Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[bis(1,3-propylenediamine)zinc(II)]-μ-naphthalene-2,6-dicarboxylato-$\kappa^2O^2:O^6$]

Rong Yu,[a] Ya-Qi Jiang[a]* and Zhao-Xiong Xie[b]

[a]Department of Chemistry, Xiamen University, Xiamen, Fujian 361005, People's Republic of China, and [b]State Key Laboratory for the Physical Chemistry of Solid Surfaces, Xiamen University, Xiamen, Fujian 361005, People's Republic of China

Correspondence e-mail: yqjiang@xmu.edu.cn

Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.105
Data-to-parameter ratio = 12.6

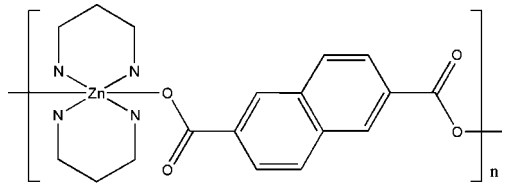
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 27 January 2006
Accepted 6 March 2006

The title compound, $[Zn(C_{12}H_6O_4)(C_3H_{10}N_2)_2]_n$, has been prepared from zinc(II), naphthalene-2,6-dicarboxylic acid (H_2napdc) and 1,3-propylenediamine (pren). The Zn atom lies on a crystallographic centre of symmetry and is coordinated by two monodentate naphthalene-2,6-dicarboxylate ligands and two chelating 1,3-propylenediamine ligands in a distorted octahedral environment. The naphthalene-2,6-dicarboxylate ligands link the Zn atoms, forming a one-dimensional chain structure.

Comment

The diverse coordination modes of carboxylate ligands result in the formation of a great number of metal carboxylates (Jiang *et al.*, 2003; Baca *et al.*, 2003). Aromatic dicarboxylate ligands have been widely used for the construction of infinite frameworks with high thermal stability (Abrahams *et al.*, 1994; Maji *et al.*, 2005; Zheng *et al.*, 2001; Kongshaug *et al.*, 2004). Here we employed naphthalene-2,6-dicarboxylic acid (H_2napdc) as the building block to design a new polymeric zinc complex, *viz*. (I).



(I)

In (I), the Zn^{II} atom lies on a crystallographic centre of symmetry and has a distorted octahedral 4 + 2 environment (Fig. 1 and Table 1). The equatorial plane is composed of four N atoms from the two propylenediamine ligands, with Zn—N bond lengths in the range 2.143 (2)–2.146 (3) Å. O atoms from two carboxylate groups occupy the axial sites, with a Zn—O distance of 2.189 (2) Å. The structure can be viewed as being composed of zinc(II) and two 1,3-propylenediamine (pren) ligands forming a $[Zn(pren)_2]^{2+}$ unit with naphthalene-2,6-dicarboxylate anions serving as bridging ligands, forming an infinite one-dimensional chain-like structure along the crystallographic direction [101] (Fig. 2). Hydrogen bond interactions among the chains help to stabilize the whole structure (Table 2).

Experimental

A mixture of $Zn(NO_3)_2{\cdot}6H_2O$, naphthalene-2,6-dicarboxylic acid, 1,3-propylenediamine and dimethyl sulfoxide in a molar ratio of

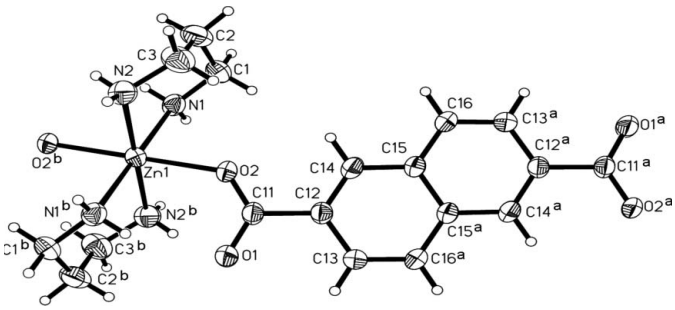


Figure 1
View of a segment of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (*a*) $2-x, 2-y, 3-z$; (*b*) $1-x, 2-y, 2-z$.]

