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Tetraaquabis(2-oxo-1,2-dihydropyridine-5-sulfonato-κO^2)zinc(II)

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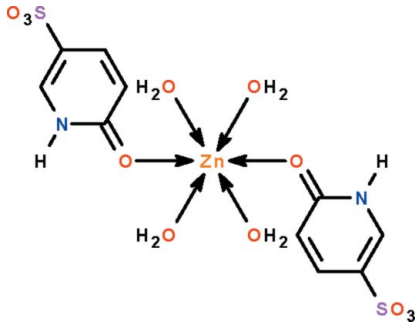
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.066; data-to-parameter ratio = 13.5.

The metal atom in the title compound, $[Zn(C_5H_4NO_4S)_2(H_2O)_4]$, lies on a center of inversion and is linked to the anionic ligand through the carbonyl O atom. In the crystal structure, the 2-oxo-1,2-dihydropyridine-5-sulfonate ligand interacts with other molecules through N—H···O and O—H···O hydrogen bonds, forming a three-dimensional network structure.

Related literature

For the crystal structure of another zwitterionic tetraaquabis(amide)–metal^{II} complex, see: Gao *et al.* (2004).



Experimental

Crystal data

$[Zn(C_5H_4NO_4S)_2(H_2O)_4]$
M_r = 485.74
Monoclinic, $P2_1/c$
a = 6.7701 (2) Å
b = 13.9725 (5) Å
c = 10.0343 (3) Å
β = 115.331 (2)°
V = 857.93 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.74 mm^{-1}
T = 293 K
0.21 × 0.16 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.711, T_{max} = 0.768
8224 measured reflections
1951 independent reflections
1866 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.066
S = 1.06
1951 reflections
144 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.85 (1)	1.99 (1)	2.790 (2)	157 (2)
O1w—H11···O2^{ii}	0.84 (1)	1.98 (1)	2.809 (2)	171 (2)
O1w—H12···O3^{iii}	0.84 (1)	1.93 (1)	2.767 (2)	172 (3)
O2w—H21···O3^{iv}	0.83 (1)	2.13 (1)	2.926 (2)	160 (3)
O2w—H22···O4^{v}	0.84 (1)	1.93 (1)	2.765 (2)	174 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2623).

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supporting information

Acta Cryst. (2009). E**65**, m1310 [https://doi.org/10.1107/S1600536809039774]

Tetraaquabis(2-oxo-1,2-dihydropyridine-5-sulfonato-κO^2)zinc(II)

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S1. Experimental

Zinc carbonate (0.25 g, 2 mmol) was added to a hot aqueous solution of 2-hydroxypyridine 5-sulfonic acid (0.35 g, 2 mmol); the pH value was adjusted to 6 with 0.1 *M* sodium hydroxide. The solution was allowed to evaporate slowly. Colorless prismatic crystals were isolated after five days. CH&N elemental analysis. Calc. for $C_{10}H_{16}N_2O_{12}S_2Zn$:*C* 24.73, H 3.32, N 5.77%; found: C 24.77, H 3.37, N 5.81%.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C). The ammonium and water H-atoms were refined with a distance restraint of N–H = O–H 0.85±0.01 Å; their temperature factors were refined.

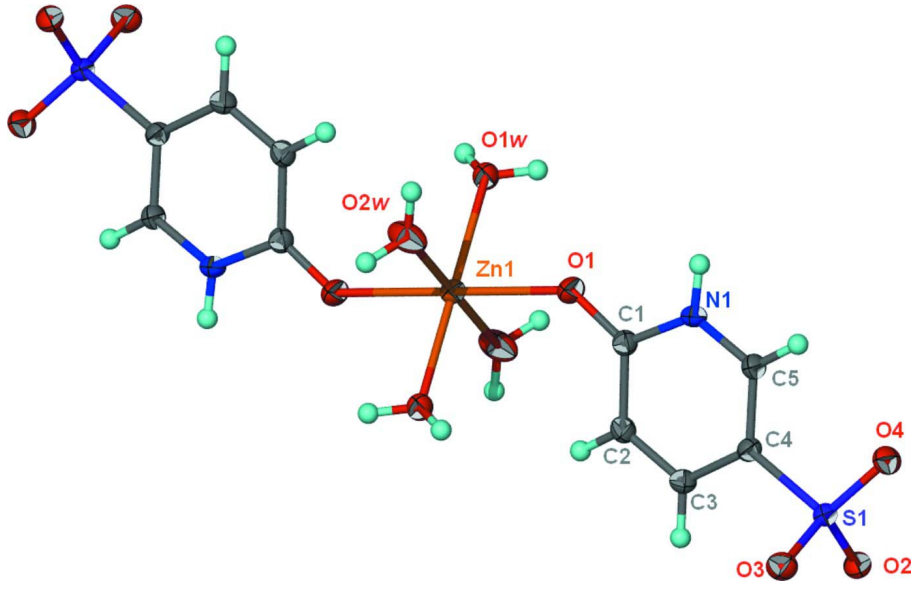

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $Zn(H_2O)_4(C_5H_4NO_4S)_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Tetraaquabis(2-oxo-1,2-dihydropyridine-5-sulfonato-κO^2)zinc(II)

