Supplementary Information (SI) for CrystEngComm.

Synthesis, Structural Analysis, and Properties of Silver-Based 1D and 3D Coordination Polymers

*Rouf Ali Dar and Athar Adil Hashmi**

Department of Chemistry, Faculty of Sciences, Jamia Millia Islamia, New-Delhi 110025, India

*Email: ahashmi@jmi.ac.in

Contents

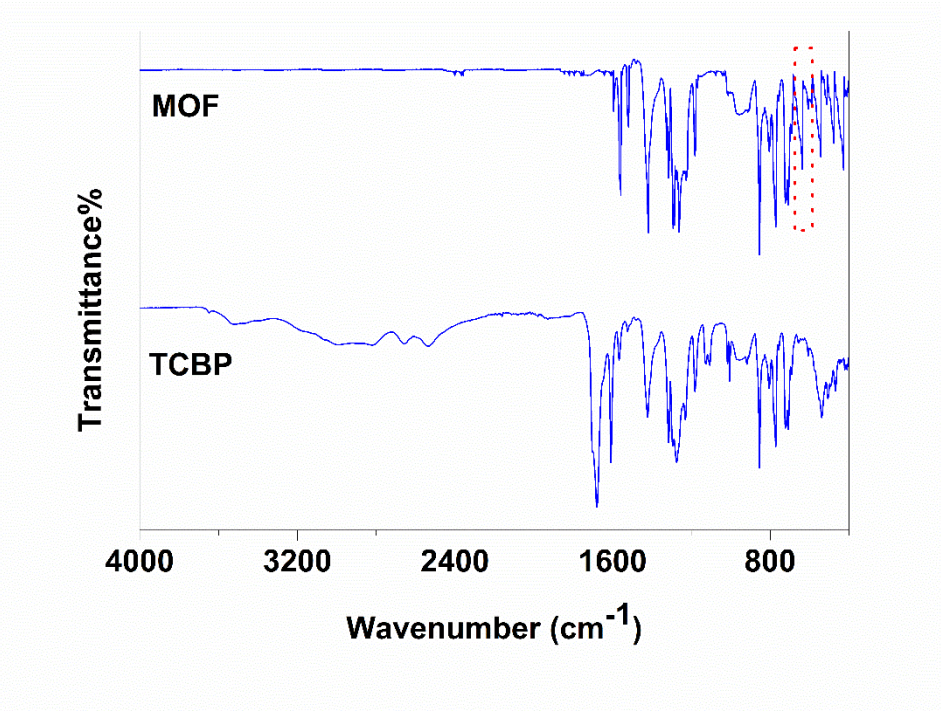
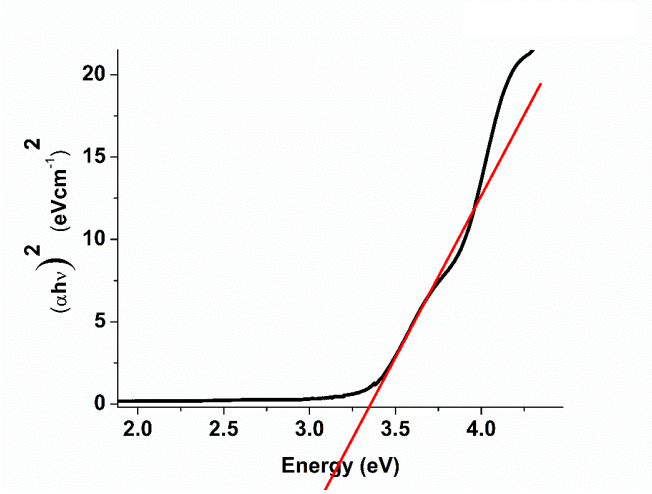


Figure S1. IR Spectra of MOF (1) and organic linker (H_4TCPB).



.

Figure S2. Calculation of optical band gap of CP-1 using UV-vis absorption spectrum.

