Crystal structure of a 1D Zn coordination polymer based on 3-(4-carboxyphenyl)-propionic acid and 2,4,6-tri(2-pyridyl)-1,3,5-triazine, $C_{28}H_{26}N_6O_7Zn$

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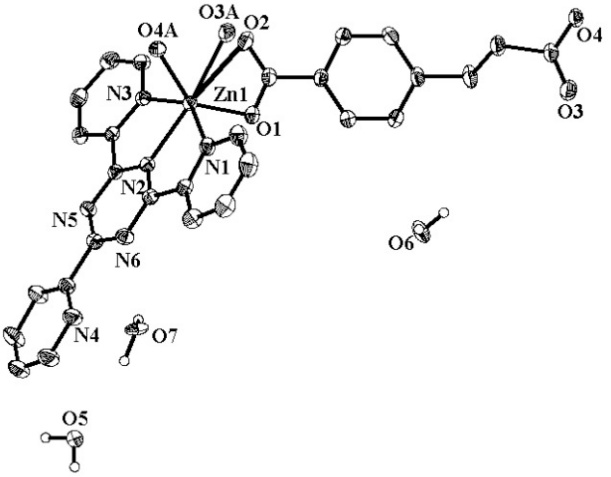

Abstract

$C_{28}H_{26}N_6O_7Zn$, monoclinic, $P2_1/c$ (no. 14), a = 7.9282(7) Å, b = 31.309(3) Å, c = 11.060(1) Å, β = 95.958(1)°, V = 2730.5 Å^3, Z = 4, $R_{gt}(F)$ = 0.0352, $wR_{ref}(F^2)$ = 0.0937, T = 296 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.16×0.22×0.30 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	9.59 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	56.66°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	21914, 6742
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 5224
$N(param)_{refined}$:	379
Programs:	SHELXS-97 [9]

Source of material

A mixture of 3-(4-carboxyphenyl)propionic acid (0.1 mmol, 19.4 mg), 2,4,6-tri-(2-pyridyl)-1,3,5-triazine (0.1 mmol, 31.2 mg), $Zn(OAc)_2{\cdot}2H_2O$ (0.1 mmol, 22.0 mg), NaOH (0.1 mmol), and H_2O (6.0 ml) were placed in a 23ml Teflon lined stainless steel reactor. The vessel was heated to 393K for 4 days, and then slowly cooled to room temperature. Colourless crystals were obtained and further crystals were filtered off, washed with the mother liquid, and dried under ambient conditions. Yield 56 %.

Discussion

It is well-known that the multi-functional carboxylate organic ligands play an important role in directing the structural extension of the resulting complexes. The latter bear potential applications in optical devices and ion exchange due to their intriguing structures [1,2] and topological features [3,4]. In this regard, a new family of benzene multicarboxylates with long-spanning carboxyl groups has been captured our attention, especially 3-(4-carboxyphenyl)-propionic acid. This ligand combined with rigid –COOH and flexible $–CH_2CH_2COOH$ carboxylate groups can probably produce new structure due to their different coordination modes and molecular flexibility [5,6]. On the other hand, the introduction of additional N-donor ligands to such systems can modify the structures and properties of the resulting materials [7,8]. The asymmetric unit of the title complex contains one Zn^{2+} ion, one 3-(4-carboxyphenyl)propionic anion, one 2,4,6-tri-(2-pyridyl)-1,3,5-triazine coligand and three crystal water molecules. The Zn ion is seven-coordinated by three N atoms of one chelating 2,4,6-tri(2-pyridyl)-1,3,5-triazine ligand and four oxygen atoms of two symmetry-related 3-(4-carboxyphenyl)propionate anions adopt-ing a bidentatly chelating mode. The Zn–N bond lengths are in the range of 2.111(2) - 2.287(2) Å and the Zn–O bond lengths are 1.9564(17) and 1.9573(18) Å, respectively. The $[ZnO_4N_3]$ environment is best described as distorted pentagonal bipyramid. Extension of the structure through the 3-(4-carboxyphenyl)-propionate anion connects the adjacent Zn^{2+} ion to result in a 1D undulating chain along the crystallographic a axis. Notably, the presences of crystal water molecules lead to the formation of extensive H-bonding interactions, which develop the total structure to form a 2D layer architecture. The adjacent 2D layers stack in a slightly off-set parallel fashion with weak van der Waals forces.