Crystal data

$[Zn(C_5H_4NO_4S)_2(H_2O)_4]$
M_r = 485.74

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

a = 6.7701 (2) Å
b = 13.9725 (5) Å
c = 10.0343 (3) Å
β = 115.331 (2)°
V = 857.93 (5) Å^3
Z = 2
F(000) = 496
D_x = 1.880 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7685 reflections
θ = 3.3–27.5°
μ = 1.74 mm^{-1}
T = 293 K
Prism, colorles
0.21 × 0.16 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.711, T_{max} = 0.768

8224 measured reflections
1951 independent reflections
1866 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −8→8
k = −17→18
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.066
S = 1.06
1951 reflections
144 parameters
5 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 0.5079P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 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	0.5000	0.5000	0.02207 (10)
S1	0.81951 (6)	0.69216 (3)	−0.07941 (4)	0.01923 (11)
O1	0.4186 (2)	0.54472 (10)	0.28771 (14)	0.0295 (3)
O3	0.9550 (2)	0.77155 (9)	0.00655 (14)	0.0290 (3)
O2	0.95353 (19)	0.61832 (9)	−0.10431 (13)	0.0264 (3)
O4	0.63570 (19)	0.72213 (9)	−0.21315 (13)	0.0271 (3)
O1W	0.20020 (19)	0.43039 (9)	0.40362 (13)	0.0252 (2)
O2W	0.3496 (2)	0.62596 (11)	0.53828 (17)	0.0406 (3)
C2	0.7484 (3)	0.55821 (12)	0.25390 (18)	0.0234 (3)
H2	0.8360	0.5271	0.3413	0.028*
C1	0.5190 (3)	0.56850 (11)	0.21274 (17)	0.0214 (3)
N1	0.4007 (2)	0.60683 (10)	0.07675 (15)	0.0229 (3)
C5	0.4880 (2)	0.64352 (13)	−0.01119 (17)	0.0221 (3)
H5	0.3979	0.6715	−0.1009	0.027*
C4	0.7072 (2)	0.63937 (11)	0.03179 (17)	0.0201 (3)
C3	0.8395 (3)	0.59340 (11)	0.16668 (18)	0.0227 (3)
H3	0.9891	0.5873	0.1956	0.027*

H1	0.2625 (16)	0.6084 (16)	0.045 (2)	0.035 (6)*
H11	0.158 (4)	0.4218 (18)	0.3125 (12)	0.048 (7)*
H12	0.166 (4)	0.3815 (12)	0.438 (3)	0.045 (7)*
H21	0.223 (2)	0.6479 (18)	0.509 (3)	0.051 (7)*
H22	0.431 (4)	0.6538 (17)	0.6168 (18)	0.049 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02021 (15)	0.02605 (16)	0.02093 (15)	−0.00103 (9)	0.00973 (11)	0.00145 (9)
S1	0.01744 (18)	0.02194 (19)	0.01890 (19)	−0.00059 (13)	0.00834 (14)	0.00027 (13)
O1	0.0244 (6)	0.0417 (7)	0.0246 (6)	−0.0023 (5)	0.0125 (5)	0.0061 (5)
O3	0.0276 (6)	0.0281 (6)	0.0320 (7)	−0.0085 (5)	0.0133 (5)	−0.0060 (5)
O2	0.0222 (5)	0.0329 (6)	0.0252 (6)	0.0046 (5)	0.0111 (5)	−0.0021 (5)
O4	0.0241 (6)	0.0313 (6)	0.0233 (6)	0.0017 (5)	0.0076 (5)	0.0071 (5)
O1W	0.0249 (6)	0.0286 (6)	0.0223 (6)	−0.0043 (5)	0.0104 (5)	0.0014 (5)
O2W	0.0268 (7)	0.0401 (8)	0.0447 (8)	0.0077 (6)	0.0056 (6)	−0.0145 (6)
C2	0.0214 (7)	0.0268 (8)	0.0198 (7)	0.0036 (6)	0.0069 (6)	0.0030 (6)
C1	0.0223 (7)	0.0218 (7)	0.0204 (7)	−0.0023 (6)	0.0094 (6)	−0.0005 (6)
N1	0.0151 (6)	0.0316 (7)	0.0216 (7)	−0.0009 (5)	0.0074 (5)	0.0019 (5)
C5	0.0203 (7)	0.0264 (8)	0.0190 (7)	0.0007 (6)	0.0079 (6)	0.0024 (5)
C4	0.0198 (7)	0.0215 (7)	0.0204 (7)	−0.0012 (6)	0.0101 (6)	−0.0006 (5)
C3	0.0178 (7)	0.0266 (8)	0.0229 (8)	0.0021 (6)	0.0078 (6)	0.0001 (6)

Geometric parameters (Å, º)