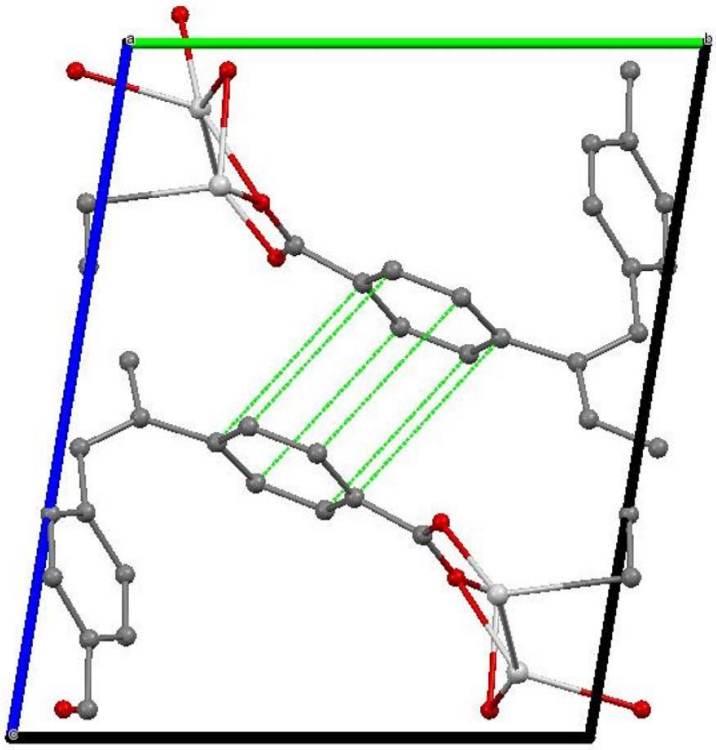


Figure S3. The π (pi)- π (pi) interactions between electron cloud of central benzene rings of adjacent TCPB linkers in a framework structure of CP-1.

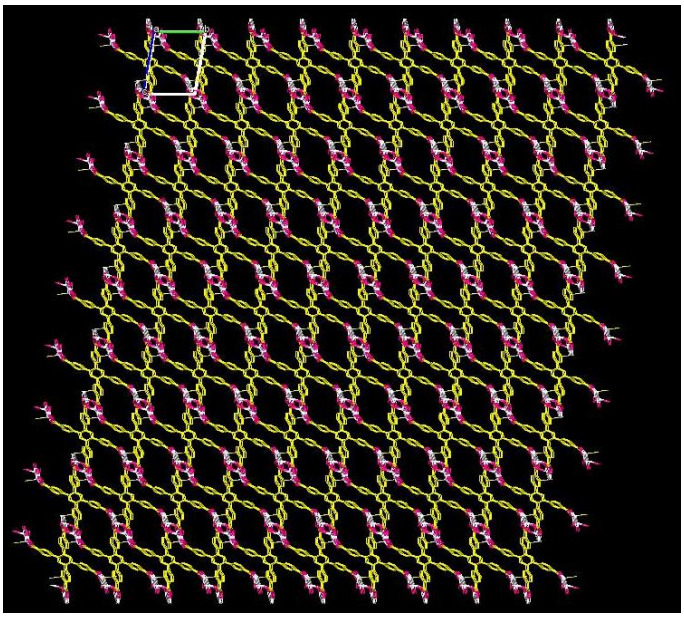


Figure S4. Total structure of CP-1 along *bc*-plane.

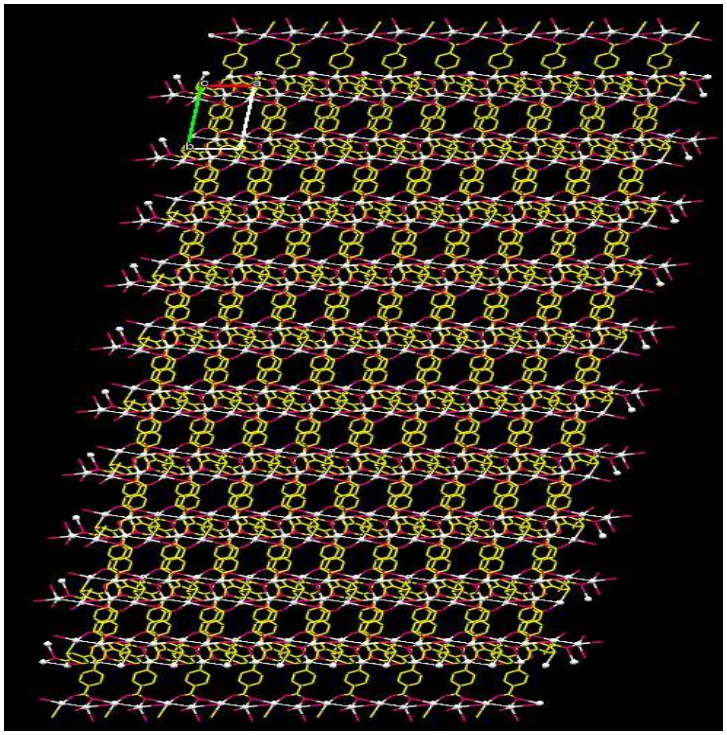


Figure S5. Total structure of CP-1 along *ac*-plane.

