Crystal structure of hexaaquatris(4,4′-bipyridine)bis{*N*-[(4-carboxyphenyl)sulfonyl]glycine}trizinc(II) octahydrate, $Zn_3(H_2O)_6(C_{10}H_8N_2)_3(C_9H_6SNO_6)_2 \cdot 8H_2O$

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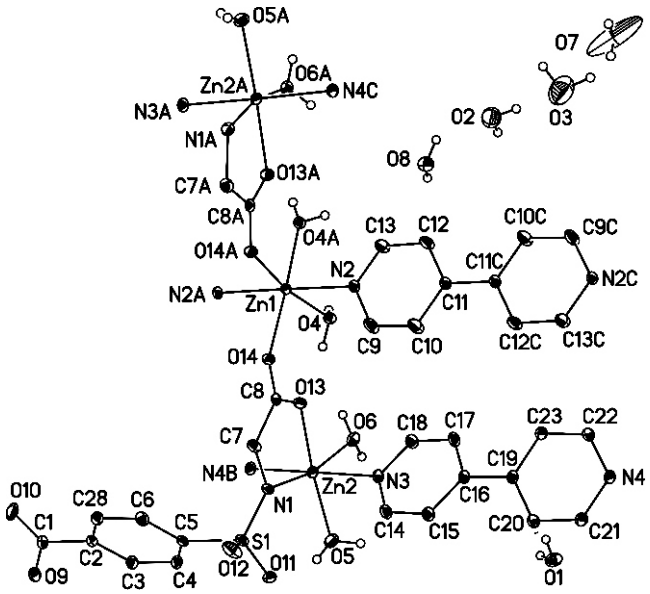

Abstract

$C_{48}H_{64}N_8O_{26}S_2Zn_3$, monoclinic, *C*12/*c*1 (no. 15), $a = 24.962(2)$ Å, $b = 15.044(1)$ Å, $c = 17.342(1)$ Å, $\beta = 117.100(1)°$, $V = 5797.6$ Å^3, $Z = 4$, $R_{gt(F)} = 0.032$, $wR_{ref(F^2)} = 0.091$, $T = 291$ K.

Source of material

The *N*-[(4-carboxyphenyl)sulfonyl]glycine acid ($cbsglyH_3$) was prepared according to the literature method [1]. The title compound was synthesized by adding $Zn(OAc)_2 \cdot 2H_2O$ (0.25 mmol, 0.061 g) to 10 mL aqueous solution containing $cbsglyH_3$ (0.5 mmol, 0.104 g) and 4,4′-bipyridine (4,4′-bipy, 0.25 mmol, 0.039 g). The mixture was stirred for 8 h at 70 °C, then filtered off. The colorless filtrate was allowed to stand at room temperature. Colorless crystals suitable for X-ray diffraction experiment were obtained after ten days.

Discussion

The realm of crystal engineering is of growing interest, and more and more efforts have been devoted to the assembly of supramolecular systems of organic molecular solids and coordination polymers through hydrogen and/or coordination bonds. The resultant crystalline materials have a wide range of potential applications [2-5]. Multidentate N- or O- donor ligands have been employed extensively as organic spacers in the construction of extended structures, such as 4,4′-bipyridine, pyrazine, 1,4-benzenedicarboxylate, and 1,3,5-benzenetricarboxylate [6-8]. Among them, the series of 1,4-benzenedicarboxylate derivatives with adjustable lengths and binding modes attract considerable interest for the modular assembly of metal-organic frameworks, as potential optical and gas absorption materials [9,10]. Recently, the multidentate ligand *N*-[(4-carboxyphenyl)sulfonyl]glycine attracted our attention because it can act not only as the hydrogen-bond donor but also as acceptor, which make it to a wonderful candidate for the construction of supramolecular structures. In the past decades, luminescent coordination compounds with amino acids have also attracted much attention due to their good performance in sensor technologies and electroluminescent devices. Several d^{10} metal-organic complexes have been found to exhibit interesting photoluminescent properties, among which luminescent zinc complexes with nitrogen-containing ligands have been considerably investigated as potential luminescent materials [11].

