New coordination polymer networks based on Copper(II) hexafluoroacetylacetonate and pyridine containing building blocks: synthesis and structureal study

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SUPPORTING INFORMATION

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Table S1. Geometric details of possible (C–)H···O/F interactions[a] and selected C···F/C inter-chain contact distances[a, b] in complex **A**.

Atoms involved	Symmetry	Distance [Å]			Angle [°]
		C···O/F/C	C–H	H··O/F	C–H··O/F
C(1)–H(1)···O(3)	*x, -y+0.5, -x+1.5*	3.074(6)	0.93	2.51	119
C(2)–H(2)···F(1)	*x–0.5, – y, –z+1*	3.448(7)	0.93	2.52	174
C(4)–H(4)···F(2)	*x–1, y, z*	3.378(7)	0.93	2.78	123
C(5)–H(5)···F(4)	*x–0.5, –y+1, z*	3.437(9)	0.93	2.68	139
C(13)–H(13)···F(2)	*–x, –y,–z+1*	3.576(7)	0.93	2.98	123
C(7)···F(1)	*x–1, y, z*	3.291(6)			
C(8)···F(1)	*x–1, y, z*	3.373(5)			
C(13)···F(1)	*–x, –y, –z+1*	3.302(7)			
C(14)···F(1)	*–x, – y,– z+1*	3.348(5)			
C(2)···C(10)	*x+0.5, –y, z*	3.562(7)			
C(7)···C(8)	*–x–0.5, y, –z+1*	3.589(6)			

[a] Esd's, where given, are in parentheses. The (C–)H atoms were held in positions calculated using geometric evidence.[47] The distances/angles have been calculated without correction or normalization of the H positions.

[b] Shorter connections with C···F < 3.4 and C···C < 3.6 Å were selected.

Table S2. Dihedral angles,[a] formed by the pyridyl rings with the central benzene ring plane within the tris(pyridylethynyl)benzene ligand moieties in compounds **C** and **D.**

Compounds		Dihedral angles [°] involving the LS planes [a] of the benzene ring and		
		pyridyl ring 1 [b]	pyridyl ring 2 [b]	pyridyl ring 3 [b]
Complex **C** [c]	A	8.20(3)	4.95(3)	7.21(3)
	B	73.69(3)	5.23(3)	11.66(3)
	C	81.77(3)	5.10(3)	13.61(3)
	D	9.06(3)	5.17(3)	7.56(3)
	E	81.67(3)	6.49(3)	13.28(3)
	F	78.59(3)	4.07(3)	11.95(3)
Complex **D**		78.1(1)	3.7(2)	22.0(7) 52.8(5) [d]

[a] The least square (LS) planes were calculated through the non-hydrogen ring atoms. Esd's are given in parentheses.

[b] Pyridyl rings 1, 2 and 3 contain the heteroatoms N(1), N(2) and N(3), respectively.

[c] Complex **C** contains six unique tris(pyridylethynyl)benzene spacer units A-F.

[d] Pyridyl ring 3 in complex **D** was found to be disordered, occupying two major disorder sites (Fig. 5) with about the same probability (*cf*. the text).

Table S3. Distances and angles in possible (C–)H···N (a) and (C–)Cl···$\pi_{ethynyl}$ interactions (b), [a, b] and selected contact distances [c] between the polymeric **D** host framework and the included chloroform guest molecule (c).