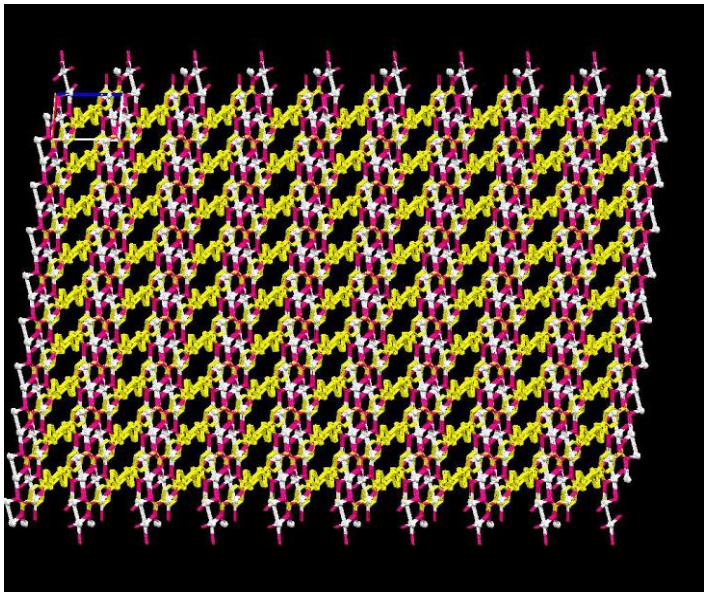


Figure S6. Total structure of CP-1 along *ab*-plane.

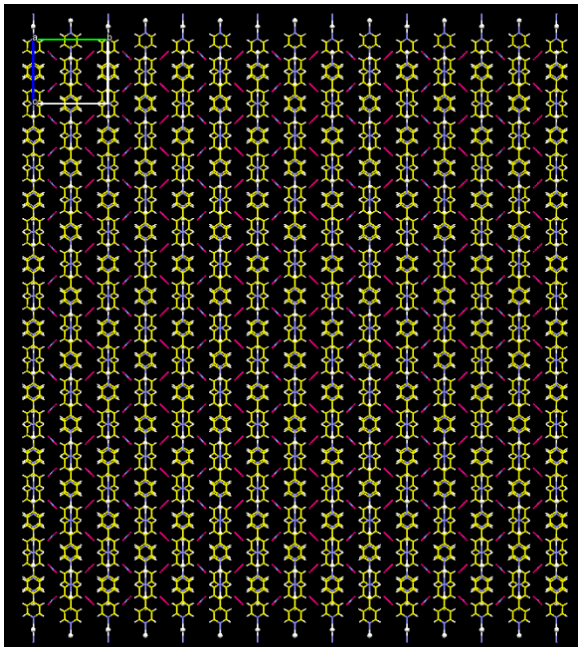


Figure S7. Packing of CP-2 along *bc*-plane.

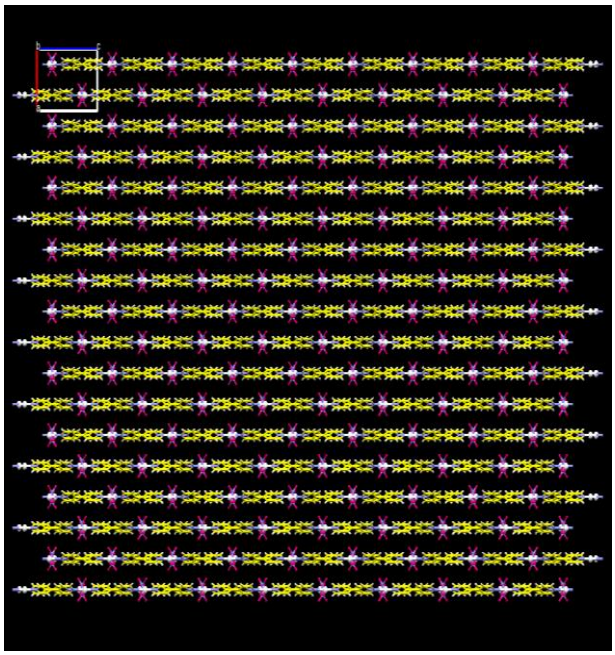


Figure S8. Packing of CP-2 along ac-plane.

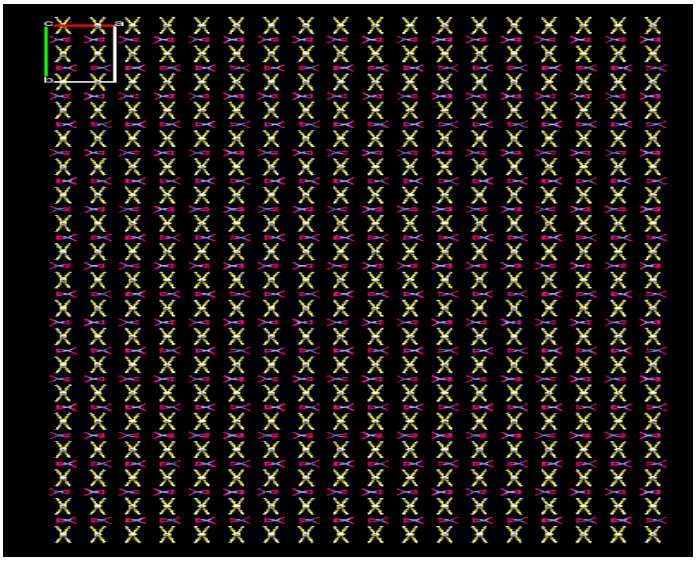


Figure S9. Packing of CP-2 along *ab*-plane.

