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Crystal structure of 4-(4'-(pyridin-4-yl)-[1,1'-biphenyl]-4-yl)pyridin-1-ium 2-carboxy-4-(3,5-dicarboxyphenoxy)benzoate hydrate, $C_{38}H_{28}N_2O_{10}$

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Abstract

$C_{38}H_{28}N_2O_{10}$, triclinic, $P\bar{1}$ (no. 2), $a = 11.3207(6)$ Å, $b = 11.9296(6)$ Å, $c = 13.6079(8)$ Å, $\alpha = 115.195(5)^\circ$, $\beta = 103.259(5)^\circ$, $\gamma = 97.356(4)^\circ$, $V = 1564.58(15)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0537$, $wR_{\text{ref}}(F^2) = 0.1286$, $T = 293(2)$ K.

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The molecular salt 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.

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Table 1: Data collection and handling.

Crystal:	Colourless
Size:	$0.41 \times 0.32 \times 0.28$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.11 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
θ_{max} , completeness:	25.5° , $>99\%$
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	18117, 5833, 0.033
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4276
$N(\text{param})_{\text{refined}}$:	460
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

Source of material

A mixture of 5-(3',4'-dicarboxylphenoxy)-isophthalic acid (50 mg, 0.1 mmol) and 4,4'-bis(pyrid-4-yl)biphenyl (6 mg, 0.1 mmol) were added to water (7 mL) in a 25 mL Teflon-lined autoclave. The mixture was heated at 413 K for 5 days and then slowly cooled down to room temperature. The colourless crystals were collected.

