Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[diaquadipyridinezinc(II)]-μ-succinato]

Tanwawan Duangthongyou and Sutatip Siripaisarnpipat*

Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10930, Thailand
Correspondence e-mail: fscists@ku.ac.th

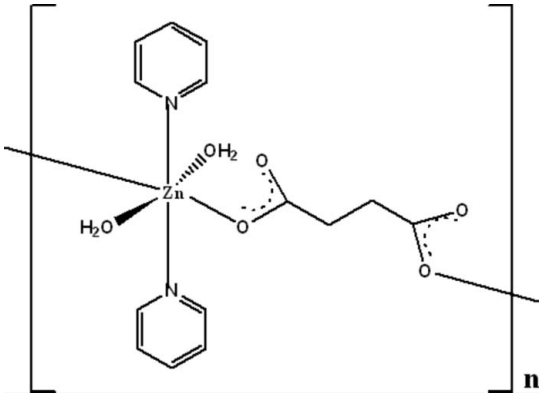
Received 12 February 2008; accepted 11 March 2008

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.008 Å; R factor = 0.066; wR factor = 0.108; data-to-parameter ratio = 13.1.

In the title compound, $[Zn(C_4H_4O_4)(C_5H_5N)_2(H_2O)_2]_n$, the Zn^{II} ion (site symmetry $\overline{1}$) is coordinated in an octahedral geometry by two pyridine molecules, two water molecules and two bridging centrosymmetric *O*-monodentate succinate dianions to create one-dimensional polymeric chains. The chains are cross-linked by O—H···O hydrogen bonds, forming sheets.

Related literature

For a related structure containing fumarate ions, see: Ohmura *et al.* (2003).



Experimental

Crystal data

$[Zn(C_4H_4O_4)(C_5H_5N)_2(H_2O)_2]$
M_r = 375.67
Orthorhombic, *Pbca*
a = 11.8142 (8) Å
b = 8.9111 (7) Å
c = 14.9705 (10) Å
V = 1576.06 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.59 mm^{-1}
T = 273 (2) K
0.08 × 0.08 × 0.04 mm

Data collection

Bruker–Nonius APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.804, T_{max} = 0.931
9256 measured reflections
1814 independent reflections
1200 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.107
S = 1.13
1814 reflections
138 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O2	2.064 (3)	Zn1—N1	2.170 (4)
Zn1—O3	2.110 (3)		
O2^{i}—Zn1—N1^{i}	88.88 (14)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O1	0.82	1.94	2.690 (5)	152
O3—H3B···O1^{ii}	0.74 (6)	1.97 (6)	2.687 (5)	164 (5)

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski and Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *Mercury* and local program.

The authors thank the Development and Promotion of Science and Technology Talents fund.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2701).

References

Hooft, R. W. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Ohmura, T., Mori, W., Hasegawa, M., Takai, T., Ikeda, T. & Hasegawa, E. (2003). *Bull. Chem. Soc. Jpn*, **76**, 1387–1395.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (2007). *SADABS*. Brucker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, m560 [doi:10.1107/S1600536808006764]

catena-Poly[[diaquadipyridinezinc(II)]-μ-succinato]

Tanwawan Duangthongyou and Sutatip Siripaisarnpipat

S1. Comment

The molecular structure of the title compound, (I), (Fig. 1), consists of zinc(II) ions linked through succinate bridges to create one-dimensional polymeric chains. Each Zn^{II} ion (site symmetry $\overline{1}$) is further coordinated by two pyridine molecules and two water molecules resulting in a slightly distorted *trans*-ZnN_2O_4 octahedral geometry (Table 1).

The coordinated water molecules form both intrachain O—H···O hydrogen bonds with the uncoordinated carboxyl group of a succinate ligand within the chain and intermolecular hydrogen bond with those in an adjacent chain (Fig. 2, Table 2). For a related structure, see Ohmura *et al.* (2003).

