Crystal structure of tetraaqua-bis(3-(3-acrylato)pyridyl-*N*)zinc(II), $Zn(H_2O)_4(C_8H_6O_2N)_2$

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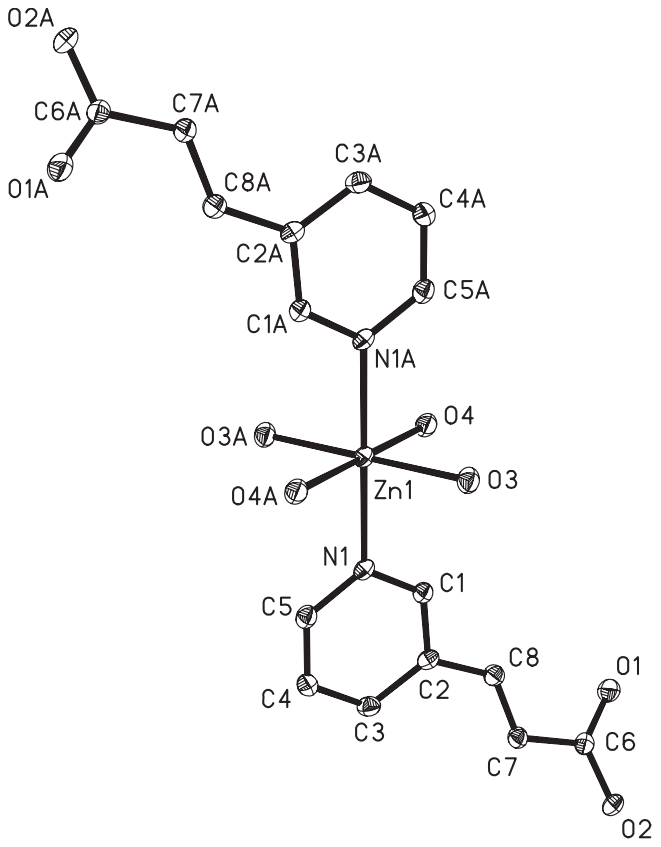

Abstract

$C_{16}H_{20}N_2O_8Zn$, monoclinic, $P12_1/n1$ (no. 14), a = 11.249(3) Å, b = 7.020(2) Å, c = 12.043(3) Å, β = 112.693(3)°, V = 877.4 Å^3, Z = 2, $R_{gt}(F)$ = 0.030, $wR_{ref}(F^2)$ = 0.078, T = 298 K.

Source of material

The title compound was synthesized by the reaction of $Zn(CH_3COO)_2 \cdot 2H_2O$ (0.110 g), 3-(3-pyridyl)acrylic acid (0.075 g) and 0.069 ml triethylamine in the molar ratio of 1:1:1 in 8 ml water. The reactions were carried out in sealed Teflon-lined stainless steel autoclave reactor at 140 °C for 5 days. After the mixture was cooled to room temperature, colorless crystals were collected.

Elemental analysis – found: C, 44.28 %; H, 4.58 %; N, 6.41 %; calc. for $C_{16}H_{20}N_2O_8Zn$: C, 44.31 %; H, 4.65 %; N, 6.46 %.

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Discussion

Weak intermolecular interactions play an important role in the formation of supramolecular structures and crystal engineering [1-3], whereas the hydrogen bonding, as a type of weak inter molecular interactions, which has attracted most interest due to its relative strength and directional properties in generating a great variety of networks with variable cavities or channels.

Within the crystal structure of title compound, the zinc atom located on the center of symmetry is coordinated by two N atoms from two 3-(3-pyridyl)acrylato ligands (d(Zn—N1) = 2.180(2) Å), four O atoms from four coordinated water molecules (d(Zn—O3) = 2.107(2) Å, d(Zn—O4) = 2.105(2) Å) to furnish a slightly distorted octahedral environment. Within the equatorial plane, the sum of the relative bond angles (∠O3–Zn–O4 = 89.35(7)° and ∠O4–Zn–O3A($-x$+1,$-y$,$-z$+1) = 90.65(7)°) around Zn(II) is consequently 360°, while the apical N1–Zn1–N1A bond angle is 180°. Through the intermolecular hydrogen bonds of the coordinated water molecules and the carboxylic groups with O–H···O (2.687 Å, 2.767 Å), the adjacent mononuclear units are linked into a two-dimensional layer structure. The layers are further linked by the intermolecular O–H···O bonds (2.753 Å, 2.803 Å) into the 3D supramolecular architecture.

