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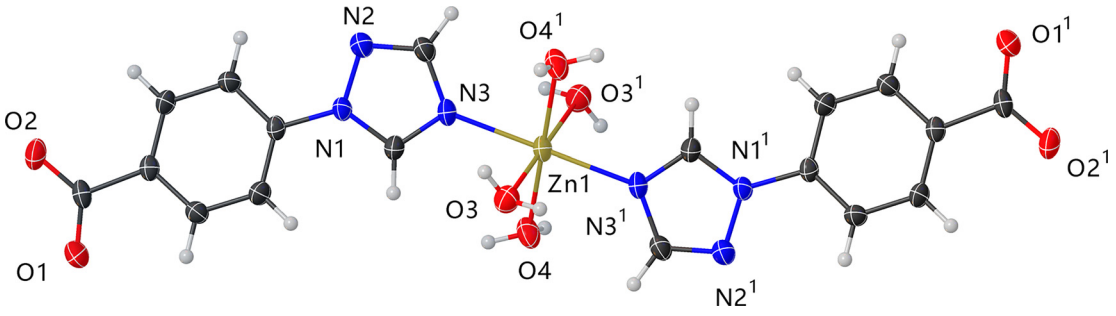
Crystal structure of tetraaqua-bis[4-(1*H*-1,2,4-triazol-1-yl)benzoato-κ^1*N*]zinc(II), $C_{18}H_{20}ZnN_6O_8$



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Abstract

$C_{18}H_{20}ZnN_6O_8$, Triclinic, $P\bar{1}$ (no. 2), a = 6.1830(5) Å, b = 7.0301(6) Å, c = 12.1369(11) Å, α = 80.665(1)°, β = 87.976(2)°, γ = 72.051(1)°, V = 495.17(7) Å^3, Z = 1, $R_{gt}(F)$ = 0.0495, $wR_{ref}(F^2)$ = 0.1243, T = 298.15 K.

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The crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Needle-like, clear light colourless
Size	0.25 × 0.22 × 0.18 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	1.30 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
θ_{max}, completeness:	28.2°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3128, 2298, 0.024
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 $\sigma(I_{obs})$, 1809
$N(param)_{refined}$:	151
Programs:	Bruker programs [1], Olex-II [2], SHELXT [3], SHELXL [4]

Source of materials

The reagents and solvents were commercially available and used without further purification. A mixture of $Zn(NO_3)_2{\cdot}6H_2O$ (0.0297 g, 0.1 mmol), Htbac (0.0189 g, 0.1 mmol) and MeOH/H_2O (10 mL, v/v = 5:5) were placed in a 15 mL Teflon-lined stainless steel vessel, heated at 120 °C for 72 h and cooled to room temperature at a rate of 10 °C/h. Colourless needle-like crystals of the title complex were obtained, yielding 43% (based on Htbac).

Experimental details

The initial structure was solved by the Shelxt program with intrinsic phasing method. The refine process was executed throughout the Shelxl program. The hydrogen atoms were placed in their idealized positions with isotropic thermal parameters.

Comment

Well known as a multidentate organic linker, 4-(1*H*-1,2,4-triazol-1-yl)benzoic acid (Htbac) has two potential coordination sites simultaneously. Due to the different coordination abilities of the carboxylic group and triazol

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	−0.0875 (4)	0.8596 (4)	0.34888 (19)	0.0239 (5)
N2	−0.3145 (4)	0.9404 (4)	0.3220 (2)	0.0339 (6)
N3	−0.1026 (4)	0.9489 (4)	0.16821 (19)	0.0290 (6)
O1	0.4830 (4)	0.4303 (4)	0.79234 (19)	0.0479 (7)
O2	0.1462 (4)	0.5174 (4)	0.87254 (17)	0.0397 (6)
O3	0.1923 (4)	1.1832 (4)	0.05081 (18)	0.0356 (5)
H3A	0.104774	1.264322	0.089903	0.043*
H3B	0.219674	1.254932	−0.008187	0.043*
O4	0.2914 (4)	0.7409 (3)	0.01930 (18)	0.0378 (6)
H4A	0.266257	0.642872	−0.005189	0.045*
H4B	0.334037	0.703952	0.087341	0.045*
Zn1	0.000000	1.000000	0.000000	0.0291 (2)
C1	0.2729 (5)	0.5111 (5)	0.7890 (2)	0.0284 (7)
C2	0.1659 (5)	0.6122 (4)	0.6750 (2)	0.0242 (6)
C3	−0.0671 (5)	0.6735 (5)	0.6540 (2)	0.0290 (7)
H3	−0.165780	0.657315	0.711860	0.035*
C4	−0.1536 (5)	0.7591 (5)	0.5463 (2)	0.0284 (7)
H4	−0.309511	0.800890	0.532299	0.034*
C5	−0.0052 (5)	0.7810 (4)	0.4609 (2)	0.0226 (6)
C6	0.2264 (5)	0.7277 (5)	0.4818 (2)	0.0315 (7)
H6	0.324629	0.750356	0.424886	0.038*
C7	0.3090 (5)	0.6406 (5)	0.5882 (2)	0.0290 (7)
H7	0.464979	0.599882	0.601894	0.035*
C8	−0.3145 (5)	0.9920 (5)	0.2135 (2)	0.0318 (7)
H8	−0.447116	1.052701	0.170853	0.038*
C9	0.0333 (5)	0.8659 (5)	0.2553 (2)	0.0305 (7)
H9	0.191023	0.818313	0.252448	0.037*

group with metal ions, Htbac can form the simple zero-dimensional (0D) complexes containing $M(tbac)_2(H_2O)_4$ (M = Co, Cu, Ni, Mn) units [5–8]. However, the isomorphous Zn(II)-complex has not been reported.

The asymmetric unit of the complex contains one $tbac^-$ ligand, half a Zn(II) ion (located on an inversion center) and two coordinated water molecules. The centre Zn(II) ion is coordinated with two N-atoms (N3, N3^1) and four O-atoms (O3, O3^1, O4, O4^1) originated from two different deprotonated Htbac ligands and four water molecules, respectively. The bond lengths between the atoms of the complex are in the normal ranges. e.g., the distances of Zn1–N3 Zn1–O3 and Zn1–O4 are 2.124(2), 2.169(2) and 2.119(2) Å, paralleled to the reported Zn-complexes with similar environment [9, 10]. The isolated 0D $Zn(tbac)_2(H_2O)_4$ units are connected to each other through O–H···O hydrogen bonds to form a three-dimensional network. What's more, the τ-π stacking interaction, distance range: 3.7823(3)–3.8454(3) Å, between the aromatic rings also have positive effects in forming the network. (symmetry code: #1: −*x*, 2−y, −z)

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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