Crystal structure of catena-[(μ_2-5-methylisophthalato)(μ_2-1,3-*bis*-(1,2,4-triazol-1-yl)propane)]zinc(II)dihydrate, $[Zn(C_9H_6O_4)(C_7H_{10}N_6)]\cdot 2H_2O$, $C_{16}H_{20}N_6O_6Zn$

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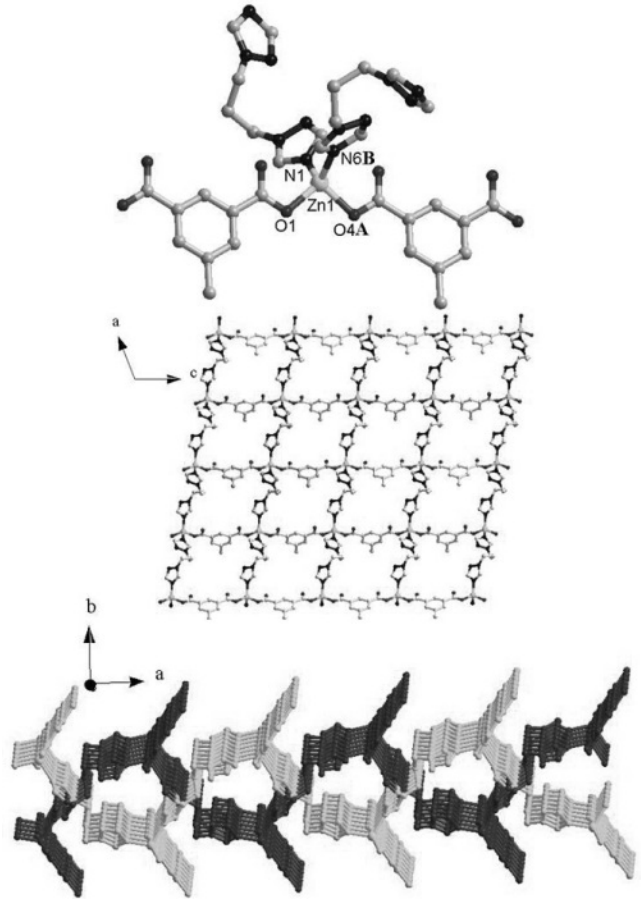

Abstract

$C_{16}H_{20}N_6O_6Zn$, monoclinic, $P2_1/c$ (no. 14), a = 9.534(1) Å, b = 21.463(3) Å, c = 10.158(1) Å, β = 110.980(1)°, V = 1940.8 Å^3, Z = 4, $R_{gt}(F)$ = 0.0331, $wR_{ref}(F^2)$ = 0.0804, T = 296 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.20×0.21×0.26 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	13.13 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	14677, 3615
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2777
$N(param)_{refined}$:	279
Programs:	SHELX [13]

Source of material

1,3-*bis*-(1,2,4-triazol-1-yl)propane (btp, 14 mg, 0.1mmol), 5-methylisophthalic acid (H_2mip, 18 mg, 0.1mmol), $Zn(OAc)_2\cdot 2H_2O$ (22 mg, 0.1mmol) and KOH (5.6 mg, 0.1mmol) were added to water (12 ml) in a Teflon-lined stainless steel vessel. The mixture was heated at 433 K for 3 d, and then slowly cooled down to room temperature. Colourless block-shaped crystals of the title complex were obtained.