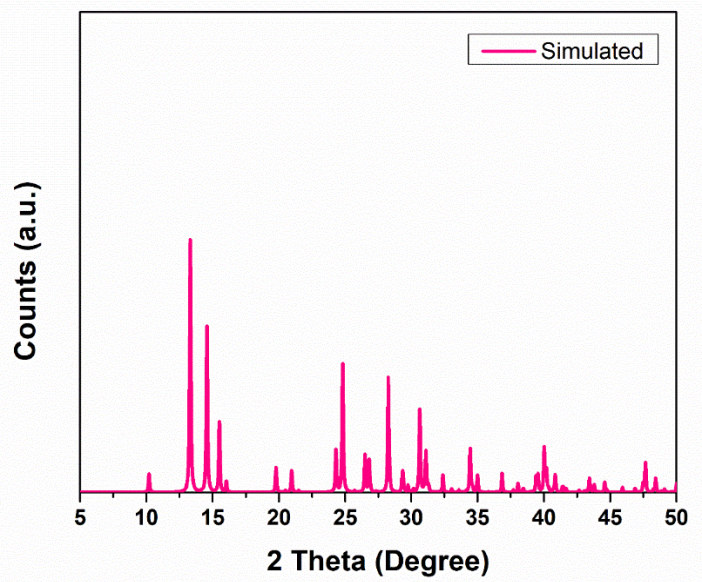


Figure S10. Simulated PXRD of CP-2.

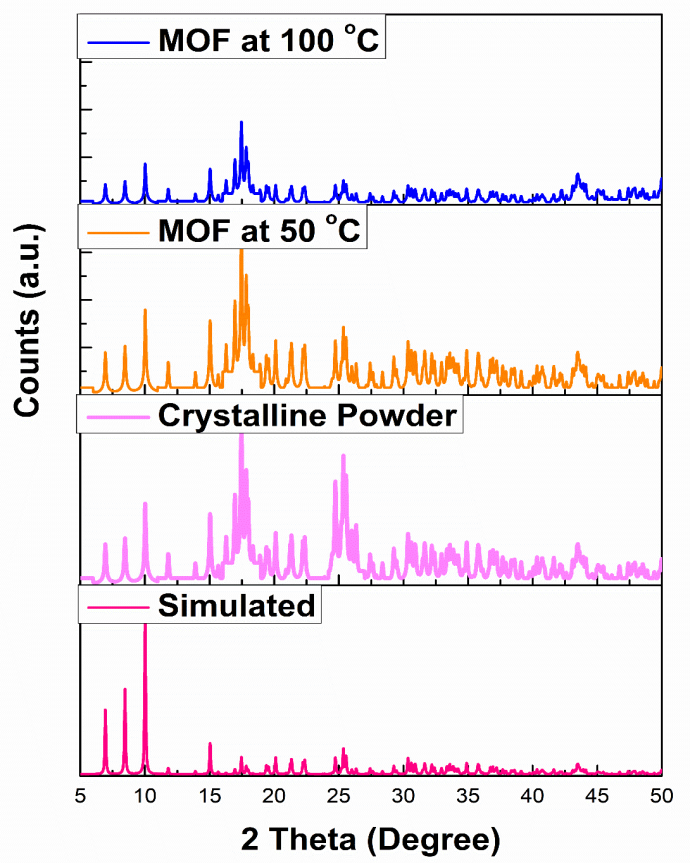


Figure S11. PXRD patterns of CP-1 at room temperature (RT), 50 °C, and 100 °C.

