

Zuo-Wei Wang,^a Yi-Zhi Li,^a Ya Cai^b and He-Gen Zheng^{a*}

^aCoordination Chemistry Institute, State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, People's Republic of China, and ^bProvincial Key Laboratory of Precious Metal Chemistry, Jiangsu Teachers University of Technology, Changzhou 213001, People's Republic of China

Correspondence e-mail: zhenghg@nju.edu.cn

Key indicators

Single-crystal X-ray study
 T = 293 K
 Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
 R factor = 0.031
 wR factor = 0.066
 Data-to-parameter ratio = 11.6

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

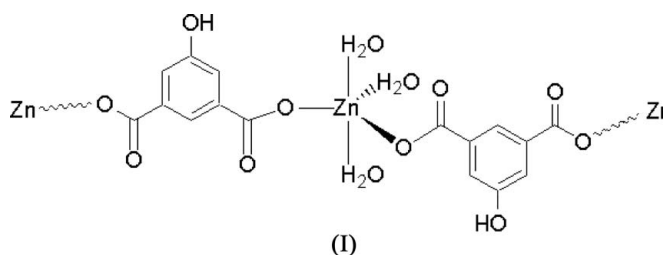
catena-Poly[[triazquazinc(II)]- μ -5-hydroxyisophthalato- $\kappa^2\text{O}:\text{O}'$]

The Zn center in the title compound, $[\text{Zn}(\text{C}_8\text{H}_4\text{O}_5)_2(\text{H}_2\text{O})_3]_n$, is in a slightly distorted trigonal-bipyramidal geometry. Each bidentate 5-hydroxyisophthalato ligand links two Zn centers, resulting in the formation of a chain structure.

Received 7 December 2005
 Accepted 6 March 2006

Comment

There has been considerable interest in metal-organic frameworks of coordination polymers due to their fascinating structures and promising applications in practical areas such as hydrogen storage and catalysis (Chen *et al.*, 2005; Biradha *et al.*, 2000). The reaction of zinc sulfate heptahydrate with the ligand 5-hydroxyisophthalic acid gives the title compound, (I).



In the structure, the local coordination geometry around the Zn atom is slightly distorted trigonal-bipyramidal, defined by three O atoms from water molecules and two O atoms from the carboxylate groups of different 5-hydroxyisophthalato ligands. Each ligand acts as a bridge linking two Zn atoms, resulting in the formation of a one-dimensional infinite chain (Fig. 1). There are hydrogen bonds between the coordinated water molecules, the hydroxy group and the carboxylate O atoms (Table 1). These interactions link the one-dimensional chains into a three-dimensional network.

This investigation was performed independently of another investigation reporting the same structure which is reported in the preceding (Xiao, 2006).

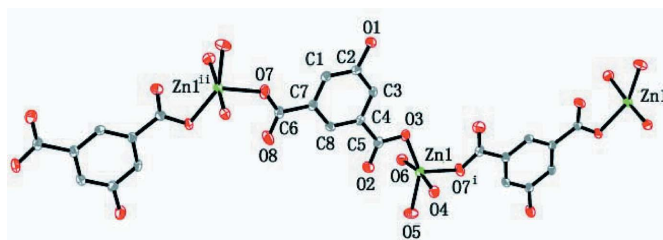


Figure 1
 A representation of the structure of the title complex, drawn with 50% probability ellipsoids. H atoms have been omitted. [Symmetry codes: (i) $-\frac{1}{2} + x, -\frac{1}{2} + y, -z$; (ii) $\frac{1}{2} + x, \frac{1}{2} + y, -z$.]

Experimental

All manipulations were carried out in air. Hydrothermal treatment of zinc sulfate tetrahydrate (0.5 mmol), 5-hydroxyisophthalic acid (0.5 mmol) and water (10.0 ml) over 3 d at 433 K yielded colorless block-shaped crystals. The yield was about 75%, based on 5-hydroxyisophthalic acid.

Crystal data

[Zn(C₈H₄O₅)₂(H₂O)₃]

M_r = 299.53

Orthorhombic, *Pccn*

a = 18.3236 (12) Å

b = 7.3975 (5) Å

c = 15.0812 (10) Å

V = 2044.2 (2) Å³

Z = 8

D_x = 1.946 Mg m⁻³

Mo *Kα* radiation

Cell parameters from 2869

reflections

θ = 2.7–28.0°

μ = 2.43 mm⁻¹

T = 293 (2) K

Block, colourless

0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-

detector diffractometer

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 2002)

T_{min} = 0.62, *T_{max}* = 0.78

10354 measured reflections

2011 independent reflections

1543 reflections with *I* > 2σ(*I*)

R_{int} = 0.085

θ_{\max} = 26.0°

h = -12 → 22

k = -9 → 9

l = -18 → 18

Refinement

Refinement on *F*²

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.066$

S = 0.95

2011 reflections

174 parameters

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.43 \text{ e } \text{Å}^{-3}$

$\Delta\rho_{\min} = -0.53 \text{ e } \text{Å}^{-3}$

Extinction correction: *SHELXTL*

Extinction coefficient: 0.0025 (3)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1—H1B···O2 ⁱ	0.82 (3)	1.82 (3)	2.646 (3)	176 (3)
O4—H4A···O8 ⁱⁱ	0.79 (4)	1.90 (4)	2.659 (2)	162 (4)
O4—H4B···O3 ⁱⁱⁱ	0.87 (4)	1.79 (4)	2.647 (2)	166 (4)
O5—H5A···O6 ^{iv}	0.83	2.19	2.971 (3)	157.0
O5—H5B···O4 ^v	0.83	1.97	2.805 (3)	177.4
O6—H6A···O8 ^{vi}	0.84 (3)	1.87 (3)	2.678 (3)	161 (3)
O6—H6B···O1 ^{vii}	0.83 (3)	1.89 (4)	2.710 (3)	172 (3)

Symmetry codes: (i) $-x + \frac{3}{2}, y, z + \frac{1}{2}$; (ii) $-x + \frac{3}{2}, -y + \frac{5}{2}, z$; (iii) $-x + 1, -y + 2, -z$; (iv) $-x + 1, y + \frac{1}{2}, -z - \frac{1}{2}$; (v) $-x + 1, y - \frac{1}{2}, -z - \frac{1}{2}$; (vi) $-x + \frac{3}{2}, -y + \frac{3}{2}, z$; (vii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$.

The three aromatic H atoms and the two H atoms on O5 were placed in calculated positions (C—H = 0.93 Å and O—H = 0.83 Å) and refined as riding, with *U_{iso}*(H) = 1.2*U_{eq}*(C,O). The other H atoms were located in a Fourier difference map and their coordinates were refined; *U_{iso}*(H) = 1.2*U_{eq}*(parent atom).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Natural Science Foundation (Nos. 20171020 and 20571039).

References

- Biradha, K., Hongo, Y. & Fujita, M. (2000). *Angew. Chem. Int. Ed.* **39**, 3843–3845.
- Bruker (2000). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Chen, B.-L., Nathan, W.-O., Anddrew, R.-M., Damacio, S.-C. & Omar, M. (2005). *Angew. Chem. Int. Ed.* **44**, 4745–4749.
- Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2002). *SADABS*. Version 2.03. University of Göttingen, Germany.
- Xiao, H.-P. (2006). *Acta Cryst.* **E62**, m731–m733.