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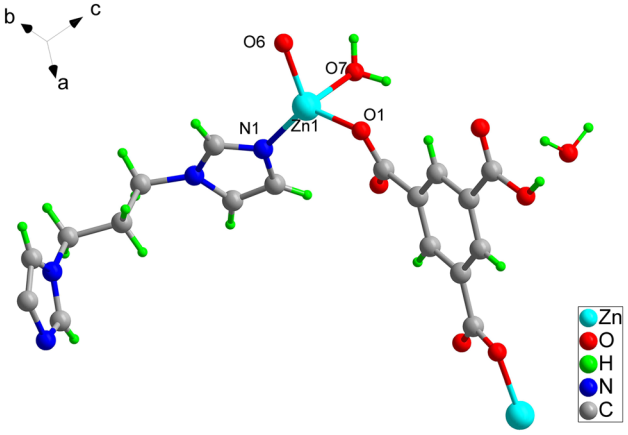
Crystal structure of poly[diaqua-(μ_2-1,3-di(1*H*-imidazol-1-yl)propane-κ^2N:*N*′)-bis(μ_2-5-carboxybenzene-1,3-dicarboxylato-*O*,*O*′:*O*″)-aqua-di-zinc dihydrate solvate], $C_{27}H_{28}N_4O_{16}Zn_2$



https://doi.org/10.1515/ncrs-2023-0315
Received July 7, 2023; accepted July 31, 2023;
published online August 10, 2023

Abstract

$C_{27}H_{28}N_4O_{16}Zn_2$, monoclinic, *C*2/*c* (no. 15), a = 13.0720(3) Å, b = 15.7589(5) Å, c = 15.7589(5) Å, β = 95.373(3)°, V = 3062.48(18) Å^3, Z = 4, $R_{gt}(F)$ = 0.0499, w$R_{ref}(F^2)$ = 0.1059, T = 294 K.

CCDC no.: 1569490

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.18 × 0.15 × 0.14 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	1.65 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	26.0°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5808, 3012, 0.026
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 2478
$N(param)_{refined}$:	229
Programs:	Bruker [1], Olex2 [2], SHELX [3,4]

1 Source of material

The mixture of copper nitrate hydrate 44.6 mg (0.15 mmol), 1,3-di(1*H*-imidazol-1-yl)propane 17.6 mg (0.10 mmol), 1,3,5-benzene tricarboxylate acid 16.6 mg (0.06 mmol), NaOH 4 mg (0.1 mmol) and ethyl alcohol (10 mL) were placed in the autoclave lined with PTFE and heated at 110 °C for 46 h, then cooled up to room temperature over 24 h. Colourless block crystals were collected after cooling to room temperature.

2 Experimental details

Using Olex2 [2], the structure was solved with the ShelXT [3] structure solution program and refined with the ShelXL [4] refinement package.

3 Comment

The crystal engineering of metal organic framework (MOFs) is one of the most rapidly developing areas of chemical science. The expansion of this research area is not only interesting in terms of structural diversity and fascinating properties but also regarding the wide range of applications for example [5,6]. N-containing ligands have received considerable attention because of their versatile coordination models for the design of multifunctional coordination polymers.

