Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Spontaneous resolution of P and M helical copper(II) MOFs built from achiral precursors

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Table S1: Crystallographic data and refinement details of **P** and **M** helical MOFs.

Complex	**M-2**	**M-3**	**M-4**	**M-5**	**M-6**
Formula	$C_{15}H_{17}CuN_5O$	$C_{15}H_{17}CuN_5O$	$C_{15}H_{17}CuN_5O$	$C_{15}H_{17}CuN_5O$	$C_{15}H_{17}CuN_5O$
Formula Weight	346.89	346.89	346.89	346.89	346.89
Temperature(K)	150	150	150	150	150
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a(Å)	8.0039(4)	8.0022(3)	8.0030(2)	8.0019(2)	7.9979(2)
b(Å)	6.8403(3)	6.8450(2)	6.8474(2)	6.8447(2)	6.8447(2)
c(Å)	14.0443(6)	14.0354(5)	14.0460(4)	14.0472(3)	14.0483(4)
β(deg)	103.686(2)	103.724(2)	103.701(2)	103.7180(10)	103.673(2)
Z	2	2	2	2	2
d_{calc} (g cm^{-3})	1.542	1.543	1.540	1.541	1.542
μ (mm^{-1})	1.471	1.471	1.469	1.470	1.470
F (000)	358	358	358	358	358
Flack Parameter	0.006(16)	0.133(16)	0.035(15)	0.014(12)	0.120(5)
Total Reflections	6085	6174	6202	12095	11461
Unique Reflections	2608	2630	2620	2849	2875
Observed data [I > 2 σ (I)]	2276	2433	2365	2641	2543
No. of parameters	199	199	199	199	199
R(int)	0.0282	0.0287	0.0266	0.0296	0.0353
R1, wR2 (all data)	0.0412, 0.0717	0.0346, 0.0771	0.0355, 0.0670	0.0280, 0.0602	0.0443, 0.0855
R1, wR2 [I > 2 σ (I)]	0.0346, 0.0692	0.0312, 0.0756	0.0303, 0.0652	0.0252, 0.0592	0.0367, 0.0821

Complex	**P-2**	**P-3**	**P-4**	**P-5**
Formula	$C_{15}H_{17}CuN_5O$	$C_{15}H_{17}CuN_5O$	$C_{15}H_{17}CuN_5O$	$C_{15}H_{17}CuN_5O$
Formula Weight	346.89	346.89	346.89	346.89
Temperature(K)	150	150	150	150
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a(Å)	8.0004(2)	8.0008(4)	8.0013(2)	8.0045(2)
b(Å)	6.8446(2)	6.8493(3)	6.8445(2)	6.8435(2)
c(Å)	14.0490(4)	14.0439(7)	14.0404(4)	14.0451(4)
β(deg)	103.671(2)	103.685(4)	103.717(2)	103.689(2)
Z	2	2	2	2
d_{calc} (g cm^{-3})	1.541	1.541	1.541	1.541
μ (mm^{-1})	1.470	1.469	1.469	1.470
F (000)	358	358	358	358
Flack Parameter	0.024(13)	-0.01(2)	0.013(12)	0.036(13)
Total Reflections	6184	10823	11314	11181
Unique Reflections	2529	2839	2842	2852
Observed data [I > 2 σ (I)]	2321	2489	2634	2626
No. of parameters	199	199	199	199
R(int)	0.0263	0.0594	0.0320	0.0332
R1, wR2 (all data)	0.0304, 0.0589	0.0505, 0.0999	0.0284, 0.0612	0.0296, 0.0626
R1, wR2 [I > 2 σ (I)]	0.0267, 0.0574	0.0429, 0.0964	0.0254, 0.0599	0.0261, 0.0611

