

catena-Poly[[[2-(2-furyl)-1*H*-imidazo[4,5-*f*][1,10]-phenanthroline]zinc(II)]- μ -benzene-1,2-dicarboxylato]**Chuan-Bi Li,^b Yan-Wei Li,^b Wei Fang,^b Bo Liu^b and De-Qian Li^{a*}**^aKey Laboratory of Rare Earth Chemistry and Physics, ChangChun Institute of Applied Chemistry, Graduate School of The Chinese Academy of Science, ChangChun, People's Republic of China, and ^bDepartment of Chemistry, Jilin Normal University, Siping 136000, People's Republic of China

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Key indicatorsSingle-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$
 R factor = 0.050
 wR factor = 0.159
Data-to-parameter ratio = 13.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

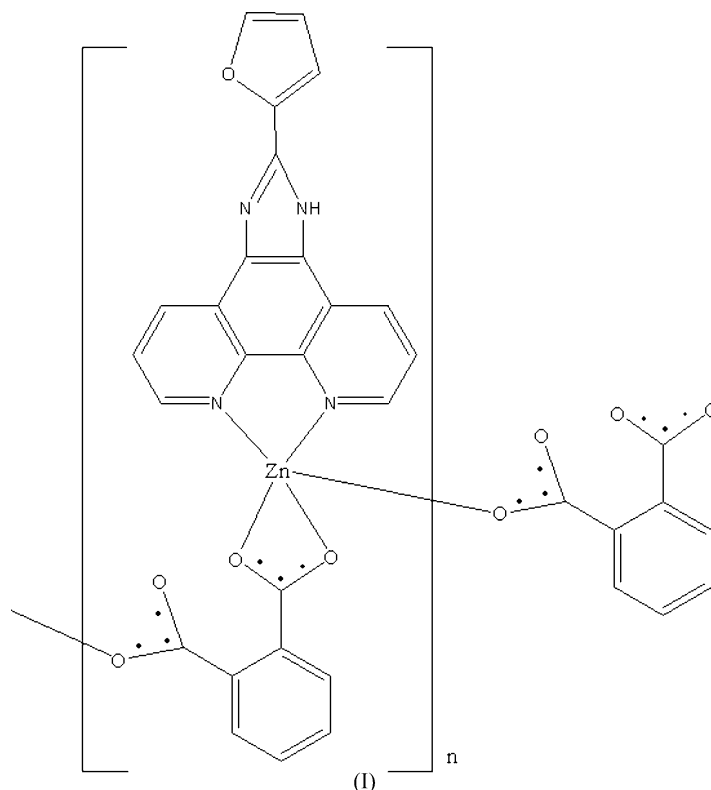
In the title compound, $[\text{Zn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{17}\text{H}_{10}\text{N}_4\text{O})]_n$, the Zn^{II} atom is five-coordinated by two N atoms from the phenanthroline-derived ligand and three O atoms from one bidentate and one monodentate benzene-1,2-dicarboxylate (1,2-BDC) dianions in a distorted trigonal-bipyramidal geometry. The Zn^{II} atoms are bridged by the 1,2-BDC ligands to form a single-chain structure. Neighboring chains interact through π - π interactions, leading to a two-dimensional network.

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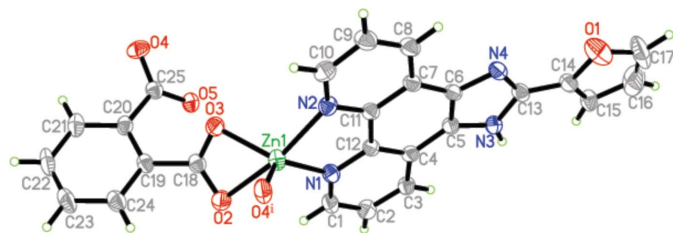
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Comment

The 1,10-phenanthroline (phen) ligand has been widely used to build novel supramolecular architectures through its aromatic π - π interactions (Chen & Liu, 2002). The phen derivative 2-(furan-2-yl)-1*H*-imidazo[4,5-*f*][1,10]phenanthroline ($\text{C}_{17}\text{H}_{10}\text{N}_4\text{O}$; *L*), was recently shown to form a coordination polymer with a distinctive supramolecular architecture (Li *et al.*, 2006).



We selected benzene-1,2-dicarboxylate ($\text{C}_8\text{H}_4\text{O}_4^{2-}$; 1,2-BDC) to act as a metal-metal linker in its deprotonated form and *L* as a secondary ligand, generating the title compound, $[\text{Zn}(1,2\text{-BDC})(L)]_n$, (I), a new coordination polymer, which is reported here.