(a)

Atoms involved	Symmetry	Distance [Å]			Angle [°]
		C···N	C–H	H···N	C–H··N
C(1G)–H(1G)···N(3)	*x, y, z*	3.12(1)	0.99	2.22	151
C(1G')–H(1G')···N(3)	*x, y, z*	3.27(2)	1.00	2.38	149
C(1G)–H(1G)···N(3')	*x, y, z*	3.04(1)	0.99	2.13	153
C(1G')–H(1G')···N(3')	*x, y, z*	3.17(2)	1.00	2.19	168
C(1G")–H(1G")···N(3)	*x, y, z*	3.35(3)	0.98	2.52	142

(b)

Atoms involved	Symmetry	Distance [Å] Cl···$\pi_{ethynyl}$ [c]	Angle [°] C–Cl···$\pi_{ethynyl}$ [c]
C(1G)–Cl(1)···$\pi_{ethynyl}$ (3) [b]	*–x – 1,–y – 1,–z – 1*	3.561(8)	151.0(8)
C(1G')–Cl(2')···$\pi_{ethynyl}$ (1) [b]	*x, y, z + 1*	3.219(6)	152.6(7)
C(1G'')–Cl (3'')···$\pi_{ethynyl}$ (3) [b]	*–x ,–y – 1,–z – 1*	3.39(1)	147(2)

(c)

Atoms involved	Symmetry	Distance [Å]
Cl(1')···F(11)	*x, y+1, z–1*	3.208(9)
C(8)···Cl(3")	*x, y, z+1*	3.67(2)
C(9)···Cl(2')	*x, y, z+1*	3.481(6)
C(12)···Cl(1')	*x+1, y, z+1*	3.477(8)
C(13)···Cl(1')	*x+1, y, z+1*	3.364(8)
C(21)···Cl(1)	*–x–1, –y–1, –z–1*	3.636(9)
C(22)···Cl(3")	*–x, –y–1, –z–1*	3.15(2)
C(22)···Cl(1)	*–x–1, –y–1, –z–1*	3.59(1)
C(29)···Cl(2")	*–x+1, –y, –z*	3.54(2)
Cl(3')···F(2)	*x–1, y–1, z–1*	3.115(8)
Cl(1)···F(2)	*x–1, y–1, z–1*	3.351(9)
Cl(2")···F(1)	*–x+1, y, z*	3.30(2)
Cl(1)···F(1)	*x–1, y–1, z–1*	3.397(7)
Cl(2")···F(2)	*–x+1, –y, –z*	3.37(2)
Cl(3)···F(4)	*x–1, y, z–1*	3.283(7)
Cl(1')···F(4)	*x, y+1, z–1*	3.474(9)
Cl(3)···F(11)	*–x–1, –y–1, –z*	3.336(7)

[a] Esd's, where given, are in parentheses. The chloroform (C–)H disorder sites were held riding on their parent C atoms during the final refinement calculations. The distances/angles have been calculated without correction or normalization of the H positions.

[b] $\pi_{ethynyl}$ means the center of gravity of the ethynyl C≡C bond,[29] where bonds (1), (2) and (3) are those between C(7) and C(8), C(14) and C(15), and C(21) and C(22), respectively (Figure 5).

[c] Shorter contacts with distances C···Cl < 3.7, Cl···F < 3.5 and Cl···π < 3.6 Å were selected, where at least one of the two connected atoms have full site occupancy.

Table S4. Geometry of possible (C–)H···F (a) and (C–)F···$\pi_{ethynyl}$ (b) interactions, [a, b, c] and selected inter-chain contact distances [b, c, d, e] (c) in complex **D**.

(a)

Atoms involved	Symmetry	Distance [Å]			Angle [°]
		C···N	C–H	H···N	C–H··N
C(10)–H(10)···F(4)	*x–1, y, z*	3.538(5)	0.93	2.93	125
C(26)–H(26)···F(5)	*x–1, y, z–1*	3.603(11)	0.93	2.83	142

(b)

Atoms involved	Symmetry	Distance [Å] F···$\pi_{ethynyl}$	Angle [°] C–F···$\pi_{ethynyl}$
C(37)–F(11) ···$\pi_{ethynyl}$ (2) [c]	*–x – 1, –y – 2, –z*	3.502(5)	119.2(4)
C(33)–F(7) ···$\pi_{ethynyl}$ (2) [c]	*–x – 1, –y – 2, –z*	3.729(5)	110.8(4)

(c)

