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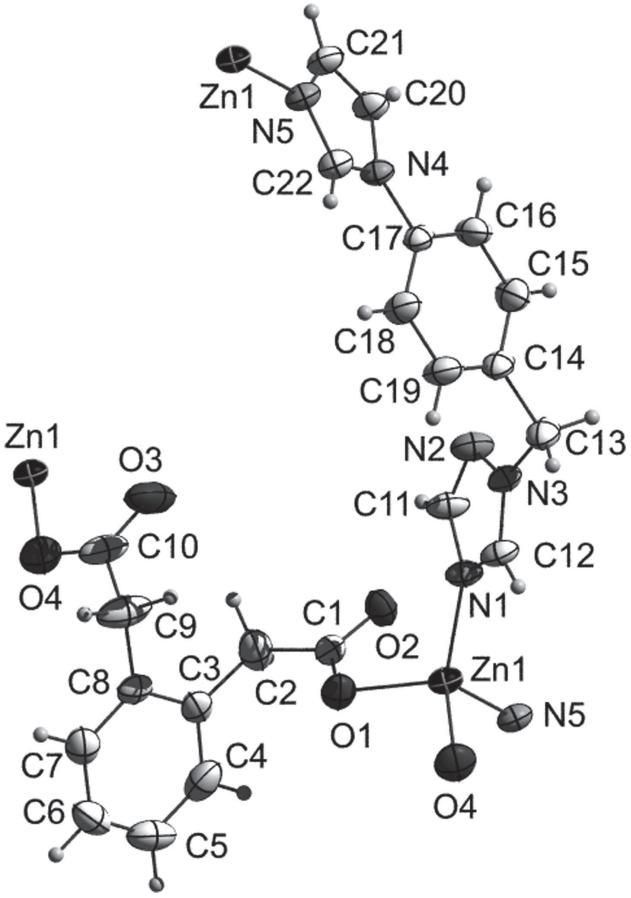
Crystal structure of poly[(μ_2-2,2′-benzene-1,2-diyldiacetato-$\kappa^2O:O'$), (μ_2-1-(4-(1*H*-imidazol-1-yl)-benzyl)-1*H*-1,2,4-triazole-$\kappa^2N:N'$)zinc(II)], $C_{22}H_{19}N_5O_4Zn$



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Abstract

$C_{22}H_{19}N_5O_4Zn$, triclinic, $P\bar{1}$ (no. 2), $a = 8.9023(6)$ Å, $b = 9.9553(7)$ Å, $c = 13.2658(10)$ Å, $\alpha = 111.048(2)°$, $\beta = 96.277(2)°$, $y = 105.763(2)°$, $V = 1027.58(13)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0371$, $wR_{ref}(F^2) = 0.0896$, $T = 293(2)$ K.

CCDC no.: 1040957

Table 1: Data collection and handling.

Crystal:	Colourless, block, size 0.18×0.27×0.32 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	12.36 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω scans
$2\theta_{max}$:	50.44°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6716, 3688
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3123
$N(param)_{refined}$:	289
Programs:	SHELX [12], Bruker programs [13]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2A)	2*i*	0.0925	0.6023	0.7463	0.068
H(2B)	2*i*	0.1937	0.6864	0.8685	0.068
H(4)	2*i*	0.3714	0.9501	0.9352	0.061
H(5)	2*i*	0.4003	1.1878	0.9386	0.062
H(6)	2*i*	0.2556	1.2107	0.7958	0.057
H(7)	2*i*	0.0806	0.9993	0.6512	0.050
H(9A)	2*i*	0.0673	0.6362	0.5716	0.068
H(9B)	2*i*	−0.0220	0.7397	0.5458	0.068
H(11)	2*i*	0.2619	0.2517	0.6138	0.045
H(12)	2*i*	0.6197	0.3030	0.4722	0.040
H(13A)	2*i*	0.4763	−0.0693	0.3658	0.049
H(13B)	2*i*	0.5262	0.0442	0.3089	0.049
H(15)	2*i*	0.2143	−0.2613	0.2982	0.050
H(16)	2*i*	−0.0126	−0.4025	0.1575	0.049
H(18)	2*i*	0.0868	−0.0848	0.0342	0.048
H(19)	2*i*	0.3182	0.0535	0.1736	0.052
H(20)	2*i*	−0.2678	−0.4919	0.0534	0.040
H(21)	2*i*	−0.4651	−0.5812	−0.1186	0.043
H(22)	2*i*	−0.0962	−0.2652	−0.1236	0.037

