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A one-dimensional herring-bone coordination polymer, *catena*-poly[[bis(1*H*-imidazole-κN^3)-zinc(II)]-μ-5-nitrobenzene-1,3-dicarboxylato-$\kappa^2 O^1:O^3$]

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In the title compound, $[Zn(C_8H_3NO_6)(C_3H_4N_2)_2]_n$, each Zn^{II} atom is four-coordinated and bridged by a 5-nitrobenzene-1,3-dicarboxylate ligand to form a one-dimensional herring-bone chain. Interchain hydrogen bonds connect the chains to produce a two-dimensional double-sheet layer. In the crystal structure, all double-sheet layers are stabilized *via* interlayer π–π interactions between adjacent benzene rings.

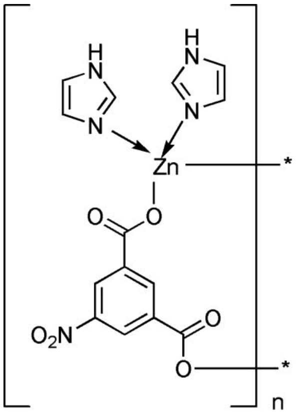
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.056
wR factor = 0.095
Data-to-parameter ratio = 15.6

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

Comment

The crystal engineering of coordination polymers with different geometric and topological characteristics has attracted much interest in view of their potential applications (Carlucci *et al.*, 2003; Janiak, 2003; Kitagawa *et al.*, 2004). In particular, the 'node and spacer' methodology has proven to be remarkably successful in the rational design of coordination polymers (Moulton & Zaworotko, 2001; Ockwig *et al.*, 2005). According to this design principle, many coordination polymers can be generated by using the organic ligands as 'spacers' for linking the metal ions or 'nodes'. Therefore, the structures of coordination polymers can be ascribed to the coordination interactions between the metal ions and ligands, as well as the conformations of the ligands. When organic carboxylate ligands are employed as spacers, the bases used to deprotonate these acids also have an important influence on the structures of the resulting coordination polymers, since the bases, as electron donors, not only accept the protons but can also coordinate to the metal ions. For example, when 5-nitrobenzene-1,3-dicarboxylic acid is deprotonated by different bases, such as NaOH, pyridine and 4,4′-bipyridine, the resulting dianion, *viz*. 5-nitrobenzene-1,3-dicarboxylate (abbreviated hereinafter as NIP), associated with the zinc(II) cation, can produce some coordination polymers with different structures (Xin *et al.*, 2002; Tao *et al.*, 2002, 2003; Xu



(I)

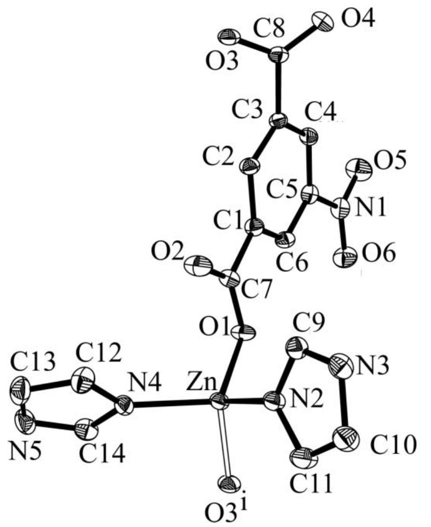


Figure 1
The asymmetric unit of (I) (solid bonds), together with completion of the coordination of Zn, with displacement ellipsoids at the 30% probability level. All H atoms have been omitted for clarity. [Symmetry code: (i) $1 + x, y, z$].

et al., 2004). Here, we report the structure of the title herringbone chain-like coordination polymer, (I), which is derived from NIP and imidazole.

As shown in Fig. 1, the asymmetric unit of (I) contains one Zn^{II} cation, an NIP dianion and two imidazole molecules. The Zn^{II} cation adopts a slightly distorted tetrahedral geometry. Two carboxyl O atoms [O1 and $O3^i$; symmetry code: (i) $1 + x, y, z$] and two imidazole N atoms (N2 and N4) occupy the four vertices. The O3/C8/O4 carboxylate group is twisted away from its parent benzene ring, with a dihedral angle of 32.6 (3)°. The dihedral angle between the two imidazole planes is 71.76 (18)°. The dihedral angles between the imidazole planes (N2/C9/N3/C10/C11 and N4/C12/N5/C13/C14) and the benzene plane of NIP are 70.66 (10) and 63.42 (16)°, respectively.

Along the *a* axis direction, the NIP dianion acts as a bridge to connect neighbouring Zn^{II} cations, generating a one-dimensional chain-like coordination polymer with a herringbone feature (Fig. 2). This herringbone chain can also be found in another zinc-containing coordination polymer derived from 1,3-benzenedicarboxylate and imidazole (Li *et al.*, 2001).

