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catena-Poly[[(2,2′-bipyridine-κ^2N,N')zinc(II)]-μ-oxalato]

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.010 Å
R factor = 0.023
wR factor = 0.021
Data-to-parameter ratio = 8.2

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

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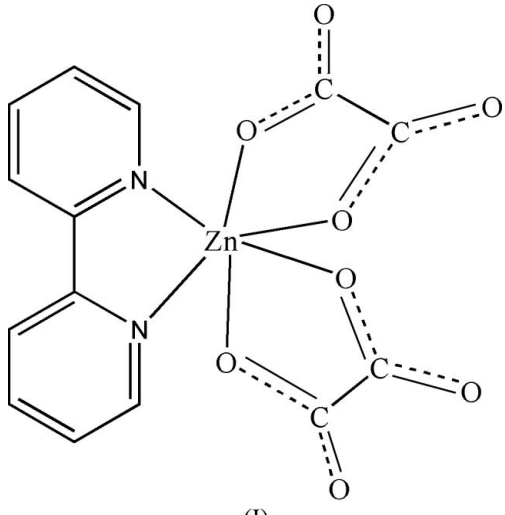
In the molecule of the title compound, $[Zn(C_2O_4)(C_{10}H_8N_2)]_n$, the coordination geometry around the zinc center can be described as slightly distorted octahedral. In the crystal structure, intermolecular C—H···O hydrogen bonds link the molecules, forming infinite chains. Hydrogen bonding and π–π stacking interactions stabilize the crystal structure.

Comment

Synthesis of metal-organic framework (MOF) structures by the modular approach is an area of intense research activity as potential zeolitic, optoelectronic, magnetic, and conducting materials (Chui *et al.*, 1999; Kiang *et al.*, 1999; Kahn & Martinez, 1998; Lin *et al.*, 1999, 2000; Munakata *et al.*, 1998). Much research has also been carried out on metal oxalate ($C_2O_4^{2-}$) compounds in the context of studies of molecular-based magnets, thermal stability, dielectricity and open framework structures (Decurtins *et al.*, 1993; Decurtins, Schmalle, Schneuwly *et al.*, 1994; Decurtins, Schmalle, Oswald *et al.*, 1994; Curtis *et al.*, 1973; Speier *et al.*, 1997; Glerup *et al.*, 1995). We present here the structure of the title complex, (I), which is analogous to the zinc(II) complex reported by Chuy *et al.* (1997).



(I)

In the molecule of the title compound, (I) (Fig. 1), the bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). Atom Zn1 is coordinated by two oxalate groups and one 2,2′-bipyridine group, forming a hexacoordination with an O_4N_2 donor set. The coordination geometry around the zinc center can be described as slightly distorted octahedral.

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 2) link the molecules, forming infinite chains (Fig. 2). In addition, there are offset face-to-face π–π stacking interactions, with centroid–centroid distances of 3.621–3.710 Å (between rings N1/C1–C5 and N2/C6–C10). These interactions may increase the stability of the crystal structure.

Experimental

A mixture of $Zn(ClO_4)_2$ (0.0661 g, 0.25 mmol), 2,3-dichloro-5,6-dicyano-*p*-benzochinon (0.05675 g, 0.25 mmol), 2,2'-bipyridine (0.0390 g, 0.25 mmol) and H_2O (12 ml) was sealed in a 23 ml Teflon-lined stainless steel autoclave to approximately 60% of capacity. The resulting mixture was heated to 383 K at a rate of *ca* 100 K h^{-1} and held at this temperature for 5 d. Subsequently, the autoclave was cooled to room temperature at a rate of *ca* 3 K h^{-1}. The resulting brown needles were filtered off and washed with water and dried at ambient temperature.