S2. Experimental

A pyridine solution (10 ml) of succinic acid (0.116 g, 1 mmol) was added to an aqueous solution (10 ml) of zinc acetate dihydrate (0.148 g, 0.673 mmol). The mixture was then allowed to stand for several days at room temperature, after which colourless blocks of (I) precipitated.

S3. Refinement

All the H atoms except H3A were located in a difference map and their positions and U_{iso} values were freely refined. H3A was geometrically placed (O—H = 0.82 Å) and refined as riding with $U_{iso}(H) = 1.5\ U_{eq}(H)$.

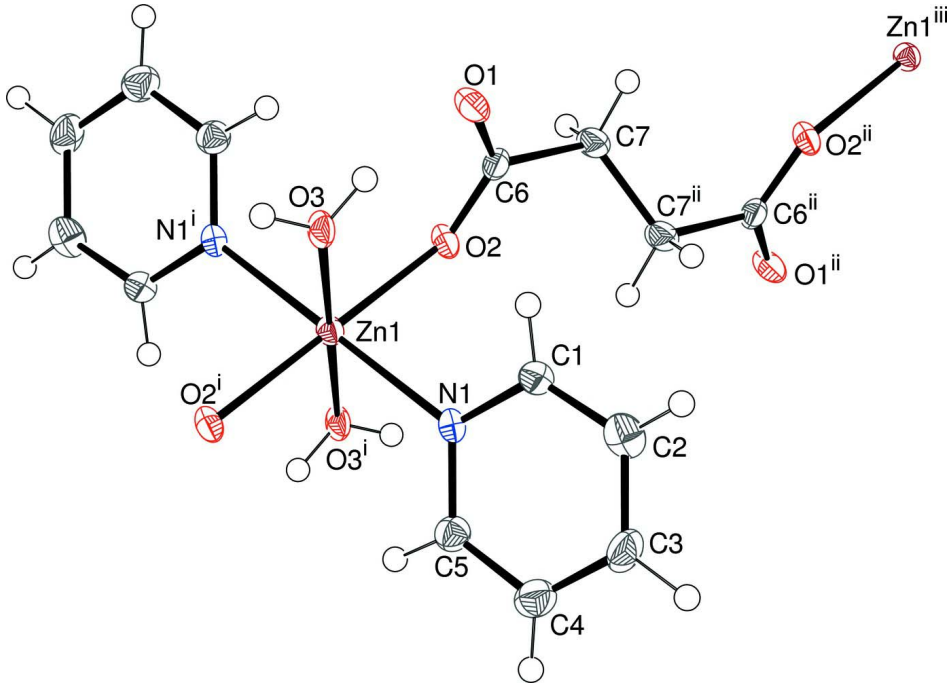


Figure 1

A fragment of the polymeric chain in (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). Symmetry codes: (i) 1 - *x*, -*y*, 1 - *z*; (ii) 1 - *x*, 1 - *y*, 1 - *z*; (iii) *x*, *y* + 1, *z*.

