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Poly[zinc(II)-μ_2-4,4′-bipyridine-di-μ_2-formato]: a chiral three-dimensional coordination polymer

Xiao-He Miao,[a] Hong-Ping Xiao[b] and Long-Guan Zhu[a]*

[a]Department of Chemistry, Zhejiang University, Hangzhou 310027, People's Republic of China, and [b]School of Chemistry and Materials Science, Wenzhou University, Wenzhou 325027, People's Republic of China

Correspondence e-mail: chezlg@zju.edu.cn

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Key indicators

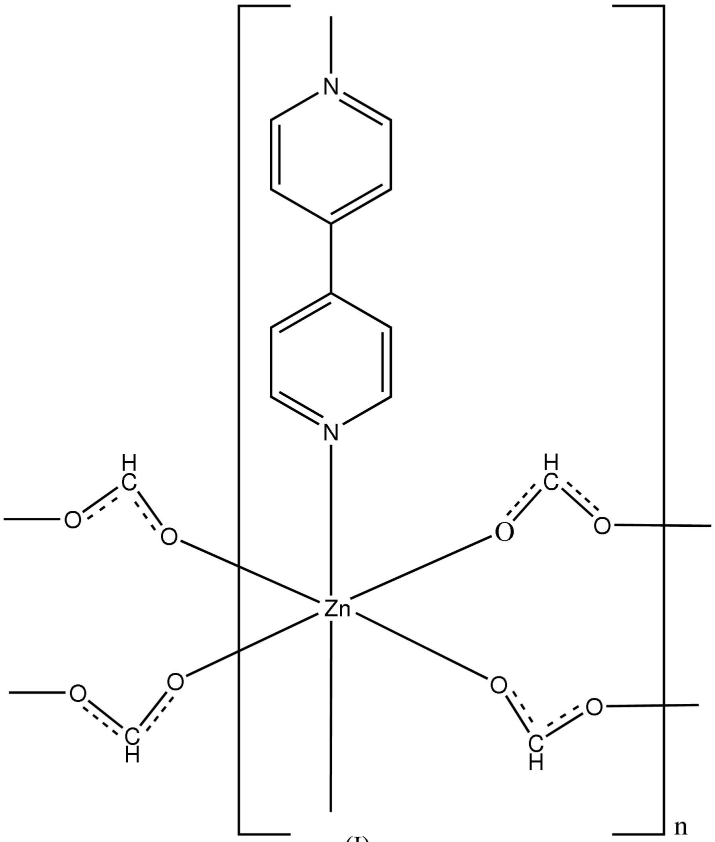
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.019
wR factor = 0.059
Data-to-parameter ratio = 13.7

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

The title compound, $[\mathrm{Zn(CHO_2)_2(C_{10}H_8N_2)}]_n$, is a chiral three-dimensional coordination polymer. The Zn atom, the two bipyridine N atoms, and the bridging bipyridine C atoms occupy special positions with site symmetry 2. In the extended structure, both the ligands act as linkers in μ_2-mode. The compound is isostructural with its copper analogue.

Comment

The reaction of copper formate and sodium formate with 4,4′-bipyridine (4,4′-bipy) in acetone solution yielded a chiral three-dimensional coordination polymer, $[\mathrm{Cu(HCOO)_2(C_{10}H_8N_2)}]_n$ (Manson *et al.*, 2003). Unexpectedly, the reaction of zinc acetate, sodium hydrogen 3-sulfobenzoate and 4,4′-bipyridine in the mixed-solvent system, water and *N*,*N*′-dimethylformamide under reflux conditions led to the title compound, (I), which is isostructural with its copper analogue (Manson *et al.* 2003).



(I)

The Zn$^{\mathrm{II}}$ atom in (I) adopts an octahedral geometry coordinated by two *trans* N-atom donors from two 4,4′-bipyridine

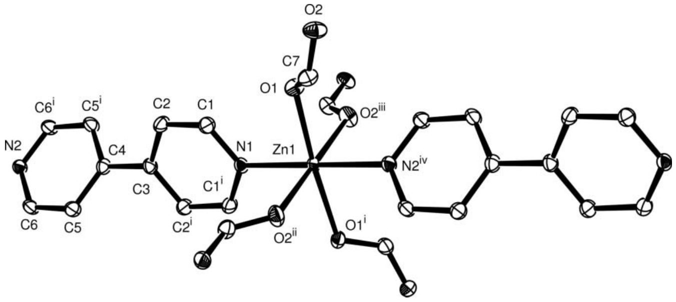


Figure 1
View of a fragment of the polymeric structure of (I), with displacement ellipsoids drawn at the 50% probability level (H atoms omitted for clarity). [Symmetry codes: (i) $y, x, -z$; (ii) $-\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{4}-z$; (iii) $\frac{1}{2}-y, x-\frac{1}{2}, \frac{1}{4}+z$; (iv) $1+x, 1+y, z$.]

molecules and four O atoms from four formate ligands (Fig. 1 and Table 1). Atoms Zn1, N1, C3, C4 and N2 occupy special positions with site symmetry 2. The [Zn(4,4′-bipy] units give rise to one-dimensional chains propagating alternately in [110] and [$\bar{1}$10]. Within a chain, the two pyridyl rings of each 4,4′-bipyridine molecule are twisted with a dihedral angle of 47.67 (6)°. The Zn⋯Zn separation *via* the 4,4′-bipyridine bridge is 11.2694 (4) Å. The formate ligands act as bridges in μ_2-mode and extend the [Zn(4,4′-bipy)] chains into a three-dimensional network. The formate C—O distances suggest delocalization of the negative charge of this ion.

Experimental

A mixture of $Zn(CH_3COO)_2\cdot 4H_2O$ (0.112 g, 0.44 mmol), sodium hydrogen 3-sulfobenzoate (0.112 g, 0.5 mmol), 4,4′-bipyridine (0.078 g, 0.5 mmol), water (30 ml) and *N*,*N*′-dimethyformamide (5 ml) was refluxed for 7 h. The resulting solution was set aside and allowed to evaporate. After two months, colorless crystals of (I) were obtained.

Crystal data

$[Zn(CHO_2)_2(C_{10}H_8N_2)]$
$M_r = 311.59$
Tetragonal, $P4_12_12$
$a = 7.9687$ (3) Å
$c = 17.7213$ (11) Å
$V = 1125.31$ (9) Å^3
$Z = 4$
$D_x = 1.839$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.19$ mm^{-1}
$T = 295$ (2) K
Block, colorless
0.39 × 0.30 × 0.22 mm

Data collection

Bruker APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.452$, $T_{max} = 0.613$
6797 measured reflections
1232 independent reflections
1206 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.059$
$S = 0.87$
1232 reflections
90 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0566P)^2 + 0.0576P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0145 (15)
Absolute structure: Flack (1983), 451 Friedel pairs
Flack parameter: 0.008 (13)

Table 1
Selected bond lengths (Å).

Zn1—N1	2.1065 (17)	Zn1—O2^{ii}	2.1831 (11)
Zn1—N2^i	2.1204 (16)	C7—O1	1.2535 (17)
Zn1—O1	2.1729 (11)	C7—O2	1.2373 (18)

Symmetry codes: (i) $x+1, y+1, z$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, -z-\frac{1}{4}$.

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

Data collection: *SMART* (Bruker, 2002); 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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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