

A series of alkaline earth metal coordination polymers constructed from two newly designed imidazole-based dicarboxylate ligands containing pyridinylmethyl group

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Supporting information

Table S1 Selected bond lengths [Å] and angles[°] for the compounds 1-7.^a

Compound 1			
Ba(1)-O(2)#1	2.655(4)	Ba(1)-O(4)#3	2.830(4)
Ba(1)-O(3)#1	2.688(4)	Ba(1)-O(2)	2.858(4)
Ba(1)-O(1)#2	2.777(4)	Ba(1)-O(3)#4	2.880(4)
Ba(1)-O(1W)	2.810(4)	Ba(1)-O(4)#4	2.942(4)
Ba(1)-O(1)	2.818(4)		
O(2)#1-Ba(1)-O(3)#1	65.33(12)	O(1W)-Ba(1)-O(2)	106.48(12)
O(2)#1-Ba(1)-O(1)#2	154.92(11)	O(1)-Ba(1)-O(2)	45.93(11)
O(3)#1-Ba(1)-O(1)#2	110.83(12)	O(4)#3-Ba(1)-O(2)	67.54(11)
O(2)#1-Ba(1)-O(1W)	91.69(12)	O(2)#1-Ba(1)-O(3)#4	118.69(12)
O(3)#1-Ba(1)-O(1W)	79.95(13)	O(3)#1-Ba(1)-O(3)#4	71.06(13)
O(1)#2-Ba(1)-O(1W)	63.53(12)	O(1)#2-Ba(1)-O(3)#4	80.23(11)
O(2)#1-Ba(1)-O(1)	74.99(11)	O(1W)-Ba(1)-O(3)#4	120.85(12)
O(3)#1-Ba(1)-O(1)	129.69(12)	O(1)-Ba(1)-O(3)#4	105.32(12)
O(1)#2-Ba(1)-O(1)	118.01(9)	O(4)#3-Ba(1)-O(3)#4	171.58(11)
O(1W)-Ba(1)-O(1)	132.29(11)	O(2)-Ba(1)-O(3)#4	104.68(11)
O(2)#1-Ba(1)-O(4)#3	64.03(11)	O(2)#1-Ba(1)-O(4)#4	138.80(12)

O(3)#1-Ba(1)-O(4)#3	116.39(11)	O(3)#1-Ba(1)-O(4)#4	115.54(11)
O(1)#2-Ba(1)-O(4)#3	99.78(11)	O(1)#2-Ba(1)-O(4)#4	66.12(11)
O(1W)-Ba(1)-O(4)#3	65.88(12)	O(1W)-Ba(1)-O(4)#4	129.51(12)
O(1)-Ba(1)-O(4)#3	67.14(11)	O(1)-Ba(1)-O(4)#4	76.19(11)
O(2)#1-Ba(1)-O(2)	114.10(10)	O(4)#3-Ba(1)-O(4)#4	127.78(7)
O(3)#1-Ba(1)-O(2)	173.56(12)	O(2)-Ba(1)-O(4)#4	60.25(10)
O(1)#2-Ba(1)-O(2)	72.53(11)	O(3)#4-Ba(1)-O(4)#4	44.50(10)

Compound 2

O(1)-Sr(1)#2	2.655(3)	O(3)-Sr(1)#1	2.785(3)
O(1)-Sr(1)	2.682(3)	O(4)-Sr(1)#4	2.742(3)
O(2)-Sr(1)#3	2.530(3)	O(4)-Sr(1)#1	2.807(3)
O(2)-Sr(1)	2.725(3)	O(1W)-Sr(1)	2.665(3)
O(3)-Sr(1)#3	2.567(3)		
O(2)#2-Sr(1)-O(3)#2	69.11(9)	O(1)#3-Sr(1)-O(4)#4	102.53(9)
O(2)#2-Sr(1)-O(1)#3	157.88(9)	O(1W)-Sr(1)-O(4)#4	67.05(9)
O(3)#2-Sr(1)-O(1)#3	107.82(9)	O(1)-Sr(1)-O(4)#4	67.37(9)
O(2)#2-Sr(1)-O(1W)	91.84(9)	O(2)-Sr(1)-O(4)#4	69.97(9)
O(3)#2-Sr(1)-O(1W)	78.00(10)	O(2)#2-Sr(1)-O(3)#5	115.70(9)
O(1)#3-Sr(1)-O(1W)	66.37(9)	O(3)#2-Sr(1)-O(3)#5	65.10(11)
O(2)#2-Sr(1)-O(1)	73.12(9)	O(1)#3-Sr(1)-O(3)#5	80.16(9)
O(3)#2-Sr(1)-O(1)	130.79(9)	O(1W)-Sr(1)-O(3)#5	118.69(9)
O(1)#3-Sr(1)-O(1)	118.78(7)	O(1)-Sr(1)-O(3)#5	106.87(9)
O(1W)-Sr(1)-O(1)	133.99(9)	O(2)-Sr(1)-O(3)#5	106.56(8)
O(2)#2-Sr(1)-O(2)	115.65(7)	O(4)#4-Sr(1)-O(3)#5	174.24(9)
O(3)#2-Sr(1)-O(2)	171.59(9)	O(2)#2-Sr(1)-O(4)#5	135.24(10)
O(1)#3-Sr(1)-O(2)	70.54(8)	O(3)#2-Sr(1)-O(4)#5	111.57(9)
O(1W)-Sr(1)-O(2)	108.13(9)	O(1)#3-Sr(1)-O(4)#5	66.79(9)
O(1)-Sr(1)-O(2)	48.81(8)	O(1W)-Sr(1)-O(4)#5	132.82(9)
O(2)#2-Sr(1)-O(4)#4	63.22(9)	O(1)-Sr(1)-O(4)#5	75.74(9)
O(3)#2-Sr(1)-O(4)#4	118.24(9)	O(2)-Sr(1)-O(4)#5	60.07(8)

