

Supporting Information for:

Four novel Zn(II)/Cd(II) metal-organic frameworks constructed from 4'-(4-pyridyl)-4,2':6',4''-terpyridine: hydrothermal synthesis, crystal structures, and luminescent properties

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Table S1. Selected bond distances /Å and bond angles /° for **1- 4^a**

Compound 1			
Zn(1)-N(1)	2.056(3)	Zn(1)-N(3)#1	2.060(3)
Zn(1)-Cl(1)	2.2373(12)	Zn(1)-Cl(2)	2.2088 (12)
N(1)-C(1)	1.336(4)	N(1)-C(5)	1.340(4)
N(2)-C(6)	1.352(4)	N(2)-C(10)	1.357(4)
N(3)-C(15)	1.332(5)	N(3)-C(11)	1.335(4)
N(3)-Zn(1)#2	2.060(3)	N(4)-C(20)	1.314(5)
N(4)-C(16)	1.323(5)		
N(1)-Zn(1)-N(3)#1	108.31(11)	N(1)-Zn(1)-Cl(2)	105.07(8)
N(3)#1-Zn(1)-Cl(2)	109.67(9)	N(1)-Zn(1)-Cl(1)	108.96(9)
N(3)#1-Zn(1)-Cl(1)	102.96(9)	Cl(2)-Zn(1)-Cl(1)	121.41(5)
C(1)-N(1)-C(5)	116.4(3)	C(1)-N(1)-Zn(1)	119.0(2)
C(5)-N(1)-Zn(1)	124.3(2)	C(6)-N(2)-C(10)	119.0(3)
C(15)-N(3)-C(11)	116.9(3)	C(15)-N(3)-Zn(1)#2	122.0(2)
C(11)-N(3)-Zn(1)#2	120.9(3)	C(20)-N(4)-C(16)	115.5(3)
N(1)-C(1)-C(2)	123.1(3)	N(1)-C(5)-C(4)	123.8(3)
N(1)-C(1)-H(1)	118.4	N(2)-C(6)-C(3)	117.7(3)
N(2)-C(6)-C(7)	121.0(3)	N(2)-C(10)-C(13)	117.4(3)
N(2)-C(10)-C(9)	121.5(3)	N(3)-C(15)-C(14)	123.4(3)
N(3)-C(11)-C(12)	123.4(3)	N(4)-C(20)-C(19)	125.2(4)
N(4)-C(16)-C(17)	124.9(4)		
Compound 2			
Zn(1)-O(1)	2.083(2)	Zn(1)-O(4)#1	2.088(2)
Zn(1)-O(3)	2.093(2)	Zn(1)-N(3)#2	2.142(3)
Zn(1)-N(1)	2.162(3)	Zn(1)-O(2)#3	2.164(2)
N(1)-C(5)	1.326(4)	N(1)-C(1)	1.337(4)
N(2)-C(10)	1.340(4)	N(2)-C(6)	1.340(4)
N(3)-C(15)	1.330(4)	N(3)-C(11)	1.332(4)
N(3)-Zn(1)#4	2.141(3)	N(4)-C(16)	1.322(6)
N(4)-C(20)	1.337(6)	O(1)-C(21)	1.256(4)
O(2)-C(21)	1.238(4)	O(2)-Zn(1)#3	2.164(2)
O(3)-C(22)	1.247(3)	O(4)-C(22)	1.250(3)
O(4)-Zn(1)#1	2.088(2)		
O(1)-Zn(1)-O(4)#1	173.44(8)	O(1)-Zn(1)-O(3)	97.70(9)
O(4)#1-Zn(1)-O(3)	80.27(8)	O(1)-Zn(1)-N(3)#2	88.11(9)
O(4)#1-Zn(1)-N(3)#2	98.29(10)	O(3)-Zn(1)-N(3)#2	96.20(9)
O(1)-Zn(1)-N(1)	96.55(10)	O(4)#1-Zn(1)-N(1)	84.63(9)
O(3)-Zn(1)-N(1)	163.40(9)	N(3)#2-Zn(1)-N(1)	92.73(10)
O(1)-Zn(1)-O(2)#3	78.57(8)	O(4)#1-Zn(1)-O(2)#3	95.03(9)
O(3)-Zn(1)-O(2)#3	85.90(9)	N(3)#2-Zn(1)-O(2)#3	166.68(9)
N(1)-Zn(1)-O(2)#3	88.61(10)	C(5)-N(1)-C(1)	116.6(3)
C(5)-N(1)-Zn(1)	122.8(2)	C(1)-N(1)-Zn(1)	120.3(2)
C(10)-N(2)-C(6)	118.5(3)	C(15)-N(3)-C(11)	115.9(3)
C(15)-N(3)-Zn(1)#4	125.2(2)	C(11)-N(3)-Zn(1)#4	118.0(2)
C(16)-N(4)-C(20)	115.3(4)	C(21)-O(1)-Zn(1)	114.7(2)

