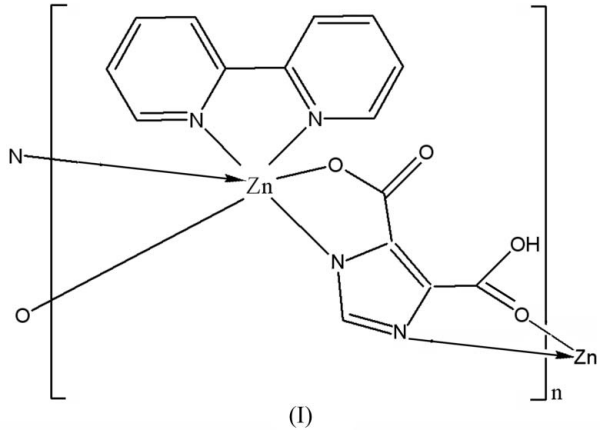
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 11 February 2007
Accepted 26 March 2007

In the title compound, $[Zn(C_5H_2N_2O_4)(C_{10}H_8N_2)]_n$, the Zn^{II} atom is six-coordinated in an octahedral geometry by two carboxylate O atoms and two N atoms from two imidazole-4,5-dicarboxylate ligands, and two N atoms from a 2,2′-bipyridine ligand. The asymmetric unit contains two formula units. The imidazole-4,5-dicarboxylate ligand bridges two Zn^{II} atoms to form a one-dimensional zigzag chain structure.

Comment

1*H*-Imidazole-4,5-dicarboxylic acid (H_3idc) has great potential for the construction of supramolecular architectures, owing to its versatile binding modes. To date, a few mononuclear (Zhang *et al.*, 2004; Xiao *et al.*, 2004; Ma *et al.*, 2003) and dinuclear complexes (Rajendiran *et al.*, 2003; Bayón *et al.*, 1987) have been reported. However, coordination polymers based on the H_3idc ligand remain largely unexplored (Wang *et al.*, 2004). In the present work, we report the crystal structure of the title one-dimensional chain Zn^{II} coordination polymer, $[Zn(2,2'\text{-bipy})(Hidc)]_n$, (I), which was obtained by hydrothermal reaction of $Zn(NO_3)_2$, H_3idc and 2,2′-bipy (2,2′-bipy = 2,2′-bipyridine).



(I)

Compound (I) has a one-dimensional chain structure, which is constructed from the basic unit [Zn(2,2′-bipy)(Hidc)], as illustrated in Fig. 1. The asymmetric unit contains two [Zn(2,2′-bipy)(Hidc)] units. The two Zn^{II} atoms have a similar distorted octahedral geometry formed by two carboxylate O atoms and four N atoms, two of which belong to a 2,2′-bipy ligand and the other two to two imidazole rings. The Zn—O and Zn—N bonds have average values of 2.209 (8) and 2.136 (1) Å, respectively. The bond angles around the Zn^{II} atoms are in the range of 74.24 (7)–172.37 (6)°, thereby indicating distorted Zn^{II} octahedra; the *cis* and *trans* angles

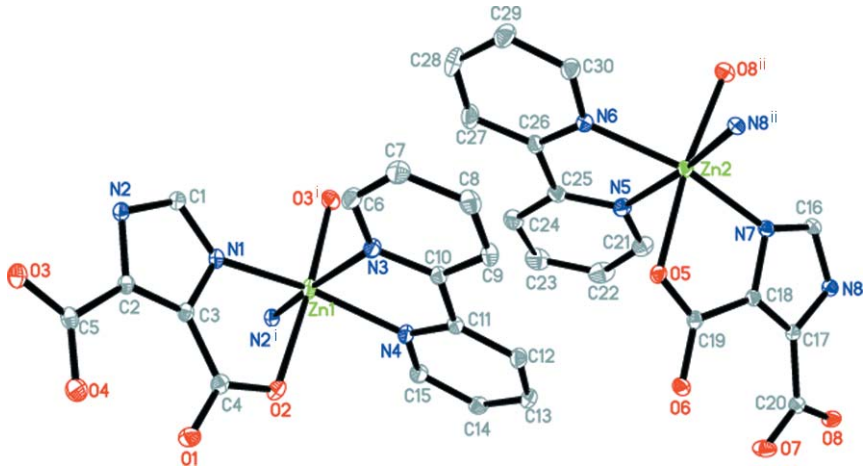


Figure 1
The asymmetric unit of (I), together with symmetry-related atoms to complete the Zn coordination. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) $-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $1-x, -\frac{1}{2}+y, \frac{3}{2}-z$.]

