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catena-Poly[[bis(2-hydroxy-2-phenylacetato- κ^2O^1, O^2)zinc(II)]- μ -1,2-di-4-pyridylethane- $\kappa^2N:N'$]

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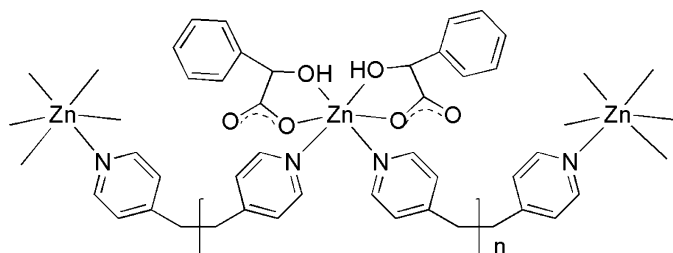
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.032; wR factor = 0.068; data-to-parameter ratio = 14.0.

The title compound, $[Zn(C_8H_6O_3)_2(C_{12}H_{12}N_2)]_n$, consists of $[Zn(Hopa)_2]$ ($H_2opa = 2$ -hydroxy-2-phenylacetic acid or mandelic acid) units bridged by 1,2-di-4-pyridylethane (bpe) ligands, forming a polymeric chain developing parallel to the b axis. The bridging bpe ligand is arranged around a twofold axis passing through the middle of the ethane C—C bond. The geometry around the Zn^{II} ion is distorted octahedral, constructed by four O atoms from two Hopa[−] ligands and two N atoms from two bridging bpe ligands. O—H...O hydrogen bonds link the chains, forming a three-dimensional network.

Related literature

Transition metal ions are the major cationic contributors to the inorganic composition of natural water and biological fluids, see: Daniele *et al.* (2008). For related structures, see: Balboa *et al.* (2008); Beghidja *et al.* (2005); Hao *et al.* (2009); Lee *et al.* (2008); Park *et al.* (2008); Shin *et al.* (2009); Wermester *et al.* (2007); Yu *et al.* (2008).



Experimental

Crystal data

 $[Zn(C_8H_6O_3)_2(C_{12}H_{12}N_2)]$
 $M_r = 551.90$
 Hexagonal, $P6_122$
 $a = 11.1360$ (6) Å
 $c = 33.110$ (3) Å
 $V = 3555.9$ (4) Å³
 $Z = 6$
 Mo $K\alpha$ radiation
 $\mu = 1.09$ mm^{−1}
 $T = 293$ K
 $0.10 \times 0.05 \times 0.05$ mm

Data collection

 Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 1997)
 $T_{min} = 0.933$, $T_{max} = 0.944$

 17715 measured reflections
 2347 independent reflections
 2045 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.077$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.068$
 $S = 1.04$
 2347 reflections
 168 parameters
 1 restraint

 H-atom parameters constrained
 $\Delta\rho_{max} = 0.22$ e Å^{−3}
 $\Delta\rho_{min} = -0.21$ e Å^{−3}
 Absolute structure: Flack (1983),
 870 Friedel pairs
 Flack parameter: -0.002 (16)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O13-H13O\cdots O12^i$	0.85	1.77	2.619 (3)	173

 Symmetry code: (i) $x - y + 1, x, z + \frac{1}{6}$.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2478).

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supplementary materials

Acta Cryst. (2009). E65, m1045-m1046 [doi:10.1107/S1600536809030281]

***catena*-Poly[[bis(2-hydroxy-2-phenylacetato- κ^2O^1,O^2)zinc(II)]- μ -1,2-di-4-pyridylethane- $\kappa^2N:N'$]**

S. M. Yu, D. H. Shin, P.-G. Kim, C. Kim and Y. Kim

Comment

A great attention has been paid to transition metal ions as the major cation contributors to the biologically active molecules such as amino acids, proteins, sugars, nucleotides *etc* (Daniele, *et al.*, 2008). This interest has driven us to study on the interaction of the transition metal ions with fulvic acids or humic acids. As models to examine the interaction, therefore, we have previously used copper(II) and zinc(II) benzoates as building blocks and reported the structures of copper(II) and zinc(II) benzoates with quinoxaline, 6-methylquinoline, 3-methylquinoline, and di-2-pyridyl ketone (Lee *et al.*, 2008; Yu *et al.*, 2008; Park *et al.*, 2008; Shin *et al.*, 2009).

