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catena-Poly[[copper(I)-di-μ-*trans*-1-(2-pyridyl)-2-(4-pyridyl)ethylene-κ^2N^2:N^4;κ^2N^4:N^2] tetrafluoroborate]

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Key indicators

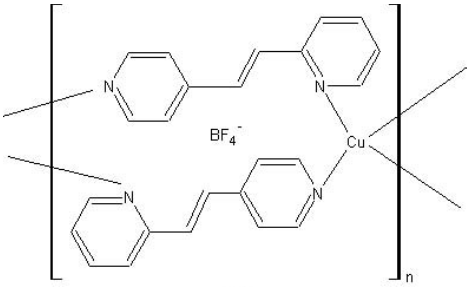
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.046
wR factor = 0.111
Data-to-parameter ratio = 13.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title complex, $\{[Cu(C_{12}H_{10}N_2)_2]BF_4\}_n$, each copper(I) centre is tetrahedrally coordinated by N atoms from four bridging *trans*-1-(2-pyridyl)-2-(4-pyridyl)ethylene (TPPE) ligands. The ligands bridge adjacent copper(I) centres to form one-dimensional folded chains. Adjacent uniform chains are further interlinked into a three-dimensional framework through weak C—H···F interactions.

Comment

Metal–organic coordination polymers have recently attracted great interest, due to their interesting structural topologies and potential application as functional materials (Batten & Robson, 1998; Eddaoudi *et al.*, 2001). In particular, the 'node and spacer' methodology has proved to be remarkably successful in the rational design of metal–organic architectures. In this context, by far the most commonly utilized linear spacer ligand for linking metal centres is 4,4′-bipyridine. More recently, bifunctional analogues with an extended backbone, such as 1,2-bis(4-pyridyl)ethane (Hong & Do, 1998), *trans*-1,2-bis(4-pyridyl)ethylene (Jung *et al.*, 1998), bis(4-pyridyl)disulfide (Tabellion *et al.*, 2001), *trans*-1-(2-pyridyl)-4-(4-pyridyl)ethylene (Raring & Zubieta, 2001) and 2,5-bis-(4-pyridyl)-1,3,4-oxadiazole (Du *et al.*, 2005), have been employed as nucleophilic linkers in self-assembly reactions with various labile metal complexes. Recently, we have utilized polydentate ligands for designing coordination networks (Lu *et al.*, 2002). Here, we report the preparation and crystal structure of the title new one-dimensional coordination polymer, $[Cu(TPPE)_2(BF_4)]_n$, (I).



(I)

The asymmetric unit of (I) contains two TPPE ligands and copper(I) tetrafluoroborate (Fig. 1). Each Cu^I centre is tetrahedrally coordinated by four neighbouring TPPE ligands, which are in turn bound to two other Cu^I centres (Fig. 2 and Table 1). The Cu—N(2-pyridyl) distances [Cu1—N1 = 2.072 (3) Å and Cu1—N3 = 2.133 (3) Å] are slightly longer than the Cu—N(4-pyridyl) distances [Cu1—N2 = 2.052 (3) Å and Cu1—N4 = 2.054 (3) Å], which are comparable with the

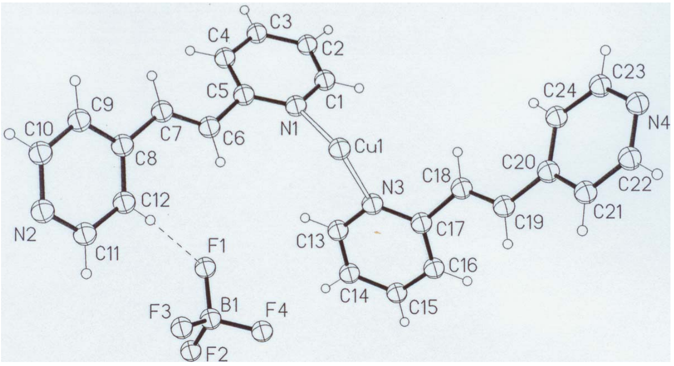


Figure 1
The asymmetric unit of (I). Displacement ellipsoids are plotted at the 30% probability level. The dashed line represents a weak C—H···F interaction.

Cu—N bond lengths in bis{[*trans*-1,2-bis(4-pyridyl)ethylene]copper(I)} tetrafluoroborate [2.003 (5)–2.084 (6) Å; Blake *et al.*, 1997]. The two pyridyl rings of the same ligand are not coplanar and subtend dihedral angles of 50.5 (2) and 56.4 (2)° in the two bipyridyl ligands, respectively.

The Cu^{I} centres are bridged by TPPE ligands to form one-dimensional corrugated chains extending along the *b* axis (Fig. 2). Adjacent uniform chains are further interlinked through the BF_4^- bridges into a three-dimensional network (Fig. 3). There are C—H···F hydrogen-bonding interactions between adjacent BF_4^- ions and pyridyl groups within each layer (Table 2).

Experimental

$[Cu(MeCN)_4]BF_4$ (0.5 mmol) and TPPE (1.0 mmol) were placed in a thick Pyrex tube with a Rotaflo stopper, and the tube was frozen using liquid nitrogen. After addition of dimethylformamide (1.0 ml) and H_2O (3.0 ml), the tube was evacuated, sealed with a stopper and heated at 383 K for 2 d to give dark-red block-like crystals of (I) in 60% yield, based on $[Cu(MeCN)_4]BF_4$. Analysis, found: C 55.63, H 3.87, N 10.73%; calculated for $C_{24}H_{20}N_4CuBF_4$: C 55.99, H 3.89, N 10.89%. FT–IR data (KBr, cm^{-1}): 3054 (*w*), 1600 (*s*), 1560 (*w*), 1493 (*w*), 1469 (*m*), 1429 (*m*), 1083 (*s*), 1030 (*s*), 970 (*w*), 814 (*m*), 768 (*w*), 543.5 (*m*).

