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(2,2′-Bipyridine)bis(hydrogen isophthalato)zinc(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.012 Å
R factor = 0.081
wR factor = 0.169
Data-to-parameter ratio = 12.0

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

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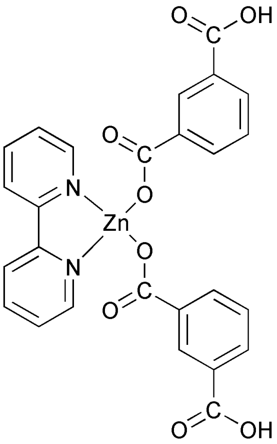
In the title compound, $[Zn(C_8H_5O_4)_2(C_{10}H_8N_2)]$, the Zn^{II} ion is located on a crystallographic twofold axis, which passes through the mid-point of the C—C bond of the bpy ligand. The Zn atom is four-coordinated by two carboxylate O atoms from two symmetry-related hydrogen isophthalate ligands [Zn—O = 1.972 (5) Å] and two N atoms from 2,2′-bipyridine ligand [Zn—N = 2.067 (5) Å] to furnish a distorted tetrahedral geometry.

Comment

The design and construction of polymeric complexes are currently of great interest owing to their intriguing network topologies and potential functions as new classes of materials (Ford *et al.*, 1999; Liu *et al.*, 2004; Li *et al.*, 2002; Xiao & Liu, 2004). Multicarboxylate and bipyridyl ligands have been widely introduced into the construction of polymeric complexes due to their diverse coordination modes. Furthermore, polynuclear d^{10} metal complexes have been found to exhibit intriguing photoluminescent properties (Zhang *et al.*, 2003; Zhou *et al.*, 2003). Taking the above factors into account, we have explored the assembling of the Zn^{II} ion, ip (Hip is hydrogen isophthalate) and bpy (bpy is 2,2′-bipyridine) in attempts to obtain luminescent coordination polymers. The coordination polymerization should be carried out under strict control, to avoid the production of unwanted mononuclear complexes. We report here the synthesis and crystal structure of the title Zn^{II} mononuclear complex, (I).



(I)

Each Zn^{II} ion is located on a crystallographic twofold axis, which passes through the mid-point of the C—C bond of the bpy ligand. The Zn atom is coordinated by two monodentate carboxylate O atoms from two Hip ligands [Zn1—O1 =

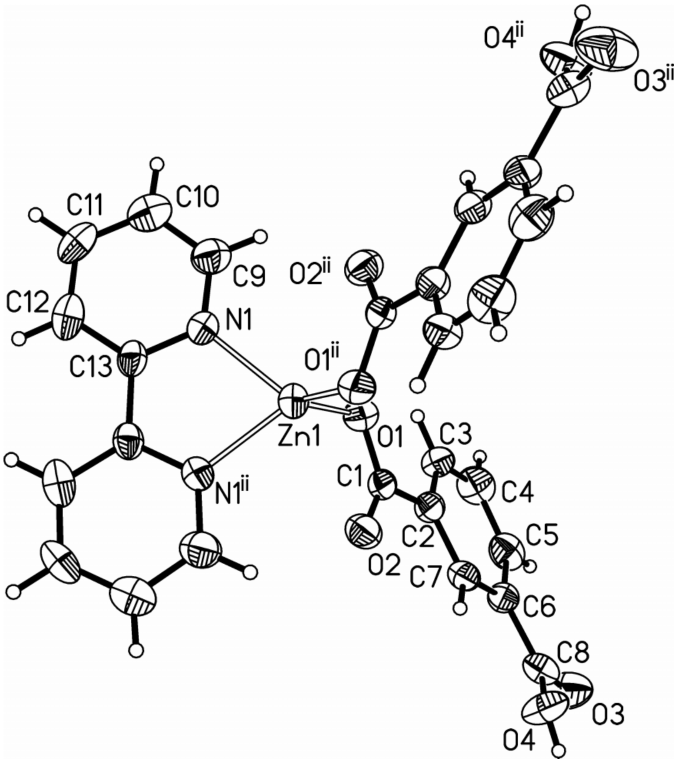


Figure 1
A view of (I), with the atom-labelling scheme [symmetry code: (ii) $1 - x, y, \frac{3}{2} - z$]. Displacement ellipsoids are drawn at the 50% probability level.

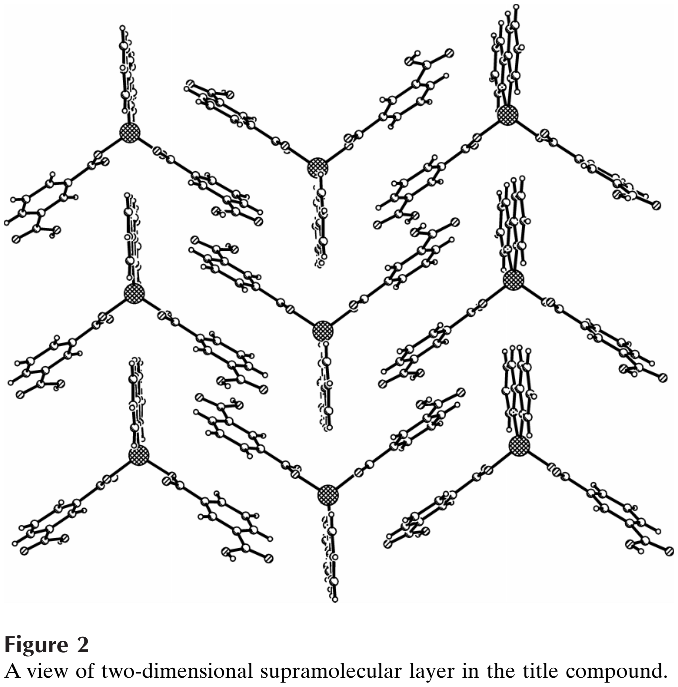


Figure 2
A view of two-dimensional supramolecular layer in the title compound.