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
N1	−0.2875(2)	0.6847(2)	0.2081(2)	0.0573(6)
N2	0.71427(18)	1.24740(18)	−0.19622(18)	0.0446(5)
H2	0.7707	1.2734	−0.2201	0.053*
O1	0.7567(2)	0.9469(2)	0.5283(3)	0.1092(9)
H1A	0.6816	0.9089	0.5152	0.164*
H1B	0.7527	1.0205	0.5355	0.164*
O2	0.12326(14)	0.36157(17)	0.34295(14)	0.0494(4)
O3	−0.08200(18)	0.3501(2)	0.75002(17)	0.0628(5)
O4	−0.21991(15)	0.20948(17)	0.58662(16)	0.0536(5)
O5	0.09728(19)	0.53173(19)	0.82137(15)	0.0654(5)
O6	0.2084(2)	0.62335(16)	0.75194(17)	0.0747(6)
O7	0.47847(16)	0.18561(18)	0.48554(18)	0.0633(5)
O8	0.63586(15)	0.26974(17)	0.44637(17)	0.0521(5)
H8	0.6758	0.2393	0.4827	0.078*
O9	0.59516(16)	0.5628(2)	0.2899(2)	0.0708(6)
H9	0.6194	0.6029	0.2589	0.106*
O10	0.40695(17)	0.54724(18)	0.18354(17)	0.0622(5)
C1	0.42198(19)	0.45077(18)	0.30505(18)	0.0319(5)
C2	0.49480(19)	0.39033(18)	0.35241(18)	0.0320(5)
H2A	0.5778	0.3970	0.3533	0.038*
C3	0.44390(19)	0.31980(18)	0.39865(17)	0.0307(5)
C4	0.32082(19)	0.31191(19)	0.40015(18)	0.0342(5)
H4	0.2872	0.2666	0.4328	0.041*
C5	0.24928(19)	0.37217(19)	0.35258(18)	0.0335(5)
C6	0.2983(2)	0.44027(19)	0.30412(18)	0.0334(5)
H6	0.2483	0.4790	0.2709	0.040*
C7	0.07899(19)	0.3430(2)	0.42363(19)	0.0350(5)
C8	0.12058(19)	0.4346(2)	0.5367(2)	0.0360(5)
H8A	0.1864	0.5053	0.5611	0.043*
C9	0.06694(19)	0.42424(18)	0.61558(19)	0.0321(5)
C10	−0.03566(19)	0.31775(19)	0.57623(19)	0.0332(5)
C11	−0.0720(2)	0.2258(2)	0.4616(2)	0.0410(6)
H11	−0.1374	0.1540	0.4354	0.049*
C12	−0.0156(2)	0.2363(2)	0.3855(2)	0.0420(6)
H12	−0.0411	0.1724	0.3097	0.050*
C13	−0.1165(2)	0.2919(2)	0.6433(2)	0.0415(6)
C14	0.1288(2)	0.5346(2)	0.7357(2)	0.0462(6)
C15	0.5192(2)	0.2515(2)	0.44782(19)	0.0365(5)
C16	0.4735(2)	0.5256(2)	0.2526(2)	0.0378(5)
C17	−0.2871(2)	0.6301(3)	0.1005(3)	0.0585(7)
H17	−0.3475	0.5541	0.0480	0.070*
C18	−0.2021(2)	0.6800(2)	0.0627(2)	0.0508(6)
H18	−0.2057	0.6378	−0.0137	0.061*
C19	−0.1105(2)	0.7938(2)	0.1384(2)	0.0386(5)
C20	−0.1131(2)	0.8507(2)	0.2503(2)	0.0535(7)
H20	−0.0553	0.9279	0.3045	0.064*
C21	−0.2005(3)	0.7937(3)	0.2814(3)	0.0600(8)
H21	−0.1989	0.8331	0.3573	0.072*
C22	−0.0146(2)	0.84990(19)	0.1021(2)	0.0353(5)
C23	−0.0270(2)	0.8068(2)	−0.0134(2)	0.0428(6)
H23	−0.0973	0.7426	−0.0687	0.051*
C24	0.0622(2)	0.8571(2)	−0.0472(2)	0.0401(5)
H24	0.0512	0.8256	−0.1250	0.048*
C25	0.16870(19)	0.95420(18)	0.03195(19)	0.0324(5)
C26	0.1809(2)	0.99723(19)	0.14722(19)	0.0391(5)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H26	0.2511	1.0617	0.2025	0.047*
C27	0.0918(2)	0.9466(2)	0.1813(2)	0.0407(6)
H27	0.1029	0.9779	0.2590	0.049*
C28	0.26451(19)	1.00712(18)	−0.00595(19)	0.0328(5)
C29	0.2829(2)	0.9330(2)	−0.10978(19)	0.0382(5)
H29	0.2353	0.8486	−0.1553	0.046*
C30	0.3699(2)	0.9823(2)	−0.14636(19)	0.0391(5)
H30	0.3791	0.9311	−0.2167	0.047*
C31	0.44468(19)	1.10763(19)	−0.07978(19)	0.0338(5)
C32	0.4289(2)	1.1806(2)	0.02509(19)	0.0394(6)
H32	0.4788	1.2638	0.0719	0.047*
C33	0.3405(2)	1.13191(19)	0.06118(19)	0.0386(5)
H33	0.3314	1.1832	0.1316	0.046*
C34	0.5378(2)	1.15933(19)	−0.12028(19)	0.0348(5)
C35	0.5175(2)	1.1191(2)	−0.2365(2)	0.0444(6)
H35	0.4428	1.0608	−0.2899	0.053*
C36	0.6068(2)	1.1649(2)	−0.2723(2)	0.0487(6)
H36	0.5923	1.1384	−0.3499	0.058*
C37	0.7371(2)	1.2907(2)	−0.0843(2)	0.0431(6)
H37	0.8124	1.3499	−0.0332	0.052*
C38	0.6506(2)	1.2488(2)	−0.0441(2)	0.0384(5)
H38	0.6669	1.2800	0.0343	0.046*
H3	0.017(4)	0.449(4)	0.796(3)	0.120(13)*

Experimental details

Coordinates of hydrogen atoms were positioned according to geometric considerations. Their U_{iso} values were set to $1.2U_{\text{eq}}$ of the parent atoms.

Comment

In the construction of CPs, multidentate organic ligands play a vital role since the structural integrity of these ligands in most cases remains unaltered throughout the mixed-ligands strategy using *N*-donor colinkers. In most situations, *N*-containing ligands are electrically neutral, while carboxylate ligands are negatively charged. Among organic aromatic multicarboxylates have been widely utilized to construct MOFs [4, 5]. On the other hand, 4,4'-bis(pyridin-4-yl)biphenyl serves as bridging ligand to coordinate to two metal ions [6, 7]. The title salt was obtained as part of our projects concerning new MOF and CP compounds.

The asymmetric unit contains one 4-(4'-(pyridin-4-yl)-[1,1'-biphenyl]-4-yl)pyridin-1-ium cation, one 2-carboxy-4-(3,5-dicarboxyphenoxy)benzoate anion and one free water molecule (see the figure). The bond lengths and angles are in the expected ranges. The monocation donates and accepts hydrogen bonds [8]. The same is true for the anion and

together with the water molecule a hydrogen-bonded network is created.

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