Mandelic acid (2-hydroxy-2-phenylacetic acid, H₂opa) is also one of the simplest bioactive molecules exhibiting a variety of coordinating and supramolecular interaction abilities (Balboa *et al.*, 2008; Beghidja *et al.*, 2005; Hao *et al.*, 2009; Wermester *et al.*, 2007). In order to study the interaction of the biologically active molecule mandelic acid with zinc(II) ion, in the present work, we have employed zinc(II) mandelate as a building block and 1,2-di-4-pyridylethane (bpe) as a ligand. We report herein the structure of new zinc(II) mandelate with 1,2-di-4-pyridylethane.

The crystal structure contains [Zn(Hopa)₂] units bridged by bpe ligands forming a polymeric chain developing parallel to the b axis. The bridging 1,2-di-4-pyridylethane (bpe) ligand is arranged around a two fold axis going through the middle of C26—C26ⁱⁱ bond (symmetry code: (ii) x, x-y+2, -z+1/6). The geometry around the Zn^{II} ion is distorted octahedral constructed by four oxygen atoms from two Hopa⁻ and two nitrogen atoms from two bridging bpe ligands (Fig. 1). The occurrence of O-H...O hydrogen bonds links the chains to form a three dimensional network.

Experimental

38.0 mg (0.125 mmol) of Zn(NO₃)₂·6H₂O and 38.4 mg (0.25 mmol) of 2-hydroxy-2-phenylacetic acid were dissolved in 4 ml water and carefully layered by 4 ml solution of a mixture of acetone, methanol and ethanol (2/2/2) of 1,2-di-4-pyridylethane ligand (46.0 mg, 0.25 mmol). Suitable crystals of the title compound for X-ray analysis were obtained in a few weeks.

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.98 Å (methyne), 0.97 Å (methylene) or 0.93 Å (aromatic) with U_{iso}(H) = 1.2U_{eq}(C). H atom attached to O was located in difference Fourier maps and included in the subsequent refinement using restraints (O-H = 0.85 (1) Å) with U_{iso}(H) = 1.5U_{eq}(O). In the last stage of refinement, it was treated as riding on its parent atom.

Figures

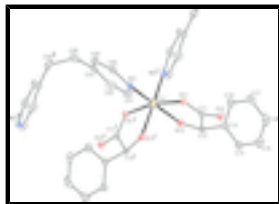


Fig. 1. View of compound I with the atom labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) $x, x-y+1, -z+1/6$; (ii) $x, x-y+2, -z+1/6$].

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Crystal data

[Zn(C₈H₆O₃)₂(C₁₂H₁₂N₂)₂]

$M_r = 551.90$

Hexagonal, $P6_122$

Hall symbol: P 61 2 (0 0 -1)

$a = 11.1360$ (6) Å

$b = 11.1360$ (6) Å

$c = 33.110$ (3) Å

$\alpha = 90^\circ$

$\beta = 90^\circ$

$\gamma = 120^\circ$

$V = 3555.9$ (4) Å³

$Z = 6$

$F_{000} = 1716$

$D_x = 1.546$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1751 reflections

$\theta = 2.2$ – 18.9°

$\mu = 1.09$ mm⁻¹

$T = 293$ K

Rod, colorless

$0.10 \times 0.05 \times 0.05$ mm

Data collection

Bruker SMART CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 1997)

$T_{\min} = 0.933$, $T_{\max} = 0.944$

17715 measured reflections

2347 independent reflections

2045 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.077$

$\theta_{\max} = 26.0^\circ$

$\theta_{\min} = 2.1^\circ$

$h = -13 \rightarrow 13$

$k = -11 \rightarrow 13$

$l = -40 \rightarrow 28$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.068$