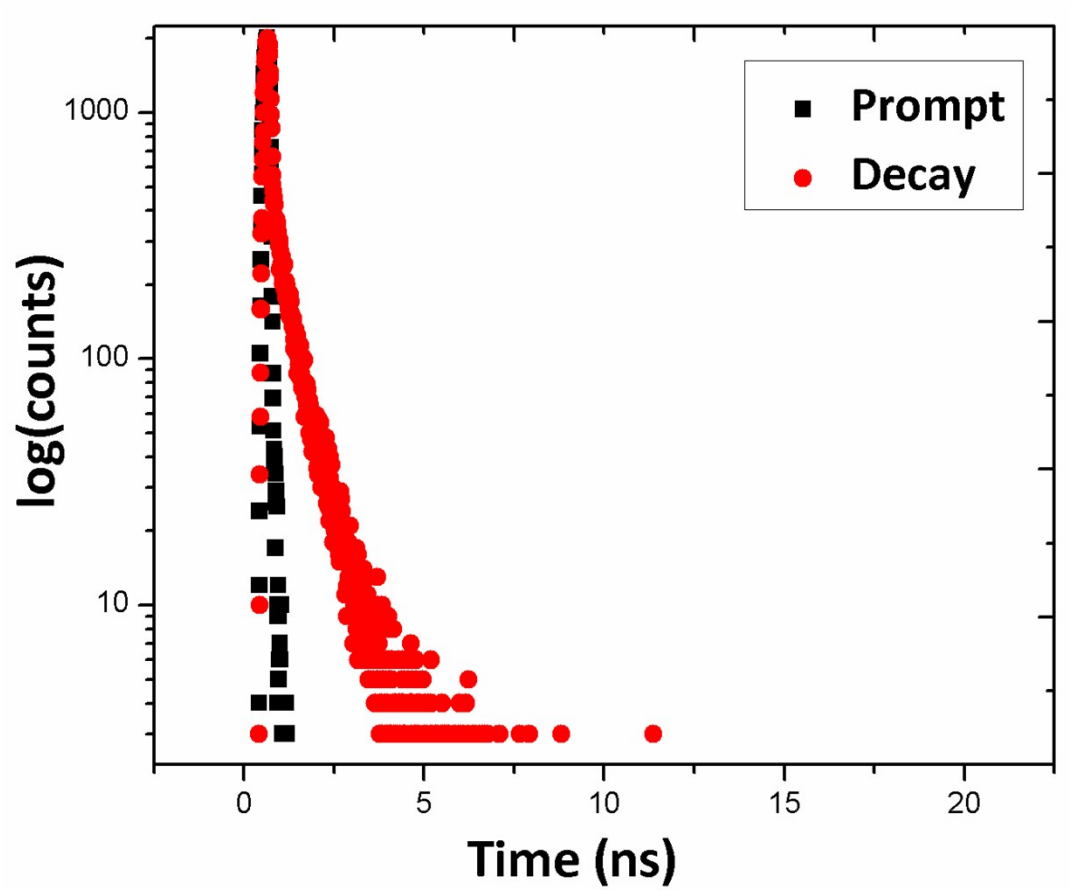

Figure S1: Time dependent photoluminescence decay profile of the complex.

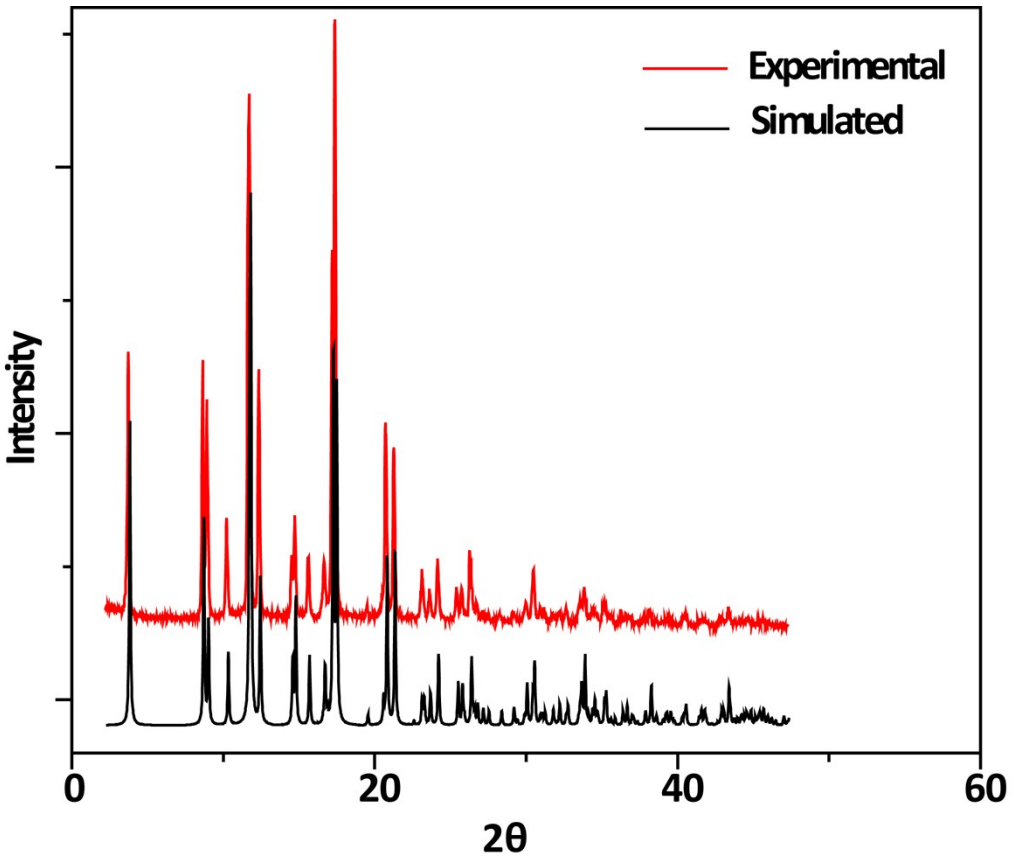

Figure S2: Experimental and simulated PXRD patterns showing the purity of the bulk material.