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Poly[diaqua-μ_4-acetylenedicarboxylato-zinc(II)]

Irena Stein and Uwe Ruschewitz*

Institut für Anorganische Chemie, Universität zu Köln, Greinstrasse 6, D-50939 Köln, Germany

Correspondence e-mail: uwe.ruschewitz@uni-koeln.de

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
R factor = 0.042
wR factor = 0.091
Data-to-parameter ratio = 14.2

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

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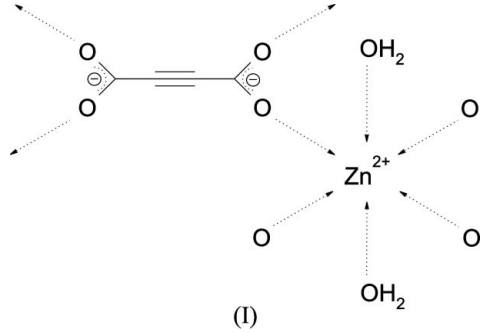
From a solution of $[Zn(H_2O)_6](NO_3)_2$ and acetylenedicarboxylic acid in deionized water, single crystals of zinc acetylenedicarboxylate dihydrate, $\{[Zn(C_4O_4)(H_2O)_2]\}_n$, were obtained by slow evaporation of the solvent. The asymmetric unit consits of one zinc cation which is located on a centre of symmetry, half of an acetylenedicarboxylate anion, the anion lying on a twofold axis, and one water molecule in a general position. Thus, zinc is octahedrally coordinated by four O atoms of acetylenedicarboxylate anions and two water molecules in *trans* positions. These octahedra are connected by dicarboxylate ligands into a three-dimensional network.

Comment

During our studies of coordination polymers based on acetylenedicarboxylic acid (*e*.g. Billetter *et al.*, 2004), we obtained colourless crystals of the title compound, (I). The crystal structure is composed of zinc ions coordinated octahedrally by four O atoms stemming from four different acetylenedicarboxylate anions [Zn—O = 2.094 (3)–2.151 (3) Å] and two water molecules in *trans* positions [Zn—O = 2.067 (4) Å]. The metal ion is located on a centre of symmetry, the anion on a twofold axis and the water molecule in a general position. These isolated, slightly distorted octahedra are connected by carboxylate groups to form a layer parallel to (011). *Via* the second carboxylate group of the bifunctional dianion these layers are linked into a three-dimensional coordination network. Compound (I) is isotypic with the analogous manganese (Robl & Hentschel, 1990), cobalt (Pantenburg & Ruschewitz, 2002) and nickel compounds (Hohn *et al.*, 2002).



(I)

Experimental

Acetylenedicarboxylic acid (0.57 g, 5 mmol) was dissolved in 5 ml of deionized water and solid $[Zn(H_2O)_6](NO_3)_2$ (1.50 g, 5 mmol) was added. The beaker with the solution was sealed with a perforated foil. After approximately two months, most of the solvent had vaporized and colourless polyhedra of (I) were isolated from the precipitate. The yield was not determined.

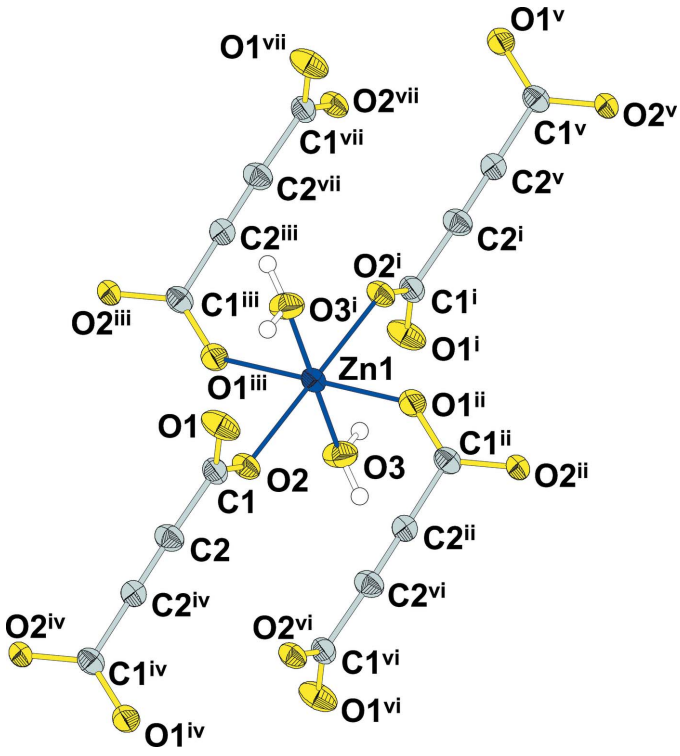


Figure 1
A view of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H-atom radii are arbitrary. [Symmetry codes: (i) $\frac{1}{2}-x,\frac{1}{2}-y,1-z$; (ii) $x,1-y,\frac{1}{2}+z$; (iii) $\frac{1}{2}-x,-\frac{1}{2}+y,\frac{1}{2}-z$; (iv) $-x,y,-\frac{1}{2}-z$; (v) $\frac{1}{2}+x,\frac{1}{2}-y,\frac{3}{2}+z$; (vi) $-x,1-y,-z$; (vii) $\frac{1}{2}+x,-\frac{1}{2}+y,1+z$.

