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Crystal structure of poly[aqua-(μ_2 -3,3',4,5'-biphenyl tetracarboxylate- $\kappa^3 O, O':O''$)-(μ_2 -4,4'-bis(pyrid-4-yl) biphenyl- $\kappa^2 N:N'$)zinc(II)], $C_{27}H_{18}NO_9Zn$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.42 × 0.35 × 0.28 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.14 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	25.5°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	12,566, 4227, 0.073
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3150
$N(\text{param})_{\text{refined}}$:	345
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

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Abstract

$C_{27}H_{18}NO_9Zn$, triclinic, $P\bar{1}$ (no. 2), $a = 8.4357(10)$ Å, $b = 10.1228(10)$ Å, $c = 13.5186(10)$ Å, $\alpha = 83.830(7)^\circ$, $\beta = 10.1228(10)^\circ$, $\gamma = 13.5186(10)^\circ$, $V = 1142.05(19)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0665$, $wR_{\text{ref}}(F^2) = 0.1427$, $T = 293(2)$ K.

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A part of the molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Zn(OAc)_2 \cdot 2H_2O$ (22 mg, 0.1 mmol), 4,4'-bis(pyrid-4-yl)biphenyl (0.06 g, 0.2 mmol) and 3,3',4,5'-biphenyl tetracarboxylic acid (H4btc) (0.1 mmol, 0.0330 g), was dissolved

in 10 mL H_2O . The solution was then heated in a 23 mL Teflon-lined autoclave under autogenous pressure at 383 K for two days. After cooling to room temperature crystals formed. The colourless crystals suitable for X-ray diffraction analysis were collected.

Experimental details

All H atoms were placed geometrically and refined as riding with $U_{\text{iso}}(H) = 1.2\text{--}1.5 U_{\text{eq}}(C, O)$ using the appropriate SHELXL AFIX commands.

Discussion

Comment

In the last two decades, a large number of mixed ligands-metal-organic frameworks (MOFs) has been reported in the literature. Mixed-ligands MOFs can be constructed from metal ions and carboxylic acid and nitrogen-containing ligands. In most situations, N-containing ligands are electrically neutral, while carboxylate ligands are negatively charged. Among organic aromatic multicarboxylates biphenyl-tetracarboxylic acids can yield predetermined networks and have been widely utilized to construct MOFs [4–8]. 4,4'-Bis(pyrid-4-yl)biphenyl often serves as a doubly bridging ligand [9–13].

