

Supporting Information

Syntheses, structures and luminescence properties of three metal–organic frameworks based on 5-(4-(2H-tetrazol-5-yl)phenoxy)isophthalic acid

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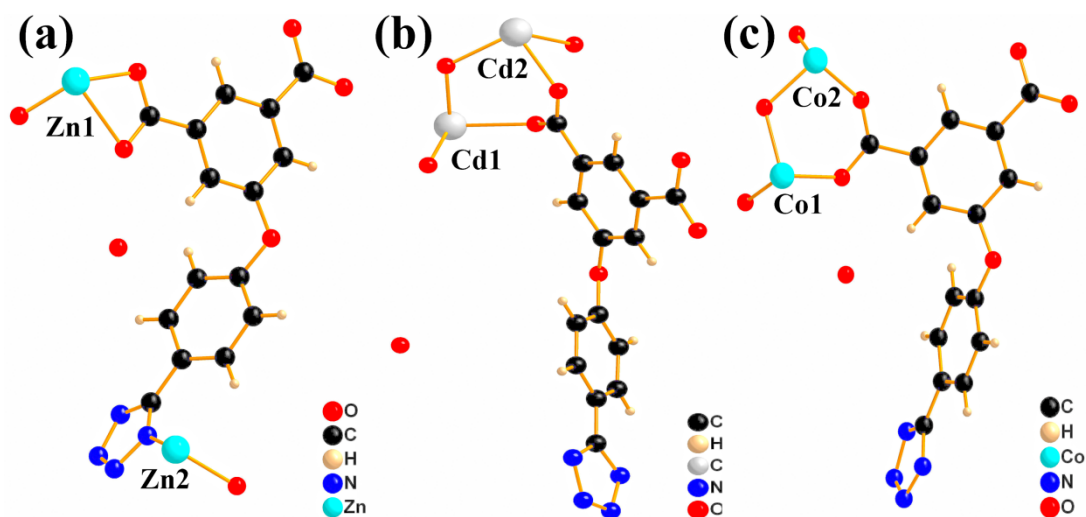


Fig. S1 The asymmetric unit of JUC-114, JUC-115 and JUC-116.

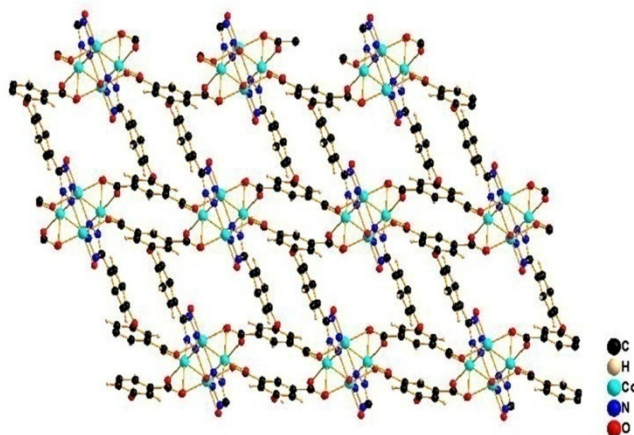


Fig. S2 View of 3D coordination framework along the a-axis of JUC-116.

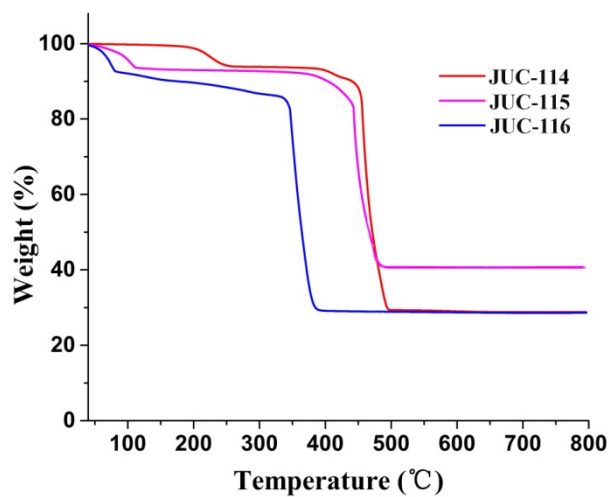


Fig. S3 The TGA curves of JUC-114, JUC-115 and JUC-116.