Compound 3

Ca(1)-O(2W)	2.284(11)	Ca(2)-O(4)#1	2.316(9)
Ca(1)-O(8)#2	2.329(9)	Ca(2)-O(7)	2.327(8)
Ca(1)-O(3)	2.332(8)	Ca(2)-O(1W)	2.331(11)
Ca(1)-O(1)#3	2.434(8)	Ca(2)-O(6)	2.411(8)
Ca(1)-O(2)	2.486(7)	Ca(2)-O(5)#3	2.442(7)
Ca(1)-O(6)	2.506(8)	Ca(2)-O(2)#3	2.489(7)
Ca(1)-O(5)	2.524(8)	Ca(2)-O(1)#3	2.537(8)
O(2W)-Ca(1)-O(8)#2	160.9(3)	O(4)#1-Ca(2)-O(7)	82.5(3)
O(2W)-Ca(1)-O(3)	78.4(3)	O(4)#1-Ca(2)-O(1W)	160.4(3)
O(8)#2-Ca(1)-O(3)	82.6(3)	O(7)-Ca(2)-O(1W)	78.6(3)
O(2W)-Ca(1)-O(1)#3	98.2(4)	O(4)#1-Ca(2)-O(6)	95.4(3)
O(8)#2-Ca(1)-O(1)#3	83.1(3)	O(7)-Ca(2)-O(6)	81.0(3)

O(3)-Ca(1)-O(1)#3	85.9(3)	O(1W)-Ca(2)-O(6)	76.7(4)
O(2W)-Ca(1)-O(2)	78.8(3)	O(4)#1-Ca(2)-O(5)#3	84.5(3)
O(8)#2-Ca(1)-O(2)	95.0(3)	O(7)-Ca(2)-O(5)#3	84.4(3)
O(3)-Ca(1)-O(2)	79.3(3)	O(1W)-Ca(2)-O(5)#3	98.7(4)
O(1)#3-Ca(1)-O(2)	165.2(3)	O(6)-Ca(2)-O(5)#3	165.3(3)
O(2W)-Ca(1)-O(6)	88.7(3)	O(4)#1-Ca(2)-O(2)#3	111.2(3)
O(8)#2-Ca(1)-O(6)	109.7(3)	O(7)-Ca(2)-O(2)#3	151.6(3)
O(3)-Ca(1)-O(6)	152.7(3)	O(1W)-Ca(2)-O(2)#3	88.1(3)
O(1)#3-Ca(1)-O(6)	72.1(3)	O(6)-Ca(2)-O(2)#3	120.4(3)
O(2)-Ca(1)-O(6)	122.0(2)	O(5)#3-Ca(2)-O(2)#3	72.9(2)
O(2W)-Ca(1)-O(5)	90.3(3)	O(4)#1-Ca(2)-O(1)#3	107.4(3)
O(8)#2-Ca(1)-O(5)	105.1(3)	O(7)-Ca(2)-O(1)#3	151.8(3)
O(3)-Ca(1)-O(5)	150.3(3)	O(1W)-Ca(2)-O(1)#3	87.5(3)
O(1)#3-Ca(1)-O(5)	123.2(3)	O(6)-Ca(2)-O(1)#3	72.0(3)
O(2)-Ca(1)-O(5)	71.6(2)	O(5)#3-Ca(2)-O(1)#3	122.2(3)
O(6)-Ca(1)-O(5)	51.9(2)	O(2)#3-Ca(2)-O(1)#3	49.8(2)

Compound 4

Ca(1)-O(5)	2.252(4)	Ca(2)-O(6)	2.276(4)
Ca(1)-O(3)#2	2.254(3)	Ca(2)-O(7)	2.309(4)
Ca(1)-O(2)#2	2.255(4)	Ca(2)-O(8)#4	2.418(4)
Ca(1)-O(4)#3	2.333(4)	Ca(2)-N(5)#4	2.546(4)
Ca(1)-O(2W)	2.352(4)	Ca(2)-N(6)#1	2.549(5)
Ca(1)-N(1)#3	2.436(4)	Ca(2)-O(1W)	2.703(6)
Ca(2)-O(1)	2.270(4)		
O(5)-Ca(1)-O(3)#2	105.63(14)	O(1)-Ca(2)-O(8)#4	74.30(13)
O(5)-Ca(1)-O(2)#2	93.49(17)	O(6)-Ca(2)-O(8)#4	113.92(13)
O(3)#2-Ca(1)-O(2)#2	83.52(14)	O(7)-Ca(2)-O(8)#4	148.70(13)
O(5)-Ca(1)-O(4)#3	85.80(13)	O(1)-Ca(2)-N(5)#4	135.95(13)
O(3)#2-Ca(1)-O(4)#3	168.35(14)	O(6)-Ca(2)-N(5)#4	94.67(14)
O(2)#2-Ca(1)-O(4)#3	93.70(14)	O(7)-Ca(2)-N(5)#4	87.38(14)
O(5)-Ca(1)-O(2W)	95.24(17)	O(8)#4-Ca(2)-N(5)#4	64.02(12)
O(3)#2-Ca(1)-O(2W)	93.92(14)	O(1)-Ca(2)-N(6)#1	88.79(15)
O(2)#2-Ca(1)-O(2W)	171.26(17)	O(6)-Ca(2)-N(6)#1	161.69(15)
O(4)#3-Ca(1)-O(2W)	87.13(15)	O(7)-Ca(2)-N(6)#1	89.81(14)
O(5)-Ca(1)-N(1)#3	153.48(14)	O(8)#4-Ca(2)-N(6)#1	83.03(15)
O(3)#2-Ca(1)-N(1)#3	100.79(14)	N(5)#4-Ca(2)-N(6)#1	99.31(14)
O(2)#2-Ca(1)-N(1)#3	87.09(16)	O(1)-Ca(2)-O(1W)	67.26(15)
O(4)#3-Ca(1)-N(1)#3	67.71(13)	O(6)-Ca(2)-O(1W)	85.91(17)
O(2W)-Ca(1)-N(1)#3	85.18(15)	O(7)-Ca(2)-O(1W)	69.86(15)
O(1)-Ca(2)-O(6)	89.35(14)	O(8)#4-Ca(2)-O(1W)	136.43(15)
O(1)-Ca(2)-O(7)	136.19(14)	N(5)#4-Ca(2)-O(1W)	156.74(14)
O(6)-Ca(2)-O(7)	79.02(13)	N(6)#1-Ca(2)-O(1W)	76.58(17)