Figure 1

The asymmetric unit of (I), expanded to show the Zn coordination. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). [Symmetry code: (i) $x, -y, z - \frac{1}{2}$]

In compound (I), the Zn^{II} atom is surrounded by two N atoms derived from the bidentate *L* ligand, two O atoms from a bidentate 1,2-BDC ligand and one O atom from a monodentate 1,2-BDC ligand. This results in a very distorted ZnN_2O_3 trigonal bipyramid with the donor atoms of both the bidentate species occupying both an equatorial and an axial site (Table 1, Fig. 1). The average Zn–O and Zn–N distances are 2.080 (3) and 2.069 (4) Å, respectively. Neighbouring Zn^{II} atoms are bridged by the 1,2-BDC ligands, forming a single-chain structure (Fig. 2). The C–O bond lengths (Table 1) indicate that the carboxylate bonding is essentially delocalized. Neighbouring single chains in (I) are connected through π – π interactions between *L* ligands with π – π stacking distances of 3.371 and 3.376 Å, resulting in a two-dimensional supramolecular structure (Noveron *et al.*, 2002). Finally, interchain N–H...O hydrogen bonds (Table 2) complete the structure of (I).

Experimental

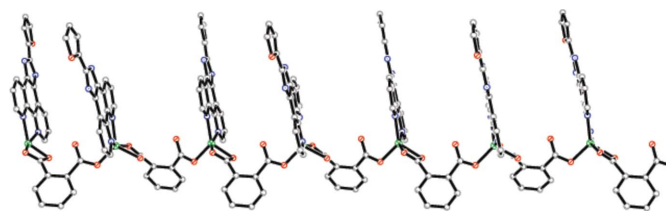
Ligand *L* was synthesized according to the literature method of Steck & Day (1943). A mixture of ZnCl_2 (0.3 mmol), *L* (0.1 mmol) and H_2 1,2-BDC (0.3 mmol) in distilled water (30 ml) was stirred thoroughly for 1 h at ambient temperature. The pH was adjusted to 7.5 with aqueous NaOH solution. The suspension was then sealed in a Teflon-lined stainless steel reaction vessel (40 ml). The reaction was performed under autogeneous pressure and static conditions in an oven at 443 K for 4.5 d. The vessel was then cooled slowly inside the oven to 298 K at a rate of 5 K h^{-1} before opening; yellow crystals of (I) were collected.

Crystal data

$[\text{Zn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{17}\text{H}_{10}\text{N}_4\text{O})]$	$Z = 8$
$M_r = 515.77$	$D_x = 1.633 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 31.852$ (13) Å	$\mu = 1.22 \text{ mm}^{-1}$
$b = 9.772$ (4) Å	$T = 293$ (2) K
$c = 13.657$ (6) Å	Block, yellow
$\beta = 99.285$ (7)°	$0.46 \times 0.14 \times 0.12 \text{ mm}$
$V = 4195$ (3) Å ³	

Data collection

Bruker APEX CCD diffractometer	11154 measured reflections
ω scans	4172 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2002)	2562 reflections with $I > 2\sigma(I)$
$T_{\text{min}} = 0.813$, $T_{\text{max}} = 0.864$	$R_{\text{int}} = 0.051$
	$\theta_{\text{max}} = 26.1^\circ$


Figure 2

View of the single-chain structure in (I). H atoms have been omitted.

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.159$
 $S = 1.03$
 4172 reflections
 316 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0803P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.68 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.38 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Zn1–O4 ⁱ	1.945 (3)	C18–O2	1.246 (5)
Zn1–O3	2.009 (3)	C18–O3	1.258 (5)
Zn1–N1	2.051 (4)	C25–O5	1.245 (5)
Zn1–N2	2.086 (4)	C25–O4	1.262 (5)
Zn1–O2	2.287 (3)		
O4 ⁱ –Zn1–O3	105.00 (14)	N1–Zn1–N2	80.13 (14)
O4 ⁱ –Zn1–N1	129.19 (14)	O4 ⁱ –Zn1–O2	98.21 (13)
O3–Zn1–N1	123.66 (14)	O3–Zn1–O2	60.44 (12)
O4 ⁱ –Zn1–N2	98.92 (14)	N1–Zn1–O2	93.96 (13)
O3–Zn1–N2	108.53 (13)	N2–Zn1–O2	161.69 (14)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N3}-\text{H3C}\cdots\text{O5}^{\text{ii}}$	0.86	1.96	2.792 (5)	162

Symmetry code: (ii) $-x, -y, -z + 2$.

All H atoms were placed geometrically (N–H = 0.86 Å, C–H = 0.93 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

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: SHELXTL-Plus (Sheldrick, 1990); software used to prepare material for publication: SHELXTL.

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