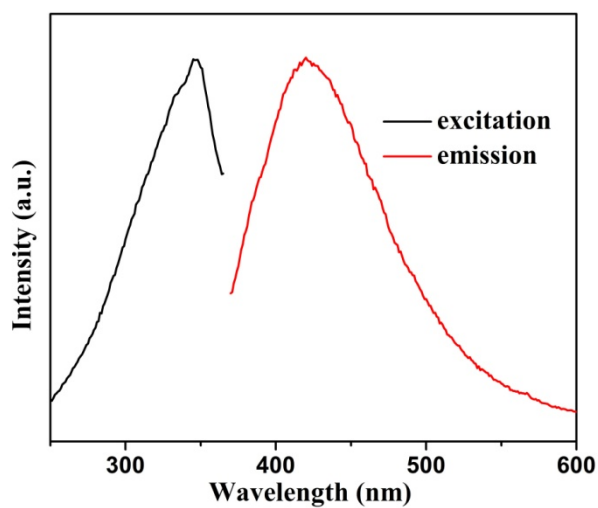


Fig. S4 Excitation (black line) and emission (red line) spectra of free H₃TPIA ligand.

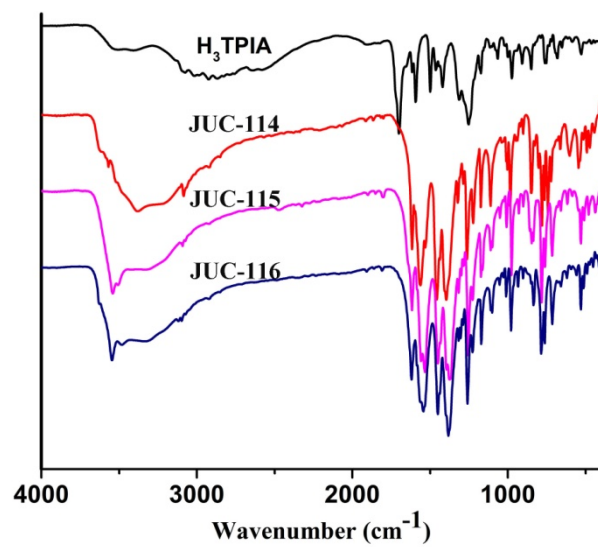
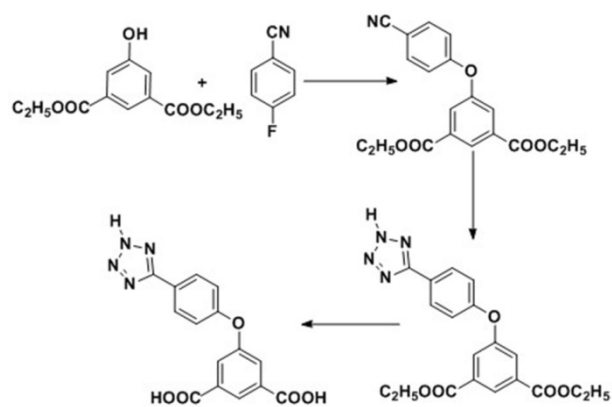


Fig. S5 IR spectra of H₃TPIA and JUC-114, JUC-115 and JUC-116.



Scheme S1 The synthetic route of H₃TPIA.

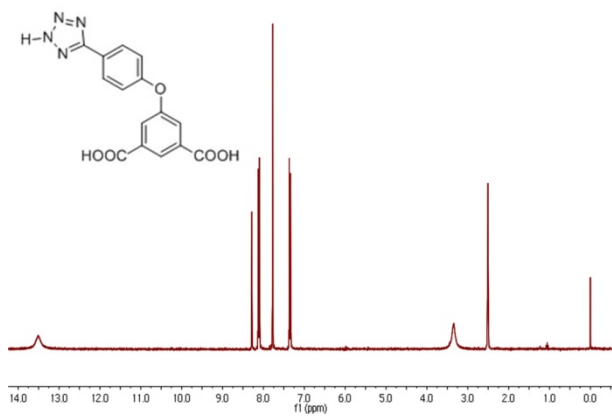
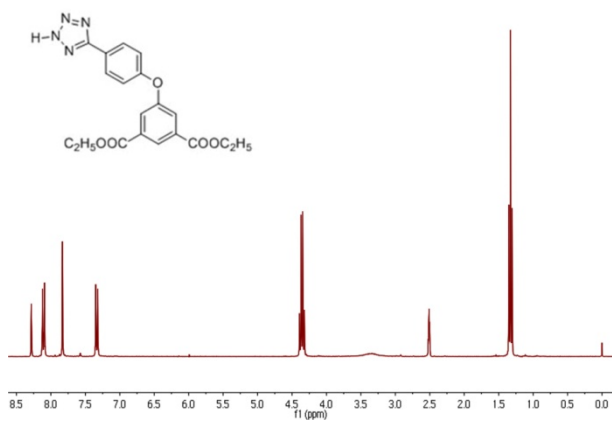


