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Crystal structure of poly[aqua(μ_3 -[2,2'-bipyridine]-3,3'-dicarboxylato- $\kappa^4 N, N': O: O'$) zinc(II)] – dimethylformamide (1/1), $C_{15}H_{15}N_3O_6Zn$

Table 1: Data collection and handling.

Crystal:	Prism, colorless
Size:	0.16 × 0.14 × 0.14 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.55 mm ⁻¹
Diffractometer, scan mode:	Rigaku Saturn, ω -scans
$\theta_{\max}$, completeness:	27.9°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	11704, 3854, 0.063
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3269
$N(\text{param})_{\text{refined}}$:	237
Programs:	CrystalClear [1], SHELX [2]

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Abstract

$C_{15}H_{15}N_3O_6Zn$, monoclinic, $P2_1/n$ (no. 14), $a = 9.607(6)$ Å, $b = 13.747(8)$ Å, $c = 12.754(8)$ Å, $\beta = 105.368(7)^\circ$, $V = 1624.2(18)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0416$, $wR_{\text{ref}}(F^2) = 0.1001$, $T = 113(2)$ K.

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A part of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

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Source of materials

2,2'-bipyridine-3,3'-bicarboxylic acid (1 mmol) was added to a solution of water (5 mL) and DMF (10 mL). A solution of $ZnCl_2$ (1 mmol) in methanol (10 mL) was then dropwise added to. The mixture was stirred at 60 °C for 3 h, then filtered. The resulting colorless filtration was allowed to evaporate by reduced pressure. The solid was dissolved in methanol and crystals of the title compound were obtained by slow evaporation within two weeks.

Experimental details

Hydrogen atoms were assigned with common isotropic displacement factors $U_{\text{iso}}(H) = 1.2$ times U_{eq} (C, pyridine ring), and $U_{\text{iso}}(H) = 1.5$ times U_{eq} (O, water) and refined as riding on their parent atom.

Comment

MOFs, as a current interest in the fields of supramolecular chemistry and crystal engineering, have been focused on the self-assembled by the metal ions and organic ligands for their exploitable magnetic [3, 4], catalytic [5], opto-electronic [6], and inclusive properties [7]. The self-assembly of suitable ligands and metal centers has been proved to be an efficient route for the formation of one- to three-dimensional networks with fascinating structural topologies [8, 9]. Recently, the interest has been focused on compounds with the picolates, because these functional groups can sustain the multi-coordinating sites and coordinating diversity [10, 11, 12].

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} [*] /U _{eq}
Zn1	0.06922(3)	0.86041(2)	0.59078(2)	0.01259(10)
N1	0.2856(2)	0.79426(15)	0.61910(17)	0.0147(4)
N2	0.0806(2)	0.76062(14)	0.71685(17)	0.0148(4)
N3	0.7063(3)	0.5459(2)	0.5634(2)	0.0350(6)
O1	0.63637(19)	0.63004(12)	0.88579(16)	0.0216(4)
O2	0.46606(18)	0.70046(13)	0.95011(15)	0.0196(4)
O3	0.35813(19)	0.51908(13)	0.73535(15)	0.0212(4)
O4	0.33048(17)	0.48742(12)	0.90077(14)	0.0157(4)
O5	−0.13282(19)	0.91525(13)	0.59834(16)	0.0184(4)
O6	0.6967(2)	0.45632(16)	0.71086(18)	0.0359(5)
C1	0.3867(3)	0.83494(17)	0.5785(2)	0.0164(5)
H1	0.3571	0.8706	0.5125	0.020*
C2	0.5323(3)	0.82717(19)	0.6286(2)	0.0205(5)
H2	0.6022	0.8559	0.5978	0.025*
C3	0.5728(2)	0.77640(18)	0.7248(2)	0.0187(5)
H3	0.6722	0.7711	0.7620	0.022*
C4	0.4699(2)	0.73262(17)	0.7686(2)	0.0151(5)
C5	0.3245(2)	0.74211(17)	0.7112(2)	0.0132(5)
C6	0.1974(2)	0.70287(17)	0.74492(19)	0.0127(4)
C7	0.1934(2)	0.61495(17)	0.7997(2)	0.0144(5)
C8	0.0686(3)	0.59312(18)	0.8312(2)	0.0188(5)
H8	0.0647	0.5354	0.8712	0.023*
C9	−0.0495(3)	0.65431(19)	0.8048(2)	0.0208(6)
H9	−0.1341	0.6402	0.8272	0.025*
C10	−0.0407(3)	0.73669(18)	0.7449(2)	0.0185(5)
H10	−0.1227	0.7778	0.7228	0.022*
C11	0.5288(2)	0.68209(17)	0.8757(2)	0.0165(5)
C12	0.3065(2)	0.53559(16)	0.8118(2)	0.0143(5)
C13	0.6477(4)	0.6241(2)	0.4880(3)	0.0452(9)
H13A	0.5584	0.6482	0.5021	0.068*
H13B	0.6272	0.5997	0.4133	0.068*
H13C	0.7181	0.6772	0.4978	0.068*
C14	0.8323(4)	0.4967(4)	0.5477(3)	0.0662(13)
H14A	0.8587	0.4431	0.5998	0.099*
H14B	0.9128	0.5428	0.5591	0.099*
H14C	0.8107	0.4709	0.4735	0.099*
C15	0.6508(3)	0.5216(2)	0.6447(2)	0.0290(6)
H15	0.5693	0.5572	0.6522	0.035*
H5A	−0.137(4)	0.945(3)	0.656(2)	0.061(12)*
H5B	−0.149(4)	0.9577(19)	0.548(2)	0.038(9)*

In this paper, we report the synthesis and crystal structure of a zinc(II) complex with the 2,2'-bipyridine-3,3'-dicarboxylato ligand. The Zn is penta-coordinated with a distorted trigonal bipyramidal geometry. The axial positions are occupied by one N atom from the ligand and the O atom from water molecule. The equatorial plane is formed by two O atoms from carboxylic ligand and a N atom from pyridine moiety. The Zn–N bond lengths (2.094(2) Å, 2.209(2) Å) and the Zn–O bond lengths (1.983(2) Å, 1.990(2) Å, 2.108(2) Å) are in agreement with the expectation. The sum of angles in the plane [122.55(8)°, 127.54(8)°, 109.20(9)°] is 359.29°.

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