Compound 5

Ba(1)-O(3)#1	2.662(4)	Ba(1)-O(1)	2.878(4)
Ba(1)-O(2)#1	2.699(3)	Ba(1)-O(2)#4	2.900(4)
Ba(1)-O(4)#2	2.776(3)	Ba(1)-O(1W)	2.905(4)
Ba(1)-O(4)#3	2.811(3)	Ba(1)-O(1)#4	2.961(3)
Ba(1)-O(3)#3	2.860(3)		
O(3)#1-Ba(1)-O(2)#1	65.63(10)	O(4)#3-Ba(1)-O(2)#4	103.41(10)
O(3)#1-Ba(1)-O(4)#2	158.61(10)	O(3)#3-Ba(1)-O(2)#4	103.76(10)
O(2)#1-Ba(1)-O(4)#2	116.03(10)	O(1)-Ba(1)-O(2)#4	168.41(10)
O(3)#1-Ba(1)-O(4)#3	72.62(9)	O(3)#1-Ba(1)-O(1W)	95.85(10)
O(2)#1-Ba(1)-O(4)#3	125.63(10)	O(2)#1-Ba(1)-O(1W)	87.23(12)
O(4)#2-Ba(1)-O(4)#3	115.60(8)	O(4)#2-Ba(1)-O(1W)	63.57(10)
O(3)#1-Ba(1)-O(3)#3	112.41(9)	O(4)#3-Ba(1)-O(1W)	131.20(11)
O(2)#1-Ba(1)-O(3)#3	168.52(10)	O(3)#3-Ba(1)-O(1W)	104.25(11)
O(4)#2-Ba(1)-O(3)#3	70.24(10)	O(1)-Ba(1)-O(1W)	67.36(11)
O(4)#3-Ba(1)-O(3)#3	45.89(10)	O(2)#4-Ba(1)-O(1W)	123.21(11)
O(3)#1-Ba(1)-O(1)	63.13(10)	O(3)#1-Ba(1)-O(1)#4	136.11(10)
O(2)#1-Ba(1)-O(1)	118.75(10)	O(2)#1-Ba(1)-O(1)#4	112.96(10)
O(4)#2-Ba(1)-O(1)	101.18(10)	O(4)#2-Ba(1)-O(1)#4	64.51(10)
O(4)#3-Ba(1)-O(1)	65.20(10)	O(4)#3-Ba(1)-O(1)#4	75.78(10)
O(3)#3-Ba(1)-O(1)	67.10(10)	O(3)#3-Ba(1)-O(1)#4	59.86(10)
O(3)#1-Ba(1)-O(2)#4	116.96(10)	O(1)-Ba(1)-O(1)#4	126.87(6)
O(2)#1-Ba(1)-O(2)#4	68.99(11)	O(2)#4-Ba(1)-O(1)#4	44.08(9)
O(4)#2-Ba(1)-O(2)#4	81.44(10)	O(1W)-Ba(1)-O(1)#4	127.99(10)

Compound 6

Mg(1)-O(4)#1	2.057(4)	Mg(3)-O(5)	2.095(4)
Mg(1)-O(2W)	2.062(6)	Mg(3)-N(4)	2.165(5)
Mg(1)-O(8)	2.102(4)	Mg(3)-N(4)#2	2.165(5)
Mg(1)-O(1W)	2.128(5)	Mg(3)-N(4)#3	2.165(5)
Mg(1)-N(5)	2.132(6)	Mg(4)-O(7W)	2.052(7)
Mg(1)-N(2)#1	2.217(6)	Mg(4)-O(4W)	2.058(6)
Mg(2)-O(3)	1.989(5)	Mg(4)-O(1)	2.071(5)
Mg(2)-O(6)	2.001(5)	Mg(4)-O(6W)	2.084(5)
Mg(2)-O(2)	2.055(4)	Mg(4)-O(5W)	2.099(6)
Mg(2)-O(3W)	2.086(4)	Mg(4)-N(1)	2.141(6)
Mg(2)-O(7)	2.109(4)	N(2)-Mg(1)#4	2.217(6)
Mg(2)-N(3)#1	2.185(7)	N(3)-Mg(2)#4	2.186(6)
Mg(3)-O(5)#2	2.095(4)	O(4)-Mg(1)#4	2.058(4)
Mg(3)-O(5)#3	2.095(4)		
O(4)#1-Mg(1)-O(2W)	93.66(19)	O(5)#2-Mg(3)-O(5)#3	88.51(16)
O(4)#1-Mg(1)-O(8)	173.1(2)	O(5)#2-Mg(3)-O(5)	88.51(17)
O(2W)-Mg(1)-O(8)	92.9(2)	O(5)#3-Mg(3)-O(5)	88.51(16)
O(4)#1-Mg(1)-O(1W)	88.41(18)	O(5)#2-Mg(3)-N(4)	93.67(15)
O(2W)-Mg(1)-O(1W)	85.6(2)	O(5)#3-Mg(3)-N(4)	165.34(17)
O(8)-Mg(1)-O(1W)	90.07(16)	O(5)-Mg(3)-N(4)	77.07(15)

