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Crystal structure of poly[(μ_2-2-carboxy-5-nitro-isophthalato-κ^2O:O')-(μ_2-4-((1*H*-imidazol-1-yl)methyl)pyridine-κ^2N:N')zinc(II)], $C_{18}H_{12}N_4O_8Zn$

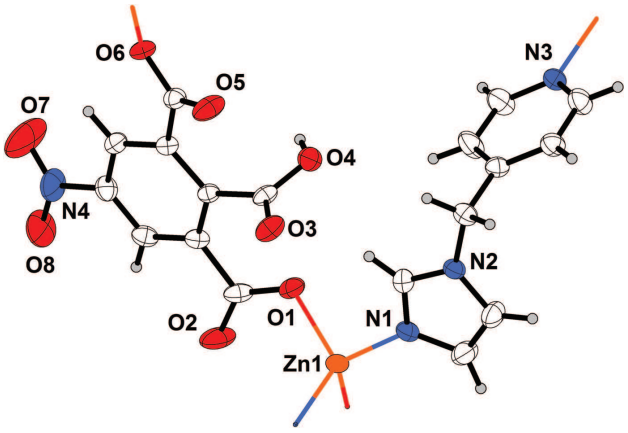

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.32 × 0.28 × 0.21 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	1.40 mm^{-1}
Diffractometer, scan mode:	SuperNova, φ and ω-scans
θ_{max}, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9731, 3218, 0.028
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2868
$N(param)_{refined}$:	281
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3], OLEX2 [4]

https://doi.org/10.1515/ncrs-2018-0156
Received April 24, 2018; accepted July 26, 2018; available online August 18, 2018

Abstract

$C_{18}H_{12}N_4O_8Zn$, monoclinic, $P2_1/n$ (no. 14), $a = 9.5472(6)$ Å, $b = 21.1662(10)$ Å, $c = 9.6909(6)$ Å, $\beta = 110.525(7)°$, $V = 1834.0(2)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0371$, $wR_{ref}(F^2) = 0.0809$, $T = 291.2(3)$ K.

CCDC no.: 1838164

The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Zn(OAc)_2 \cdot 2H_2O$ (22.0 mg, 0.1 mmol), 1,2,3-benzenetricarboxylic acid (25.5 mg, 0.1 mmol), N-(4-pyridylmethyl)imidazole (15.9 mg, 0.1 mmol) and 6 mL distilled water in a 25 mL Teflon-lined autoclave was kept under autogenous pressure at 413 K for 5 days. After cooling to room temperature at a rate of 5 K h^{-1}, colourless block crystals were collected by filtration and washed with distilled water in 27% yield. Elemental analysis calc: C 45.26%, H 2.53%, N 11.73%.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Discussion

For decades, coordination polymers have been investigated due to their intriguing topological variety and potential applications [5–7]. In general, the structures of coordination polymers are totally dependent on organic ligands with different binding sites, metal ions with various coordination abilities, and reaction conditions such as temperature, pH, solvent, and reaction time. Multicarboxylic acids and the deprotonated products are employed to construct many coordination polymers with interesting structures. From a structural point of view, the anions of the 5-nitro-1,2,3-benzenetricarboxylic acid (H_3nbta) may act as good ligands bearing up to three carboxylate groups and non-coordinating electron-withdrawing nitro-group on the aromatic backbone [8]. In addition, the flexible 4-((1*H*-imidazol-1-yl)methyl)pyridine (pyim) ligand possesses flexibility owing to the presence of a –CH_2– spacer between the pyridyl ring and imidazole moiety, which makes it a useful bridge to construct coordination polymers [9].