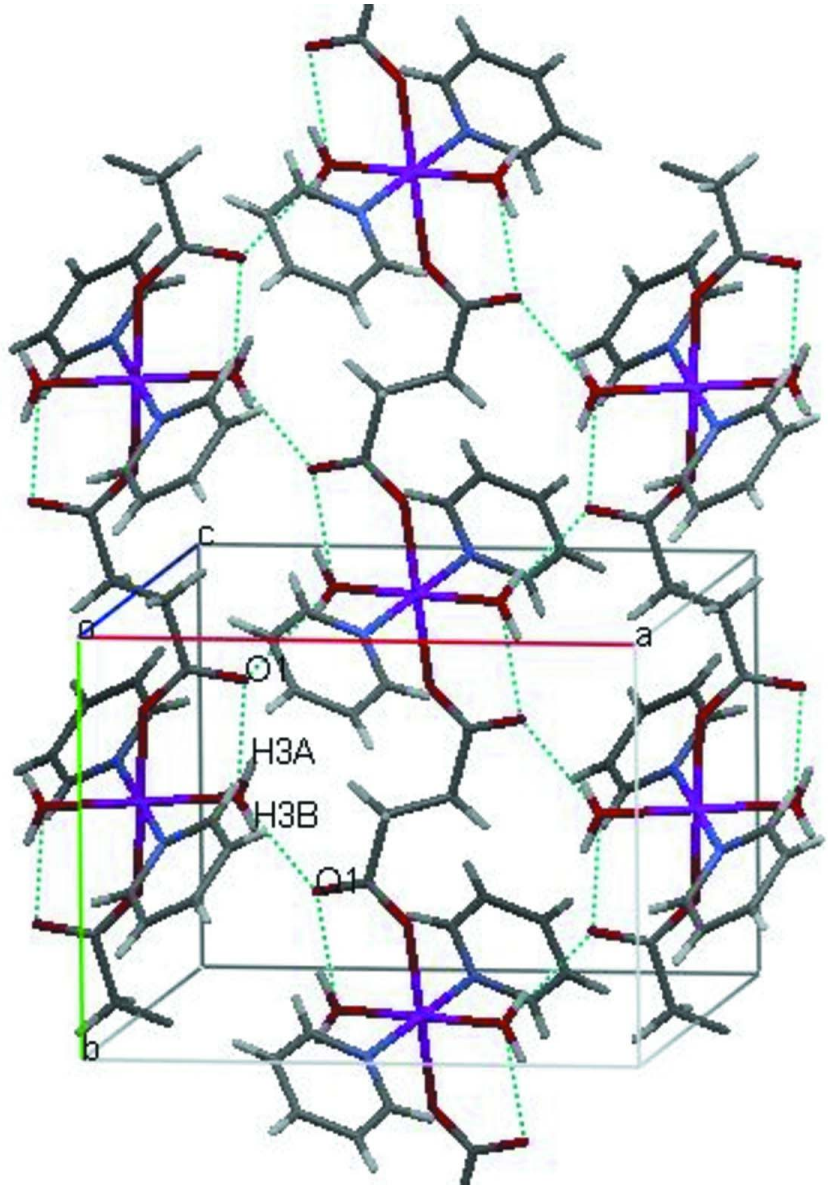


Figure 2

The packing in (I) viewed along the *b* axis with hydrogen bonds indicated by dashed lines.

catena-Poly[[diaquadipyridinezinc(II)]-μ-succinato]

Crystal data

$[Zn(C_4H_4O_4)(C_5H_5N)_2(H_2O)_2]$
$M_r = 375.67$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 11.8142\ (8)$ Å
$b = 8.9111\ (7)$ Å
$c = 14.9705\ (10)$ Å
$V = 1576.06\ (19)$ Å^3
$Z = 4$
$F(000) = 776$
$D_x = 1.583$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2052 reflections
$\theta = 2.9$–$27.5°$
$\mu = 1.59$ mm^{-1}
$T = 273$ K
Block, colourless
0.08 × 0.08 × 0.04 mm

