

Supplementary Information for the Manuscript:

“UNUSUAL TRINUCLEAR COMPLEX OF COPPER (II) CONTAINING A 4'-(3-METHYL-2-THIENYL)-4,2':6',4''-TERPYRIDINE LIGAND. STRUCTURAL, SPECTROSCOPIC, ELECTROCHEMICAL AND MAGNETIC PROPERTIES”

By the authors:

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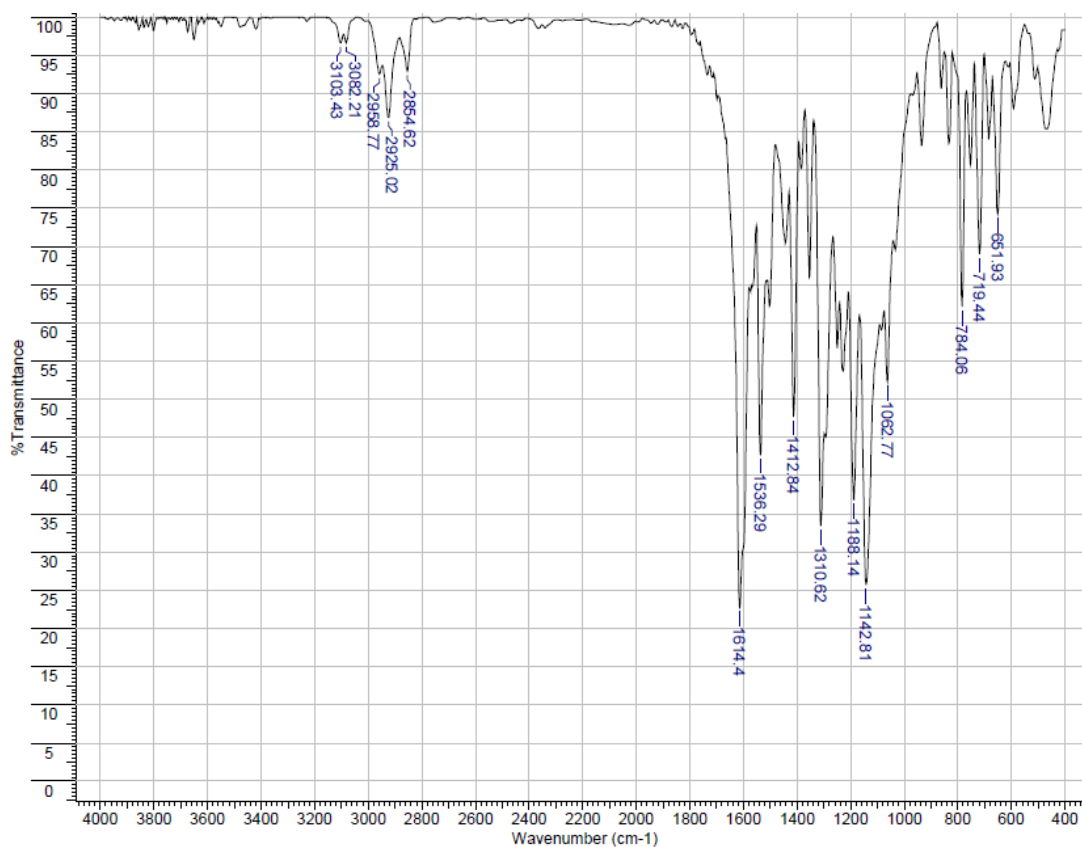


Fig. S1. FT-IR spectra of complex 1.

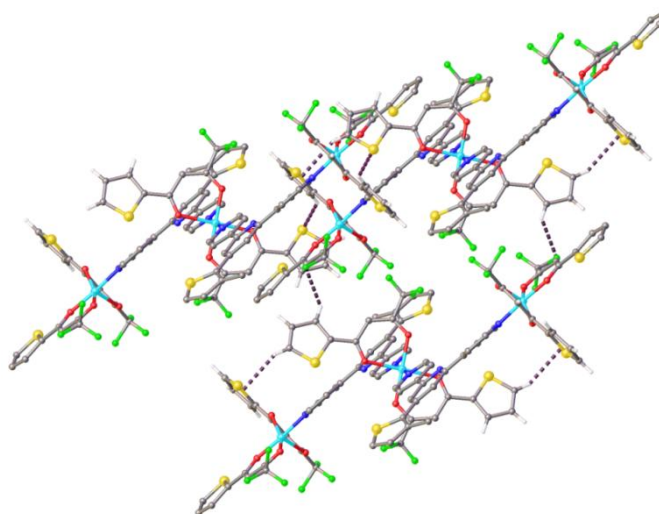


Fig. S2. Packing view of intermolecular Hydrogen Bonds in complex **1** projected along the [001] direction.

Table S1. Intermolecular hydrogen bonds in complex **1**.