$S = 1.04$

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.016P)^2 + 1.0575P]$

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

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

$\Delta\rho_{\max} = 0.22$ e Å⁻³

2347 reflections	$\Delta\rho_{\min} = -0.21 \text{ e \AA}^{-3}$
168 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 870 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: $-0.002 (16)$
Secondary atom site location: difference Fourier map	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.73603 (4)	0.86802 (2)	0.0833	0.01944 (12)
O11	0.76202 (18)	0.84579 (18)	0.02239 (5)	0.0216 (4)
O12	0.89644 (18)	0.82448 (18)	-0.02384 (5)	0.0245 (5)
O13	0.89365 (17)	0.81243 (17)	0.08319 (5)	0.0233 (4)
H13O	0.9568	0.8433	0.1013	0.035*
N21	0.5928 (2)	0.9386 (2)	0.07376 (7)	0.0223 (5)
C11	0.8619 (3)	0.8302 (2)	0.01183 (8)	0.0191 (6)
C12	0.9540 (3)	0.8194 (3)	0.04470 (8)	0.0179 (6)
H12	1.0448	0.9043	0.0438	0.022*
C13	0.9761 (3)	0.6975 (3)	0.03869 (8)	0.0201 (6)
C14	1.1078 (3)	0.7159 (3)	0.03588 (9)	0.0284 (7)
H14	1.1839	0.8052	0.0368	0.034*
C15	1.1293 (4)	0.6038 (4)	0.03167 (10)	0.0394 (8)
H15	1.2189	0.6185	0.0295	0.047*
C16	1.0181 (4)	0.4716 (4)	0.03078 (10)	0.0423 (9)
H16	1.0316	0.3960	0.0283	0.051*
C17	0.8862 (4)	0.4520 (3)	0.03359 (9)	0.0382 (8)
H17	0.8105	0.3624	0.0328	0.046*
C18	0.8639 (3)	0.5636 (3)	0.03754 (8)	0.0280 (6)
H18	0.7741	0.5486	0.0394	0.034*
C21	0.6235 (3)	1.0429 (3)	0.04786 (9)	0.0310 (8)
H21	0.7018	1.0742	0.0317	0.037*
C22	0.5445 (3)	1.1057 (3)	0.04412 (10)	0.0357 (8)
H22	0.5682	1.1757	0.0252	0.043*
C23	0.4294 (3)	1.0642 (3)	0.06862 (10)	0.0289 (7)
C24	0.4001 (3)	0.9599 (3)	0.09618 (9)	0.0288 (7)
H24	0.3251	0.9299	0.1136	0.035*

supplementary materials

C25	0.4832 (3)	0.9009 (3)	0.09751 (8)	0.0252 (6)
H25	0.4613	0.8304	0.1161	0.030*
C26	0.3364 (3)	1.1263 (3)	0.06523 (12)	0.0520 (11)
H26A	0.2422	1.0517	0.0607	0.062*
H26B	0.3641	1.1857	0.0416	0.062*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0209 (2)	0.01972 (17)	0.0181 (2)	0.01044 (12)	0.000	-0.00108 (18)
O11	0.0248 (10)	0.0247 (10)	0.0185 (10)	0.0148 (8)	-0.0010 (8)	0.0008 (8)
O12	0.0311 (12)	0.0325 (11)	0.0154 (10)	0.0200 (9)	0.0007 (9)	0.0017 (8)
O13	0.0270 (10)	0.0352 (10)	0.0135 (9)	0.0198 (9)	-0.0050 (9)	-0.0048 (8)
N21	0.0218 (12)	0.0224 (12)	0.0213 (14)	0.0101 (10)	0.0011 (10)	0.0006 (10)
C11	0.0231 (13)	0.0141 (14)	0.0176 (15)	0.0074 (12)	-0.0024 (13)	-0.0004 (11)
C12	0.0190 (13)	0.0189 (13)	0.0142 (14)	0.0083 (10)	-0.0012 (11)	-0.0025 (11)
C13	0.0274 (15)	0.0231 (15)	0.0113 (13)	0.0137 (12)	-0.0034 (11)	0.0004 (12)
C14	0.0297 (17)	0.0309 (16)	0.0296 (18)	0.0189 (14)	-0.0055 (13)	-0.0065 (14)
C15	0.048 (2)	0.057 (2)	0.0319 (19)	0.040 (2)	-0.0055 (17)	-0.0054 (17)
C16	0.080 (3)	0.049 (2)	0.0260 (18)	0.053 (2)	-0.0044 (18)	-0.0044 (16)
C17	0.062 (2)	0.0242 (17)	0.0226 (17)	0.0172 (17)	-0.0001 (16)	-0.0020 (14)
C18	0.0350 (16)	0.0237 (16)	0.0215 (15)	0.0117 (14)	-0.0015 (14)	-0.0003 (13)
C21	0.0241 (16)	0.0359 (18)	0.0286 (18)	0.0118 (14)	0.0005 (13)	0.0089 (14)
C22	0.0329 (18)	0.0310 (18)	0.0393 (19)	0.0131 (16)	-0.0083 (15)	0.0094 (14)
C23	0.0298 (17)	0.0265 (15)	0.0344 (19)	0.0172 (14)	-0.0179 (14)	-0.0153 (14)
C24	0.0275 (17)	0.0359 (18)	0.0293 (17)	0.0206 (14)	0.0010 (13)	-0.0039 (14)
C25	0.0306 (16)	0.0239 (16)	0.0219 (15)	0.0143 (12)	0.0033 (13)	0.0018 (12)
C26	0.039 (2)	0.0319 (17)	0.093 (3)	0.0242 (16)	-0.0356 (19)	-0.0234 (19)

Geometric parameters (\AA , $^\circ$)