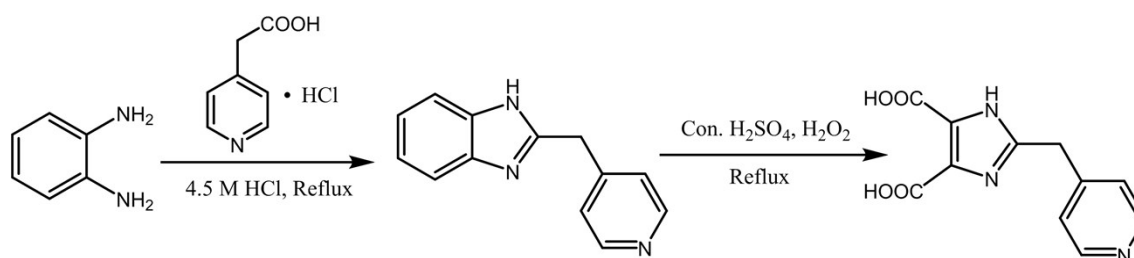
O(4)#1-Mg(1)-N(5)	97.31(18)	O(5)#2-Mg(3)-N(4)#2	77.07(15)
O(2W)-Mg(1)-N(5)	168.9(2)	O(5)#3-Mg(3)-N(4)#2	93.68(15)
O(8)-Mg(1)-N(5)	76.07(17)	O(5)-Mg(3)-N(4)#2	165.34(17)
O(1W)-Mg(1)-N(5)	92.8(2)	N(4)-Mg(3)-N(4)#2	100.94(17)
O(4)#1-Mg(1)-N(2)#1	77.53(19)	O(5)#2-Mg(3)-N(4)#3	165.34(17)
O(2W)-Mg(1)-N(2)#1	87.71(18)	O(5)#3-Mg(3)-N(4)#3	77.07(15)
O(8)-Mg(1)-N(2)#1	104.78(17)	O(5)-Mg(3)-N(4)#3	93.68(15)
O(1W)-Mg(1)-N(2)#1	164.0(2)	N(4)-Mg(3)-N(4)#3	100.95(17)
N(5)-Mg(1)-N(2)#1	96.46(17)	N(4)#2-Mg(3)-N(4)#3	100.94(17)
O(3)-Mg(2)-O(6)	177.03(17)	O(7W)-Mg(4)-O(4W)	88.6(3)
O(3)-Mg(2)-O(2)	93.80(19)	O(7W)-Mg(4)-O(1)	92.3(2)
O(6)-Mg(2)-O(2)	87.9(2)	O(4W)-Mg(4)-O(1)	92.5(2)
O(3)-Mg(2)-O(3W)	90.1(2)	O(7W)-Mg(4)-O(6W)	84.9(2)
O(6)-Mg(2)-O(3W)	87.4(2)	O(4W)-Mg(4)-O(6W)	169.9(3)
O(2)-Mg(2)-O(3W)	91.6(2)	O(1)-Mg(4)-O(6W)	95.5(2)
O(3)-Mg(2)-O(7)	89.10(19)	O(7W)-Mg(4)-O(5W)	95.1(3)
O(6)-Mg(2)-O(7)	89.33(19)	O(4W)-Mg(4)-O(5W)	84.2(3)
O(2)-Mg(2)-O(7)	176.17(18)	O(1)-Mg(4)-O(5W)	171.9(3)
O(3W)-Mg(2)-O(7)	90.9(2)	O(6W)-Mg(4)-O(5W)	88.6(2)
O(3)-Mg(2)-N(3)#1	90.03(18)	O(7W)-Mg(4)-N(1)	167.4(2)
O(6)-Mg(2)-N(3)#1	92.42(17)	O(4W)-Mg(4)-N(1)	99.8(3)
O(2)-Mg(2)-N(3)#1	89.83(18)	O(1)-Mg(4)-N(1)	78.0(2)
O(3W)-Mg(2)-N(3)#1	178.6(2)	O(6W)-Mg(4)-N(1)	87.9(2)
O(7)-Mg(2)-N(3)#1	87.66(17)	O(5W)-Mg(4)-N(1)	95.1(3)

Compound 7

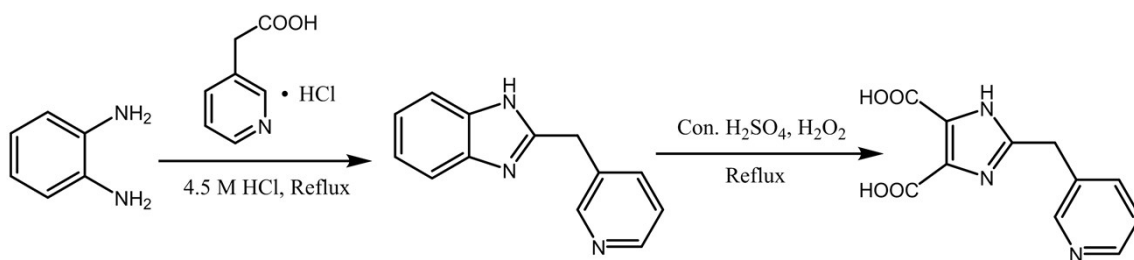
Sr(1)-O(4)#1	2.515(5)	Sr(1)-O(1)	2.625(5)
Sr(1)-O(4)#2	2.515(5)	Sr(1)-O(1)#3	2.625(5)
Sr(1)-O(5)	2.539(7)	Sr(1)-N(1)	2.779(5)
Sr(1)-O(5)#3	2.539(7)	Sr(1)-N(1)#3	2.779(5)
O(4)#1-Sr(1)-O(4)#2	133.2(3)	O(1)-Sr(1)-O(1)#3	125.9(2)
O(4)#1-Sr(1)-O(5)	71.5(3)	O(4)#1-Sr(1)-N(1)	133.18(17)
O(4)#2-Sr(1)-O(5)	76.2(2)	O(4)#2-Sr(1)-N(1)	86.4(2)
O(4)#1-Sr(1)-O(5)#3	76.2(2)	O(5)-Sr(1)-N(1)	103.4(3)
O(4)#2-Sr(1)-O(5)#3	71.5(3)	O(5)#3-Sr(1)-N(1)	149.9(2)
O(5)-Sr(1)-O(5)#3	91.2(4)	O(1)-Sr(1)-N(1)	61.42(16)
O(4)#1-Sr(1)-O(1)	72.30(17)	O(1)#3-Sr(1)-N(1)	76.46(17)
O(4)#2-Sr(1)-O(1)	131.69(18)	O(4)#1-Sr(1)-N(1)#3	86.4(2)
O(5)-Sr(1)-O(1)	77.5(2)	O(4)#2-Sr(1)-N(1)#3	133.18(17)
O(5)#3-Sr(1)-O(1)	148.5(2)	O(5)-Sr(1)-N(1)#3	149.9(2)
O(4)#1-Sr(1)-O(1)#3	131.69(18)	O(5)#3-Sr(1)-N(1)#3	103.4(3)
O(4)#2-Sr(1)-O(1)#3	72.30(17)	O(1)-Sr(1)-N(1)#3	76.46(17)
O(5)-Sr(1)-O(1)#3	148.5(2)	O(1)#3-Sr(1)-N(1)#3	61.42(16)
O(5)#3-Sr(1)-O(1)#3	77.5(2)	N(1)-Sr(1)-N(1)#3	76.8(3)