D-H...A		d(D...H)(Å)	d(H...A)(Å)	d(D...A)(Å)	<(D-H...A) (°)
C(8A)-H(8A)	Cg(9) ⁱⁱ	0.95	2.95	3.795(6)	148
C(6C)-H(6C)	F(4BC) ⁱⁱⁱ	0.95	2.54	3.469(11)	167
C(6B)-H(6B)	S(2) ^{iv}	0.95	2.87	3.591(6)	134

Symmetry codes: (ii) 2-X,1-Y,-1-Z ; (iii) -x,2-y,-1-z ; (iv) -1+x,1+y,-1+z

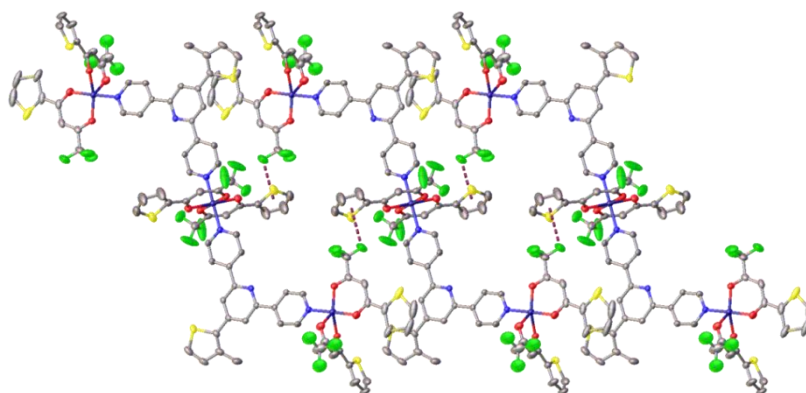
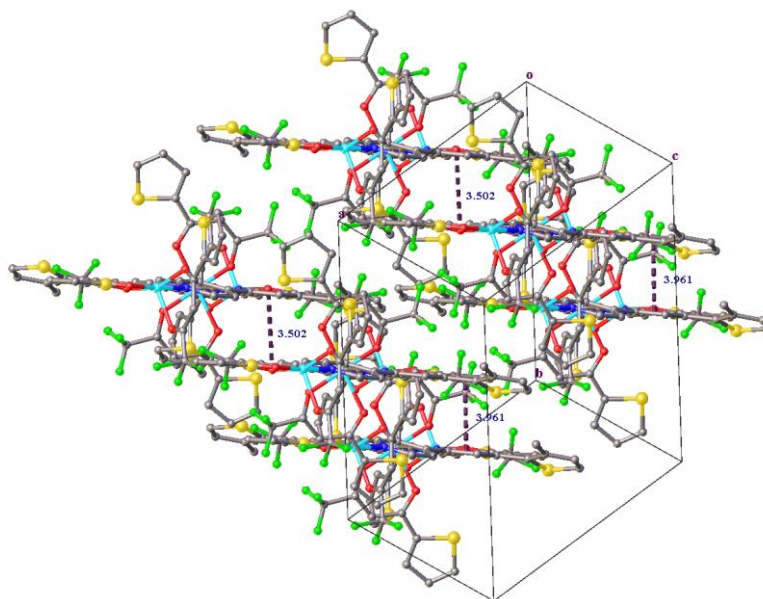


Fig. S3. Packing view of C-F... π Interactions in complex **1** projected along the [110] direction. Hydrogen atoms are omitted for clarity.

Table S2. C-F... π Interactions in complex **1**.

D-F...A	d(D...F)(Å)	d(F...A)(Å)	<(D-F...A) (°)
C(4C)-F(4CC)---Cg(8) ^v	1.321(5)	3.741(4)	103.5(3)

Symmetry codes: (v) -1+X,1+Y,Z

**Fig. S4.** Packing view of π - π interactions in complex **1**. Hydrogen atoms are omitted for clarity.**Table S3.** π - π interactions in complex **1**.

Group 1/Group2	ccd (Å)	da (°)	ipd (Å)	sa(°)
Cg(18)...Cg(18) ⁱⁱ	3.502(4)	0.0(4)	3.337(3)	1.063(5)
Cg(10)...Cg(18) ^{vi}	3.961(3)	2.38(19)	3.467(4)	1.804(13)

Cg(18) is the centroid of the N2 /C6-C10 pyridine ring and Cg(10) is the centroid of the S4/ C5B-C8B thienyl ring. Symmetry codes; (ii) 2-X,1-Y,-1-Z ; (vi):- 1-X,2-Y,-1-Z.

Note: ccd is the centre-to-centre distance (distance between ring centroids); da is the dihedral angle between rings; ipd is the interplanar distance (distance from one plane to the neighbouring centroid), sa is the slippage angle (angle subtended by the intercentroid vector to the normal plane) [1].

[1] C. Janiak, J. Chem. Soc., Dalton Trans. (2000) 3885-3896.