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

Atom	Site	x	y	z	U_{iso}
H(1W)	4*e*	0.5521	0.3886	0.1748	0.108
H(2W)	4*e*	0.4012	0.3942	0.1259	0.108
H(3W)	4*e*	0.0486	0.7564	0.5510	0.177
H(4W)	4*e*	0.0650	0.7478	0.4369	0.177
H(5W)	4*e*	0.6048	0.4956	0.4215	0.241
H(6W)	4*e*	0.5355	0.4741	0.3149	0.241
H(3)	4*e*	0.9116	0.7161	1.2145	0.049
H(4)	4*e*	0.7113	0.7500	1.3158	0.053
H(6)	4*e*	0.3450	0.6840	1.1245	0.061
H(7)	4*e*	0.5465	0.6490	1.0245	0.056
H(8A)	4*e*	0.2629	0.7319	1.2682	0.065
H(8B)	4*e*	0.3957	0.7397	1.3812	0.065
H(9A)	4*e*	0.3759	0.7951	1.1822	0.059
H(9B)	4*e*	0.4690	0.8039	1.3116	0.059
H(11)	4*e*	0.8185	0.6907	0.6800	0.059
H(12)	4*e*	0.6421	0.6957	0.5024	0.071

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Table 2. continued.

Atom	Site	*x*	*y*	*z*	U_{iso}
H(13)	4*e*	0.5731	0.635	0.3901	0.072
H(14)	4*e*	0.6773	0.5691	0.4625	0.06
H(22)	4*e*	1.0265	0.4054	0.7451	0.062
H(23)	4*e*	0.9572	0.3394	0.6574	0.078
H(24)	4*e*	0.7903	0.3365	0.4753	0.077

Table 2. continued.

Atom	Site	*x*	*y*	*z*	U_{iso}
H(25)	4*e*	0.6933	0.3992	0.3851	0.073
H(27)	4*e*	1.2429	0.4681	0.9649	0.046
H(28)	4*e*	1.4156	0.4833	1.1432	0.053
H(29)	4*e*	1.4316	0.5529	1.2135	0.055
H(30)	4*e*	1.2722	0.605	1.1095	0.049