Crystal data

$[Cu(C_{12}H_{10}N_2)_2]BF_4$
$M_r = 514.79$
Monoclinic, $P2_1/n$
$a = 9.9969\ (6)$ Å
$b = 16.5736\ (10)$ Å
$c = 14.6322\ (9)$ Å
$\beta = 109.2480\ (10)°$
$V = 2288.8\ (2)$ Å^3
$Z = 4$

$D_x = 1.494$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10795 reflections
$\theta = 3–23°$
$\mu = 1.01$ mm^{-1}
$T = 293\ (2)$ K
Block, dark red
0.39 × 0.25 × 0.14 mm

Data collection

Bruker SMART CCD 1K area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.696$, $T_{max} = 0.869$
12314 measured reflections

4045 independent reflections
2273 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 25.0°$
$h = -11 \rightarrow 11$
$k = -17 \rightarrow 19$
$l = -17 \rightarrow 17$

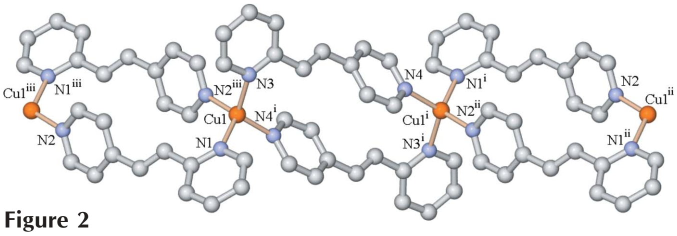


Figure 2
Diagram showing the one-dimensional zigzag polymeric chain running parallel to the *b* axis. [Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $x, 1 + y, z$; (iii) $1 - x, -y, 1 - z$.] H atoms have been omitted.

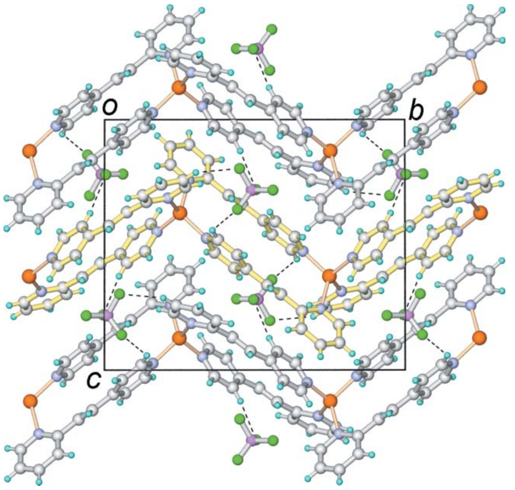


Figure 3
Diagram showing the neighbouring zigzag polymeric chains interlinked by tetrafluoroborate anions *via* very weak C—H···F interactions, shown as dashed lines.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.111$
$S = 1.00$
4045 reflections
307 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2^{i}	2.052 (3)	N2—C11	1.332 (4)
Cu1—N4^{ii}	2.054 (3)	N2—Cu1^{i}	2.052 (3)
Cu1—N1	2.072 (3)	N3—C13	1.335 (5)
Cu1—N3	2.133 (3)	N3—C17	1.347 (4)
N1—C1	1.343 (4)	N4—C23	1.334 (4)
N1—C5	1.360 (4)	N4—C22	1.337 (5)
N2—C10	1.323 (4)	N4—Cu1^{ii}	2.054 (3)
N2^{i}—Cu1—N4^{ii}	102.70 (12)	C11—N2—Cu1^{i}	121.3 (3)
N2^{i}—Cu1—N1	120.96 (11)	N1—C1—C2	124.8 (3)
N4^{ii}—Cu1—N1	109.40 (12)	C13—N3—C17	117.9 (4)
N2^{i}—Cu1—N3	105.74 (12)	C13—N3—Cu1	115.5 (3)
N4^{ii}—Cu1—N3	120.31 (11)	C17—N3—Cu1	123.5 (3)
N1—Cu1—N3	98.91 (11)	C23—N4—C22	116.5 (3)
C1—N1—C5	116.6 (3)	C23—N4—Cu1^{ii}	119.7 (3)
C1—N1—Cu1	114.2 (2)	C22—N4—Cu1^{ii}	123.6 (3)
C5—N1—Cu1	128.0 (2)	N3—C13—C14	123.5 (4)
C10—N2—C11	116.1 (3)	N3—C17—C16	121.3 (4)
C10—N2—Cu1^{i}	122.2 (3)	N3—C17—C18	115.3 (3)

Symmetry codes: (i) $-x + 1, -y, -z + 1$; (ii) $-x + 1, -y + 1, -z + 1$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*A*···F1	0.93	2.48	3.409 (5)	173
C22—H22*A*···F2^{iii}	0.93	2.54	3.195 (5)	128
C2—H2*A*···F3^{iv}	0.93	2.43	3.192 (4)	139
C3—H3*A*···F4^{v}	0.93	2.47	3.174 (5)	133

Symmetry codes: (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $x-1, y, z$.

The H atoms were positioned geometrically, with C—H = 0.93 Å and $U_{\rm iso}$(H)= 1.2$U_{\rm eq}$(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

The X-ray data were collected at the Chinese University of Hong Kong.

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