Crystal data

$[Zn(C_2O_4)(C_{10}H_8N_2)]$
M_r = 309.57
Orthorhombic, $Pna2_1$
a = 9.1922 (5) Å
b = 9.1265 (5) Å
c = 14.1060 (7) Å
V = 1183.39 (11) Å^3
Z = 4
D_x = 1.738 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.09 mm^{-1}
T = 294 (2) K
Needle, brown
0.41 × 0.06 × 0.03 mm

Data collection

Rigaku Weissenberg IP diffractometer
ω scans
Absorption correction: multi-scan (*TEXSAN*; Molecular Structure Corporation, 1998)
T_{min} = 0.819, T_{max} = 0.939
11070 measured reflections
1405 independent reflections
766 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.021
S = 0.97
1405 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.001P)^2 + 0.0046P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), with 544 Friedel pairs
Flack parameter: 0.02 (4)

Table 1
Selected geometric parameters (Å, °).

Zn1—O2	2.094 (3)	N2—C10	1.320 (7)
Zn1—O1	2.110 (5)	O2—C12	1.258 (6)
Zn1—N1	2.129 (5)	O3—C12	1.227 (7)
Zn1—N2	2.133 (5)	O4—C11	1.247 (5)
N1—C1	1.336 (7)	C5—C6	1.485 (5)
N1—C5	1.352 (8)	C11—C12	1.556 (4)
N2—C6	1.317 (8)		
O2—Zn1—O1	79.72 (16)	C6—N2—C10	118.6 (6)
O2—Zn1—N1	97.26 (16)	N2—C6—C7	123.8 (7)
O1—Zn1—N1	94.71 (19)	N2—C6—C5	115.1 (7)
O2—Zn1—N2	94.31 (15)	N2—C10—C9	122.3 (6)
O1—Zn1—N2	168.85 (18)	O4—C11—O1	125.5 (6)
N1—Zn1—N2	76.59 (13)	O3—C12—O2	127.4 (6)
C1—N1—C5	119.1 (6)		

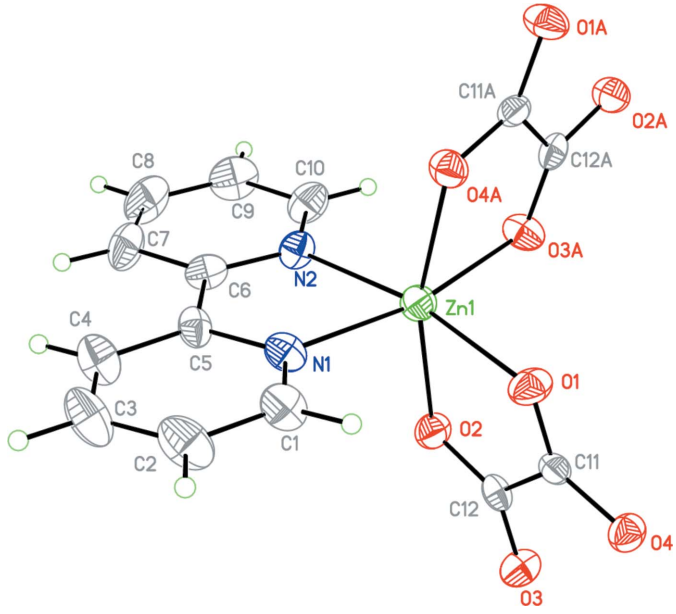


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

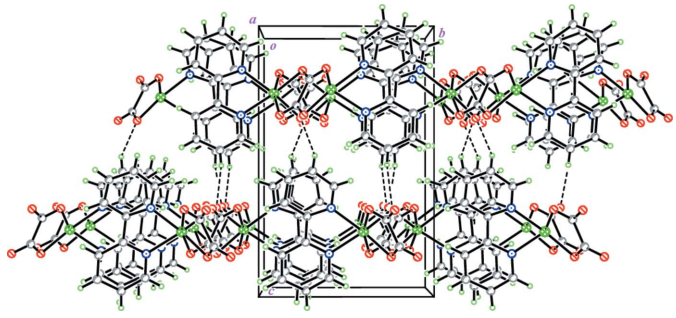


Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O1^{i}	0.93	2.41	3.279 (8)	155
C2—H2C···O3^{ii}	0.93	2.48	3.395 (9)	170

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

H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *TEXSAN* (Molecular Structure Corporation, 1998); cell refinement: *TEXSAN*; data reduction: *TEXSAN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL97*.

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