Along the *b*-axis direction, adjacent chains are connected together to form a two-dimensional single-sheet layer through an interchain hydrogen bond, $N5—H5\cdots O4^{ii}$, while another inter-chain hydrogen bond, $N3—H3\cdots O2^{iii}$, links two adjacent two-dimensional single-sheet layers to produce a two-dimensional double-sheet layer (symmetry codes as in Table 2). Moreover, three weak hydrogen bonds, $C10—H10\cdots O3^{iii}$, $C13—H13\cdots N3^{iv}$ and $C14—H14\cdots O1^{v}$, also contribute to the two-dimensional double-sheet layer. Neighbouring chains in two adjacent double-sheet layers are related by inversion centres.

The centroid–centroid distance between the two anti-parallel benzene rings of two inter-layer pairs of NIP dianions is 3.820 (11) Å, indicating the presence of a π–π interaction between two adjacent layers (Janiak, 2000). In the crystal structure, all double-sheet layers are stabilized by π–π interactions.

Experimental

$Zn(ClO_4)_2\cdot 6H_2O$ (186.2 mg, 0.5 mmol), 5-nitrobenzene-1,3-dicarboxylic acid (105.7 mg, 0.5 mmol) and imidazole (204.0 mg, 3.0 mmol) were dissolved in water (10 ml). The solution was placed in a 25 ml Teflon-lined stainless steel vessel, which was sealed and heated at 423 K for 72 h. After cooling to room temperature, colourless block crystals of (I) were collected by filtration and washed with water and ethanol (125.0 mg, yield *ca* 60%).

Crystal data

$[Zn(C_8H_3NO_6)(C_3H_4N_2)_2]$
$M_r = 410.65$
Monoclinic, $P2_1/n$
$a = 9.5225$ (16) Å
$b = 8.6825$ (15) Å
$c = 19.210$ (3) Å
$\beta = 99.91$ (3)°
$V = 1564.6$ (5) Å^3
$Z = 4$
$D_x = 1.743$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1610 reflections
$\theta = 2.6$–24.0°
$\mu = 1.62$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.18 × 0.14 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.762$, $T_{max} = 0.890$
27420 measured reflections
3659 independent reflections
2916 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 28.0°$
$h = -11 \rightarrow 12$
$k = -8 \rightarrow 11$
$l = -25 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.095$
$S = 1.07$
3659 reflections
235 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.011P)^2 + 4.62P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N2—Zn	1.989 (3)	O1—Zn	1.964 (2)
N4—Zn	1.987 (3)	Zn—$O3^i$	1.959 (2)
$O3^i$—Zn—O1	112.43 (11)	$O3^i$—Zn—N2	107.94 (12)
$O3^i$—Zn—N4	96.94 (12)	O1—Zn—N2	111.31 (12)
O1—Zn—N4	111.63 (12)	N4—Zn—N2	115.76 (13)

Symmetry code: (i) $x + 1, y, z$.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
$N5—H5\cdots O4^{ii}$	0.86	1.96	2.820 (4)	176
$N3—H3\cdots O2^{iii}$	0.86	1.96	2.799 (4)	163
$C10—H10\cdots O3^{iii}$	0.93	2.58	3.491 (5)	168
$C13—H13\cdots N3^{iv}$	0.93	2.57	3.462 (5)	161
$C14—H14\cdots O1^{v}$	0.93	2.34	3.233 (5)	161

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

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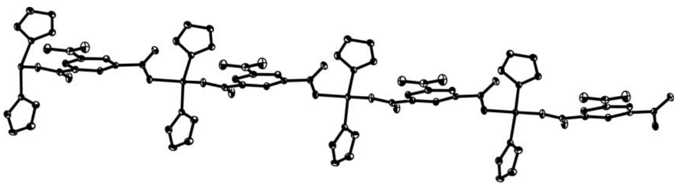

Figure 2
An illustration of the herringbone chain formed by bridging NIP ligands. H atoms have been omitted.

H atoms were introduced in calculated positions and refined using a riding model, with C—H distances of 0.93 Å and N—H distances of 0.86 Å, and with $U_{\rm iso}(\rm H) = 1.2U_{\rm eq}(\rm C)$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 1997); 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* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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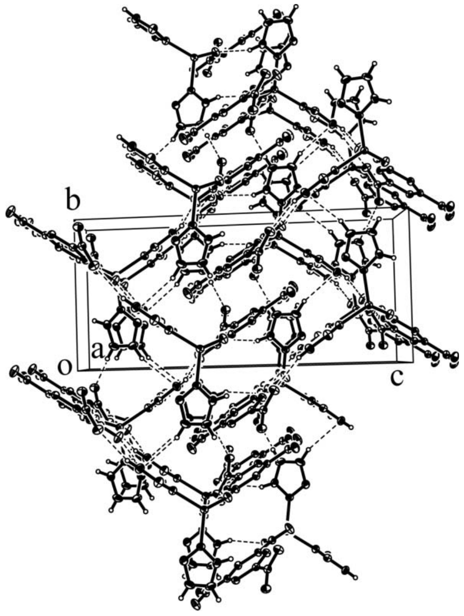

Figure 3
A packing diagram of the title compound, viewed down the *a* axis. All H atoms not involved in the hydrogen-bonding have been omitted for clarity. Dashed lines indicate hydrogen bonds.

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