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Hexaaquazinc(II) bis(6-hydroxypyridine-3-carboxylate)

Xue-Li Zhang,[a] Yu-Juan Lu,[a] Ji-Zhen Li[b] and Seik Weng Ng[c]*

[a]Normal College, Shenzhen University, Shenzhen 518060, People's Republic of China, [b]Chemistry College, Jilin University, Changchun 130012, People's Republic of China, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(n–O) = 0.003 Å
Disorder in main residue
R factor = 0.038
wR factor = 0.107
Data-to-parameter ratio = 8.8

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

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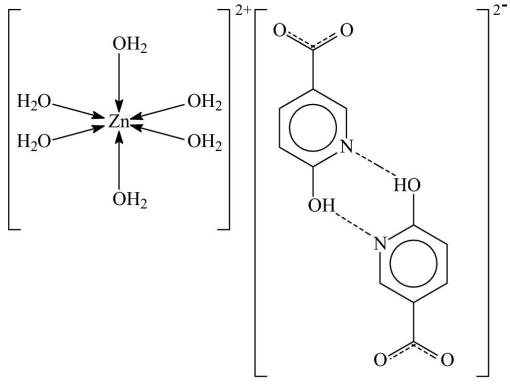
The Zn atom in the title compound, $[Zn(H_2O)_6](C_6H_4NO_3)_2$, lies on a special position of 2/*m* site symmetry in an octahedron made up of water molecules. The anion is disordered across a mirror plane. The cation interacts with the anion indirectly through hydrogen bonds to form a three-dimensional network.

Comment

A number of syntheses of the zinc(II) derivatives of organic acids have yielded the hexaaquazinc(II) cation, the deprotonated acid remaining in the outer coordination sphere of the coordination octahedron as noted in, for example, the dihydrogen-1,2,4,5-benzenetetracarboxylate (Sun *et al.*, 2002), the bis[(4-oxo-4*H*-pyridin-1-yl)acetate] dihydrate (Gao *et al.*, 2004), the 1,5-naphthalenedisulfonate (Huo *et al.*, 2005) and the 3-carboxy-4-hydroxybenzenesulfonate tetrahydrate (Ma *et al.*, 2003). The reaction of the zinc cation and the 6-hydroxypyridine-3-carboxylate anion in a 1:1 molar stoichiometry yielded a similar compound, (I), with a hexaaquazinc(II) cation and an uncoordinated 6-hydroxypyridine-3-carboxylate anion (Fig. 1). As the O1*w* water molecule lies on a general position, whereas atom Zn1 lies on a special position of 2/*m* site symmetry, atom Zn1 exists within a square made up of the four equivalent water molecules; the other two sites are occupied by the O2*w* (which lies on a mirror plane) and O2w^{ii} water molecules [symmetry code: (ii) $1-x, 1-y, 1-z$]. The two ions interact through hydrogen bonds to lead to a tightly held three-dimensional framework (Table 2). The anion lies on a mirror plane bisecting the carboxyl group; its two C—O distances are equal. The hydroxypyridine portion is disordered across this mirror plane. Pairs of adjacent anions are linked by hydrogen bonds to furnish a hydrogen-bonded dianion (Fig. 1).



(I)

