Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[aqua(phenanthroline)zinc(II)]-μ-cyclohexanedicarboxylato]

Wenhua Bi,* Daofeng Sun, Rong Cao and Yanqin Wang

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Fuzhou, Fujian 350002, People's Republic of China

Correspondence e-mail: whbi@fjirsm.ac.cn

Received 5 April 2004
Accepted 20 April 2004
Online 8 May 2004

Key indicators

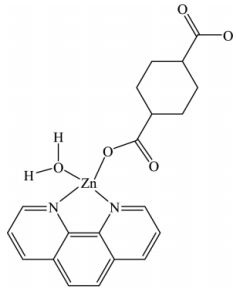
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.056
wR factor = 0.141
Data-to-parameter ratio = 9.3

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

The title complex, $[Zn(C_8H_{10}O_4)(C_{12}H_8N_2)(H_2O)]_n$, has a chain structure. The central Zn^{II} ion is coordinated by four water and carboxylate O atoms and two N atoms from 1,10-phenanthroline. All the cyclohexanedicarboxylate ligands are in an *e,a-cis*-conformation and each is linked to two Zn^{II} ions in chelating and monodentate modes. The most interesting feature of the structure is that it possesses a 2_1 helical axis in the chain.

Comment

The title compound, (I), is isostructural with its nickel analog (Qi *et al.*, 2003).



(I)

Experimental

$Zn(NO_3)_2(H_2O)_6$ (0.089 g, 0.3 mmol), 1,4-cyclohexanedicarboxylic acid (0.103 g, 0.6 mmol) and 1,10-phenanthroline (0.054 g, 0.3 mmol) were dissolved in 20 ml of a mixture of ethanol and water (1:1) and

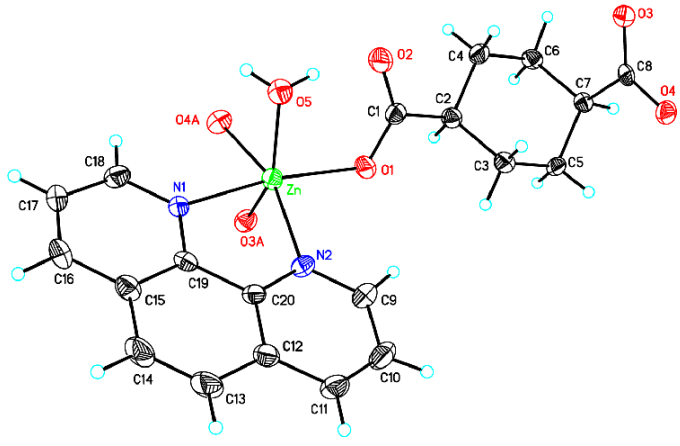


Figure 1
The coordination environment of the Zn^{II} atom in the title complex, shown with 30% probability displacement ellipsoids. The suffix A corresponds to symmetry code (i) in Table 1.

the solution was heated in a 25 ml capacity Teflon-lined reaction vessel at 403 K for 72 h and then cooled to room temperature over a period of 12 h. Colorless block-shaped crystals of (I) were collected (yield 58.6%).

Crystal data

$[Zn(C_8H_{10}O_4)(C_{12}H_8N_2)(H_2O)]$	D_x = 1.607 Mg m^{-3}
M_r = 433.75	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1910 reflections
a = 10.0974 (3) Å	θ = 2.0–25.0°
b = 8.8974 (4) Å	μ = 1.41 mm^{-1}
c = 20.2619 (10) Å	T = 293 (2) K
β = 99.997 (2)°	Block, colorless
V = 1792.70 (13) Å^3	0.30 × 0.24 × 0.16 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	3098 independent reflections
ω scans	2153 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.044
T_{min} = 0.649, T_{max} = 0.798	θ_{max} = 25.0°
5355 measured reflections	$h = -6 \rightarrow 12$
	$k = -6 \rightarrow 10$
	$l = -24 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 5.0293P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.056	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.141	$\Delta\rho_{max}$ = 0.44 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.49 e Å^{-3}
3098 reflections	Extinction correction: *SHELXL*97 (Sheldrick, 1997)
333 parameters	Extinction coefficient: 0.0040 (4)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn—O1	2.047 (4)	Zn—O4^{i}	2.239 (4)
Zn—O5	2.068 (4)	O1—C1	1.274 (6)
Zn—N2	2.129 (4)	O2—C1	1.246 (6)
Zn—O3^{i}	2.172 (4)	O3—C8	1.247 (6)
Zn—N1	2.179 (4)	O4—C8	1.264 (6)
O1—Zn—O5	92.12 (19)	O3^{i}—Zn—N1	96.62 (16)
O1—Zn—N2	91.22 (17)	O1—Zn—O4^{i}	99.16 (16)
O5—Zn—N2	108.49 (18)	O5—Zn—O4^{i}	89.87 (16)
O1—Zn—O3^{i}	89.20 (16)	N2—Zn—O4^{i}	158.61 (17)
O5—Zn—O3^{i}	148.78 (16)	O3^{i}—Zn—O4^{i}	59.18 (14)
N2—Zn—O3^{i}	102.66 (16)	N1—Zn—O4^{i}	93.29 (15)
O1—Zn—N1	167.52 (16)	Zn—O1—C1	126.6 (4)
O5—Zn—N1	88.60 (19)	Zn^{ii}—O3—C8	91.4 (3)
N2—Zn—N1	76.76 (17)	Zn^{ii}—O4—C8	87.9 (3)

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

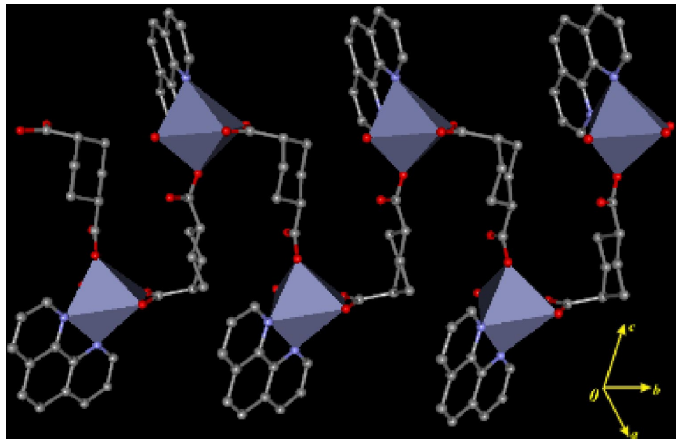


Figure 2
The chain structure of the title complex. All H atoms have been omitted for clarity.

All H atoms were positioned geometrically (C—H = 0.97 Å) and refined using a riding model [U_{iso}(H) = 1.2U_{eq}(parent atom].

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994); program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the Natural Science Foundation of China and the Natural Science Foundation of Fujian Province.

References

Qi, Y. J., Wang, Y. H., Hu, C. W., Cao, M. H. & Wang, E. B. (2003). *Inorg. Chem.* **42**, 8519–8523.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Siemens (1994). *SAINT* and *SHELXTL* (Version 5). Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.