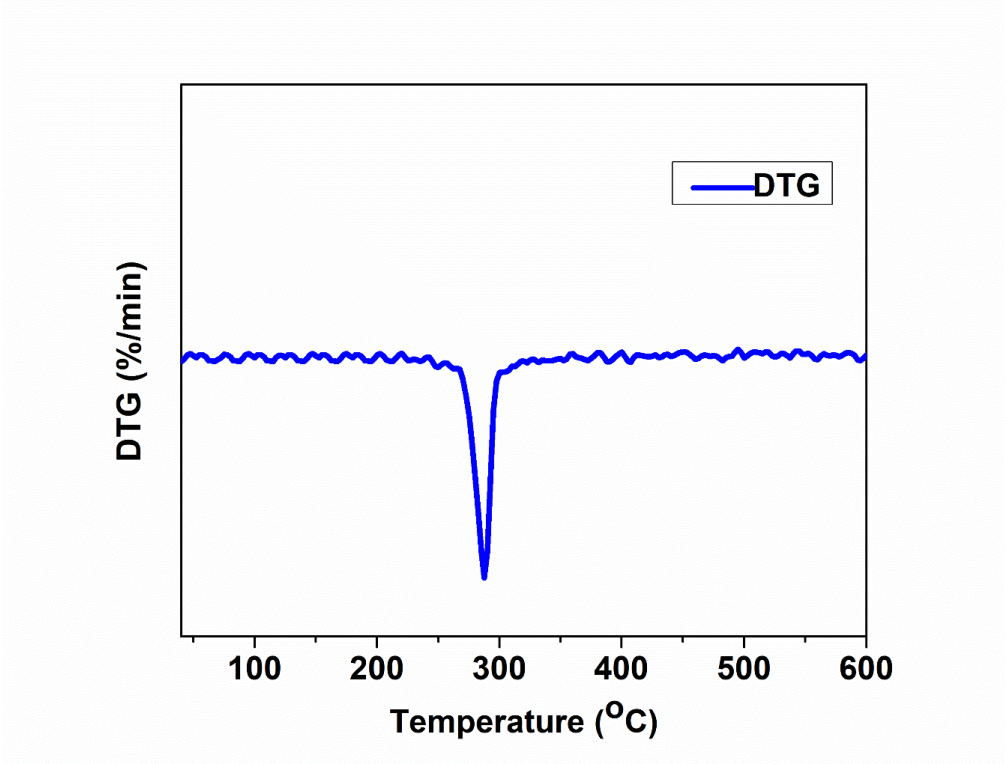


Figure S12. DTG curve of CP-1.

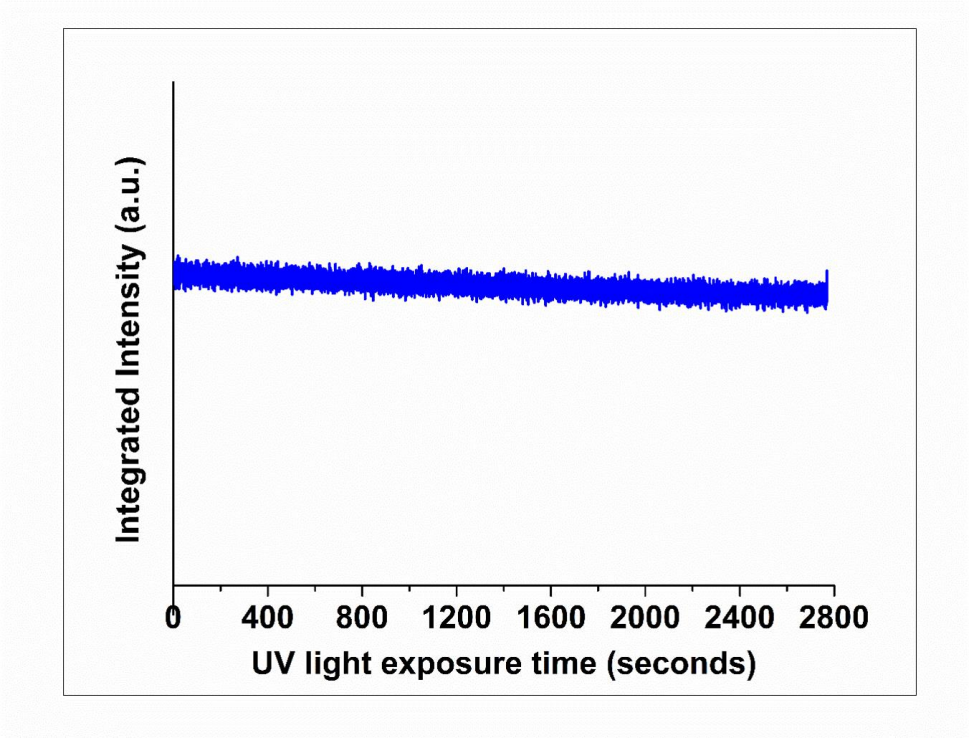


Figure S13. UV exposure of CP-1.