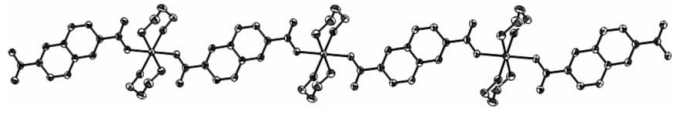


Figure 2
View of the chain in (I). H atoms have been omitted for clarity.

1:1:2:140 was sealed in a 30 ml Teflon-lined stainless steel autoclave and heated at 393 K for 72 h. After cooling to room temperature, colorless plate-like crystals of (I) were obtained.

Crystal data

$[Zn(C_{12}H_6O_4)(C_3H_{10}N_2)_2]$
$M_r = 427.80$
Monoclinic, $P2_1/c$
$a = 9.7497\ (5)$ Å
$b = 10.1560\ (5)$ Å
$c = 10.2458\ (5)$ Å
$\beta = 96.521\ (1)^\circ$
$V = 1007.95\ (9)$ Å^3
$Z = 2$
$D_x = 1.410$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2311 reflections
$\theta = 2.1$–28.4°
$\mu = 1.25$ mm^{-1}
$T = 273\ (2)$ K
Plate, colorless
0.32 × 0.25 × 0.12 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.691$, $T_{max} = 0.865$
7588 measured reflections
1771 independent reflections
1701 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0^\circ$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.105$
$S = 1.14$
1771 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0521P)^2 + 0.9274P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.143 (2)	Zn1—O2	2.189 (2)
Zn1—N2	2.146 (3)		
N1—Zn1—N1^{i}	180	N2—Zn1—O2^{i}	89.9 (1)
N1—Zn1—N2^{i}	94.7 (1)	N1—Zn1—O2	88.7 (1)
N1—Zn1—N2	85.3 (1)	N2—Zn1—O2	90.1 (1)
N2^{i}—Zn1—N2	180	O2^{i}—Zn1—O2	180.
N1—Zn1—O2^{i}	91.3 (1)		

Symmetry code: (i) $-x+1, -y+2, -z+2$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H12···O1^{i}	0.85 (1)	2.28 (2)	3.047 (3)	150 (3)
N1—H11···O1^{ii}	0.85 (1)	2.21 (2)	3.046 (3)	167 (3)
N2—H21···O1^{i}	0.85 (1)	2.49 (2)	3.232 (4)	146 (3)
N2—H22···O1^{iii}	0.85 (1)	2.17 (2)	2.988 (3)	164 (3)

Symmetry codes: (i) $-x+1, -y+2, -z+2$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{5}{2}$; (iii) $x, -y+\frac{5}{2}, z-\frac{1}{2}$.

All C-bound H atoms were positioned geometrically and refined as riding, with C—H = 0.93 and 0.97 Å in napdc and pren, respectively, and with $U_{iso}(H) = 1.2U_{eq}(C)$. All N-bound H atoms were located in a difference Fourier map and refined with the following restraints: N—H distances of 0.85 (1) Å and H···H distances of 1.39 (1) Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank the National Science Foundation of China (No. 20473069) and the Science Foundation of Fujian Province (No. E0410006) for supporting this work.

References

Abrahams, B. F., Hoskins, B. F., Michail, D. M. & Robson, R. (1994). *Nature* (London), **369**, 727–729.
Baca, S. G., Filippova, I. G., Gerbeleu, N. V., Simonov, Y. A., Gdaniec, M., Timco, G. A., Gherco, O. A. & Malaestean, Y. L. (2003). *Inorg. Chim. Acta*, **344**, 109–116.
Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Jiang, Y.-Q. & Xie, Z.-X. (2003). *Chin. J. Struct. Chem.* **24**, 457–461.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Kongshaug, K. O. & Fjellvåg, H. (2004). *J. Solid State Chem.* **177**, 1852–1857.
Maji, T. K., Ohba, M. & Kitagawa, S. (2005). *Inorg. Chem.* **44**, 9225–9231.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zheng, S.-L., Tong, M.-L., Tan, S.-D., Wang, Y., Shi, J.-X., Tong, Y.-X., Lee, H. K. & Chen, X.-M. (2001). *Organometallics*, **20**, 5319–5325.