Data collection

Bruker–Nonious APEXII CCD camera on κ-goniostat diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 4096x4096pixels / 62x62mm pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.804, T_{max} = 0.931
9256 measured reflections
1814 independent reflections
1200 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 27.6°, θ_{min} = 3.2°
h = −15→15
k = −11→10
l = −19→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.108
S = 1.13
1814 reflections
138 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difmap and geom
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 9.8897P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.0000	0.5000	0.0147 (2)
O3	0.6625 (3)	0.0017 (4)	0.4416 (2)	0.0186 (7)
H3A	0.6910	0.0850	0.4477	0.028*
O2	0.5136 (3)	0.2237 (4)	0.5340 (2)	0.0179 (7)
O1	0.6873 (3)	0.2905 (4)	0.4901 (2)	0.0229 (8)
C3	0.3411 (5)	0.1656 (6)	0.2097 (4)	0.0290 (13)
C2	0.4391 (5)	0.2285 (6)	0.2438 (4)	0.0254 (12)
C5	0.3356 (4)	0.0065 (7)	0.3386 (3)	0.0206 (10)
C6	0.5888 (4)	0.3201 (5)	0.5168 (3)	0.0172 (10)
N1	0.4308 (3)	0.0673 (4)	0.3719 (3)	0.0156 (8)
C1	0.4810 (4)	0.1762 (6)	0.3235 (3)	0.0199 (11)
C7	0.5529 (4)	0.4835 (6)	0.5275 (4)	0.0224 (11)
C4	0.2892 (5)	0.0528 (7)	0.2586 (4)	0.0279 (13)
H4	0.224 (5)	0.010 (6)	0.243 (3)	0.025 (15)*
H1	0.549 (4)	0.205 (6)	0.345 (3)	0.018 (13)*
H3	0.308 (5)	0.199 (7)	0.154 (4)	0.035 (17)*
H5	0.304 (4)	−0.066 (6)	0.376 (4)	0.026 (15)*
H2	0.476 (5)	0.295 (6)	0.209 (4)	0.028 (16)*
H7A	0.540 (4)	0.492 (6)	0.591 (4)	0.018 (13)*
H7	0.616 (4)	0.549 (5)	0.514 (3)	0.014 (13)*
H3B	0.694 (5)	−0.064 (7)	0.459 (4)	0.04 (2)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0146 (3)	0.0125 (3)	0.0169 (4)	0.0005 (4)	0.0010 (3)	0.0002 (4)
O3	0.0190 (16)	0.0113 (16)	0.0254 (18)	0.0048 (18)	0.0012 (13)	0.0012 (17)
O2	0.0192 (16)	0.0116 (16)	0.0229 (16)	−0.0006 (14)	0.0033 (14)	0.0022 (14)
O1	0.0160 (15)	0.0137 (18)	0.039 (2)	−0.0010 (17)	0.0048 (15)	0.0000 (13)
C3	0.041 (3)	0.026 (3)	0.020 (3)	0.004 (2)	−0.012 (2)	0.001 (3)
C2	0.036 (3)	0.021 (3)	0.019 (3)	0.000 (2)	0.004 (2)	−0.006 (2)
C5	0.019 (2)	0.022 (3)	0.021 (2)	0.000 (3)	0.0002 (18)	0.001 (2)
C6	0.019 (2)	0.015 (2)	0.018 (3)	0.003 (2)	−0.0046 (18)	0.0011 (19)
N1	0.0181 (19)	0.012 (2)	0.017 (2)	0.0011 (17)	0.0012 (16)	0.0016 (17)
C1	0.020 (3)	0.018 (3)	0.022 (3)	−0.001 (2)	−0.002 (2)	−0.001 (2)
C7	0.020 (2)	0.014 (3)	0.034 (3)	−0.001 (2)	−0.005 (2)	−0.003 (2)
C4	0.028 (3)	0.026 (3)	0.029 (3)	0.003 (3)	−0.007 (2)	−0.005 (3)

Geometric parameters (Å, º)