In this work, we report a two-dimensional coordination polymer constructed from central Zn(II) ions, dianionic

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.35765(4)	0.59229(2)	0.62976(4)	0.02586(12)
O1	0.3705(2)	0.55468(10)	0.4510(2)	0.0358(5)
O2	0.1724(3)	0.49616(12)	0.4314(3)	0.0580(7)
O3	0.3570(2)	0.64236(9)	0.2231(2)	0.0374(5)
O4	0.5573(2)	0.58564(9)	0.2528(2)	0.0346(5)
H4	0.5773	0.5493	0.2370	0.052*
O5	0.3879(3)	0.61246(10)	−0.0691(2)	0.0454(6)
O6	0.3546(2)	0.53056(9)	−0.2195(2)	0.0290(5)
O7	0.0709(5)	0.35134(18)	−0.1497(4)	0.1197(16)
O8	−0.0079(3)	0.34853(14)	0.0300(3)	0.0704(9)
N1	0.5235(3)	0.65433(12)	0.6663(3)	0.0309(6)
N2	0.6750(3)	0.71635(11)	0.6043(3)	0.0275(5)
N3	1.1663(3)	0.64316(11)	0.5877(3)	0.0282(5)
N4	0.0620(4)	0.37272(15)	−0.0377(4)	0.0547(8)
C1	0.2644(4)	0.51812(14)	0.3822(3)	0.0321(7)
C2	0.2502(3)	0.50062(13)	0.2260(3)	0.0271(6)
C3	0.1636(3)	0.44850(14)	0.1630(3)	0.0324(7)
H3	0.1165	0.4256	0.2162	0.039*
C4	0.1474(3)	0.43068(14)	0.0229(3)	0.0337(7)
C5	0.2096(3)	0.46461(14)	−0.0626(3)	0.0317(7)
H5	0.1951	0.4520	−0.1586	0.038*
C6	0.2941(3)	0.51778(13)	−0.0033(3)	0.0246(6)
C7	0.3518(3)	0.55754(14)	−0.1008(3)	0.0274(6)
C8	0.3169(3)	0.53560(12)	0.1429(3)	0.0229(6)
C9	0.4109(3)	0.59256(13)	0.2089(3)	0.0267(6)
C10	0.5695(3)	0.67202(15)	0.5597(3)	0.0348(7)
H10	0.5330	0.6556	0.4647	0.042*
C11	0.6045(4)	0.68971(15)	0.7860(4)	0.0407(8)
H11	0.5965	0.6877	0.8788	0.049*
C12	0.6974(4)	0.72790(15)	0.7476(3)	0.0395(8)
H12	0.7644	0.7568	0.8083	0.047*
C13	0.7555(3)	0.74302(14)	0.5143(3)	0.0313(7)
H13A	0.7758	0.7874	0.5384	0.038*
H13B	0.6936	0.7400	0.4110	0.038*
C14	0.9005(3)	0.70865(13)	0.5402(3)	0.0284(7)
C15	1.0360(3)	0.73869(14)	0.5923(3)	0.0329(7)
H15	1.0404	0.7817	0.6125	0.040*
C16	1.1654(3)	0.70527(14)	0.6149(4)	0.0378(8)
H16	1.2562	0.7266	0.6504	0.045*
C17	1.0338(4)	0.61408(15)	0.5379(4)	0.0423(8)
H17	1.0317	0.5709	0.5194	0.051*
C18	0.9009(4)	0.64492(15)	0.5127(4)	0.0427(8)
H18	0.8112	0.6228	0.4771	0.051*

Hnbta and pyim ligands. The title compound, $C_{18}H_{12}N_4O_8Zn$, was prepared under hydrothermal condition. The asymmetric unit of the crystal structure consists of one Zn(II) ion, one $Hnbta^{2-}$ anion and one pyim ligand. Each Zn(II) ion is four-coordinated with distorted tetrahedral geometry and defined by two carboxylate oxygen atoms from two Hnbta anionic ligands (Zn–O bond lengths are 1.949(2), and 1.9675(19) Å) and two N-atoms donor from two pyim ligands (Zn–N bond lengths are 1.991(2), and 2.035(2) Å). Both Zn–O and Zn–N bond lengths are well-matched to those in similar complexes [10, 11]. The 1- and 3-positions in the Hnbta ligand are deprotonated and coordinated to two Zn(II), while the 2-position is still protonated. The Hnbta anions link the Zn(II) ions into a one-dimensional chain structure, and the pyim ligands further connect adjacent chanis to generate a two-dimensional layer.

Acknowledgements: We thank the Natural Science Foundation of Henan Province (No. 172102210410) for the financial support.

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