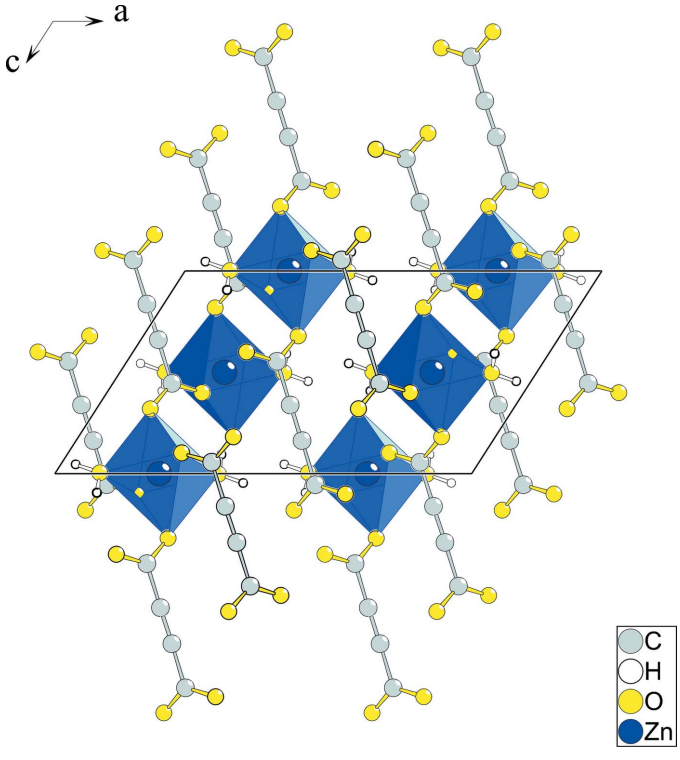


Figure 2
View of the crystal structure of (I), in a projection along [010].

Crystal data

$[Zn(C_4O_4)(H_2O)_2]$
M_r = 213.44
Monoclinic, $C2/c$
a = 13.245 (3) Å
b = 7.223 (2) Å
c = 7.649 (2) Å
β = 122.66 (1)°
V = 616.1 (3) Å^3
Z = 4
D_x = 2.301 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2482 reflections
θ = 6.3–59.2°
μ = 3.96 mm^{-1}
T = 295 (2) K
Block, colourless
0.1 × 0.1 × 0.07 mm

Data collection

Stoe IPDS-II diffractometer
φ scans
Absorption correction: numerical [*X-RED* (Stoe & Cie, 2001); the crystal shape was optimized using *X-SHAPE* (Stoe & Cie, 1999)]
T_{min} = 0.690, T_{max} = 0.766
5711 measured reflections
868 independent reflections
551 reflections with $I > 2\sigma(I)$
R_{int} = 0.092
θ_{max} = 29.6°
$h = -18 \rightarrow 18$
$k = -9 \rightarrow 10$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.091
S = 1.02
868 reflections
61 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 0.4994P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −1.30 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0066 (14)

Table 1
Selected geometric parameters (Å, °).

Zn1—O3^{i}	2.067 (3)	O1—C1	1.245 (5)
Zn1—O3	2.067 (3)	O2—C1	1.262 (5)
Zn1—O2^{i}	2.094 (3)	C1—C2	1.462 (6)
Zn1—O2	2.094 (3)	C2—C2^{iv}	1.199 (9)
Zn1—O1^{ii}	2.151 (3)	O3—H1	0.82 (2)
Zn1—O1^{iii}	2.151 (3)	O3—H2	0.81 (2)
O1—C1—O2	126.4 (4)	C2^{iv}—C2—C1	177.7 (4)
O1—C1—C2	118.1 (4)	H1—O3—H2	110 (7)
O2—C1—C2	115.5 (4)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1···O2^{viii}	0.82 (2)	2.06 (2)	2.871 (5)	171 (7)
O3—H2···O1^{i}	0.81 (2)	2.04 (4)	2.771 (5)	150 (7)

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

The H atoms of the water molecule were located in a difference Fourier maps and were refined isotropically. The maximum electron-density peak is located 1 Å from atom O2.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

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