Zn1—O11	2.0707 (17)	C15—C16	1.371 (5)
Zn1—O11 ⁱ	2.0707 (17)	C15—H15	0.9300
Zn1—N21	2.125 (2)	C16—C17	1.376 (5)
Zn1—N21 ⁱ	2.125 (2)	C16—H16	0.9300
Zn1—O13 ⁱ	2.1332 (17)	C17—C18	1.390 (4)
Zn1—O13	2.1332 (17)	C17—H17	0.9300
O11—C11	1.258 (3)	C18—H18	0.9300
O12—C11	1.254 (3)	C21—C22	1.376 (4)
O13—C12	1.425 (3)	C21—H21	0.9300
O13—H13O	0.8543	C22—C23	1.386 (4)
N21—C25	1.332 (3)	C22—H22	0.9300
N21—C21	1.344 (3)	C23—C24	1.381 (4)
C11—C12	1.541 (4)	C23—C26	1.511 (4)
C12—C13	1.509 (4)	C24—C25	1.378 (4)
C12—H12	0.9800	C24—H24	0.9300
C13—C14	1.379 (4)	C25—H25	0.9300
C13—C18	1.387 (4)	C26—C26 ⁱⁱ	1.519 (7)

C14—C15	1.390 (4)	C26—H26A	0.9700
C14—H14	0.9300	C26—H26B	0.9700
O11—Zn1—O11 ⁱ	166.10 (10)	C13—C14—H14	119.3
O11—Zn1—N21	94.27 (8)	C15—C14—H14	119.3
O11 ⁱ —Zn1—N21	94.75 (8)	C16—C15—C14	119.8 (3)
O11—Zn1—N21 ⁱ	94.75 (8)	C16—C15—H15	120.1
O11 ⁱ —Zn1—N21 ⁱ	94.27 (8)	C14—C15—H15	120.1
N21—Zn1—N21 ⁱ	98.92 (11)	C15—C16—C17	119.3 (3)
O11—Zn1—O13 ⁱ	92.80 (7)	C15—C16—H16	120.4
O11 ⁱ —Zn1—O13 ⁱ	77.21 (7)	C17—C16—H16	120.4
N21—Zn1—O13 ⁱ	86.60 (7)	C16—C17—C18	121.2 (3)
N21 ⁱ —Zn1—O13 ⁱ	170.28 (8)	C16—C17—H17	119.4
O11—Zn1—O13	77.21 (7)	C18—C17—H17	119.4
O11 ⁱ —Zn1—O13	92.80 (7)	C13—C18—C17	119.8 (3)
N21—Zn1—O13	170.28 (8)	C13—C18—H18	120.1
N21 ⁱ —Zn1—O13	86.60 (7)	C17—C18—H18	120.1
O13 ⁱ —Zn1—O13	89.11 (9)	N21—C21—C22	123.1 (3)
C11—O11—Zn1	118.26 (16)	N21—C21—H21	118.5
C12—O13—Zn1	114.85 (15)	C22—C21—H21	118.5
C12—O13—H13O	109.5	C21—C22—C23	119.8 (3)
Zn1—O13—H13O	120.8	C21—C22—H22	120.1
C25—N21—C21	116.5 (2)	C23—C22—H22	120.1
C25—N21—Zn1	122.35 (18)	C24—C23—C22	117.2 (3)
C21—N21—Zn1	120.11 (19)	C24—C23—C26	120.4 (3)
O12—C11—O11	125.7 (3)	C22—C23—C26	122.4 (3)
O12—C11—C12	115.4 (2)	C25—C24—C23	119.3 (3)
O11—C11—C12	118.9 (2)	C25—C24—H24	120.4
O13—C12—C13	110.7 (2)	C23—C24—H24	120.4
O13—C12—C11	108.8 (2)	N21—C25—C24	124.0 (3)
C13—C12—C11	113.0 (2)	N21—C25—H25	118.0
O13—C12—H12	108.1	C24—C25—H25	118.0
C13—C12—H12	108.1	C23—C26—C26 ⁱⁱ	115.7 (3)
C11—C12—H12	108.1	C23—C26—H26A	108.4
C14—C13—C18	118.5 (3)	C26 ⁱⁱ —C26—H26A	108.4
C14—C13—C12	121.0 (3)	C23—C26—H26B	108.4
C18—C13—C12	120.4 (2)	C26 ⁱⁱ —C26—H26B	108.4
C13—C14—C15	121.4 (3)	H26A—C26—H26B	107.4

Symmetry codes: (i) $x, x-y+1, -z+1/6$; (ii) $x, x-y+2, -z+1/6$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O13—H13O \cdots O12 ⁱⁱⁱ	0.85	1.77	2.619 (3)	173

Symmetry codes: (iii) $x-y+1, x, z+1/6$.

Fig. 1