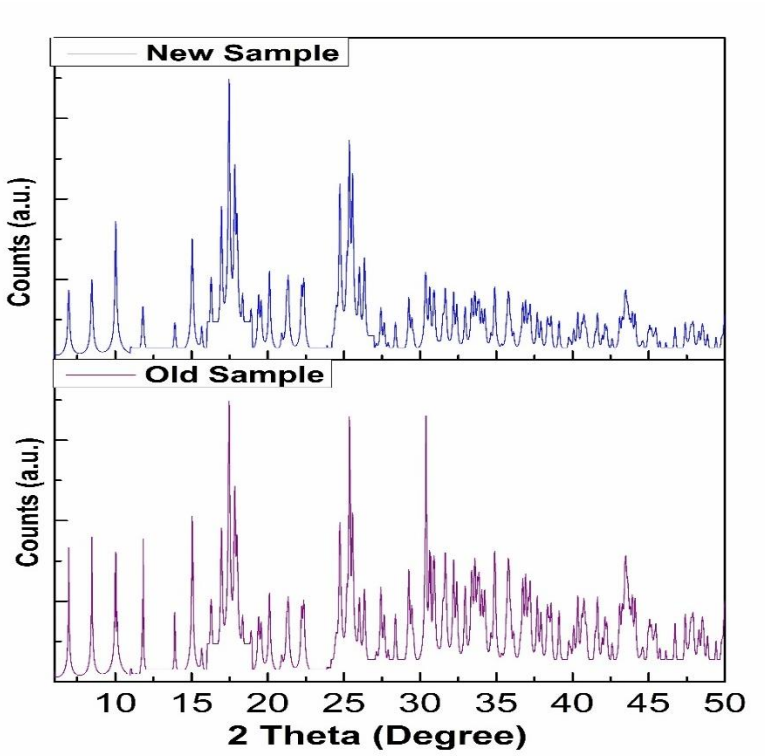


Figure S14. PXRD of a new and old sample.

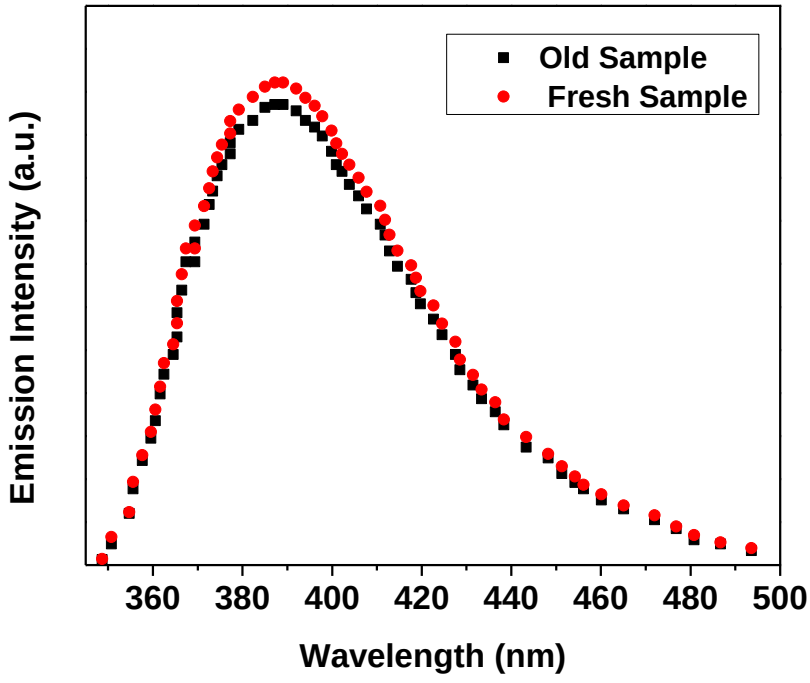


Figure S15. PL of a new and old sample.

Table S1. Bond lengths [Å] and angles [°] for CP-1.

Ag(1)-O(3)	2.231(5)
Ag(1)-O(2)#1	2.257(5)
Ag(1)-O(2)#2	2.494(5)
Ag(1)-Ag(2)	2.8937(10)
Ag(2)-O(4)	2.167(5)
Ag(2)-O(1)#1	2.235(5)
Ag(2)-O(3)#3	2.548(5)
Ag(2)-C(13)#4	2.647(7)
C(1)-O(3)	1.260(9)
C(1)-O(4)	1.262(9)
C(1)-C(2)	1.501(10)
C(2)-C(3)	1.371(11)
C(2)-C(7)	1.384(10)
C(3)-C(4)	1.398(10)
C(3)-H(3)	0.9300
C(4)-C(5)	1.379(11)
C(4)-H(4)	0.9300
C(5)-C(6)	1.390(10)
C(5)-C(8)	1.499(10)
C(6)-C(7)	1.387(10)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-C(9)	1.393(9)
C(8)-C(10)#5	1.417(10)
C(9)-C(10)	1.399(9)
C(9)-H(9)	0.9300
C(10)-C(8)#5	1.417(10)
C(10)-C(11)	1.496(9)
C(11)-C(12)	1.391(10)
C(11)-C(16)	1.405(10)
C(12)-C(13)	1.400(9)
C(12)-H(12)	0.9300
C(13)-C(14)	1.389(10)
C(13)-Ag(2)#4	2.647(7)
C(13)-H(13)	0.9300