C(21)-O(2)-Zn(1)#3	112.22(19)	C(22)-O(3)-Zn(1)	112.43(18)
C(22)-O(4)-Zn(1)#1	112.65(18)	N(1)-C(1)-C(2)	123.7(3)
N(1)-C(5)-C(4)	123.2(3)	N(2)-C(6)-C(7)	122.2(3)
N(2)-C(6)-C(3)	114.5(3)	N(2)-C(10)-C(9)	122.4(3)
N(2)-C(10)-C(13)	113.8(3)	N(3)-C(11)-C(12)	123.7(3)
N(3)-C(15)-C(14)	124.2(3)	N(4)-C(16)-C(17)	125.0(4)
N(4)-C(20)-C(19)	124.1(4)	O(2)-C(21)-O(1)	125.5(3)
O(2)-C(21)-C(21)#3	117.7(3)	O(1)-C(21)-C(21)#3	116.8(3)
O(3)-C(22)-O(4)	125.7(3)	O(3)-C(22)-C(22)#1	117.3(3)
O(4)-C(22)-C(22)#1	117.0(3)		

Compound 3

Cd(1)-N(1)	2.318(5)	Cd(1)-O(1)#1	2.323(4)
Cd(1)-N(3)#2	2.360(5)	Cd(1)-O(5)#3	2.384(5)
Cd(1)-O(1)	2.418(5)	Cd(1)-O(3)	2.446(5)
Cd(1)-O(4)#3	2.515(6)	N(1)-C(5)	1.317(8)
N(1)-C(1)	1.341(8)	N(2)-C(6)	1.348(8)
N(2)-C(10)	1.366(8)	N(3)-C(15)	1.320(8)
N(3)-C(11)	1.323(8)	N(3)-Cd(1)#4	2.360(5)
N(4)-C(16)	1.328(10)	N(4)-C(20)	1.333(10)
O(1)-C(21)	1.259(8)	O(1)-Cd(1)#1	2.323(4)
O(2)-C(21)	1.234(8)	O(3)-C(22)	1.422(8)
O(4)-C(24)	1.237(9)	O(4)-Cd(1)#5	2.515(6)
O(5)-C(24)	1.227(9)	O(5)-Cd(1)#5	2.384(5)