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*	1.02012(3)	0.618159(7)	0.85702(2)	0.0301(1)	0.0297(1)	0.0429(1)	–0.00191(9)	0.01036(9)	–0.00221(9)
N(1)	4*e*	0.8536(2)	0.62875(5)	0.6779(2)	0.0391(9)	0.0333(9)	0.0419(9)	0.0051(7)	0.0073(7)	0.0053(7)
N(2)	4*e*	0.9819(2)	0.55823(5)	0.7715(1)	0.0298(7)	0.0300(8)	0.0322(8)	–0.0003(6)	0.0027(6)	0.0021(6)
N(3)	4*e*	1.1688(2)	0.56943(5)	0.9770(1)	0.0301(8)	0.0331(8)	0.0355(8)	–0.0030(6)	0.0024(6)	–0.0007(7)
N(4)	4*e*	0.7957(2)	0.43867(6)	0.5074(2)	0.053(1)	0.051(1)	0.045(1)	–0.0076(9)	–0.0005(8)	–0.0121(9)
O(1)	4*e*	0.8329(2)	0.63353(5)	0.9509(1)	0.0356(7)	0.0492(9)	0.0485(8)	0.0022(6)	0.0127(6)	–0.0105(7)
O(2)	4*e*	1.0355(2)	0.66348(5)	1.0749(1)	0.0319(8)	0.067(1)	0.061(1)	0.0052(7)	0.0086(7)	–0.0110(8)
O(3)	4*e*	0.0801(2)	0.79482(5)	1.3132(2)	0.0430(9)	0.0405(9)	0.094(1)	0.0040(7)	0.0203(8)	0.0027(8)
O(4)	4*e*	0.2302(2)	0.85456(4)	1.3184(1)	0.0377(7)	0.0315(7)	0.0528(8)	0.0070(6)	0.0107(6)	–0.0003(6)
O(5)	4*e*	0.4715(2)	0.40624(6)	0.1785(2)	0.058(1)	0.059(1)	0.099(1)	0.0037(9)	0.007(1)	–0.019(1)
O(6)	4*e*	0.0603(4)	0.73525(7)	0.5046(2)	0.184(3)	0.072(2)	0.106(2)	0.018(2)	0.053(2)	0.007(1)
O(7)	4*e*	0.5822(4)	0.4977(1)	0.3652(3)	0.164(3)	0.158(3)	0.137(2)	–0.069(2)	–0.092(2)	0.078(2)
C(1)	4*e*	0.8848(2)	0.65737(6)	1.0416(2)	0.037(1)	0.037(1)	0.042(1)	0.0049(8)	0.0095(8)	0.0018(9)
C(2)	4*e*	0.7510(2)	0.67885(6)	1.1076(2)	0.033(1)	0.034(1)	0.042(1)	0.0050(8)	0.0081(8)	0.0016(8)
C(3)	4*e*	0.7976(3)	0.70935(7)	1.1960(2)	0.036(1)	0.040(1)	0.046(1)	0.0031(8)	0.0046(9)	–0.0002(9)
C(4)	4*e*	0.6772(3)	0.72979(7)	1.2566(2)	0.053(1)	0.033(1)	0.047(1)	0.0021(9)	0.011(1)	–0.0043(9)
C(5)	4*e*	0.5067(3)	0.72075(6)	1.2308(2)	0.045(1)	0.029(1)	0.054(1)	0.0093(9)	0.0184(9)	0.0040(9)
C(6)	4*e*	0.4592(3)	0.69050(8)	1.1432(2)	0.032(1)	0.047(1)	0.076(2)	0.0014(9)	0.013(1)	–0.008(1)
C(7)	4*e*	0.5806(3)	0.66954(7)	1.0826(2)	0.039(1)	0.046(1)	0.057(1)	0.0003(9)	0.009(1)	–0.015(1)
C(8)	4*e*	0.3733(3)	0.74405(7)	1.2942(2)	0.059(1)	0.039(1)	0.070(2)	0.014(1)	0.029(1)	0.002(1)
C(9)	4*e*	0.3692(3)	0.79092(7)	1.2684(2)	0.044(1)	0.037(1)	0.070(2)	0.0092(9)	0.016(1)	–0.001(1)
C(10)	4*e*	0.2137(3)	0.81397(6)	1.3036(2)	0.040(1)	0.034(1)	0.045(1)	0.0086(8)	0.0091(9)	0.0019(9)
C(11)	4*e*	0.7902(3)	0.66602(7)	0.6357(2)	0.054(1)	0.040(1)	0.053(1)	0.009(1)	0.007(1)	0.008(1)
C(12)	4*e*	0.6846(3)	0.66928(8)	0.5291(2)	0.063(2)	0.053(2)	0.062(2)	0.021(1)	0.005(1)	0.021(1)
C(13)	4*e*	0.6428(3)	0.63329(9)	0.4629(2)	0.060(2)	0.067(2)	0.051(1)	0.011(1)	–0.008(1)	0.018(1)
C(14)	4*e*	0.7052(3)	0.59416(8)	0.5052(2)	0.050(1)	0.054(1)	0.043(1)	0.004(1)	–0.003(1)	0.007(1)
C(15)	4*e*	0.8102(2)	0.59354(6)	0.6130(2)	0.034(1)	0.040(1)	0.037(1)	0.0030(8)	0.0049(8)	0.0068(8)
C(16)	4*e*	0.8849(2)	0.55367(6)	0.6659(2)	0.0328(9)	0.035(1)	0.0321(9)	–0.0019(8)	0.0045(7)	0.0031(8)
N(6)	4*e*	0.8546(2)	0.51641(5)	0.6104(1)	0.0432(9)	0.0382(9)	0.0362(9)	–0.0022(7)	–0.0016(7)	0.0002(7)
C(17)	4*e*	0.9299(2)	0.48269(6)	0.6672(2)	0.038(1)	0.034(1)	0.0341(9)	–0.0018(8)	0.0052(8)	–0.0010(8)
N(5)	4*e*	1.0329(2)	0.48428(5)	0.7713(1)	0.0398(9)	0.0303(8)	0.0377(8)	0.0006(7)	0.0021(7)	–0.0018(7)
C(18)	4*e*	1.0547(2)	0.52279(6)	0.8196(2)	0.0280(9)	0.030(1)	0.0329(9)	–0.0004(7)	0.0059(7)	0.0019(7)
C(28)	4*e*	0.8946(3)	0.43971(7)	0.6136(2)	0.042(1)	0.039(1)	0.038(1)	–0.0038(9)	0.0086(8)	–0.0063(8)
C(27)	4*e*	0.9577(3)	0.40360(7)	0.6718(2)	0.063(2)	0.040(1)	0.050(1)	–0.000(1)	–0.001(1)	–0.007(1)
C(26)	4*e*	0.9170(4)	0.36437(8)	0.6193(3)	0.083(2)	0.037(1)	0.073(2)	0.000(1)	0.004(2)	–0.011(1)
C(25)	4*e*	0.8185(4)	0.36262(9)	0.5123(3)	0.072(2)	0.050(2)	0.072(2)	–0.013(1)	0.010(1)	–0.027(1)
C(24)	4*e*	0.7606(3)	0.40049(9)	0.4590(2)	0.065(2)	0.065(2)	0.052(1)	–0.012(1)	0.003(1)	–0.023(1)
C(19)	4*e*	1.1636(2)	0.52894(6)	0.9355(2)	0.0273(8)	0.033(1)	0.0322(9)	–0.0013(7)	0.0053(7)	0.0016(7)
C(20)	4*e*	1.2519(2)	0.49585(6)	0.9952(2)	0.037(1)	0.035(1)	0.043(1)	0.0033(8)	0.0023(8)	0.0016(8)
C(21)	4*e*	1.3538(3)	0.50487(7)	1.1011(2)	0.036(1)	0.050(1)	0.046(1)	0.0087(9)	–0.0005(9)	0.009(1)
C(22)	4*e*	1.3625(3)	0.54605(7)	1.1431(2)	0.039(1)	0.058(1)	0.039(1)	–0.002(1)	–0.0052(9)	–0.000(1)
C(23)	4*e*	1.2672(3)	0.57725(7)	1.0794(2)	0.039(1)	0.041(1)	0.042(1)	–0.0050(9)	0.0014(9)	–0.0041(9)

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