Discussion

Photoluminescent properties of coordination compounds which contain d^{10} metal centers have been attracting increasing interest [1-7]. Major reasons for this interest stem from the d^{10} metal ions not only possessing various coordination numbers and geometries, but also exhibiting photoluminescent properties when bound to functional ligands. Organic aromatic multicarboxylate, such as 1,*n*-benzenedicarboxylate (n = 2, 3, or 4), 1,2,3-benzenetricarboxylate, and 1,2,4,5-benzenetetracarboxylate, as the linkers between the metal centers, present versatile coordination modes, can yield predetermined networks and have been widely utilized to construct coordination polymers[8-12]. 5-methylisophthalic acid (H_2mip), a derivative of isophthalic acid, has a substituent, a subtle difference to H_2ip, and the difference may significantly influence the resulting metal-organic frameworks, although substituents will not be involved in metal coordination. We report herein a new zinc(II) coordination polymers based on 5-methylisophthalic acid and a flexible *N*-donor ligand, 1,3-*bis*-(1,2,4-triazol-1-yl)propane (btp). The crystal structure of the title complex comprises a 5-methylisophthalate anion (mip), a Zn(II) ion and a 1,3-*bis*-(1,2,4-triazol-1-yl)propane molecule (btp) as well as two free water per asymmetric unit (figure, top). Both of the carboxylate groups of the acid are deprotonated. The Zn(II) ion has the distorted tetrahedral coordination which is composed of two nitrogen atoms from two btp ligands and two oxygen atoms from two mip. The bond lengths of Zn–O are 1.9825(18) and 1.9914(17) Å and the ones of Zn–N are 2.011(2) and 2.046(2) Å, respectively. The bond angles around the central Zn(II) ion range from 98.04(7)° to 110.51(9)°. Zn(II) ions are linked by μ_2-mip and μ_2-btp ligands to form a 2-D (4,4) layer (figure middle). The single layers are interlocked and form a 2-fold interpenetrated architecture (figure, bottom). There are also hydrogen bonding interactions among mip O atom and free water molecules. These hydrogen bonding interactions bring further stability for the structure.

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1W)	4*e*	0.104(5)	0.263(2)	0.627(4)	0.08(2)
H(2W)	4*e*	0.030(6)	0.312(3)	0.585(6)	0.15(3)
H(3W)	4*e*	0.051(5)	0.179(2)	0.761(5)	0.11(2)
H(4W)	4*e*	0.123(6)	0.206(3)	0.892(6)	0.16(3)
H(2)	4*e*	–0.0776	0.4006	0.4121	0.036
H(4)	4*e*	–0.2930	0.5345	0.5371	0.049
H(6)	4*e*	–0.3016	0.5327	0.1410	0.047
H(9A)	4*e*	–0.4353	0.6119	0.2031	0.135
H(9B)	4*e*	–0.3674	0.6327	0.3613	0.135
H(9C)	4*e*	–0.5091	0.5894	0.3101	0.135
H(10)	4*e*	0.2042	0.4359	0.1713	0.045
H(11)	4*e*	0.1595	0.3264	–0.1419	0.057
H(12A)	4*e*	0.5105	0.4272	0.2858	0.056
H(12B)	4*e*	0.5770	0.3722	0.2252	0.056
H(13A)	4*e*	0.5894	0.3496	0.4530	0.059
H(13B)	4*e*	0.4155	0.3578	0.4072	0.059
H(14A)	4*e*	0.4487	0.2554	0.4220	0.055
H(14B)	4*e*	0.3896	0.2685	0.2597	0.055
H(15)	4*e*	0.8199	0.2126	0.1916	0.067
H(16)	4*e*	0.6658	0.1787	0.4883	0.048

