Crystal structure of aqua-(2,2′-bipyridyl)-(2,5-thiophenedicarboxylato)-zinc(II) dihydrate, $Zn(H_2O)(C_{10}H_8N_2)(C_6H_2O_4S) \cdot 2H_2O$

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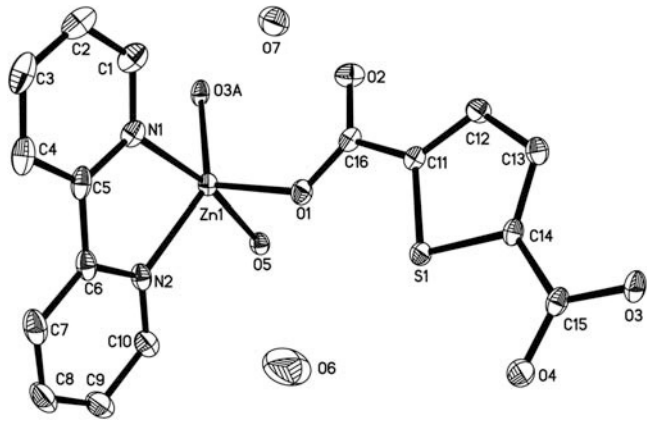

Abstract

$C_{16}H_{16}N_2O_7SZn$, triclinic, $P\bar{1}$ (No. 2), a = 8.5356(7) Å, b = 9.5342(8) Å, c = 12.670(1) Å, α = 69.377(1)°, β = 86.236(1)°, γ = 67.666(1)°, V = 889.8 Å^3, Z = 2, $R_{gt}(F)$ = 0.037, $wR_{ref}(F^2)$ = 0.106, T = 292 K.

Source of material

A mixture of $Zn(NO_3)_2 \cdot 6H_2O$ (0.5 mmol, 0.150 g), 2,2′-bipyridine (bipy, 0.5 mmol, 0.078 g), 2,5-thiophenedicarboxylic acid (tdc, 0.5 mmol, 0.085 g) and H_2O (18 mL) was kept in a 30 mL Teflon-lined autoclave under autogenous pressure at 423 K for five days. After cooling to room temperature, colorless block-shaped crystals were collected by filtration and washed with distilled water in 35 % yield (based on Zn). Chemical analysis — found: C, 42.9 %; H, 3.5 %; N, 6.2 %; S, 7.1 %.; calculated for $C_{16}H_{16}N_2O_7SZn$: C, 43.1 %; H, 3.6 %; N, 6.3 %; S, 7.2 %.

Discussion

The versatility of metal-organic chemistry offers a unique opportunity to construct multifunctional materials based on the assembly of molecular building blocks. Such an approach can lead to the design of coordination polymers with intriguing architectures and potential applications [1,2]. Particularly attractive is the ability of organic moiety to diversify structural arrangements associated with the wide-ranging properties of transition metals (e.g., magnetic and optical properties, electronic conductivity and ferroelectricity) [3,4]. In this regard, much attention has been devoted to the deliberate design and control of self-assembly infinite coordination networks *via* selecting the chemistry structures of ligands [5,6]. Among these, the employment of symmetrical ligands is a successful paradigm owing to their high symmetry and structural predictability [7,8]. 2,5-Thiophenedicarboxylic acid, as a member of them, has been less studied up to now [9-12].