C(14)-C(15)	1.376(10)
C(14)-C(17)	1.507(9)
C(15)-C(16)	1.375(10)
C(15)-H(15)	0.9300
C(16)-H(16)	0.9300
C(17)-O(2)	1.245(9)
C(17)-O(1)	1.260(9)
O(1)-Ag(2)#6	2.235(5)
O(2)-Ag(1)#6	2.257(5)
O(2)-Ag(1)#2	2.494(5)
O(3)-Ag(2)#7	2.548(5)
O(5)-C(18)	1.35(2)
O(5)-C(19)#8	1.86(6)
O(5)-C(18)#9	1.93(7)
O(6)-C(19)	1.36(2)
C(18)-C(19)#7	1.32(5)
C(18)-C(18)#9	1.60(11)
C(18)-O(5)#9	1.93(7)
C(19)-C(18)#3	1.32(5)
C(19)-O(5)#8	1.86(6)

O(3)-Ag(1)-O(2)#1	155.3(2)
O(3)-Ag(1)-O(2)#2	123.80(19)
O(2)#1-Ag(1)-O(2)#2	80.76(19)
O(3)-Ag(1)-Ag(2)	83.15(14)
O(2)#1-Ag(1)-Ag(2)	81.15(14)
O(2)#2-Ag(1)-Ag(2)	120.66(13)
O(4)-Ag(2)-O(1)#1	138.0(2)
O(4)-Ag(2)-O(3)#3	112.24(19)
O(1)#1-Ag(2)-O(3)#3	78.28(19)
O(4)-Ag(2)-C(13)#4	127.0(2)
O(1)#1-Ag(2)-C(13)#4	93.4(2)
O(3)#3-Ag(2)-C(13)#4	84.9(2)
O(4)-Ag(2)-Ag(1)	79.36(15)
O(1)#1-Ag(2)-Ag(1)	79.39(15)
O(3)#3-Ag(2)-Ag(1)	155.96(14)
C(13)#4-Ag(2)-Ag(1)	105.29(16)
O(3)-C(1)-O(4)	124.3(7)

O(3)-C(1)-C(2)	119.3(7)
O(4)-C(1)-C(2)	116.4(7)
C(3)-C(2)-C(7)	118.6(7)
C(3)-C(2)-C(1)	123.0(7)
C(7)-C(2)-C(1)	118.2(7)
C(2)-C(3)-C(4)	121.3(7)
C(2)-C(3)-H(3)	119.4
C(4)-C(3)-H(3)	119.4
C(5)-C(4)-C(3)	120.1(7)
C(5)-C(4)-H(4)	119.9
C(3)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	118.4(7)
C(4)-C(5)-C(8)	121.6(6)
C(6)-C(5)-C(8)	120.0(6)
C(7)-C(6)-C(5)	121.0(7)
C(7)-C(6)-H(6)	119.5
C(5)-C(6)-H(6)	119.5
C(2)-C(7)-C(6)	120.3(7)
C(2)-C(7)-H(7)	119.8
C(6)-C(7)-H(7)	119.8
C(9)-C(8)-C(10)#5	119.3(6)
C(9)-C(8)-C(5)	119.2(6)
C(10)#5-C(8)-C(5)	121.5(6)
C(8)-C(9)-C(10)	122.2(6)
C(8)-C(9)-H(9)	118.9
C(10)-C(9)-H(9)	118.9
C(9)-C(10)-C(8)#5	118.6(6)
C(9)-C(10)-C(11)	118.5(6)
C(8)#5-C(10)-C(11)	122.8(6)
C(12)-C(11)-C(16)	117.8(6)
C(12)-C(11)-C(10)	121.7(6)
C(16)-C(11)-C(10)	120.3(6)
C(11)-C(12)-C(13)	120.5(7)
C(11)-C(12)-H(12)	119.7
C(13)-C(12)-H(12)	119.7
C(14)-C(13)-C(12)	120.8(7)
C(14)-C(13)-Ag(2)#4	103.2(5)
C(12)-C(13)-Ag(2)#4	82.2(4)