around the Zn^{II} atom are in the ranges 74.24 (7)–102.90 (7) and 158.35 (7)–172.37 (6)°, respectively. Both carboxylate groups of the Hidc ligand, one of which is protonated and the other deprotonated, show monodentate coordination to Zn^{II} atoms. The connectivity between the Zn^{II} atoms and the Hidc ligands gives rise to one-dimensional zigzag chains. The 2,2′-bipy molecules act as chelating ligands to the Zn^{II} atoms and occupy the interchain spaces. A three-dimensional network is built up *via* C—H···O hydrogen bonds (Table 1).

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O6	0.82	1.67	2.486 (2)	180
O4—H4A···O1	0.82	1.67	2.485 (2)	179
C9—H9···O5	0.93	2.57	3.387 (3)	148
C12—H12···O5	0.93	2.48	3.246 (3)	139
C12—H12···O6	0.93	2.50	3.182 (3)	130
C13—H13···O8^{iii}	0.93	2.45	3.077 (3)	124
C16—H16···O7^{iv}	0.93	2.30	3.204 (2)	165

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

Experimental

Compound (I) was prepared from a mixture of $Zn(NO_3)_2{\cdot}6H_2O$ (0.149 g, 0.5 mmol), H_3idc (0.085 g, 0.5 mmol), 2,2′-bipy (0.156 g, 1.0 mmol) and H_2O (18 ml) in a 30 ml Teflon-lined autoclave under autogenous pressure at 413 K for 5 d. After cooling to room temperature, colorless block crystals suitable for X-ray structure analysis were obtained. Analysis calculated for $C_{15}H_{10}N_4O_4Zn$: C 48.0, H 2.7, N 14.9%; found: C 47.9, H 2.5, N 14.8%.

Crystal data

$[Zn(C_5H_2N_2O_4)(C_{10}H_8N_2)]$
M_r = 375.64
Monoclinic, $P2_1/c$
a = 20.470 (1) Å
b = 9.6494 (5) Å
c = 14.7843 (7) Å
β = 101.783 (1)°
V = 2858.7 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.75 mm^{-1}
T = 292 (2) K
0.27 × 0.23 × 0.21 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SAINT-Plus*; Bruker, 2001)
T_{min} = 0.629, T_{max} = 0.691
15264 measured reflections
5621 independent reflections
4913 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.074
S = 1.05
5621 reflections
433 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

All H atoms were positioned geometrically and refined as riding atoms, with C—H= 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) and with O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001) and Mercury (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

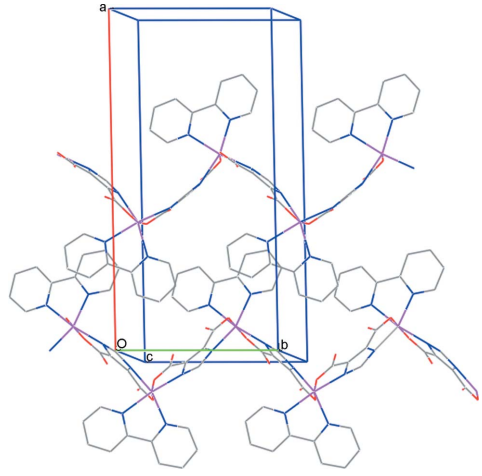


Figure 2
A view of the crystal packing. H atoms have been omitted for clarity.

The authors thank Mr Heng-Qing Jia at Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, for the data collection.

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