^aSymmetry transformations used to generate equivalent atoms: #1 $-x+1,y+1/2,-z-1/2$ #2 $-x+1,y-1/2,-z-1/2$ #3 $-x+1,-y+1,-z$ #4 $x,-y+1/2,z-1/2$ for compound **1**; #1 $x,-y+1/2,z-1/2$ #2 $-x+2,y+1/2,-z+3/2$ #3 $-x+2,y-1/2,-z+3/2$ #4 $-x+2,-y+1,-z+1$ #5 $x,-y+1/2,z+1/2$ for compound **2**; #1 $x+1/2,-y+3,z$ #2 $x-1/2,-y+3,z$ #3 $x,y+1,z$ for compound **3**; #1 $x-1,-y+1,z+1/2$ #2 $x+1,y,z$ #3 $x+1,-y,z-1/2$ #4 $x,-y+1,z+1/2$ for compound **4**; #1 $x,-y+1/2,z+1/2$ #2 $x,-y+3/2,z+1/2$ #3 $-x+1,-y+1,-z$ #4 $-x+1,y+1/2,-z+1/2$ for compound **5**; #1 $-x+y+5/3,y+1/3,z-1/6$ #2 $-y+1,x-y,z$ #3 $-x+y+1,-x+1,z$ #4 $-x+y+4/3,y-1/3,z+1/6$ for compound **6**; #1 $x-1/2,-y+3/2,-z+1/4$ #2 $-y+3/2,x-1/2,z-1/4$ #3 $y,x,-z$ for compound **7**.

Scheme S1: Synthetic Route of Ligand $H_3pPyMIDC$.



Scheme S2: Synthetic Route of Ligand $H_3mPyMIDC$.



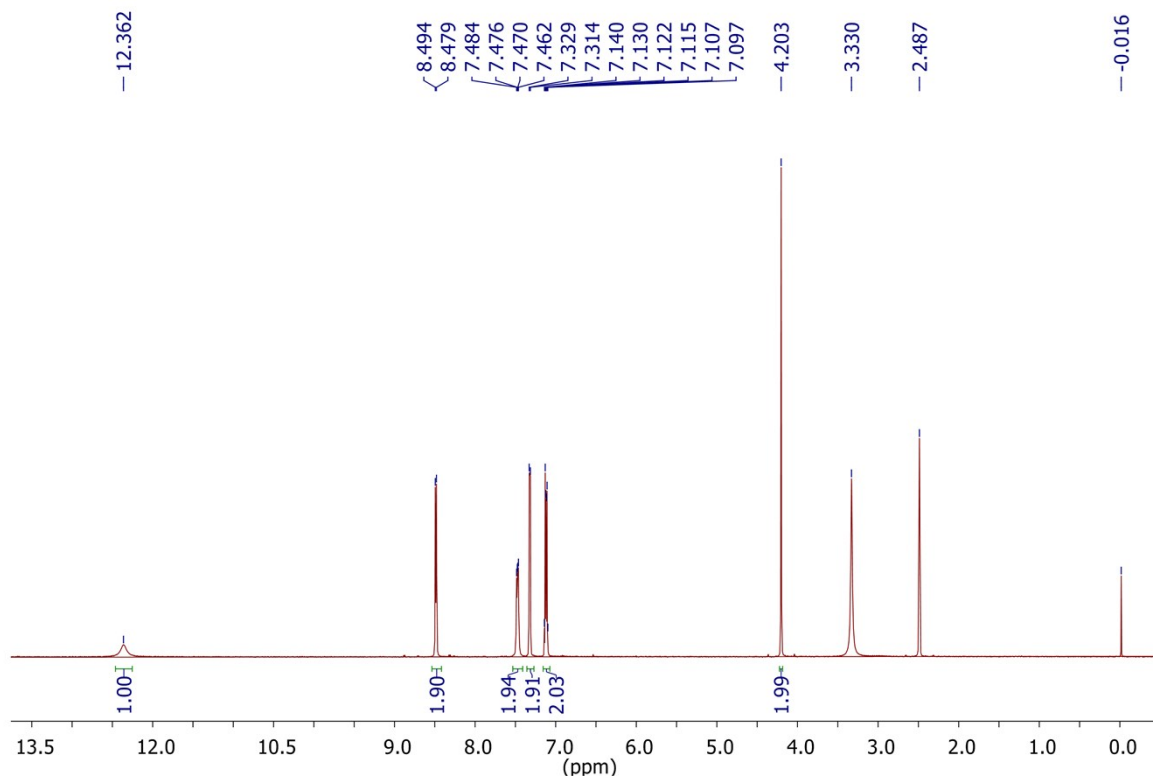


Figure S1. ^1H NMR spectrum (DMSO- d_6 , 298 K, 400 MHz) of 2-(pyridin-4-ylmethyl)-1H-benzimidazole.