Zn1—O1^{i}	2.0560 (12)	O2W—H21	0.833 (10)
Zn1—O1	2.0560 (12)	O2W—H22	0.838 (10)
Zn1—O1W^{i}	2.0788 (12)	C2—C3	1.360 (2)
Zn1—O1W	2.0788 (12)	C2—C1	1.434 (2)
Zn1—O2W	2.1487 (14)	C2—H2	0.9300
Zn1—O2W^{i}	2.1487 (14)	C1—N1	1.362 (2)
S1—O4	1.4477 (12)	N1—C5	1.356 (2)
S1—O3	1.4626 (12)	N1—H1	0.850 (10)
S1—O2	1.4643 (12)	C5—C4	1.358 (2)
S1—C4	1.7588 (15)	C5—H5	0.9300
O1—C1	1.2553 (19)	C4—C3	1.418 (2)
O1W—H11	0.841 (10)	C3—H3	0.9300
O1W—H12	0.841 (10)		
O1^{i}—Zn1—O1	180.0	Zn1—O1W—H12	125.1 (18)
O1^{i}—Zn1—O1W^{i}	83.37 (5)	H11—O1W—H12	108 (2)
O1—Zn1—O1W^{i}	96.63 (5)	Zn1—O2W—H21	137.0 (19)
O1^{i}—Zn1—O1W	96.63 (5)	Zn1—O2W—H22	112.2 (18)
O1—Zn1—O1W	83.37 (5)	H21—O2W—H22	109 (3)
O1W^{i}—Zn1—O1W	180.00 (6)	C3—C2—C1	120.81 (15)
O1^{i}—Zn1—O2W	90.07 (6)	C3—C2—H2	119.6
O1—Zn1—O2W	89.93 (6)	C1—C2—H2	119.6

O1W^{i}—Zn1—O2W	88.66 (5)	O1—C1—N1	117.88 (14)
O1W—Zn1—O2W	91.34 (5)	O1—C1—C2	126.76 (15)
O1^{i}—Zn1—O2W^{i}	89.93 (6)	N1—C1—C2	115.35 (14)
O1—Zn1—O2W^{i}	90.07 (6)	C5—N1—C1	124.58 (13)
O1W^{i}—Zn1—O2W^{i}	91.34 (5)	C5—N1—H1	117.5 (16)
O1W—Zn1—O2W^{i}	88.66 (5)	C1—N1—H1	118.0 (16)
O2W—Zn1—O2W^{i}	180.0	N1—C5—C4	119.93 (14)
O4—S1—O3	113.63 (8)	N1—C5—H5	120.0
O4—S1—O2	113.28 (7)	C4—C5—H5	120.0
O3—S1—O2	110.91 (7)	C5—C4—C3	118.76 (14)
O4—S1—C4	106.01 (7)	C5—C4—S1	119.40 (12)
O3—S1—C4	106.05 (7)	C3—C4—S1	121.84 (12)
O2—S1—C4	106.28 (7)	C2—C3—C4	120.17 (14)
C1—O1—Zn1	136.67 (11)	C2—C3—H3	119.9
Zn1—O1W—H11	112.6 (17)	C4—C3—H3	119.9
O1W^{i}—Zn1—O1—C1	28.28 (18)	N1—C5—C4—C3	2.1 (2)
O1W—Zn1—O1—C1	−151.72 (18)	N1—C5—C4—S1	−177.08 (12)
O2W—Zn1—O1—C1	116.92 (17)	O4—S1—C4—C5	−6.85 (15)
O2W^{i}—Zn1—O1—C1	−63.08 (17)	O3—S1—C4—C5	114.25 (14)
Zn1—O1—C1—N1	−171.26 (12)	O2—S1—C4—C5	−127.66 (13)
Zn1—O1—C1—C2	9.9 (3)	O4—S1—C4—C3	173.98 (13)
C3—C2—C1—O1	−175.15 (17)	O3—S1—C4—C3	−64.92 (15)
C3—C2—C1—N1	6.0 (2)	O2—S1—C4—C3	53.17 (15)
O1—C1—N1—C5	173.90 (16)	C1—C2—C3—C4	−1.2 (2)
C2—C1—N1—C5	−7.1 (2)	C5—C4—C3—C2	−3.0 (2)
C1—N1—C5—C4	3.2 (3)	S1—C4—C3—C2	176.21 (13)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{ii}	0.85 (1)	1.99 (1)	2.790 (2)	157 (2)
O1w—H11···O2^{iii}	0.84 (1)	1.98 (1)	2.809 (2)	171 (2)
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O2w—H22···O4^{vi}	0.84 (1)	1.93 (1)	2.765 (2)	174 (3)

Symmetry codes: (ii) *x*−1, *y*, *z*; (iii) −*x*+1, −*y*+1, −*z*; (iv) −*x*+1, *y*−1/2, −*z*+1/2; (v) *x*−1, −*y*+3/2, *z*+1/2; (vi) *x*, *y*, *z*+1.