C(14)-C(13)-H(13)	119.6
C(12)-C(13)-H(13)	119.6
Ag(2)#4-C(13)-H(13)	84.6
C(15)-C(14)-C(13)	118.3(6)
C(15)-C(14)-C(17)	120.0(6)
C(13)-C(14)-C(17)	121.7(6)
C(16)-C(15)-C(14)	121.7(7)
C(16)-C(15)-H(15)	119.1
C(14)-C(15)-H(15)	119.1
C(15)-C(16)-C(11)	120.7(7)
C(15)-C(16)-H(16)	119.6
C(11)-C(16)-H(16)	119.6
O(2)-C(17)-O(1)	125.0(7)
O(2)-C(17)-C(14)	119.6(7)
O(1)-C(17)-C(14)	115.4(6)
C(17)-O(1)-Ag(2)#6	125.9(5)
C(17)-O(2)-Ag(1)#6	122.3(5)
C(17)-O(2)-Ag(1)#2	127.4(5)
Ag(1)#6-O(2)-Ag(1)#2	99.24(19)
C(1)-O(3)-Ag(1)	119.8(5)
C(1)-O(3)-Ag(2)#7	143.4(5)
Ag(1)-O(3)-Ag(2)#7	96.36(18)
C(1)-O(4)-Ag(2)	128.1(5)
C(18)-O(5)-C(19)#8	96(4)
C(18)-O(5)-C(18)#9	55(4)
C(19)#8-O(5)-C(18)#9	40.8(17)
C(19)#7-C(18)-O(5)	167(6)
C(19)#7-C(18)-C(18)#9	110(5)
O(5)-C(18)-C(18)#9	81(4)
C(19)#7-C(18)-O(5)#9	67(4)
O(5)-C(18)-O(5)#9	125(4)
C(18)#9-C(18)-O(5)#9	44(2)
C(18)#3-C(19)-O(6)	148(6)
C(18)#3-C(19)-O(5)#8	72(3)
O(6)-C(19)-O(5)#8	138(4)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y+1,z+1 #2 -x+2,-y+1,-z+1 #3 x-1,y,z

#4 -x+1,-y+1,-z+1 #5 -x+1,-y,-z+1 #6 x+1,y-1,z-1
#7 x+1,y,z #8 -x+1,-y-1,-z #9 -x+2,-y-1,-z

Table S2. Bond lengths [Å] and angles [°] for CP-2.

Ag(1)-N(1)	2.171(6)
Ag(1)-N(2)#1	2.194(8)
C(1)-N(1)	1.330(8)
C(1)-C(2)	1.389(9)
C(1)-H(1)	0.9300
C(2)-C(3)	1.371(8)
C(2)-H(2)	0.9300
C(3)-C(4)	1.481(11)
C(4)-C(5)	1.382(8)
C(4)-C(5)#2	1.382(8)
C(5)-C(6)	1.383(9)
C(5)-H(5)	0.9300
C(6)-N(2)	1.333(8)
C(6)-H(6)	0.9300
N(3)-O(1)	1.220(8)
N(3)-O(1)#3	1.220(8)
N(3)-O(2)#3	1.241(13)
N(3)-O(2)	1.241(13)
O(2)-O(2)#3	1.06(3)

N(1)-Ag(1)-N(2)#1	180.0
N(1)-C(1)-C(2)	123.2(7)
N(1)-C(1)-H(1)	118.4
C(2)-C(1)-H(1)	118.4
C(3)-C(2)-C(1)	119.4(7)
C(3)-C(2)-H(2)	120.3
C(1)-C(2)-H(2)	120.3
C(2)#2-C(3)-C(2)	117.9(8)
C(2)#2-C(3)-C(4)	121.1(4)
C(2)-C(3)-C(4)	121.1(4)
C(5)-C(4)-C(5)#2	117.6(8)
C(5)-C(4)-C(3)	121.2(4)

C(5)#2-C(4)-C(3)	121.2(4)
C(4)-C(5)-C(6)	119.6(7)
C(4)-C(5)-H(5)	120.2
C(6)-C(5)-H(5)	120.2
N(2)-C(6)-C(5)	122.5(7)
N(2)-C(6)-H(6)	118.8
C(5)-C(6)-H(6)	118.8
C(1)#2-N(1)-C(1)	117.0(7)
C(1)#2-N(1)-Ag(1)	121.5(4)
C(1)-N(1)-Ag(1)	121.5(4)
C(6)-N(2)-C(6)#2	118.3(8)
C(6)-N(2)-Ag(1)#4	120.9(4)
C(6)#2-N(2)-Ag(1)#4	120.9(4)
O(1)-N(3)-O(1)#3	109.2(12)
O(1)-N(3)-O(2)#3	150.6(10)
O(1)#3-N(3)-O(2)#3	100.2(8)
O(1)-N(3)-O(2)	100.2(8)
O(1)#3-N(3)-O(2)	150.6(10)
O(2)#3-N(3)-O(2)	50.4(13)
O(2)#3-O(2)-N(3)	64.8(6)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1 #2 -x+3/2,-y+1,z #3 x,-y+1/2,-z+3/2

#4 x,y,z-1