N(1)-Cd(1)-O(1)#1	90.02(17)	N(1)-Cd(1)-N(3)#2	177.58(19)
O(1)#1-Cd(1)-N(3)#2	89.28(17)	N(1)-Cd(1)-O(5)#3	89.3(2)
O(1)#1-Cd(1)-O(5)#3	102.99(19)	N(3)#2-Cd(1)-O(5)#3	93.1(2)
N(1)-Cd(1)-O(1)	90.55(17)	O(1)#1-Cd(1)-O(1)	71.65(16)
N(3)#2-Cd(1)-O(1)	87.03(17)	O(5)#3-Cd(1)-O(1)	174.64(17)
N(1)-Cd(1)-O(3)	89.16(18)	O(1)#1-Cd(1)-O(3)	135.94(17)
N(3)#2-Cd(1)-O(3)	89.72(18)	O(5)#3-Cd(1)-O(3)	121.05(19)
O(1)-Cd(1)-O(3)	64.31(16)	N(1)-Cd(1)-O(4)#3	98.45(19)
O(1)#1-Cd(1)-O(4)#3	153.11(17)	N(3)#2-Cd(1)-O(4)#3	83.18(19)
O(5)#3-Cd(1)-O(4)#3	52.02(18)	O(1)-Cd(1)-O(4)#3	133.25(16)
O(3)-Cd(1)-O(4)#3	70.03(17)	C(5)-N(1)-C(1)	116.5(6)
C(5)-N(1)-Cd(1)	120.2(4)	C(1)-N(1)-Cd(1)	123.1(4)
C(6)-N(2)-C(10)	119.1(5)	C(15)-N(3)-C(11)	115.8(6)
C(15)-N(3)-Cd(1)#4	121.7(4)	C(11)-N(3)-Cd(1)#4	122.3(5)
C(16)-N(4)-C(20)	116.0(7)	C(21)-O(1)-Cd(1)#1	125.5(5)
C(21)-O(1)-Cd(1)	125.5(4)	Cd(1)#1-O(1)-Cd(1)	108.35(17)
C(22)-O(3)-Cd(1)	122.5(4)	C(24)-O(4)-Cd(1)#5	89.7(5)
C(24)-O(5)-Cd(1)#5	96.3(5)	N(1)-C(1)-C(2)	123.2(6)
N(1)-C(5)-C(4)	123.9(6)	N(2)-C(6)-C(7)	121.1(6)
N(2)-C(6)-C(3)	117.4(5)	N(2)-C(10)-C(9)	120.9(5)
N(2)-C(10)-C(13)	117.0(5)	N(3)-C(11)-C(12)	123.7(7)
N(3)-C(15)-C(14)	125.0(6)	N(4)-C(16)-C(17)	124.1(8)
N(4)-C(20)-C(19)	123.8(8)	O(2)-C(21)-C(22)	117.7(6)
O(1)-C(21)-C(22)	116.7(6)	O(3)-C(22)-C(23)	112.8(6)

O(3)-C(22)-C(21)	109.8(5)	O(4)-C(24)-C(23)	117.9(7)
O(5)-C(24)-C(23)	120.4(7)	O(5)-C(24)-O(4)	121.7(8)