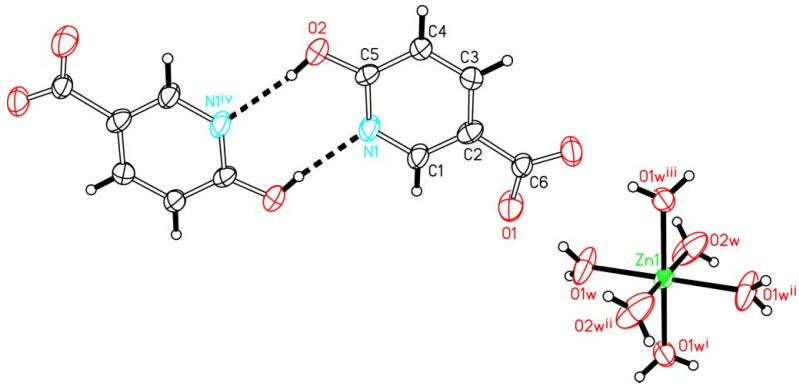


Figure 1
ORTEPII (Johnson, 1976) plot showing the numbering scheme for (I). Displacement ellipsoids are shown at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii. [Symmetry codes: (i) $1-x, y, 1-z$; (ii) $1-x, 1-y, 1-z$; (iii) $x, 1-y, z$; (iv) $\frac{5}{2}-x, \frac{3}{2}-y, 2-z$.]

Experimental

A mixture of zinc nitrate trihydrate (0.298 g, 1 mmol), 6-hydroxypyridine-3-carboxylic acid (0.139 g, 1 mmol), sodium hydroxide (0.040 g, 1 mmol) and water (10 ml) were sealed in a 23 ml Teflon-lined stainless steel Parr bomb. The bomb was heated to 433 K for 2 d. It was cooled to room temperature at 10 K h^{-1} to yield colorless crystals.

Crystal data

$[Zn(H_2O)_6](C_6H_4NO_3)_2$
$M_r = 449.67$
Monoclinic, $C2/m$
$a = 11.568$ (1) Å
$b = 9.780$ (1) Å
$c = 7.6255$ (7) Å
$\beta = 91.286$ (3)°
$V = 862.5$ (1) $Å^3$
$Z = 2$
$D_x = 1.732$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1640 reflections
$\theta = 2.7$–27.5°
$\mu = 1.49$ mm^{-1}
$T = 295$ (2) K
Block, colorless
0.34 × 0.31 × 0.24 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.211$, $T_{max} = 0.716$
2428 measured reflections
992 independent reflections
979 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 27.5°$
$h = -14 \rightarrow 14$
$k = -12 \rightarrow 12$
$l = -7 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.107$
$S = 1.12$
992 reflections
113 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 1.9207P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e $Å^{-3}$
$\Delta\rho_{min} = -0.35$ e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

Zn1—O1w^{i}	2.037 (2)	Zn1—O2w	2.121 (4)
Zn1—O1w^{ii}	2.037 (2)	Zn1—O2w^{ii}	2.121 (4)
Zn1—O1w^{iii}	2.037 (2)		
O1w—Zn1—O1w^{i}	92.1 (2)	O1w—Zn1—O2w	91.4 (1)
O1w—Zn1—O1w^{ii}	180	O1w—Zn1—O2w^{ii}	88.7 (1)
O1w—Zn1—O1w^{iii}	87.9 (2)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w1···O1	0.84 (1)	1.82 (1)	2.655 (3)	174 (3)
O1w—H1w2···O1^{viii}	0.84 (1)	1.89 (1)	2.706 (3)	166 (3)
O2w—H2w1···O2^{v}	0.85 (1)	2.01 (2)	2.788 (5)	153 (3)
O2w—H2w1···O2^{v}	0.85 (1)	2.01 (2)	2.788 (5)	153 (3)
O2w—H2w2···O2^{vi}	0.85 (1)	1.96 (1)	2.758 (6)	157 (1)
O2w—H2w2···O2^{vii}	0.85 (1)	1.96 (1)	2.758 (6)	157 (1)
O2—H2o···N1^{iv}	0.85	2.03	2.86 (1)	165

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

The carboxylate anion is disordered over a mirror plane. The C—C distances were restrained to 1.39 (1) Å, and the two N—C distances were restrained to within 0.01 Å of each other. Additionally, the ring was restrained to near planarity. C-bound H atoms were placed at calculated positions (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with U_{iso}(H) set to $1.2U_{eq}$(C). The water H atoms were located in difference Fourier maps, and were refined with a distance restraint of O—H = 0.85 (1) Å. The hydroxy group was allowed to rotate about the C—O bond, with O—H = 0.85 Å and U_{iso}(H) = $1.2U_{eq}$(O).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997; program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976).

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