The title crystal structure possesses a one-dimensional architecture in which the asymmetric unit contains one Zn(II) atom, one tdc ligand, one bipy ligand, one coordinated water molecule and two lattice water molecules. The Zn(II) atom is five-coordinated by two nitrogen atoms from bipy ligand, one oxygen atom from coordinated water molecule and one oxygen atom from tdc ligand in the equatorial plane (d(Zn1—N1) = 2.128(2), d(Zn1—N2) = 2.109(2), d(Zn1—O5) = 2.079(2), d(Zn1—O3A) = 2.075(2) Å) and one oxygen atoms from different tdc ligand at the axial sites (d(Zn1—O1) = 2.028(2) Å) in a distorted square-pyramidal ZnO_3N_2 coordination environment with the O(N)–Zn–O(N) angles ranging from 77.1(1)° to 169.42(9)°. The bipy ligand acts as a typical chelating ligand terminally coordinating the Zn(II) metal center, while each tdc anion is coordinating the Zn(II) atom in a μ_2-bridging mode, which is similar to reported in [11]. The most interesting feature of the crystal structure is that each tdc ligand links two symmetry related zinc atoms into an infinite 1D chain along [100] with Zn···Zn distance of about 10.095 Å. The bipy molecules are parallel to each other. The adjacent polymeric chains are stacked into an infinite two-dimensional network *via* C–H···O, O–H···S and O–H···O hydrogen bonding between the coordinated water molecules, sulfur atoms, carbon atoms and carboxylate oxygen atoms, and π-π interactions between the neighboring bipy ligands with the contacting distances in the range of 3.563 - 3.589 Å.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.068 × 0.126 × 0.358 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	15.40 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	52.04°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5039, 3426
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3100
$N(param)_{refined}$:	244
Programs:	SHELXS-97 [13], SHELXL-97 [14], SHELXTL [15]

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

Atom	Site	x	y	z	U_{iso}
H(5B)	2*i*	–0.2541	1.1152	0.9088	0.032
H(5A)	2*i*	–0.3366	1.0305	0.9886	0.040
H(7)	2*i*	–0.3684	1.3534	0.3998	0.053
H(3)	2*i*	–0.7751	1.1671	0.3778	0.057
H(4)	2*i*	–0.5676	1.2662	0.3815	0.051
H(9)	2*i*	–0.0913	1.4010	0.6170	0.053

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Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(12A)	2*i*	–0.3062	0.4063	0.9661	0.034
H(8)	2*i*	–0.1713	1.4465	0.4330	0.057
H(2)	2*i*	–0.8756	1.0465	0.5454	0.057
H(1)	2*i*	–0.7590	1.0202	0.7150	0.048
H(13A)	2*i*	–0.0364	0.1979	0.9517	0.034
H(10)	2*i*	–0.2096	1.2585	0.7640	0.043
H(7B)	2*i*	–0.6150	0.6111	0.8478	0.057
H(7A)	2*i*	–0.7688	0.7058	0.7828	0.071
H(6B)	2*i*	0.0261	1.0036	0.6961	0.192
H(6A)	2*i*	0.0164	0.9237	0.8102	0.240