Compound 4

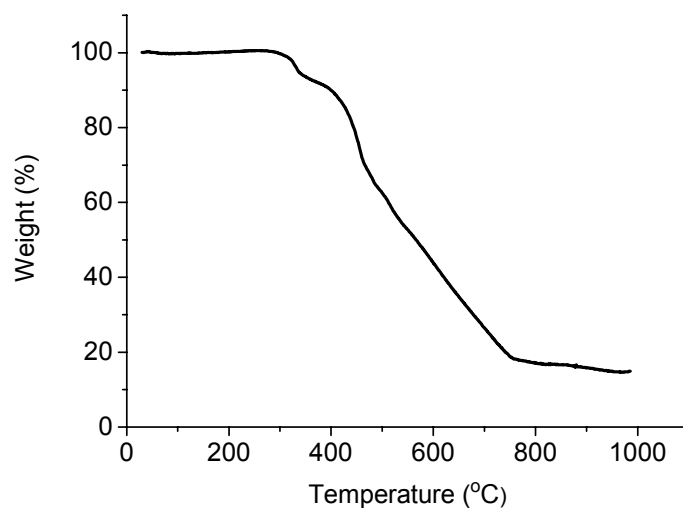
Zn(1)-O(7)	1.919(4)	Zn(1)-O(2)	1.993(4)
Zn(1)-O(6)#1	1.997(5)	Zn(1)-N(1)	2.035(4)
Zn(1)-O(1)	2.447(4)	Zn(2)-O(7)	1.911(4)
Zn(2)-O(5)#1	1.980(5)	Zn(2)-O(3)#2	2.051(5)
Zn(2)-N(3)#3	2.075(5)	Zn(2)-O(4)#2	2.431(6)
N(1)-C(14)	1.355(7)	N(1)-C(10)	1.338(7)
N(2)-C(15)	1.369(9)	N(2)-C(19)	1.315(9)
N(3)-C(20)	1.314(8)	N(3)-C(24)	1.308(8)
N(4)-C(27)	1.37(3)	N(3)-Zn(2)#4	2.075(5)
N(4')-C(27')	1.30(4)	N(4)-C(28)	1.40(3)
O(1)-C(1)	1.243(7)	O(2)-C(1)	1.264(7)
O(3)-C(2)	1.236(8)	O(3)-Zn(2)#5	2.051(5)
O(4)-C(2)	1.223(8)	O(4)-Zn(2)#5	2.431(5)
O(5)-C(3)	1.275(7)	O(5)-Zn(2)#6	1.980(5)
O(6)-C(3)	1.222(7)	O(6)-Zn(1)#6	1.997(5)
C(2)-Zn(2)#5	2.538(7)		
O(7)-Zn(1)-O(2)	114.09(19)	O(7)-Zn(1)-O(6)#1	103.51(18)
O(2)-Zn(1)-O(6)#1	94.42(18)	O(7)-Zn(1)-N(1)	104.42(18)
O(2)-Zn(1)-N(1)	132.60(19)	O(6)#1-Zn(1)-N(1)	102.63(19)
O(7)-Zn(1)-O(1)	92.84(17)	O(2)-Zn(1)-O(1)	58.02(15)
O(6)#1-Zn(1)-O(1)	152.12(16)	N(1)-Zn(1)-O(1)	94.78(16)
O(7)-Zn(2)-O(5)#1	106.02(19)	O(7)-Zn(2)-O(3)#2	113.3(2)
O(5)#1-Zn(2)-O(3)#2	104.2(2)	O(7)-Zn(2)-N(3)#3	108.5(2)
O(5)#1-Zn(2)-N(3)#3	97.1(2)	O(3)#2-Zn(2)-N(3)#3	124.8(2)
O(7)-Zn(2)-O(4)#2	95.49(18)	O(5)#1-Zn(2)-O(4)#2	155.96(19)
O(3)#2-Zn(2)-O(4)#2	56.22(18)	N(3)#3-Zn(2)-O(4)#2	85.91(18)
O(7)-Zn(2)-C(2)#2	100.8(2)	O(5)#1-Zn(2)-C(2)#2	133.0(2)
O(3)#2-Zn(2)-C(2)#2	28.84(19)	N(3)#3-Zn(2)-C(2)#2	110.2(2)
O(4)#2-Zn(2)-C(2)#2	28.40(18)	C(10)-N(1)-C(14)	117.8(5)
C(10)-N(1)-Zn(1)	119.2(4)	C(14)-N(1)-Zn(1)	122.2(4)
C(19)-N(2)-C(15)	118.1(5)	C(24)-N(3)-C(20)	117.8(5)
C(24)-N(3)-Zn(2)#4	122.5(4)	C(20)-N(3)-Zn(2)#4	119.1(5)
C(27)-N(4)-C(28)	115(2)		
C(1)-O(1)-Zn(1)	79.6(4)	C(1)-O(2)-Zn(1)	99.8(3)
C(2)-O(3)-Zn(2)#5	98.0(4)	C(2)-O(4)-Zn(2)#5	80.6(4)
C(3)-O(5)-Zn(2)#6	129.9(5)	C(3)-O(6)-Zn(1)#6	134.5(4)
Zn(2)-O(7)-Zn(1)	118.2(2)	O(1)-C(1)-O(2)	121.7(5)
O(1)-C(1)-C(4)	119.4(6)	O(2)-C(1)-C(4)	118.9(5)
O(4)-C(2)-O(3)	120.8(6)	O(4)-C(2)-C(6)	119.6(7)
O(3)-C(2)-C(6)	119.4(6)	O(4)-C(2)-Zn(2)#5	71.0(4)
O(3)-C(2)-Zn(2)#5	53.2(3)	C(6)-C(2)-Zn(2)#5	155.6(5)
O(6)-C(3)-O(5)	126.2(6)	O(6)-C(3)-C(8)	117.7(5)
O(5)-C(3)-C(8)	116.2(6)	N(1)-C(10)-C(11)	123.4(6)
N(1)-C(14)-C(13)	120.8(6)	N(2)-C(15)-C(25)	119.1(6)