The asymmetric unit of the title crystal structure consists of one and a half zinc(II) ions, one *N*-[(4-carboxyphenyl)sulfonyl]-glycine ligand, one and a half 4,4′-bipy ligands, three coordinating water molecules and four lattice water molecules. Two crystallographically independent Zn(II) ions are both six-coordinated in distorted octahedral environment. Zn1 is coordinated by two oxygen atoms (O4 and O4A) of two water molecules, two nitrogen atoms (N2 and N2A) of two different bipy ligands, and two carboxylic oxygen atoms (O14 and O14A) from two glycinato moieties of different 4-$cbsgly^{3-}$ ligands. The oxygen atoms (O4, O4A, O14 and O14A) occupy the equatorial sites, while the nitrogen atoms (N2 and N2A) locate in the axial positions. Zn2 is coordinated by two oxygen atoms (O5 and O6) of water molecules, one oxygen atom (O13) and one nitrogen atom (N1) of glycinato group in the equatorial sites, and two nitrogen atoms (N3 and N4B) from 4,4′-bipy molecules in the axial positions. The 4-$cbsgly^{3-}$ anion acts as a bidentate ligand. Both carboxylic oxygen atoms of $C_6H_5COO^-$ keep free. Zn1 and two Zn2 are linked by the carboxylic oxygen atoms of glycinato part in *syn-anti* mode which is similar to [12], forming a trinuclear complex. The bond lengths of Zn1—O14 and Zn2—O13 are 2.104(2) Å and 2.097(2) Å, respectively.

Unlike to the reported structure [13], the zinc trinuclear units are further bridged by bipy molecules to construct trinal chain polymer. The nearest Zn···Zn separation within the chain is 11.510 Å, while the nearest Zn···Zn separation between the neighboring chain is 5.394 Å. In addition, there exist a series of hydrogen bonds between the adjacent chains, which contribute to the stability of the system.

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Table 1. Data collection and handling.

Crystal:	colorless block, size 0.22 × 0.29 × 0.44 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	13.96 cm^{-1}
Diffractometer, scan mode:	CCD, φ/ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	18934, 5400
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4463
$N(param)_{refined}$:	394
Programs:	SHELXS-97, SHELXL-97 [14]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1W)	8*f*	0.0653	0.4476	0.8886	0.077
H(2W)	8*f*	0.1050	0.5016	0.8766	0.077
H(3W)	8*f*	0.6887	0.0122	0.6029	0.130
H(4W)	8*f*	0.7344	0.0645	0.6047	0.130
H(5W)	8*f*	0.8191	0.0460	0.6321	0.238
H(6W)	8*f*	0.8698	0.0513	0.7091	0.238
H(7W)	8*f*	–0.0241	0.6541	0.3527	0.044
H(8W)	8*f*	–0.0266	0.5795	0.3069	0.044
H(9W)	8*f*	–0.1045	0.7840	0.6082	0.072
H(10W)	8*f*	–0.0673	0.7134	0.6442	0.072
H(11W)	8*f*	–0.0754	0.5753	0.5281	0.057
H(12W)	8*f*	–0.0740	0.5786	0.4503	0.057
H(13W)	8*f*	0.9942	0.0391	0.7699	0.517
H(14W)	8*f*	0.4841	0.1061	0.7676	0.076
H(3)	8*f*	–0.3250	0.9015	0.3753	0.040
H(4)	8*f*	–0.2261	0.8826	0.4782	0.042
H(6A)	8*f*	–0.1715	1.0423	0.3425	0.041
H(7A)	8*f*	–0.0262	0.9425	0.4351	0.040
H(7B)	8*f*	–0.0918	0.9341	0.3592	0.040
H(9)	8*f*	0.0853	0.8159	0.4296	0.067
H(10)	8*f*	0.1837	0.8240	0.5307	0.073
H(12)	8*f*	0.2251	0.6696	0.3796	0.052
H(13)	8*f*	0.1260	0.6679	0.2822	0.051
H(14)	8*f*	0.0113	0.8637	0.6507	0.044
H(15)	8*f*	0.1103	0.8791	0.7506	0.040
H(17)	8*f*	0.1478	0.6637	0.6475	0.044
H(18)	8*f*	0.0475	0.6520	0.5543	0.045
H(20)	8*f*	0.1993	0.8537	0.8672	0.041
H(21)	8*f*	0.2994	0.8520	0.9643	0.043
H(22)	8*f*	0.3371	0.7052	0.8113	0.042
H(23)	8*f*	0.2389	0.7038	0.7087	0.040
H(28)	8*f*	–0.2697	1.0555	0.2370	0.041