Zn1—O2	2.064 (3)	C2—C1	1.374 (7)
Zn1—O2^{i}	2.064 (3)	C2—H2	0.90 (6)
Zn1—O3^{i}	2.110 (3)	C5—N1	1.345 (6)
Zn1—O3	2.110 (3)	C5—C4	1.379 (7)
Zn1—N1^{i}	2.170 (4)	C5—H5	0.93 (6)
Zn1—N1	2.170 (4)	C6—C7	1.525 (7)
O3—H3A	0.8200	N1—C1	1.348 (6)
O3—H3B	0.74 (6)	C1—H1	0.90 (5)
O2—C6	1.263 (6)	C7—C7^{ii}	1.526 (9)
O1—C6	1.258 (5)	C7—H7A	0.97 (5)
C3—C2	1.383 (8)	C7—H7	0.97 (5)
C3—C4	1.387 (8)	C4—H4	0.89 (6)
C3—H3	0.96 (6)		
O2—Zn1—O2^{i}	180.0	C1—C2—H2	123 (4)
O2—Zn1—O3^{i}	88.60 (13)	C3—C2—H2	118 (4)
O2^{i}—Zn1—O3^{i}	91.40 (13)	N1—C5—C4	122.2 (5)
O2—Zn1—O3	91.40 (13)	N1—C5—H5	113 (3)
O2^{i}—Zn1—O3	88.60 (13)	C4—C5—H5	125 (3)
O3^{i}—Zn1—O3	180.0	O1—C6—O2	124.9 (4)
O2—Zn1—N1^{i}	91.12 (14)	O1—C6—C7	119.4 (4)
O2^{i}—Zn1—N1^{i}	88.88 (14)	O2—C6—C7	115.7 (4)
O3^{i}—Zn1—N1^{i}	88.53 (14)	C5—N1—C1	117.3 (4)
O3—Zn1—N1^{i}	91.47 (14)	C5—N1—Zn1	122.1 (3)
O2—Zn1—N1	88.88 (14)	C1—N1—Zn1	120.5 (3)
O2^{i}—Zn1—N1	91.12 (14)	N1—C1—C2	123.5 (5)
O3^{i}—Zn1—N1	91.47 (14)	N1—C1—H1	114 (3)
O3—Zn1—N1	88.53 (14)	C2—C1—H1	122 (3)
N1^{i}—Zn1—N1	180	C6—C7—C7^{ii}	110.8 (5)
Zn1—O3—H3A	109.5	C6—C7—H7A	103 (3)

Zn1—O3—H3B	108 (5)	C7^{ii}—C7—H7A	112 (3)
H3A—O3—H3B	118.2	C6—C7—H7	110 (3)
C6—O2—Zn1	131.5 (3)	C7^{ii}—C7—H7	114 (3)
C2—C3—C4	118.0 (5)	H7A—C7—H7	106 (4)
C2—C3—H3	122 (3)	C5—C4—C3	120.0 (5)
C4—C3—H3	120 (3)	C5—C4—H4	116 (3)
C1—C2—C3	118.9 (5)	C3—C4—H4	124 (4)
O3^{i}—Zn1—O2—C6	−174.6 (4)	O3—Zn1—N1—C5	137.5 (4)
O3—Zn1—O2—C6	5.4 (4)	O2—Zn1—N1—C1	47.0 (4)
N1^{i}—Zn1—O2—C6	96.9 (4)	O2^{i}—Zn1—N1—C1	−133.0 (4)
N1—Zn1—O2—C6	−83.1 (4)	O3^{i}—Zn1—N1—C1	135.6 (4)
C4—C3—C2—C1	0.5 (8)	O3—Zn1—N1—C1	−44.4 (4)
Zn1—O2—C6—O1	−16.8 (7)	C5—N1—C1—C2	1.0 (7)
Zn1—O2—C6—C7	161.3 (3)	Zn1—N1—C1—C2	−177.2 (4)
C4—C5—N1—C1	−0.5 (7)	C3—C2—C1—N1	−1.0 (8)
C4—C5—N1—Zn1	177.6 (4)	O1—C6—C7—C7^{ii}	123.7 (6)
O2—Zn1—N1—C5	−131.1 (4)	O2—C6—C7—C7^{ii}	−54.5 (7)
O2^{i}—Zn1—N1—C5	48.9 (4)	N1—C5—C4—C3	0.1 (9)
O3^{i}—Zn1—N1—C5	−42.5 (4)	C2—C3—C4—C5	−0.1 (9)

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O1	0.82	1.94	2.690 (5)	152
O3—H3*B*···O1^{iii}	0.74 (6)	1.97 (6)	2.687 (5)	164 (5)

Symmetry code: (iii) −*x*+3/2, *y*−1/2, *z*.