Table 3: Fractional coordinates and atomic displacement parameters (Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(1)	2*i*	0.58265(4)	0.55239(4)	0.69065(3)	0.0264(2)	0.0285(2)	0.0257(2)	0.0033(1)	0.0026(1)	0.0085(2)
N(1)	2*i*	0.4706(3)	0.3370(3)	0.5743(2)	0.031(1)	0.030(1)	0.023(1)	0.001(1)	0.002(1)	0.009(1)
N(2)	2*i*	0.2965(3)	0.0986(3)	0.4820(2)	0.035(1)	0.037(2)	0.038(2)	−0.001(1)	0.008(1)	0.011(1)
N(3)	2*i*	0.4234(3)	0.1218(3)	0.4347(2)	0.028(1)	0.031(1)	0.023(1)	0.004(1)	−0.000(1)	0.005(1)
N(4)	2*i*	−0.1273(3)	−0.3460(3)	−0.0050(2)	0.027(1)	0.028(1)	0.022(1)	0.004(1)	0.0016(9)	0.008(1)
N(5)	2*i*	−0.3088(3)	−0.4287(3)	−0.1607(2)	0.025(1)	0.032(1)	0.026(1)	0.003(1)	0.002(1)	0.008(1)
O(1)	2*i*	0.4290(2)	0.6683(2)	0.7164(2)	0.033(1)	0.045(1)	0.050(1)	0.013(1)	0.017(1)	0.030(1)
O(2)	2*i*	0.3197(2)	0.4895(2)	0.7741(2)	0.044(1)	0.037(1)	0.047(1)	0.018(1)	0.014(1)	0.024(1)
O(3)	2*i*	−0.1614(3)	0.4846(3)	0.6194(2)	0.045(1)	0.043(2)	0.096(2)	−0.003(1)	0.022(1)	0.008(2)
O(4)	2*i*	−0.2414(3)	0.6844(3)	0.6555(2)	0.040(1)	0.054(2)	0.056(2)	0.012(1)	0.023(1)	0.030(1)
C(1)	2*i*	0.3240(3)	0.6063(3)	0.7583(2)	0.027(2)	0.031(2)	0.034(2)	0.007(1)	0.002(1)	0.012(1)
C(2)	2*i*	0.1953(4)	0.6751(4)	0.7929(4)	0.038(2)	0.054(2)	0.103(3)	0.022(2)	0.033(2)	0.051(2)
C(3)	2*i*	0.2093(3)	0.8262(3)	0.7882(3)	0.024(1)	0.037(2)	0.063(2)	0.011(1)	0.020(2)	0.027(2)
C(4)	2*i*	0.3129(4)	0.9588(4)	0.8767(3)	0.030(2)	0.070(3)	0.056(2)	0.009(2)	0.005(2)	0.036(2)
C(5)	2*i*	0.3302(4)	1.1011(4)	0.8794(3)	0.046(2)	0.038(2)	0.048(2)	−0.003(2)	0.013(2)	0.004(2)
C(6)	2*i*	0.2438(4)	1.1144(4)	0.7947(3)	0.051(2)	0.031(2)	0.065(2)	0.015(2)	0.028(2)	0.019(2)
C(7)	2*i*	0.1399(4)	0.9876(4)	0.7078(3)	0.038(2)	0.047(2)	0.052(2)	0.017(2)	0.017(2)	0.029(2)
C(8)	2*i*	0.1207(3)	0.8416(3)	0.7019(2)	0.022(1)	0.036(2)	0.037(2)	0.006(1)	0.014(1)	0.012(1)
C(9)	2*i*	0.0092(4)	0.7053(4)	0.6020(3)	0.040(2)	0.059(2)	0.044(2)	−0.005(2)	0.020(2)	0.002(2)
C(10)	2*i*	−0.1428(4)	0.6166(4)	0.6255(3)	0.035(2)	0.045(2)	0.036(2)	−0.006(2)	0.008(1)	−0.000(2)
C(11)	2*i*	0.3290(3)	0.2315(3)	0.5654(3)	0.033(2)	0.035(2)	0.032(2)	−0.003(1)	0.009(1)	0.010(2)
C(12)	2*i*	0.5244(3)	0.2623(3)	0.4900(2)	0.027(1)	0.035(2)	0.025(2)	−0.001(1)	−0.001(1)	0.010(1)
C(13)	2*i*	0.4425(4)	−0.0002(4)	0.3401(3)	0.035(2)	0.037(2)	0.035(2)	0.012(1)	−0.003(1)	0.002(1)
C(14)	2*i*	0.2901(3)	−0.0899(3)	0.2502(2)	0.029(2)	0.030(2)	0.025(2)	0.008(1)	−0.001(1)	0.003(1)
C(15)	2*i*	0.1898(4)	−0.2260(4)	0.2445(3)	0.049(2)	0.038(2)	0.033(2)	0.010(2)	−0.006(1)	0.015(2)
C(16)	2*i*	0.0539(4)	−0.3104(3)	0.1606(3)	0.043(2)	0.029(2)	0.040(2)	0.001(1)	−0.005(1)	0.015(2)
C(17)	2*i*	0.0162(3)	−0.2583(3)	0.0812(2)	0.025(1)	0.026(2)	0.025(2)	0.005(1)	0.001(1)	0.004(1)
C(18)	2*i*	0.1133(3)	−0.1215(4)	0.0866(3)	0.036(2)	0.041(2)	0.038(2)	0.002(1)	−0.001(1)	0.023(2)
C(19)	2*i*	0.2512(4)	−0.0382(4)	0.1707(3)	0.035(2)	0.037(2)	0.042(2)	−0.004(1)	−0.003(1)	0.016(2)
C(20)	2*i*	−0.2572(3)	−0.4573(3)	−0.0028(2)	0.030(2)	0.036(2)	0.033(2)	0.004(1)	0.007(1)	0.018(1)
C(21)	2*i*	−0.3654(3)	−0.5057(3)	−0.0980(2)	0.026(1)	0.036(2)	0.037(2)	−0.001(1)	0.003(1)	0.015(2)
C(22)	2*i*	−0.1639(3)	−0.3328(3)	−0.1013(2)	0.027(1)	0.032(2)	0.027(2)	0.005(1)	0.004(1)	0.010(1)

Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The mixtures of 1,2-phenylenediacetic acid (0.1 mmol, 19.4 mg), 1-(imidazo-1-ly)-4-(1,2,4-triazol-1-yl-methyl)benzene (0.1 mmol, 22.5 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 23 mL Teflon liner stainless steel reactor. The vessel was heated to 393 K for 4 days, and then slowly cooled to room temperature. Colorless crystals were obtained, filtered off, washed with mother liquid, and dried under ambient conditions. Yield: 67%.

Experimental details

The hydrogen atoms were placed on calculated positions using a riding model (AFIX 23 or 43 option of the SHELX program [12].

Discussion

Design and construction of novel coordination networks or metal organic frameworks (MOFs) continue to receive researchers attention, due to its structural diversity [1, 2], intriguing topology architecture [3, 4], and potential applications in areas such as gas storage, fluorescence, catalysis, and magnetism etc. [5–9]. The effective and facile approach for the synthesis of such complexes is still the appropriate choice of well-designed organic ligands as bridges or terminal groups (building blocks) with metal ions or clusters as nodes. It is to be noted that the flexibility of the ligand can afford a good opportunity to enrich the structural and functional diversities of MOFs. It is because that flexible molecules can easily adjust their conformations to meet the coordination requirement of the metal ion [10] and may be prone to promote helical or looped structural motifs through which other organic linkers can penetrate. Thus, the flexibility of the ligand can afford a good opportunity to enrich the structural and functional diversities of MOFs and provide the further understanding of

the directional synthesis of target coordination polymers. It is therefore an important aspect worthwhile paying attention to, and is the potential for erecting some signposts toward future research on predicted and pre-designed coordination polymers [11].

Herein, a 2D grid zinc coordinated polymer assemblied from flexible carboxylate ligand, 2,2′-benzene-1,2-diyldiacetate (H_2phda) and the coligand, 1-(imidazo-1-ly)-4-(1,2,4-triazol-1-yl-methyl)benzene (itmb). The asymmetric unit contains one Zn ion, one phda dianion and one itmb molecule. Each Zn(II) is coordinated by two carboxylate oxygen atoms from two different phda ligands (Zn(1)—O(4)#1 = 1.970(2) (#1 = $1+x$, y, z) and Zn(1)—O(1) = 1.999(2) Å) and two nitrogen atoms from two different itmb molecules (Zn(1)—N(5)#2 = 2.019(2) (#2 = $1+x$, $1+y$, $1+z$) and Zn(1)—N(1) = 2.024(2) Å) to form a distorted tetrahedral geometry (see the figure). Each phda coordinates adjacent Zn(II) in a mondentate bridging mode to yield an undulating $[Zn(phda)]_n$ chain with a Zn···Zn distance of 8.9023(6) Å, which is further cross-linked by itmb ligands to develop a 2D open layer containing rhombic grids, wherein each phda anion is located above or below the layer plane as dangling lateral arms. The parallel layers stack in a AB sequence with each dangling lateral arm deeply interpenerating into the cavity of the adjacent layers, that is, these 2D open layers exist in a mutually embedded mode. Interestingly, no hydrogen bonding is observed between the layers, which stack in a slightly off-set parallel fashion and are cohered only by the weak van der Waals force to complish its entire 3D supramolecular structure.

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