

Supporting Information

Three novel zinc(II) metal-organic frameworks based on three tetrazolate ligands: synthesis, structures and photoluminescence

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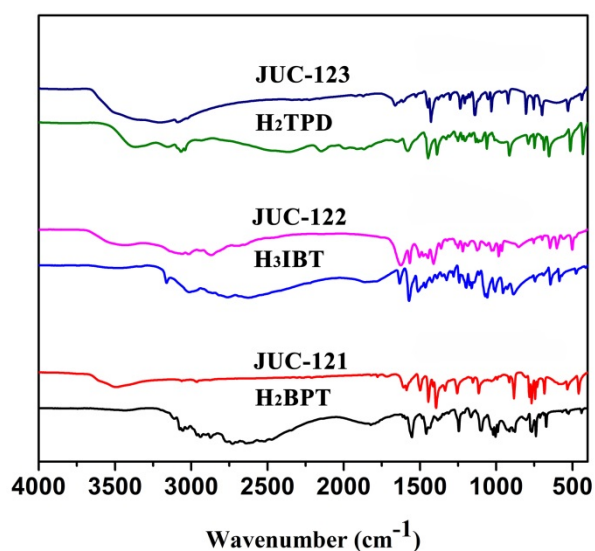


Fig. S1 The FT-IR spectra of the free ligands, JUC-121, JUC-122 and JUC-123.

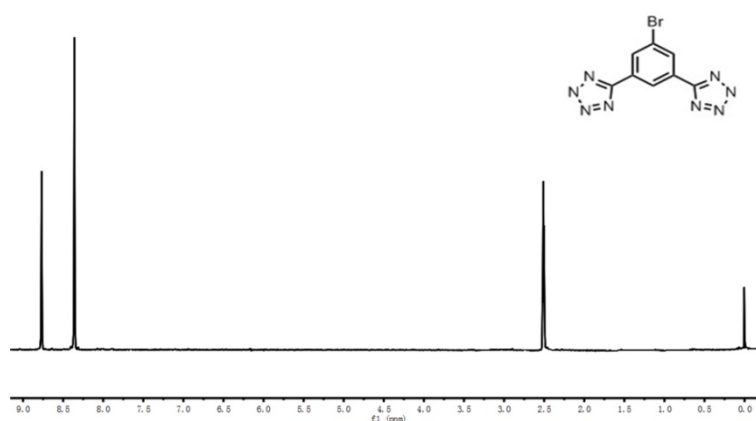


Fig. S2 The ¹H NMR spectra of H₂BPT.

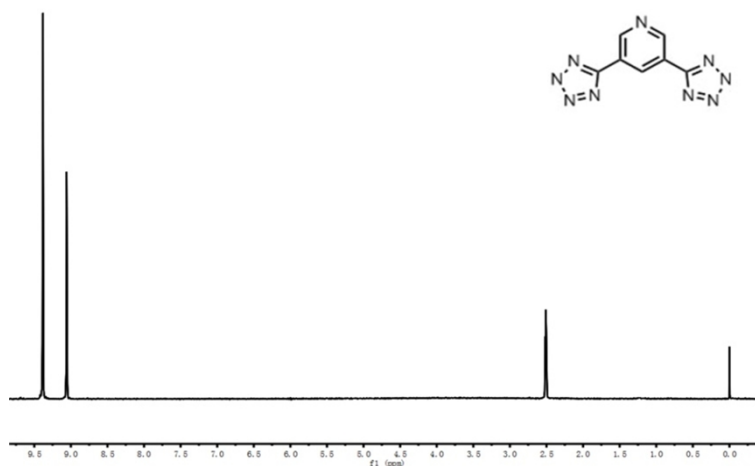


Fig. S3 The ^1H NMR spectra of H_2TPD .

Table S1 Selected bond lengths (\AA) and angles (deg) for JUC-121, JUC-122 and JUC-123