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Zn1	0.73694 (6)	0.40771 (5)	0.63134 (4)	0.0302 (2)
N1	0.5822 (5)	0.5138 (4)	0.7193 (3)	0.0335 (9)
O1	0.7959 (4)	0.5500 (3)	0.5131 (2)	0.0394 (8)
H1A	0.8218	0.6364	0.5295	0.059*
H1B	0.8441	0.5614	0.4437	0.059*
O2	0.8153 (4)	0.2579 (3)	0.4861 (3)	0.0498 (10)
O3	0.5868 (3)	0.3044 (3)	0.5661 (2)	0.0335 (8)
O4	0.0985 (4)	0.2047 (4)	0.4415 (3)	0.0675 (13)
H4	0.0014	0.2087	0.4410	0.101*
O5	0.0718 (4)	0.0409 (4)	0.3507 (3)	0.0606 (12)
O6	0.8345 (4)	−0.3967 (4)	0.0045 (2)	0.0563 (11)
H6	0.8890	−0.4460	−0.0294	0.084*
O7	1.0200 (4)	−0.4456 (3)	0.1097 (2)	0.0449 (9)
O8	1.0010 (5)	−0.4326 (4)	0.3377 (2)	0.0652 (12)
O9	1.1544 (4)	−0.2730 (4)	0.2639 (3)	0.0547 (10)
C1	0.9012 (6)	−0.3829 (5)	0.0854 (3)	0.0340 (10)
C2	0.8206 (5)	−0.2867 (4)	0.1487 (3)	0.0290 (9)
C3	0.6861 (5)	−0.2219 (4)	0.1186 (3)	0.0332 (9)
H3	0.6490	−0.2385	0.0587	0.040*
C4	0.6053 (5)	−0.1324 (4)	0.1758 (3)	0.0337 (9)
H4A	0.5139	−0.0908	0.1547	0.040*
C5	0.6604 (5)	−0.1050 (4)	0.2644 (3)	0.0268 (8)
C6	0.7973 (5)	−0.1691 (4)	0.2942 (3)	0.0266 (8)
H6A	0.8358	−0.1500	0.3533	0.032*
C7	0.8780 (5)	−0.2606 (4)	0.2385 (3)	0.0271 (8)
C8	0.5764 (5)	−0.0066 (4)	0.3247 (3)	0.0252 (8)
C9	0.4110 (5)	0.0087 (4)	0.3270 (3)	0.0263 (8)
H9	0.3538	−0.0422	0.2896	0.032*
C10	0.3313 (5)	0.0991 (4)	0.3846 (3)	0.0260 (8)
C11	0.4172 (5)	0.1751 (4)	0.4411 (3)	0.0259 (8)
H11	0.3642	0.2353	0.4800	0.031*
C12	0.5803 (5)	0.1614 (4)	0.4394 (3)	0.0270 (8)
C13	0.6590 (5)	0.0715 (4)	0.3814 (3)	0.0250 (8)
H13	0.7690	0.0631	0.3803	0.030*
C14	0.1549 (5)	0.1101 (4)	0.3882 (3)	0.0301 (9)
C15	0.6686 (5)	0.2450 (4)	0.5010 (3)	0.0294 (8)
C16	1.0215 (6)	−0.3276 (5)	0.2804 (3)	0.0342 (9)
C17	0.4285 (6)	0.5237 (5)	0.7034 (3)	0.0356 (9)
H17	0.3934	0.4761	0.6546	0.043*
C18	0.3190 (6)	0.5992 (4)	0.7541 (3)	0.0372 (9)
H18	0.2140	0.6024	0.7385	0.045*
C19	0.3645 (6)	0.6712 (5)	0.8287 (3)	0.0352 (10)
C20	0.5232 (6)	0.6585 (5)	0.8468 (3)	0.0472 (10)
H20	0.5601	0.7032	0.8966	0.057*
C21	0.6283 (6)	0.5806 (5)	0.7922 (3)	0.0447 (10)
H21	0.7338	0.5746	0.8067	0.054*
C22	0.2535 (6)	0.7624 (5)	0.8816 (3)	0.0390 (10)
C23	0.1242 (6)	0.8189 (5)	0.8387 (3)	0.0396 (10)
H23	0.1013	0.7937	0.7775	0.048*
C24	0.0267 (6)	0.9115 (5)	0.8826 (3)	0.0426 (10)
H24	−0.0567	0.9494	0.8493	0.051*
C25	0.0519 (6)	0.9488 (5)	0.9762 (3)	0.0377 (10)
C26	0.1764 (6)	0.8866 (5)	1.0223 (4)	0.0486 (11)
H26	0.1945	0.9064	1.0859	0.058*

Table 2: (continued)

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
C27	0.2749 (6)	0.7957 (5)	0.9765 (3)	0.0484 (11)
H27	0.3571	0.7561	1.0100	0.058*

The asymmetric unit of the title complex contains a Zn(II) cation, one coordinated water molecule, one 3,3',4,5'-biphenyl tetracarboxylate ligand and one half of the 4,4' bis(pyrid-4-yl) biphenyl ligand. The cation is five-coordinated with a distorted octahedral geometry by three O atoms from two H4btc units, one water molecule, and one N atom from the 4,4'-bis(pyrid-4-yl)biphenyl ligand (see the figure). All bond lengths and angles are within the expected ranges. All hydrogen-bond donors and acceptors participate in several hydrogen bonds giving rise to a three-dimensional supramolecular structure.

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