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*	–0.09845(3)	0.40609(1)	–0.09406(3)	0.0414(2)	0.0386(2)	0.0223(2)	0.0042(2)	0.0120(1)	–0.0002(1)
O(1)	4*e*	–0.1717(2)	0.45845(9)	0.0288(2)	0.071(1)	0.047(1)	0.0246(9)	0.012(1)	0.0248(9)	0.0058(8)
O(2)	4*e*	–0.0825(3)	0.3791(1)	0.1680(2)	0.113(2)	0.059(1)	0.040(1)	0.036(1)	0.040(1)	0.009(1)
O(3)	4*e*	–0.0589(2)	0.38350(9)	0.6618(2)	0.064(1)	0.048(1)	0.0279(9)	0.015(1)	0.0184(9)	0.0080(9)
O(4)	4*e*	–0.1651(2)	0.46038(9)	0.7357(2)	0.056(1)	0.049(1)	0.0204(8)	0.0065(9)	0.0187(8)	0.0009(8)
O(5)	4*e*	0.0860(6)	0.2867(2)	0.5738(4)	0.202(5)	0.089(3)	0.088(3)	0.064(3)	0.081(3)	0.014(2)
O(6)	4*e*	0.1254(4)	0.2055(1)	0.8114(4)	0.091(2)	0.075(2)	0.087(2)	–0.032(2)	0.044(2)	–0.022(2)
N(1)	4*e*	0.1229(2)	0.3881(1)	–0.0095(2)	0.040(1)	0.036(1)	0.027(1)	0.001(1)	0.012(1)	–0.0034(9)
N(2)	4*e*	0.3422(3)	0.3413(1)	0.0243(2)	0.054(2)	0.058(2)	0.038(1)	0.017(1)	0.008(1)	–0.012(1)
N(3)	4*e*	0.3536(2)	0.3801(1)	0.1327(2)	0.040(1)	0.036(1)	0.032(1)	–0.002(1)	0.011(1)	–0.003(1)
N(4)	4*e*	0.6058(2)	0.2430(1)	0.3362(2)	0.043(1)	0.041(1)	0.038(1)	0.002(1)	0.017(1)	0.005(1)
N(5)	4*e*	0.6563(3)	0.2562(1)	0.2299(3)	0.066(2)	0.067(2)	0.059(2)	0.020(2)	0.038(1)	0.027(1)
N(6)	4*e*	0.7815(2)	0.1752(1)	0.3578(2)	0.040(1)	0.043(1)	0.030(1)	0.003(1)	0.013(1)	0.004(1)
C(1)	4*e*	–0.1824(3)	0.4625(1)	0.2587(2)	0.035(1)	0.036(2)	0.020(1)	–0.003(1)	0.012(1)	–0.000(1)
C(2)	4*e*	–0.1364(3)	0.4364(1)	0.3926(2)	0.032(1)	0.036(2)	0.024(1)	0.001(1)	0.010(1)	–0.002(1)
C(3)	4*e*	–0.1773(3)	0.4633(1)	0.4973(2)	0.034(1)	0.037(2)	0.020(1)	–0.003(1)	0.010(1)	–0.001(1)
C(4)	4*e*	–0.2659(3)	0.5162(1)	0.4667(3)	0.058(2)	0.046(2)	0.027(1)	0.006(1)	0.023(1)	–0.002(1)
C(5)	4*e*	–0.3154(3)	0.5427(1)	0.3326(3)	0.065(2)	0.044(2)	0.037(2)	0.017(2)	0.026(1)	0.007(1)
C(6)	4*e*	–0.2710(3)	0.5152(1)	0.2306(3)	0.055(2)	0.043(2)	0.025(1)	0.006(1)	0.020(1)	0.007(1)
C(7)	4*e*	–0.1415(3)	0.4311(1)	0.1459(3)	0.044(2)	0.040(2)	0.026(1)	0.002(1)	0.015(1)	–0.002(1)
C(8)	4*e*	–0.1289(3)	0.4335(1)	0.6410(2)	0.037(2)	0.044(2)	0.021(1)	–0.003(1)	0.010(1)	–0.001(1)
C(9)	4*e*	–0.4159(5)	0.5993(2)	0.2987(4)	0.142(4)	0.084(3)	0.061(2)	0.072(3)	0.058(3)	0.030(2)
C(10)	4*e*	0.2229(3)	0.4074(1)	0.1108(3)	0.044(2)	0.037(2)	0.032(1)	0.000(1)	0.014(1)	–0.006(1)
C(11)	4*e*	0.2017(3)	0.3479(1)	–0.0573(3)	0.055(2)	0.050(2)	0.031(2)	0.009(2)	0.006(1)	–0.012(1)
C(12)	4*e*	0.4944(3)	0.3843(1)	0.2542(3)	0.042(2)	0.042(2)	0.048(2)	–0.004(1)	0.006(1)	–0.005(1)
C(13)	4*e*	0.4947(3)	0.3434(1)	0.3757(3)	0.047(2)	0.057(2)	0.036(2)	0.011(2)	0.007(1)	–0.003(1)
C(14)	4*e*	0.4739(3)	0.2747(1)	0.3470(3)	0.043(2)	0.051(2)	0.048(2)	0.006(1)	0.021(1)	0.007(1)
C(15)	4*e*	0.7623(4)	0.2148(2)	0.2486(3)	0.060(2)	0.064(2)	0.056(2)	0.019(2)	0.036(2)	0.022(2)
C(16)	4*e*	0.6810(3)	0.1956(1)	0.4102(3)	0.048(2)	0.041(2)	0.032(1)	–0.001(1)	0.014(1)	0.005(1)

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