Atoms involved	Symmetry	Distance [Å]
C(9)···F(11)	*x+1, y+1, z*	3.353(5)
C(10)···F(12)	*x+1, y+1, z*	3.182(6)
C(10)···F(6)	*x–1, y, z*	3.479(5)
C(11)···F(6)	*x–1, y, z*	3.277(5)
C(11)···F(12)	*x+1, y+1, z*	3.154(5)
C(13)···F(11)	*x+1, y+1, z*	3.329(5)
C(17)···F(7)	*–x–1, –y–2, –z*	3.201(5)
C(20)···F(10)	*–x–1,–y–2,–z*	3.226(5)
C(21)···F(9)	*x+1, y+1, z*	3.368(5)
C(22)···F(9)	*x+1, y+1, z*	3.212(6)
C(23)···F(1)	*–x, – y, – z*	3.40(2)
C(24)···F(1)	*–x, – y, – z*	3.21(2)
C(25)···F(1)	*–x, – y, – z*	3.27(2)
C(25)···F(1)	*x+1, y+1, z+1*	3.305(9)
C(27)···F(3)	*–x, – y, – z*	3.30(2)
C(27')···F(3)	*–x, – y, – z*	3.42(2)

Table S4 (cont.)

Atoms involved	Symmetry	Distance [Å]
C(29)···F(12)	*x+1, y+1, z*	3.278(5)
C(30)···F(12)	*x+1, y+1, z*	3.416(6)
C(10)···O(4)	*x+1, y+1, z*	3.376(5)
C(1)···C(6)	*–x, –y–1, –z*	3.469(5)
C(1)···C(5)	*–x, –y–1, –z*	3.559(5)
C(1)···C(20)	*–x–1, –y–1, –z*	3.484(5)
C(1)···C(16)	*–x–1, –y–1, –z*	3.584(5)
C(2)···C(6)	*–x, –y–1, –z*	3.528(5)
C(3)···C(15)	*–x–1, –y–1, –z*	3.543(5)
C(4)···C(7)	*–x, –y–1, –z*	3.572(5)
C(5)···C(7)	*–x, –y–1, –z*	3.508(5)
C(5)···C(17)	*–x–1, –y–1, –z*	3.405(5)
C(6)···C(17)	*–x–1, –y–1, –z*	3.462(5)
C(6)···C(18)	*–x–1, –y–1, –z*	3.456(5)
C(7)···C(19)	*–x–1, –y–1, –z*	3.504(5)
C(7)···C(20)	*–x–1, –y–1, –z*	3.568(5)
C(14)···C(14)	*–x–1, –y–1, –z*	3.576(7)
π_{aryl} (1)···π_{aryl} (3) [e]	*x, y+1, z–1*	3.743
$\pi_{ethynryl}$ (2)···$\pi_{ethynryl}$ (2) [c]	*–x–1, –y–1, –z*	3.804

[a] Only the most probable C–H··F bonds, with C··F < 3.61 Å and C–H··F angle >120^{o} were selected.

[b] Esd's, where given, are in parentheses. The (C–)H atoms were held in positions calculated using geometric evidence. [47] The distances/angles have been calculated without correction or normalization of the H positions.

[c] $\pi_{ethynyl}$ means the center of gravity of the ethynyl C≡C bond, [29] where bonds (1), (2) and (3) are those between C(7) and C(8), C(14) and C(15), and C(21) and C(22), respectively (Figure 5).

[d] Shorter contacts with distances C···F < 3.4, C···O < 3.5 and C···C < 3.6 Å were selected, where at least one of the two connected atoms has full site occupancy.

[e] π_{aryl} means the ring center of gravity, [29] here calculated for the six-membered rings (1) and (3), where ring (1) is the C(1)–C(2)–C(3)–C(4)–C(5)–C(6) benzene ring; and ring (3) is the C(16)–C(17)–C(18)–N(2)–C(19)–C(20) pyridine ring (Fig. 5).