JUC-121			
Zn(1)-N(3)	2.131(3)	Zn(1)-N(3)#1	2.131(3)
Zn(1)-N(3)#2	2.131(3)	Zn(1)-N(3)#3	2.131(3)
Zn(1)-O(1)#2	2.138(3)	Zn(1)-O(1)	2.138(3)
Zn(2)-N(1)#4	2.016(3)	Zn(2)-N(1)#5	2.016(3)
Zn(2)-N(1)#6	2.016(3)	Zn(2)-N(1)	2.016(3)
N(3)-Zn(1)-N(3)#1	84.58(15)	N(3)-Zn(1)-N(3)#2	180.0
N(3)#1-Zn(1)-N(3)#2	95.42(15)	N(3)-Zn(1)-N(3)#3	95.42(15)
N(3)#1-Zn(1)-N(3)#3	180.0	N(3)#2-Zn(1)-N(3)#3	84.58(15)
N(3)-Zn(1)-O(1)#2	91.85(10)	N(3)#1-Zn(1)-O(1)#2	88.15(10)
N(3)#2-Zn(1)-O(1)#2	88.15(10)	N(3)#3-Zn(1)-O(1)#2	91.85(10)
N(3)-Zn(1)-O(1)	88.15(10)	N(3)#1-Zn(1)-O(1)	91.85(10)
N(3)#2-Zn(1)-O(1)	91.85(10)	N(3)#3-Zn(1)-O(1)	88.15(10)
O(1)#2-Zn(1)-O(1)	180.00(11)	N(1)#4-Zn(2)-N(1)#5	110.63(7)
N(1)#4-Zn(2)-N(1)#6	110.63(8)	N(1)#5-Zn(2)-N(1)#6	107.18(15)
N(1)#4-Zn(2)-N(1)	107.18(15)	N(1)#5-Zn(2)-N(1)	110.63(8)
N(1)#6-Zn(2)-N(1)	110.63(7)		

Symmetry transformations used to generate equivalent atoms:

#1 $y+1/2, x-1/2, -z+2$; #2 $-x+1, -y, -z+2$; #3 $-y+1/2, -x+1/2, z$; #4 $-x+3/2, -y+1/2, z$; #5 $-y+1, x-1/2, -z+3/2$; #6 $+1/2, -x+1, -z+3/2$; #7 y, x, z .

JUC-122

N(1)-Zn(1)	2.162(3)	N(4)-Zn(2)	1.983(3)
N(5)-Zn(1)	2.162(3)	N(10)-Zn(2)	1.988(3)
Zn(1)-N(1)#1	2.162(3)	Zn(1)-N(1)#2	2.162(3)
Zn(1)-N(5)#2	2.162(3)	Zn(1)-N(5)#1	2.163(3)
Zn(2)-N(4)#3	1.982(3)	Zn(2)-N(10)#3	1.988(3)
N(1)#1-Zn(1)-N(1)#2	98.01(9)	N(1)#1-Zn(1)-N(1)	98.00(9)
N(1)#2-Zn(1)-N(1)	98.00(9)	N(1)#1-Zn(1)-N(5)#2	93.99(11)
N(1)#2-Zn(1)-N(5)#2	76.42(10)	N(1)-Zn(1)-N(5)#2	167.40(10)
N(1)#1-Zn(1)-N(5)	167.40(10)	N(1)#2-Zn(1)-N(5)	93.99(11)
N(1)-Zn(1)-N(5)	76.42(10)	N(5)#2-Zn(1)-N(5)	92.55(10)
N(1)#1-Zn(1)-N(5)#1	76.42(10)	N(1)#2-Zn(1)-N(5)#1	167.40(10)
N(1)-Zn(1)-N(5)#1	93.99(11)	N(5)#2-Zn(1)-N(5)#1	92.55(10)
N(5)-Zn(1)-N(5)#1	92.55(10)	N(4)#3-Zn(2)-N(4)	114.59(17)
N(4)#3-Zn(2)-N(10)	112.30(13)	N(4)-Zn(2)-N(10)	103.55(11)
N(4)#3-Zn(2)-N(10)#3	103.55(11)	N(4)-Zn(2)-N(10)#3	112.30(13)
N(10)-Zn(2)-N(10)#3	110.8(2)		

Symmetry transformations used to generate equivalent atoms:

#1 -y,x-y,z; #2 -x+y,-x,z; #3 x-y+1/3,-y+2/3,-z+1/6.

JUC-123

N(2)-Zn(1)	2.028(3)	N(5)-Zn(1)	2.059(3)
N(7)-Zn(1)	2.002(3)	O(1)-Zn(1)	2.149(3)
O(2)-Zn(1)	2.154(3)		
N(7)-Zn(1)-N(2)	131.05(11)	N(7)-Zn(1)-N(5)	114.25(11)
N(2)-Zn(1)-N(5)	114.68(10)	N(7)-Zn(1)-O(1)	91.41(11)
N(2)-Zn(1)-O(1)	88.17(11)	N(5)-Zn(1)-O(1)	91.99(11)
N(7)-Zn(1)-O(2)	91.00(12)	N(2)-Zn(1)-O(2)	88.98(11)
N(5)-Zn(1)-O(2)	88.55(11)	O(1)-Zn(1)-O(2)	177.06(10)