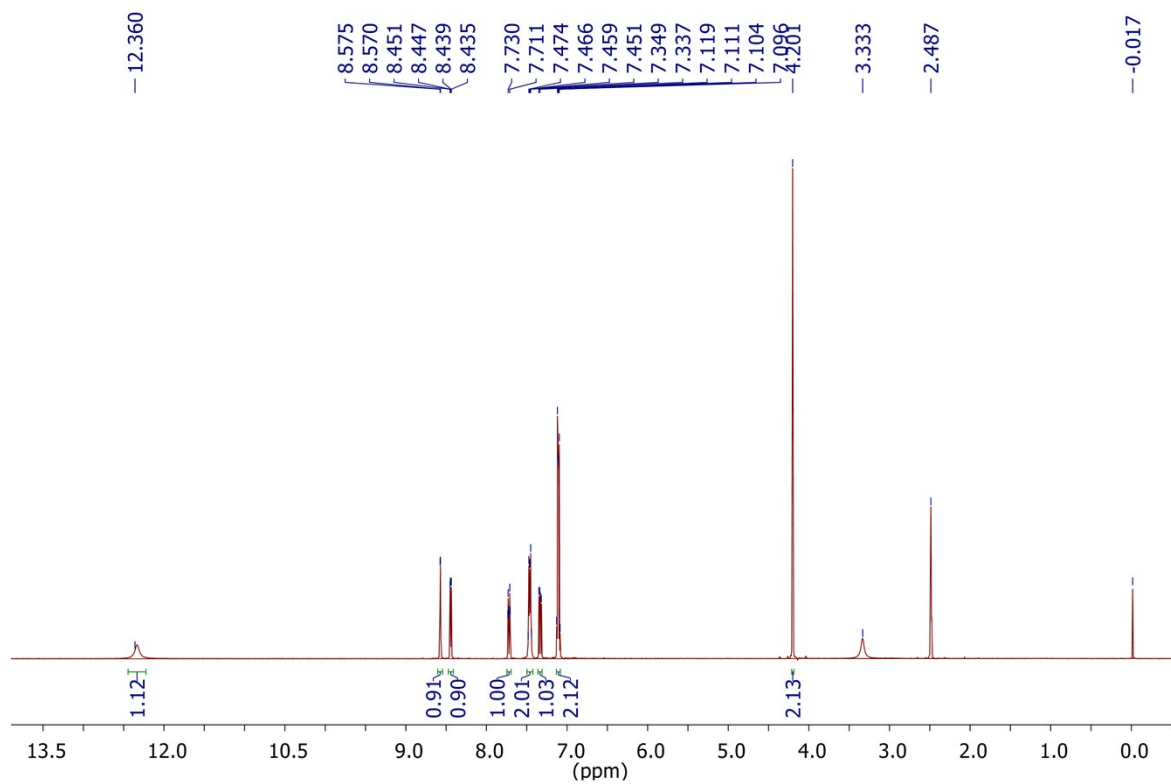


Figure S2. ^1H NMR spectrum (DMSO- d_6 , 298 K, 400 MHz) of 2-(pyridin-3-ylmethyl)-1H-benzimidazole.

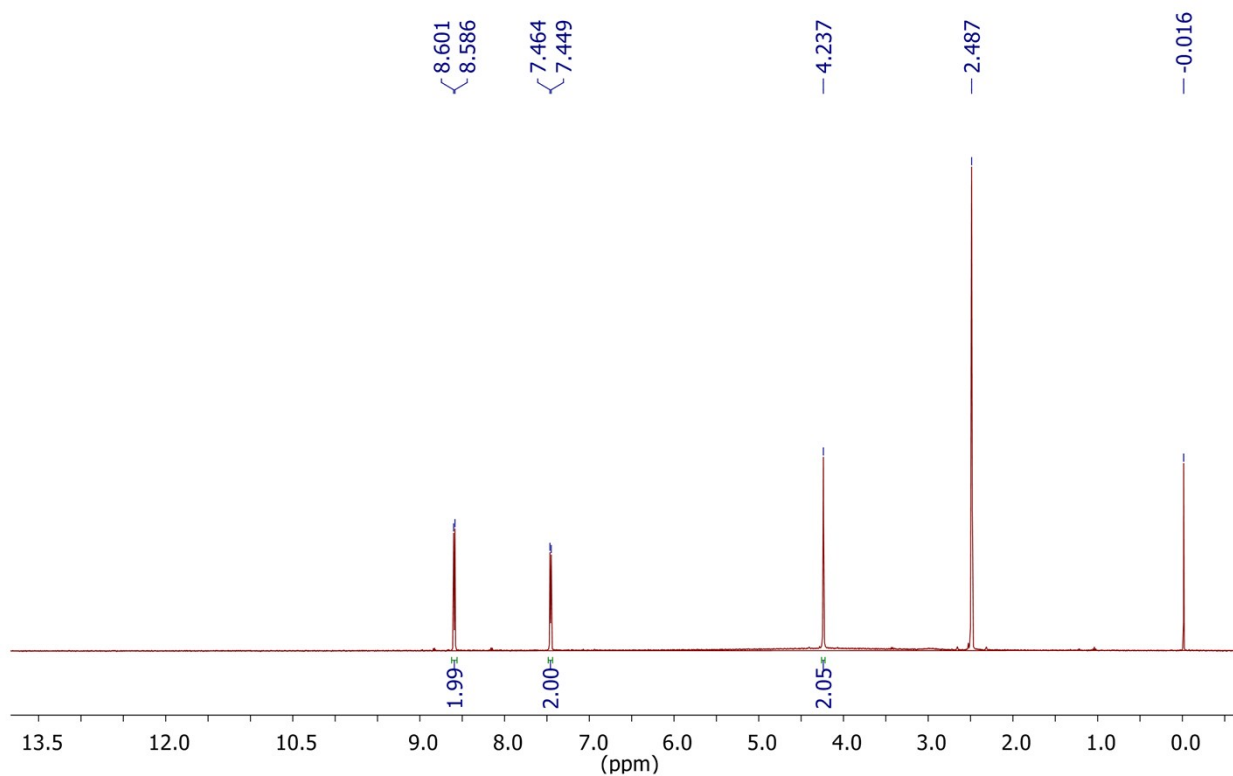


Figure S3. ^1H NMR spectrum ($\text{DMSO-}d_6$, 298 K, 400 MHz) of the $\text{H}_3\text{pPyMIDC}$ ligand

