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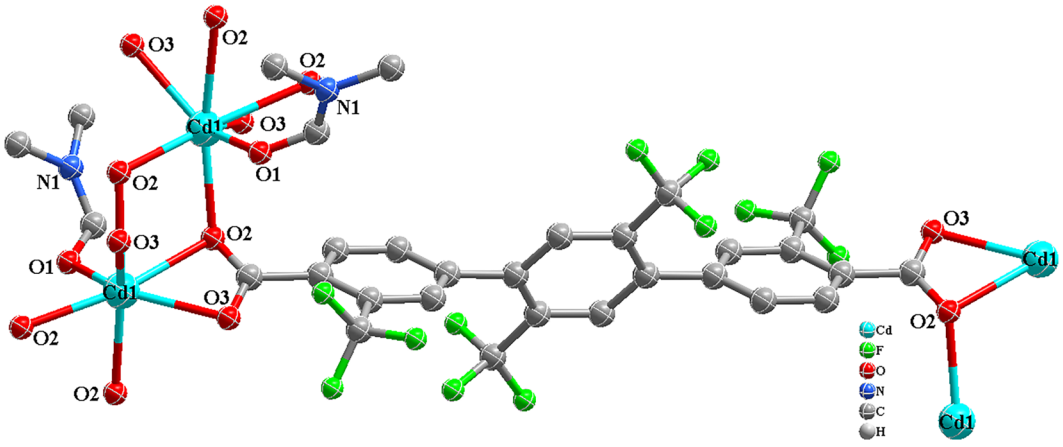
The crystal structure of poly [bis(dimethylformamide-κ^{1}N)-(μ$_4$-2′,3,3″,5′-tetrakis(trifluoromethyl)-[1,1′:4′,1″-terphenyl]-4,4″-dicarboxylato-κ^4*O*,*O*′:*O*″,*O*‴)dicadmium(II)], $C_{27}H_{15}CdF_{12}NO_5$



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Abstract

$C_{27}H_{15}CdF_{12}NO_5$, orthorhombic, *Pnma* (no. 62), a = 7.6643(3) Å, b = 31.5516(10) Å, c = 11.1830(4) Å, V = 2704.28(17) Å^3, Z = 4, $R_{gt}(F)$ = 0.0359, w$R_{ref}(F^2)$ = 0.0906, T = 100 K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of material

The reagents were purchased from standard commercial sources and used without further purification. The

Table 1: Data collection and handling.

Crystal:	Clear whitish block
Size:	0.20 × 0.14 × 0.1 0mm
Wavelength:	CuKα radiation (1.54184 Å)
μ:	7.63 mm^{-1}
Diffractometer, scan mode:	Rigaku synergy R, ω scans
θ_{max}, completeness:	76.2°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9169, 2754, 0.028
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2734
$N(param)_{refined}$:	268
Programs:	Rigaku,[1] Shelx,[2] Olex2[3]

2′,3,3″,5′-tetrakis(trifluoromethyl)-[1,1′:4′,1″-terphenyl]-4,4″-dicarboxylic acid (H_2TPDC-4CF_3) was synthesized according to literature.[4] The preparation of the title crystal is similar to the previously reported literature procedure.[5,6] A mixture of H_2TPDC-4CF_3 (6.0 mg 0.01 mmol) and $Cd(NO_3)_2{\cdot}4H_2O$ (6.0 mg 0.02 mmol) were dispersed in a mixed solution of *N*,*N*-dimethyl formamide (1.5 mL) and methyl alcohol (1.5 mL) and sealed in a caped glass bottle at 375 K for 72 h. The colourless block crystals suitable for X-ray single crystal diffraction analysis were prepared with the yield of 60 % based on H_2TPDC-4CF_3.

2 Experimental details

The initial crystal structure was solved and refined by Olex2 and SHELXS.[2,3] Anisotropic displacement parameters were assigned to all non-hydrogen atoms. Hydrogen atoms were located at geometrically calculated positions and refined with fixed thermal factors.

3 Comment

Metal-organic frameworks (MOFs) have attracted tremendous interest as a promising class of functional crystalline porous materials.[7–10] With the development of crystal engineering, the structures of MOFs can be predesigned and predicted according to several useful strategies such as reticular chemistry and soft/hard acid/base principle. In addition, the performance and structures of MOFs also could be significantly improved by introducing functional ligands containing F-carboxylic acids.[11–14] Recently, the LZPU-3 was obtained by using H_2TPDC-4CF_3 and $Cd(NO_3)_2{\cdot}4H_2O$ under solvothermal conditions.

The asymmetric structural unit consists of one Cd atoms, one half of a deprotonated H_2TPDC-4CF_3 ligand, and one coordinated DMF molecule. The Cd(II) atom is coordinated with six oxygen atoms from four deprotonated H_2TPDC-4CF_3 ligands and one oxygen atom from coordinated DMF molecule, which form a seven-coordinated monocapped trigonal prism configuration. This deprotonated H_2TPDC-4CF_3 ligand adopts a tridentate bridging coordination mode. The Cd–O bond lengths fall in the range 2.267(3)–2.496(2) Å. In LZPU-3, the three benzene rings of the H_2TPDC-4CF_3 ligand are respectively located on two planes. Among them, R_1 and R_3 are on one plane while R_2 is on the other plane. The angle between the two planes is 68.34° and this phenomenon is rare in previously reported MOFs materials.[15,16]

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

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