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*i*	–0.47682(4)	1.09898(4)	0.80056(2)	0.0246(2)	0.0225(2)	0.0203(2)	–0.0046(1)	0.0037(1)	–0.0081(1)
S(1)	2*i*	–0.02417(8)	0.58002(8)	0.83227(6)	0.0213(3)	0.0200(3)	0.0325(4)	–0.0040(3)	0.0046(3)	–0.0077(3)
O(5)	2*i*	–0.3502(2)	1.1127(2)	0.9290(2)	0.030(1)	0.026(1)	0.0214(9)	–0.0089(8)	0.0044(8)	–0.0076(8)
C(5)	2*i*	–0.5413(4)	1.1962(3)	0.5528(2)	0.037(2)	0.025(1)	0.022(1)	0.004(1)	–0.001(1)	–0.009(1)
O(2)	2*i*	–0.4845(3)	0.7338(3)	0.9274(2)	0.028(1)	0.037(1)	0.047(1)	–0.0117(9)	0.0138(9)	–0.027(1)
C(7)	2*i*	–0.3362(5)	1.3361(4)	0.4735(3)	0.055(2)	0.038(2)	0.024(2)	–0.008(2)	0.009(1)	–0.005(1)
O(3)	2*i*	0.2944(2)	0.1376(2)	0.8755(2)	0.028(1)	0.023(1)	0.024(1)	0.0012(8)	0.0023(8)	–0.0067(8)
C(3)	2*i*	–0.7311(5)	1.1573(4)	0.4465(3)	0.049(2)	0.044(2)	0.035(2)	0.005(2)	–0.013(2)	–0.020(2)
O(1)	2*i*	–0.3168(3)	0.8642(2)	0.8380(2)	0.027(1)	0.020(1)	0.034(1)	–0.0030(8)	0.0014(8)	–0.0102(8)
C(6)	2*i*	–0.4079(4)	1.2538(3)	0.5647(2)	0.038(2)	0.023(1)	0.023(1)	–0.002(1)	0.005(1)	–0.006(1)
O(4)	2*i*	0.3119(3)	0.3762(3)	0.7888(2)	0.028(1)	0.030(1)	0.041(1)	–0.0067(9)	0.0100(9)	–0.0110(9)
N(2)	2*i*	–0.3586(3)	1.2254(3)	0.6720(2)	0.034(1)	0.023(1)	0.022(1)	–0.005(1)	0.005(1)	–0.0069(9)
N(1)	2*i*	–0.5982(3)	1.1236(3)	0.6499(2)	0.026(1)	0.034(1)	0.027(1)	–0.005(1)	0.002(1)	–0.015(1)
C(4)	2*i*	–0.6070(5)	1.2153(4)	0.4484(3)	0.053(2)	0.033(2)	0.027(2)	–0.001(2)	–0.007(1)	–0.010(1)
C(15)	2*i*	0.2320(3)	0.2929(3)	0.8432(2)	0.024(1)	0.027(1)	0.019(1)	–0.002(1)	–0.002(1)	–0.009(1)
C(14)	2*i*	0.0567(3)	0.3732(3)	0.8709(2)	0.024(1)	0.020(1)	0.023(1)	–0.002(1)	–0.001(1)	–0.009(1)
C(11)	2*i*	–0.2135(3)	0.5818(3)	0.8872(2)	0.022(1)	0.025(1)	0.020(1)	–0.005(1)	0.001(1)	–0.010(1)
C(9)	2*i*	–0.1704(5)	1.3637(4)	0.6023(3)	0.045(2)	0.037(2)	0.050(2)	–0.019(2)	0.016(2)	–0.011(2)
C(12)	2*i*	–0.2139(4)	0.4287(3)	0.9329(2)	0.028(1)	0.027(1)	0.032(2)	–0.010(1)	0.008(1)	–0.013(1)
C(8)	2*i*	–0.2186(5)	1.3909(4)	0.4933(3)	0.053(2)	0.038(2)	0.040(2)	–0.018(2)	0.018(2)	–0.002(2)
C(2)	2*i*	–0.7904(4)	1.0846(5)	0.5459(3)	0.033(2)	0.056(2)	0.056(2)	–0.007(2)	–0.005(2)	–0.033(2)
C(16)	2*i*	–0.3496(3)	0.7378(3)	0.8845(2)	0.023(1)	0.026(1)	0.023(1)	–0.004(1)	–0.001(1)	–0.014(1)
C(1)	2*i*	–0.7200(4)	1.0695(4)	0.6473(3)	0.032(2)	0.048(2)	0.040(2)	–0.008(1)	0.004(1)	–0.023(2)
C(13)	2*i*	–0.0582(4)	0.3082(3)	0.9243(2)	0.032(2)	0.021(1)	0.030(1)	–0.007(1)	0.002(1)	–0.010(1)
C(10)	2*i*	–0.2430(4)	1.2788(4)	0.6899(3)	0.041(2)	0.031(2)	0.034(2)	–0.013(1)	0.008(1)	–0.011(1)
O(7)	2*i*	–0.6614(3)	0.6677(3)	0.7811(2)	0.057(2)	0.052(2)	0.035(1)	–0.029(1)	–0.002(1)	–0.010(1)
O(6)	2*i*	0.0010(6)	0.9279(5)	0.7433(6)	0.080(3)	0.056(2)	0.294(8)	–0.026(2)	0.042(4)	–0.010(3)

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