Table 1. Data collection and handling.

Crystal:	colorless platelet, size 0.11 × 0.32 × 0.35 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	14.49 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	50.02°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4410, 1543
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1260
$N(param)_{refined}$:	124
Programs:	SHELXS-97 [4], SHELXL-97 [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(9)	4*e*	0.3895	–0.3251	0.4037	0.047
H(10)	4*e*	0.3034	–0.2187	0.4295	0.047
H(11)	4*e*	0.3532	0.2702	0.3664	0.047
H(12)	4*e*	0.2781	0.1133	0.3363	0.047
H(1)	4*e*	0.2589	0.0532	0.5559	0.033
H(3A)	4*e*	0.3398	0.1444	0.9045	0.035
H(4A)	4*e*	0.5566	0.1256	0.9369	0.036
H(5)	4*e*	0.6169	0.0659	0.7795	0.034
H(7)	4*e*	0.1148	0.0636	0.8432	0.034
H(8)	4*e*	0.0846	0.1266	0.6100	0.033

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(1)	2*c*	½	0	½	0.0193(2)	0.0309(3)	0.0256(2)	0.0000(2)	0.0108(2)	–0.0002(2)
N(1)	4*e*	0.4443(2)	0.0534(3)	0.6517(2)	0.021(1)	0.034(1)	0.029(1)	–0.001(1)	0.014(1)	–0.0002(9)
O(1)	4*e*	–0.1334(2)	0.1543(3)	0.6106(2)	0.024(1)	0.053(1)	0.036(1)	0.001(1)	0.0112(9)	0.006(1)
O(2)	4*e*	–0.1293(2)	0.0133(3)	0.7775(2)	0.024(1)	0.034(1)	0.036(1)	–0.0015(9)	0.0169(9)	0.0009(8)
O(3)	4*e*	0.3832(2)	–0.2455(3)	0.4542(2)	0.025(1)	0.035(1)	0.035(1)	–0.0025(9)	0.0122(9)	–0.0055(8)
O(4)	4*e*	0.3399(2)	0.1645(3)	0.3940(2)	0.025(1)	0.035(1)	0.033(1)	–0.0014(9)	0.0092(8)	0.0072(8)
C(1)	4*e*	0.3193(3)	0.0663(4)	0.6342(2)	0.023(1)	0.033(2)	0.026(1)	–0.004(1)	0.011(1)	–0.003(1)
C(2)	4*e*	0.2738(2)	0.0977(4)	0.7243(2)	0.025(1)	0.025(1)	0.029(1)	0.001(1)	0.015(1)	0.001(1)
C(3)	4*e*	0.3651(3)	0.1213(4)	0.8409(2)	0.031(2)	0.033(2)	0.027(1)	0.001(1)	0.016(1)	0.000(1)
C(4)	4*e*	0.4940(3)	0.1098(4)	0.8599(2)	0.026(2)	0.038(2)	0.025(1)	–0.002(1)	0.007(1)	–0.000(1)
C(5)	4*e*	0.5296(3)	0.0749(4)	0.7647(2)	0.022(1)	0.030(1)	0.032(2)	0.000(1)	0.010(1)	0.002(1)
C(6)	4*e*	–0.0738(3)	0.0848(4)	0.7123(2)	0.025(1)	0.025(1)	0.030(2)	–0.001(1)	0.013(1)	–0.007(1)
C(7)	4*e*	0.0696(3)	0.0817(4)	0.7611(2)	0.023(1)	0.035(2)	0.027(1)	–0.002(1)	0.010(1)	–0.003(1)
C(8)	4*e*	0.1340(3)	0.1040(4)	0.6908(2)	0.024(1)	0.033(2)	0.027(1)	0.001(1)	0.010(1)	–0.001(1)

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