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)	4*e*	0	0.73822(3)	¼	0.0159(2)	0.0289(2)	0.0218(2)	0	0.0071(2)	0
Zn(2)	8*f*	–0.07583(1)	0.74137(2)	0.49575(2)	0.0182(2)	0.0431(2)	0.0221(2)	0.0002(1)	0.0068(1)	–0.0010(1)
S(1)	8*f*	–0.11248(3)	0.94797(5)	0.50108(4)	0.0200(3)	0.0508(4)	0.0313(3)	0.0063(3)	0.0078(3)	–0.0135(3)
O(1)	8*f*	0.09508(9)	0.4809(2)	0.9129(1)	0.051(1)	0.061(2)	0.046(1)	–0.017(1)	0.025(1)	–0.016(1)
O(2)	8*f*	0.6975(1)	0.0540(2)	0.5797(2)	0.079(2)	0.096(2)	0.080(2)	–0.001(2)	0.033(2)	0.006(2)
O(3)	8*f*	0.8300(2)	0.0503(3)	0.6853(3)	0.146(4)	0.198(5)	0.111(3)	–0.024(3)	0.041(3)	0.032(3)
O(4)	8*f*	–0.00853(7)	0.6274(1)	0.3261(1)	0.0271(9)	0.0303(9)	0.0316(9)	–0.0020(7)	0.0150(7)	–0.0037(7)
O(5)	8*f*	–0.09801(9)	0.7313(2)	0.6017(1)	0.033(1)	0.080(2)	0.031(1)	0.002(1)	0.0141(9)	0.002(1)
O(6)	8*f*	–0.06282(8)	0.6039(1)	0.4985(1)	0.037(1)	0.042(1)	0.029(1)	–0.0061(8)	0.0094(8)	–0.0003(8)
O(7)	4*e*	0	–0.0096(4)	¾	0.84(3)	0.082(5)	0.127(6)	0	0.23(1)	0
O(8)	4*e*	½	0.1440(2)	¾	0.056(2)	0.048(2)	0.052(2)	0	0.029(2)	0
O(9)	8*f*	–0.41367(8)	0.9859(1)	0.2496(1)	0.0252(9)	0.051(1)	0.039(1)	0.0078(9)	0.0113(8)	0.0041(9)
O(10)	8*f*	–0.37970(9)	1.0230(2)	0.1553(1)	0.043(1)	0.077(2)	0.034(1)	0.014(1)	0.012(1)	0.022(1)
O(11)	8*f*	–0.11637(9)	0.9127(2)	0.5765(1)	0.036(1)	0.094(2)	0.026(1)	0.022(1)	0.0127(9)	–0.004(1)
O(12)	8*f*	–0.08588(9)	1.0346(2)	0.5100(2)	0.032(1)	0.054(1)	0.078(2)	–0.005(1)	0.018(1)	–0.035(1)
O(13)	8*f*	–0.04758(8)	0.7459(1)	0.3989(1)	0.034(1)	0.032(1)	0.033(1)	0.0028(8)	0.0202(8)	–0.0011(8)
O(14)	8*f*	–0.02062(7)	0.8345(1)	0.3204(1)	0.0275(9)	0.034(1)	0.0301(9)	0.0011(7)	0.0171(8)	–0.0012(7)
N(1)	8*f*	–0.08204(9)	0.8758(2)	0.4695(1)	0.020(1)	0.041(1)	0.028(1)	0.0051(9)	0.0115(9)	–0.0043(9)
N(2)	8*f*	0.09495(9)	0.7417(1)	0.3448(1)	0.018(1)	0.028(1)	0.025(1)	–0.0013(8)	0.0064(8)	–0.0032(8)
N(3)	8*f*	0.0190(1)	0.7556(2)	0.5934(1)	0.019(1)	0.041(1)	0.028(1)	0.0012(9)	0.0042(9)	–0.0018(9)
N(4)	8*f*	0.32835(9)	0.7774(2)	0.8991(1)	0.019(1)	0.046(1)	0.026(1)	–0.0004(9)	0.0052(9)	–0.002(1)
C(1)	8*f*	–0.3719(1)	0.9974(2)	0.2276(2)	0.030(1)	0.036(2)	0.030(1)	0.008(1)	0.009(1)	0.004(1)
C(2)	8*f*	–0.3079(1)	0.9813(2)	0.2954(2)	0.026(1)	0.032(1)	0.027(1)	0.007(1)	0.013(1)	0.003(1)
