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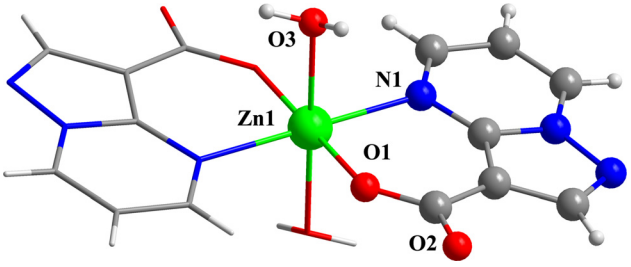
The crystal structure of diaqua-bis(pyrazolo [1,5-*a*]-pyrimidine-3-carboxylato-κ^2*N*,*O*)zinc(II), $C_{14}H_{12}N_6O_6Zn$



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Abstract

$C_{14}H_{12}N_6O_6Zn$, monoclinic, $P2_1/n$, a = 7.0347(6) Å, b = 12.8467(7) Å, c = 9.0017(6) Å, β = 112.525(9)°, V = 751.45 (10) Å^3, Z = 2, $R_{gt}(F)$ = 0.029, $wR_{ref}(F^2)$ = 0.074, T = 293 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.

Source of material

All reagents and chemicals were purchased and used without further purification. $Zn(NO_3)_2{\cdot}6H_2O$ (29.5 mg, 0.1 mmol) pyrazolo[1,5-a]pyrimidine-3-carboxylic acid (16.3 mg, 0.1 mmol) and DMF/H_2O (5 mL, 2.5:2.5, v/v) were placed in a 15 mL capped glass vial. The vial was then heated at 358 K for three days and cooled to room temperature at a rate of 5 °C/h. Colourless block crystals of the title complex were obtained.

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Table 1: Data collection and handling.

Crystal:	Block, colourless
Size	0.33 × 0.31 × 0.29 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	1.69 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω-scans
θ_{max}, completeness:	29.3°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7881, 1858, 0.025
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1614
$N(param)_{refined}$:	125
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3], OLEX2 [4]

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Discussion

Metal complexes constructed from metal centers and carboxylate-type ligands containing N-based heterocycles have developed rapidly owing to their applications in many areas [5–8]. As a rigid organic ligand, pyrazolo-[1,5-a]pyrimidine-3-carboxylate bearing both O and N coordinated sites, has been applied to synthesize metal complexes. Also similar complexes have been synthesized [9, 10]. To further enrich the family of pyrazolo[1,5-a]pyrimidine-3-carboxylate-based metal complexes, the title complex was synthesized.

Single crystal X-ray structural analysis shows that the title complex crystallizes in the monoclinic space group $P2_1/n$ with Z = 2. The asymmetric unit consists of half a Zn(II) cation, one fully deprotonated pyrazolo[1,5-a] pyrimidine-3-carboxylate anion and one coordinated water molecule. The central Zn(II) cation is six-coordinated to form a distorted octahedral geometry by two nitrogen atoms and two carboxylate O atoms from two pyrazolo-[1,5-*a*]pyrimidine-3-carboxylate ligands, and two O atoms from two coordinating water molecules. The Zn–O/N distances are within the normal ranges [11, 12]. The pyrazolo[1,5-*a*]pyrimidine-3-carboxylate anion coordinates

Table 2: 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	0.02399 (11)
O1	0.4595 (2)	0.38661 (10)	0.33097 (16)	0.0299 (3)
O2	0.4185 (2)	0.23201 (10)	0.21556 (15)	0.0304 (3)
O3	0.1787 (2)	0.54026 (11)	0.38789 (17)	0.0318 (3)
H3A	0.1118	0.4956	0.3119	0.048*
H3B	0.1626	0.5992	0.3353	0.048*
N1	0.4263 (3)	0.39225 (12)	0.65348 (18)	0.0237 (3)
N2	0.4139 (3)	0.21378 (12)	0.71741 (18)	0.0240 (3)
N3	0.4150 (3)	0.11670 (13)	0.6565 (2)	0.0311 (4)
C1	0.4348 (3)	0.28890 (14)	0.3313 (2)	0.0210 (4)
C2	0.4255 (3)	0.24077 (14)	0.4775 (2)	0.0217 (4)
C3	0.4218 (3)	0.13561 (15)	0.5132 (2)	0.0285 (4)
H3	0.4239	0.0830	0.4429	0.034*
C4	0.4217 (3)	0.29054 (14)	0.6130 (2)	0.0204 (4)
C5	0.4144 (3)	0.41378 (16)	0.7931 (2)	0.0295 (4)
H5	0.4132	0.4833	0.8215	0.035*
C6	0.4034 (3)	0.33743 (17)	0.9009 (2)	0.0309 (5)
H6	0.3953	0.3564	0.9979	0.037*
C7	0.4049 (3)	0.23605 (16)	0.8619 (2)	0.0283 (4)
H7	0.4000	0.1835	0.9314	0.034*

with a N, O chelating mode to form a discrete structure. The complex molecules are connected to each other through classical O–H···O and O–H···N hydrogen bonds between the coordinated water molecules and the pyrazolo[1,5-*a*]pyrimidine-3-carboxylate ligands to form a two-dimensional structure.

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

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