**Supplementary Information for the Manuscript:**

**“COMPARATIVE STUDY ON STRUCTURAL, MAGNETIC AND SPECTROSCOPIC PROPERTIES OF FOUR NEW COPPER(II) COORDINATION POLYMERS WITH 4’-substituted TERPYRIDINE LIGANDS”**

By the authors:

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**Figure S1.** 1H NMR spectrum of **3-qtpy** ligand

**Figure S2.** 13C NMR spectrum of **3-qtpy** ligand

**IR- Compounds I-IV**



**Figure S3.** IR spectrum of Compound **I-IV**

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**Fig. S4**: **a)** Packing view of **I**, projected along the chains direction [100]. Contiguous chains drawn in different blackness, for clarity. **b)** Packing view of **II**, projected perpendicular to the chains direction. Vertical lines at y ≈ 0.25, 0.75. The *c* glide planes shown in projection. Solvates not shown to clarify the position and size of the central focus (labelled (A)) occupied by the solvates in disordered manner.

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**Fig. S5: a)** The wavy (001) arrays in **III**, made up by the interaction of parallel [100] chains through a set of  C-H···N bonds (encircled). **b)**  Neighbouring chains in **IV**, related by the set of screw axis directed along b. Note their internal structure, alternating peaks and troughs in projection, and generating a set of double undulating sheets parallel to the (-101) plane.

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| **Table S 1**  Hydrogen Bonds for **I, II, III and IV.** | | | | | |
| Compd | D-H···A | d(D···H)(Å) | d(H···A)(Å) | d(D···A)(Å) | <(D-H···A) (°) |
| **I** | C20–H20C···F5BAii | 0.96 | 2.47 | 3.4065 (7) | 167 |
| **II** | C1S–H1SA..N4ii | 0.98 | 2.47 | 3.229 (18) | 134 |
|  | C1S -Cl3S···Cg2iii | 1.35 | 3.405 (6) |  | 145 |
| **III** | C7–H7···N4ii | 0.95 | 2.51 | 3.218 (4) | 131 |
|  | C20–H20···Cl2Siii | 0.95 | 2.75 | 3.635 (4) | 155.2(3) |
| **IV** | C12 –H12···O1Aiii | 0.95 | 2.53 | 3.377(5) | 149 |
| Symmetry codes for **I**: (ii) -1/2+x,1/2-y,1/2+z; for **II**: (ii) -1-x,-1/2+y,-1/2-z; (iii) -x,2-y,-z ; for **III** (ii): -x,-y,-z (iii):-x,-y,1-z ; for **IV**: (iii):1/2-x,-1/2+y,3/2-z | | | | | |

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| **Table S 2**  π-π contacts for **III** | | | | |
| Group 1/Group2 | ccd (Å) | da (°) | ipd (Å) | sa(°) |
| Cg4···Cg4ii | 3.730 (3) | 0 | 3.612(3) | 0.929 |
| Cg4···Cg5ii | 3.974(2) | 1.36(12) | 3.622(4) | 1.636 |
| Ring codes: as in Fig 2. Symmetry codes (ii):-x,-y,-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 plane normal).[51](#_ENREF_51) | | | | |

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| **Table S 3**  F ··F contacts in **I**, **II**. | | |
| Compd | F···F | d(F···F)(Å) |
| **I** | F5AB···.F5BCiii | 2.9292 (6) |
| **II** | F5AB···F5BBiii | 2.72 (2) |
|  | F4BB···F4BBiv | 2.56 (2) |
| Only distances shorter than the sum of Van der Waals radii (2.94 Å). Only major fractions of the disordered F' have been considered. | | |
| Symmetry codes : For **I** : (iii) -x, -y, -z ; for **II** : (iii) -x, - y, -z, (iv) - x, - y, -z | | |

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| **Table S 4.**  C-F···π bonds in **I** | | | | |
| Compound | C-F··· | d(C-F)(Å) | d(F···)(Å) | <(C-F),)> (°) |
| **I** | C4A-F4AA···Cg2iv | 1.344 (8) | 3.5391 (7) | 26.85 |
|  | C4A-F4AC···Cg2iv | 1.304 (3) | 3.3022 (6) | 13.70 |
|  | C5A-F5AC···Cg1v | 1.304 (3) | 3.3461 (6) | 14.61 |
|  | C4B-F4BA···Cg1vi | 1.307 (3) | 3.0828 (6) | 14.36 |
|  | C5B-F5BC···Cg2vii | 1.311 (3) | 3.4468 (7) | 11.53 |
| Ring codes as in Fig. 1 Symmetry codes : (iv) 1/2 + x, 1/2 - y, 1/2 + z ; (v) 1/2 - x, -1/2 + y, 1/2 – z ; (vi) -x, -y, -z; (vii) 1/2 + x, 1/2 - y, -1/2 + z | | | | |

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| **Cu(4-stpy)(hfacac)2 (I)** | **Cu(4-qtpy)(hfacac)2 (II)** |
| **Cu(3-qtpy)(hfacac)2 (III)** | **Cu(4-cntpy)(hfacac)2 (IV)** |
| **Figure S6.** TGA and DTG curves for Compounds **I-IV** | |

 

**Figure S7.** TGA/DTG curve of **3-qtpy** (left)and **4-cntpy** (right) ligands.



**Figure S8.** TGA/DTG curve of precursor **Cu(hfacac)2** complex.

**XRPD**

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**Figure S9.** The peak positions of simulated and experimental XRPD patterns are in agreement with each other, confirming the crystal structure of the compounds **I-IV**. The differences in intensity may be due to the preferred orientation of the crystalline powder sample.



**Figure S10.** Emissionspectra of compounds **I-IV** in the solid state. (λexc: 280 nm)

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| Compound **I** | Compound **II** |
| Compound **III** | Compound **IV** |

**Figure S11.** Calculated Absorptionspectra for compounds **I-IV:** optimized (black line) and solid state(red line).

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**Fig. S12:** Temperature dependence of χM-1for compounds: Cu(4-stpy)(hfacac)2, (I), Cu(4-qtpy)(hfacac)2, (II) and Cu(3-qtpy)(hfacac)2, (III)