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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	0.36003 (3)	0.27105 (3)	0.07953 (3)	0.03562 (16)
O1	0.37396 (19)	0.14900 (16)	0.10835 (18)	0.0346 (6)
O2	0.5418 (2)	0.17188 (18)	0.1313 (3)	0.0529 (9)
O3	0.25454 (19)	−0.14186 (19)	0.1835 (2)	0.0445 (8)
O4	0.3666 (2)	−0.24817 (18)	0.1828 (3)	0.0500 (9)
O5	0.7704 (2)	−0.07203 (19)	0.0851 (3)	0.0549 (9)
O6	0.71197 (18)	−0.20362 (15)	0.07798 (18)	0.0306 (6)
O7	0.39887 (18)	0.31195 (17)	0.21395 (19)	0.03562 (16)
H7A	0.408285	0.268808	0.251839	0.053*
H7B	0.349283	0.343592	0.232647	0.053*
N1	0.4541 (2)	0.33569 (19)	0.0095 (2)	0.0271 (7)
N2	0.5015 (3)	0.4289 (2)	−0.0871 (2)	0.0343 (8)
C1	0.4675 (3)	0.1234 (2)	0.1208 (3)	0.0308 (9)
C2	0.4836 (3)	0.0290 (2)	0.1230 (2)	0.0245 (8)
C3	0.4059 (3)	−0.0259 (2)	0.1412 (2)	0.0259 (8)
H3	0.341784	−0.004387	0.151522	0.031*
C4	0.4226 (3)	−0.1131 (2)	0.1442 (2)	0.0244 (8)
C5	0.5175 (3)	−0.1457 (2)	0.1246 (2)	0.0249 (8)
H5	0.528149	−0.204044	0.124566	0.030*
C6	0.5954 (2)	−0.0913 (2)	0.1052 (2)	0.0224 (7)
C7	0.5785 (3)	−0.0041 (2)	0.1054 (2)	0.0240 (8)
H7	0.631377	0.032612	0.093678	0.029*
C8	0.3394 (3)	−0.1689 (2)	0.1711 (3)	0.0305 (9)
C9	0.7004 (3)	−0.1227 (2)	0.0875 (3)	0.0268 (8)
C10	0.4228 (3)	0.3874 (3)	−0.0568 (3)	0.0347 (9)
H10	0.354630	0.394111	−0.079524	0.042*
C11	0.5882 (3)	0.4023 (3)	−0.0375 (3)	0.0428 (11)
H11	0.655056	0.420089	−0.043657	0.051*
C12	0.5586 (3)	0.3454 (3)	0.0220 (3)	0.0344 (9)
H12	0.602214	0.317090	0.064891	0.041*
C13	0.4963 (4)	0.4852 (3)	−0.1658 (3)	0.0457 (11)
H13A	0.553511	0.524573	−0.160021	0.055*
H13B	0.433059	0.517713	−0.169243	0.055*
C14	0.500000	0.4334 (4)	−0.250000	0.0454 (16)
H14A[a]	0.560104	0.397052	−0.243062	0.054*
H14B[a]	0.439893	0.397055	−0.256939	0.054*
O8	0.2287 (3)	−0.3549 (2)	0.2277 (3)	0.0590 (10)
H8A	0.173 (3)	−0.348 (4)	0.190 (3)	0.10 (3)*
H8B	0.208 (5)	−0.354 (5)	0.282 (2)	0.12 (3)*
H4	0.318 (3)	−0.282 (3)	0.199 (4)	0.11 (2)*

[a]Occupancy: 0.5.

Meanwhile, the bis(imidazole)propane bearing alkyl spacers are a good choice [7,8], in which the flexible nature of spacers allows the ligands to bend and rotate when it coordinates to metal centres, and 1,3-di(1*H*-imidazol-1-yl)propane(diim) is known to serve as bridging ligand [9–11].

The asymmetric unit of the title structure contains one Zn(II), one half of a 1,3-di(1*H*-imidazol-1-yl)propane, one 1,3,5-benzene tricarboxylate anion, an unidentate coordinated water molecule and one free water molecule. As shown in Figure, Zinc(II) ions exhibit a distorted tetrahedral geometry, with two oxygen atoms from two 1,3,5-benzene tricarboxylate acid anions, one nitrogen atom from one 1,3-di(1*H*-imidazol-1-yl) propane ligand, and one oxygen atom from one unidentate coordinated water molecule. Two carboxyl groups of 1,3,5-benzene tricarboxylate acid ligands are deprotonated and two carboxylate oxygen atoms connect adjacent Zn(II) cations to form a one-dimensional chain. Meanwhile, 1,3-di(1*H*-imidazol-1-yl)propane, as a bridging ligand connects two adjacent Zn(II) of the above-mentioned one dimensional chains forming an interesting 3D framework. The title structure exhibit an interesting 3D non-interpenetrated structure [12,13]

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

Research funding: The Innovation Team of Shaanxi Universities (No. 2022–94), Research project of Shaanxi University of Science and Technology (SLGKYXM2304).

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