Fig. S6 The ¹H NMR spectra of the ligand.

Table S1. Selected bond lengths (Å) and angles (deg) for JUC-114, JUC-115 and JUC-116.

JUC-114			
N(1)-Zn(1)#1	2.027(3)	N(4)-Zn(2)	2.018(3)
O(1)-Zn(2)#2	1.887(3)	O(1)-Zn(1)	1.918(3)
O(2)-Zn(1)	2.366(3)	O(3)-Zn(1)	1.993(3)
O(4)-Zn(1)#3	2.004(2)	O(5)-Zn(2)#4	1.952(3)
O(7)-Zn(2)	2.003(3)	Zn(1)-O(4)#3	2.005(2)
Zn(1)-N(1)#5	2.027(3)	Zn(2)-O(1)#6	1.887(3)
Zn(2)-O(5)#7	1.952(3)		
O(1)-Zn(1)-O(4)#3	95.57(12)	O(1)-Zn(1)-O(3)	126.15(13)
O(1)-Zn(1)-N(1)#5	109.42(14)	O(3)-Zn(1)-O(4)#3	104.72(11)
O(4)#3-Zn(1)-N(1)#5	103.30(12)	O(3)-Zn(1)-N(1)#5	113.30(12)
O(3)-Zn(1)-O(2)	59.25(10)	O(1)-Zn(1)-O(2)	88.87(11)
N(1)#5-Zn(1)-O(2)	91.65(12)	O(4)#3-Zn(1)-O(2)	161.90(11)
O(1)#6-Zn(2)-O(7)	108.23(12)	O(1)#6-Zn(2)-O(5)#7	118.02(14)
O(1)#6-Zn(2)-N(4)	119.15(14)	O(5)#7-Zn(2)-O(7)	101.69(11)
O(7)-Zn(2)-N(4)	103.02(13)	O(5)#7-Zn(2)-N(4)	104.41(12)
Symmetry transformations used to generate equivalent atoms:			
#1 x-1,y+1,z	#2 x,y-1,z	#3 -x+1,-y-1,-z+1	#4 x,y-1,z+1
#5 x+1,y-1,z	#6 x,y+1,z	#7 x,y+1,z-1	
JUC-115			
Cd(1)-O(7)	2.237(2)	Cd(1)-O(4)#1	2.274(3)
Cd(1)-O(6)	2.326(3)	Cd(1)-N(2)#2	2.340(3)
Cd(1)-O(1)	2.376(3)	Cd(1)-N(3)#3	2.389(3)
O(7)-Cd(2)#4	2.243(2)	Cd(2)-O(2)	2.205(3)
Cd(2)-O(3)#5	2.234(3)	Cd(2)-O(7)#4	2.243(2)
Cd(2)-O(7)	2.274(2)	Cd(2)-N(4)#6	2.383(3)
Cd(2)-O(8)	2.768(4)	N(2)-Cd(1)#2	2.340(3)
N(3)-Cd(1)#7	2.389(3)	N(4)-Cd(2)#6	2.383(3)
O(3)-Cd(2)#5	2.234(3)	O(4)-Cd(1)#8	2.274(3)
O(7)-Cd(1)-O(4)#1	99.99(10)	O(7)-Cd(1)-O(6)	88.32(11)