C(3)	8*f*	–0.2942(1)	0.9293(2)	0.3682(2)	0.024(1)	0.045(2)	0.034(1)	0.004(1)	0.015(1)	0.008(1)
C(4)	8*f*	–0.2350(1)	0.9187(2)	0.4304(2)	0.026(1)	0.052(2)	0.030(1)	0.010(1)	0.014(1)	0.013(1)
C(5)	8*f*	–0.1890(1)	0.9616(2)	0.4214(2)	0.021(1)	0.036(1)	0.029(1)	0.007(1)	0.011(1)	–0.005(1)
C(6)	8*f*	–0.2022(1)	1.0134(2)	0.3489(2)	0.027(1)	0.036(2)	0.043(2)	0.001(1)	0.019(1)	0.004(1)
C(7)	8*f*	–0.0602(1)	0.9025(2)	0.4071(2)	0.027(1)	0.035(2)	0.040(2)	0.000(1)	0.017(1)	–0.006(1)
C(8)	8*f*	–0.04127(9)	0.8219(2)	0.3730(1)	0.011(1)	0.034(1)	0.023(1)	0.0007(9)	0.0028(9)	–0.002(1)
C(9)	8*f*	0.1138(1)	0.7863(3)	0.4187(2)	0.023(1)	0.079(2)	0.051(2)	0.011(2)	0.004(1)	–0.032(2)
C(10)	8*f*	0.1734(1)	0.7913(3)	0.4803(2)	0.028(2)	0.089(3)	0.048(2)	0.012(2)	0.001(1)	–0.041(2)
C(11)	8*f*	0.2177(1)	0.7484(2)	0.4678(2)	0.020(1)	0.033(1)	0.027(1)	0.001(1)	0.007(1)	–0.004(1)
C(12)	8*f*	0.1977(1)	0.7010(2)	0.3916(2)	0.022(1)	0.058(2)	0.043(2)	0.003(1)	0.010(1)	–0.023(1)
C(13)	8*f*	0.1376(1)	0.6999(2)	0.3332(2)	0.024(1)	0.057(2)	0.038(2)	–0.002(1)	0.008(1)	–0.024(1)
C(14)	8*f*	0.0391(1)	0.8222(2)	0.6510(2)	0.023(1)	0.042(2)	0.038(2)	0.006(1)	0.007(1)	–0.005(1)
C(15)	8*f*	0.0988(1)	0.8325(2)	0.7111(2)	0.025(1)	0.034(2)	0.034(1)	–0.001(1)	0.007(1)	–0.006(1)
C(16)	8*f*	0.1414(1)	0.7727(2)	0.7118(2)	0.019(1)	0.032(1)	0.026(1)	–0.001(1)	0.006(1)	0.001(1)
C(17)	8*f*	0.1209(1)	0.7046(2)	0.6504(2)	0.021(1)	0.040(2)	0.040(2)	0.003(1)	0.007(1)	–0.005(1)
C(18)	8*f*	0.0603(1)	0.6985(2)	0.5941(2)	0.024(1)	0.043(2)	0.038(2)	–0.001(1)	0.006(1)	–0.011(1)
C(19)	8*f*	0.2059(1)	0.7771(2)	0.7757(2)	0.020(1)	0.032(1)	0.025(1)	–0.001(1)	0.007(1)	0.002(1)

Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(20)	8*f*	0.2263(1)	0.8225(2)	0.8542(2)	0.020(1)	0.048(2)	0.032(1)	0.003(1)	0.009(1)	–0.005(1)
C(21)	8*f*	0.2869(1)	0.8209(2)	0.9127(2)	0.024(1)	0.050(2)	0.028(1)	–0.001(1)	0.007(1)	–0.007(1)
C(22)	8*f*	0.3090(1)	0.7352(2)	0.8228(2)	0.021(1)	0.051(2)	0.031(1)	0.004(1)	0.009(1)	–0.004(1)
C(23)	8*f*	0.2498(1)	0.7337(2)	0.7607(2)	0.024(1)	0.047(2)	0.026(1)	0.002(1)	0.008(1)	–0.004(1)
C(28)	8*f*	–0.2611(1)	1.0219(2)	0.2863(2)	0.037(1)	0.036(2)	0.034(1)	0.009(1)	0.019(1)	0.010(1)

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