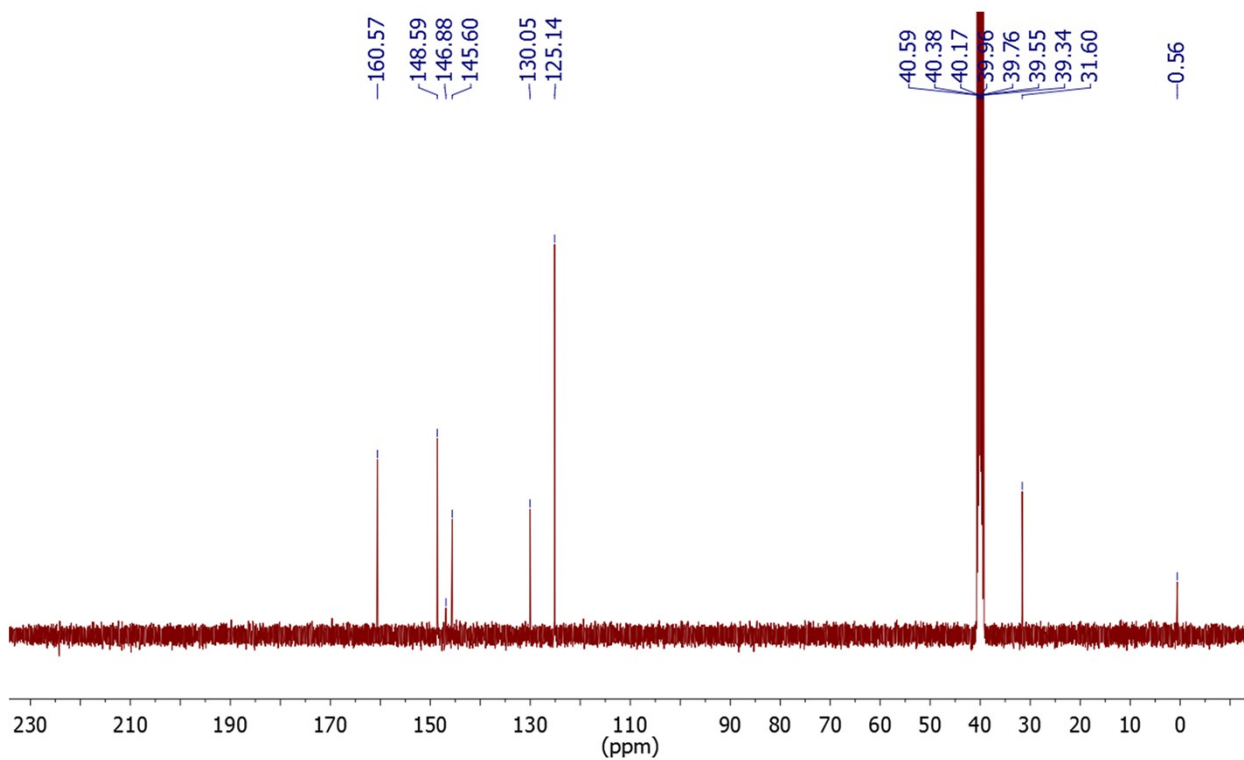


Figure S4. ^{13}C NMR spectrum ($\text{DMSO-}d_6$, 298 K, 400 MHz) of the $\text{H}_3\text{pPyMIDC}$ ligand

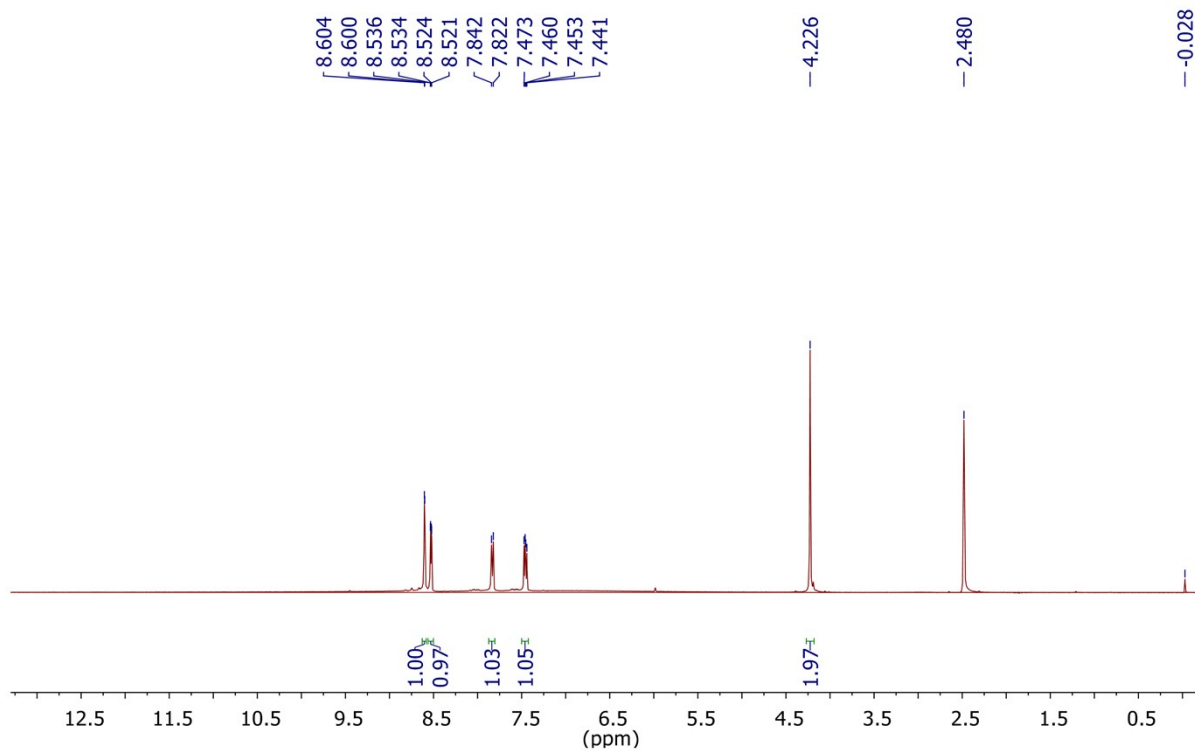


Figure S5. ^1H NMR spectrum ($\text{DMSO-}d_6$, 298 K, 400 MHz) of the $\text{H}_3\text{mPyMIDC}$ ligand