N(3)-C(20)-C(21)	120.8(6)	N(3)-C(24)-C(23)	124.0(6)
N(4)-C(27)-C(26)	128(2)	N(4')-C(27')-C(26')	124 (2)

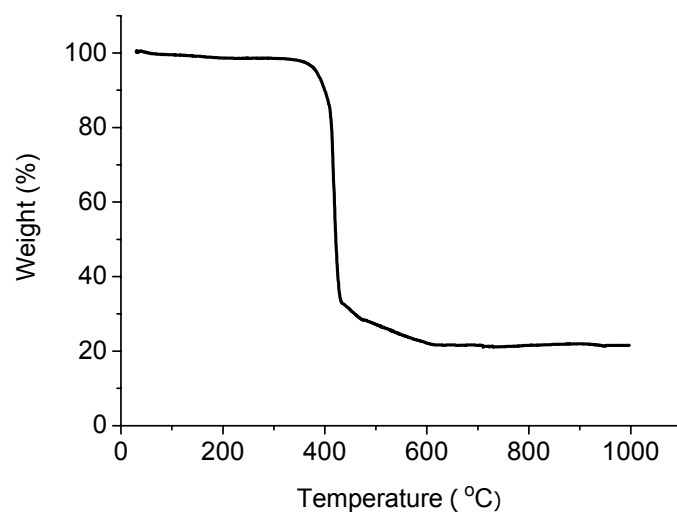
^aSymmetry code for **1**: #1 (-x+1/2, y+1/2, -z+1/2), #2 (-x+1/2, y-1/2, -z+1/2); for **2**: #1 (-x, -y, -z), #2 (-x+1/2, y-1/2, -z+1/2), #3 (-x, -y+1, -z), #4 (-x+1/2, y+1/2, -z+1/2); for **3**: #1 (-x+1/2, -y+5/2, -z+2), #2 (x+1/2, -y+5/2, z+1/2), #3 (-x+1/2, y+1/2, z+5/2), #4 (x-1/2, -y+5/2, -1/2), #5 (-x+1/2, y-1/2, -z+5/2); for **4**: #1 (x, -y+2, -1/2), #2 (x, y-1, z), #3 (x-1/2, -y+3/2, z-1/2), #4 (x+1/2, -y+3/2, z+1/2), #5 (x, y+1, z), #6 (x, -y+2, z+1/2).

Fig. S1 TGA curves of compounds **1-4** (a, b, c, d).

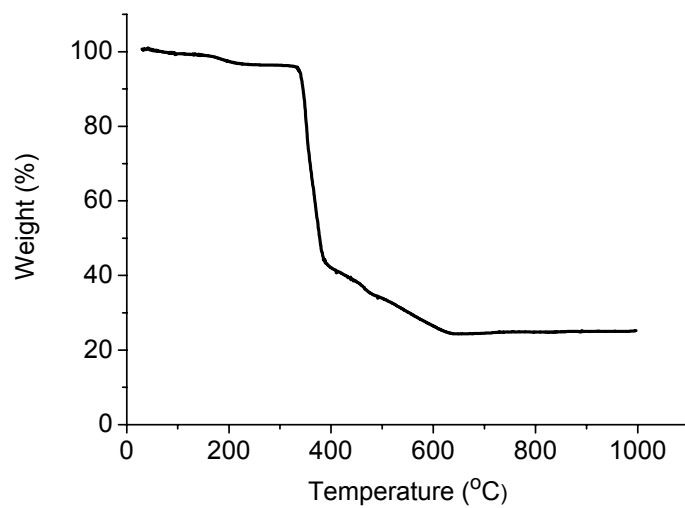
(a)



(b)



(c)



(d)