O(4)#1-Cd(1)-O(6)	95.49(13)	O(7)-Cd(1)-N(2)#2	164.82(10)
O(4)#1-Cd(1)-N(2)#2	93.73(11)	O(6)-Cd(1)-N(2)#2	83.91(12)
O(7)-Cd(1)-O(1)	83.43(9)	O(4)#1-Cd(1)-O(1)	171.29(11)
O(6)-Cd(1)-O(1)	92.60(13)	N(2)#2-Cd(1)-O(1)	83.92(10)
O(7)-Cd(1)-N(3)#3	88.70(10)	O(4)#1-Cd(1)-N(3)#3	86.87(11)
O(6)-Cd(1)-N(3)#3	176.48(12)	N(2)#2-Cd(1)-N(3)#3	98.57(10)
O(1)-Cd(1)-N(3)#3	85.20(10)	O(2)-Cd(2)-O(3)#5	91.66(10)
O(2)-Cd(2)-O(7)#4	156.38(10)	O(3)#5-Cd(2)-O(7)#4	89.18(10)
O(2)-Cd(2)-O(7)	97.26(10)	O(3)#5-Cd(2)-O(7)	171.08(10)
O(7)#4-Cd(2)-O(7)	82.77(9)	O(2)-Cd(2)-N(4)#6	112.58(10)
O(3)#5-Cd(2)-N(4)#6	87.19(11)	O(7)#4-Cd(2)-N(4)#6	91.03(10)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 -x+1,-y+1,-z+1 #3 x-1,y-1,z-1 #4 -x,-y-1,-z #5 -x,-y-1,-z+1 #6 -x+1,-y,-z+1 #7
 x+1,y+1,z+1 #8 x,y,z+1

JUC-116

Co(1)-O(2)	2.080(5)	Co(1)-O(4)	2.093(5)
Co(1)-O(6)#1	2.146(5)	Co(1)-N(3)#2	2.163(5)
Co(1)-O(1)	2.196(5)	Co(1)-N(2)#3	2.205(6)
Co(2)-O(3)	2.019(5)	Co(2)-O(5)#4	2.073(5)
Co(2)-O(2)	2.080(4)	Co(2)-O(2)#5	2.123(4)
Co(2)-N(4)#2	8 2.230(5)	N(2)-Co(1)#3	2.204(6)
N(3)-Co(1)#6	2.163(5)	N(4)-Co(2)#6	2.230(5)
O(2)-Co(2)#5	2.123(4)	O(5)-Co(2)#4	2.073(4)
O(6)-Co(1)#7	2.146(5)	O(2)-Co(1)-O(4)	96.42(15)
O(2)-Co(1)-O(6)#1	88.26(14)	O(4)-Co(1)-O(6)#1	174.80(14)
O(2)-Co(1)-N(3)#2	88.28(15)	O(4)-Co(1)-N(3)#2	88.2(2)
O(6)#1-Co(1)-N(3)#2	89.7(2)	O(2)-Co(1)-O(1)	88.42(15)
O(4)-Co(1)-O(1)	92.5(2)	O(6)#1-Co(1)-O(1)	89.9(2)
N(3)#2-Co(1)-O(1)	176.68(14)	O(2)-Co(1)-N(2)#3	168.91(15)

O(4)-Co(1)-N(2)#3	91.81(17)	O(6)#1-Co(1)-N(2)#3	83.85(17)
N(3)#2-Co(1)-N(2)#3	99.43(15)	O(1)-Co(1)-N(2)#3	83.80(15)
O(3)-Co(2)-O(5)#4	89.7(2)	O(3)-Co(2)-O(2)	93.89(19)
O(5)#4-Co(2)-O(2)	162.04(14)	O(3)-Co(2)-O(2)#5	177.17(14)
O(5)#4-Co(2)-O(2)#5	92.77(19)	O(2)-Co(2)-O(2)#5	83.32(19)
O(3)-Co(2)-N(4)#2	89.7(2)	O(5)#4-Co(2)-N(4)#2	108.10(17)
O(2)-Co(2)-N(4)#2	89.52(16)	O(2)#5-Co(2)-N(4)#2	90.72(19)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 x+1,y+1,z #3 -x,-y,-z #4 -x+2,-y+1,-z+1 #5 -x+2,-y+1,-z #6 x-1,y-1,z #7 x,y,z+1