1.972 (5) Å] and two N atoms from the chelating bpy ligand [Zn1—N1 = 2.067 (5) Å] to furnish a distorted tetrahedral geometry (Table 1 and Fig. 1). The two Hip ligands are attached to the Zn^{II} ion in a V shape, the dihedral angle between the benzene rings being 70.2 (8)°.

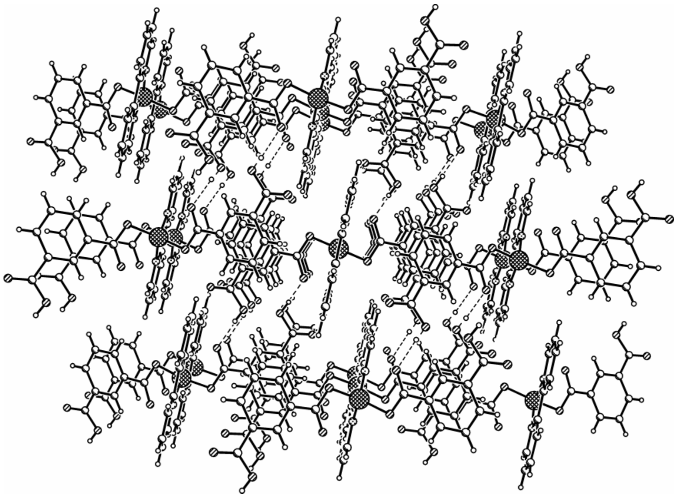


Figure 3
The crystal packing, viewed down the *b* axis. Dashed lines indicate hydrogen bonds.

Adjacent mononuclear units are consolidated through van der Waals forces, the face-to-face distances between the benzene rings being 4.05 or 4.15 Å, resulting in two-dimensional supramolecular layers parallel to the *ab* plane (Fig. 2). The hydroxyl O atom of the Hip carboxylic group forms a hydrogen bond with the carbonyl O atom of the Hip carboxylate group in the adjacent layer (Table 2). The inter-layer hydrogen bonds link the layers into a three-dimensional supramolecular network (Fig. 3).

Experimental

The hydrothermal reaction of $Zn(NO_3)_2\cdot 4H_2O$ (52 mg, 0.20 mmol), isophthalic acid (42 mg, 0.25 mmol), 2,2′-bipyridine (31 mg, 0.20 mmol) and water (10 ml) was carried out at 443 K for 3 d. After cooling to room temperature at a rate of 5 K h^{-1}, colorless crystals of the title compound were isolated by filtration and washed with distilled water (yield 41%, based on H_2ip). IR (KBr, ν cm^{-1}): 1599, 1473, 1444, 1319, 1030, 771, 733. Elemental analysis calculated for $C_{26}H_{18}N_2O_8Zn$: C 56.59, H 3.29, N 5.08%; found: C 56.34, H 3.00, N 4.99%.

Crystal data

$[Zn(C_8H_5O_4)_2(C_{10}H_8N_2)]$
$M_r = 551.81$
Monoclinic, $C2/c$
$a = 21.731$ (2) Å
$b = 8.1038$ (7) Å
$c = 15.1428$ (16) Å
$\beta = 121.595$ (2)°
$V = 2271.4$ (4) Å^3
$Z = 4$
$D_x = 1.614$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1383 reflections
$\theta = 2.2$–25.1°
$\mu = 1.14$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.24 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.761$, $T_{max} = 0.796$
3608 measured reflections
2026 independent reflections
1446 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 25.1°$
$h = -25 \rightarrow 25$
$k = -9 \rightarrow 7$
$l = -18 \rightarrow 14$

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Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0098P)^2 + 22.9335P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.081$	$(\Delta/\sigma)_{\max} < 0.001$
$wR(F^2) = 0.169$	$\Delta\rho_{\max} = 0.47$ e Å^{-3}
$S = 1.28$	$\Delta\rho_{\min} = -0.65$ e Å^{-3}
2026 reflections	
168 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.972 (5)	Zn1—N1	2.067 (5)
O1—Zn1—O1^{ii}	111.0 (3)	O1^{ii}—Zn1—N1	121.8 (2)
O1—Zn1—N1^{ii}	121.8 (2)	N1^{ii}—Zn1—N1	79.0 (3)

Symmetry code: (ii) $1 - x, y, \frac{3}{2} - z$.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O4—H4$B\cdots$O2^{i}	0.82	1.86	2.684 (7)	177

Symmetry code: (i) $\frac{1}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$.

The H atoms were found in a difference Fourier map, placed in idealized positions (C—H = 0.93 Å) and refined as riding, with $U_{\rm iso}(\rm H) = 1.2U_{\rm eq}(\rm C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Siemens, 1996); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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