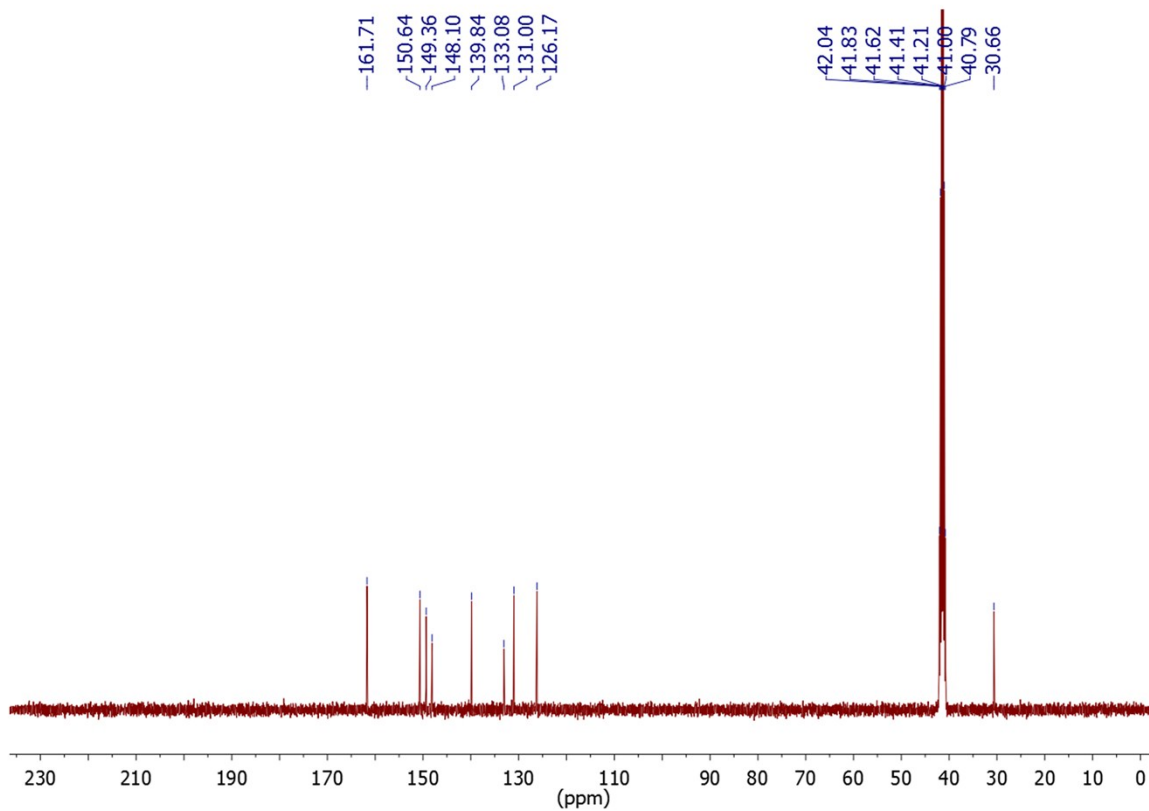


Figure S6. ^{13}C NMR spectrum ($\text{DMSO-}d_6$, 298 K, 400 MHz) of the $\text{H}_3\text{mPyMIDC}$ ligand

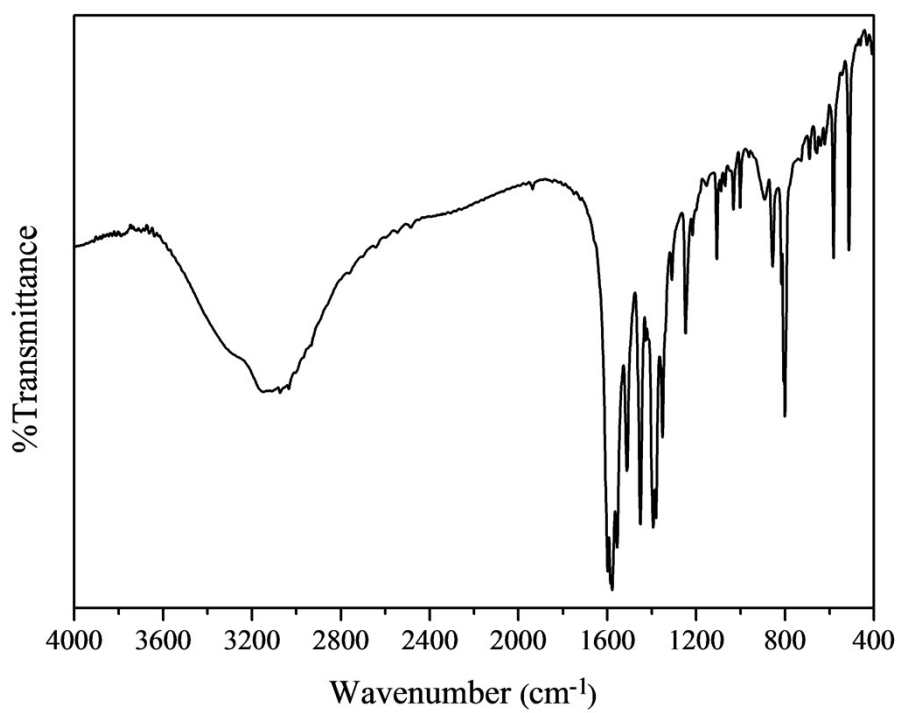


Figure S7. FT-IR spectrum of compound 1.

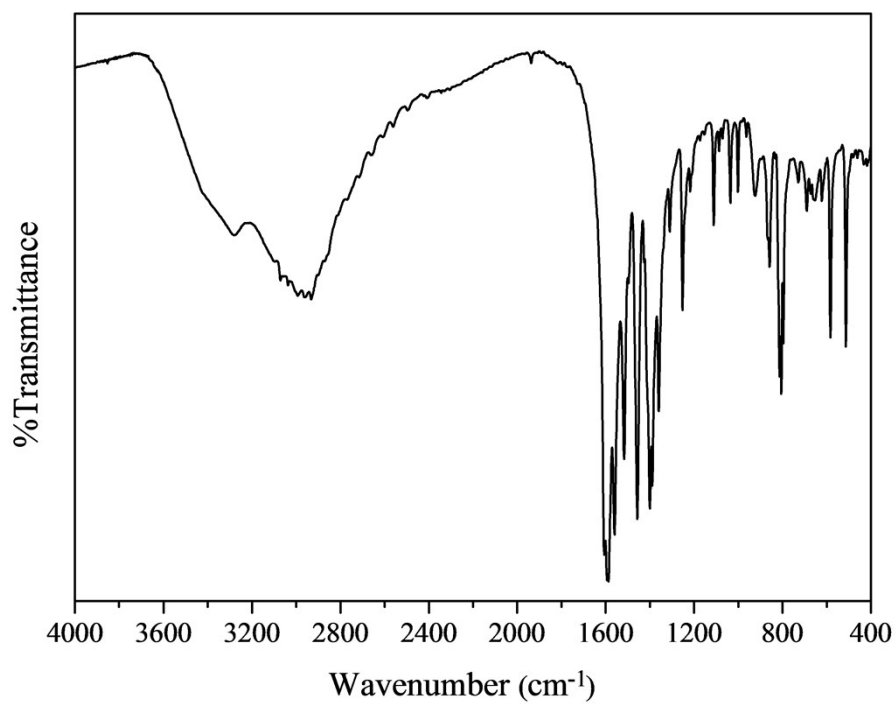


Figure S8. FT-IR spectrum of compound 2.

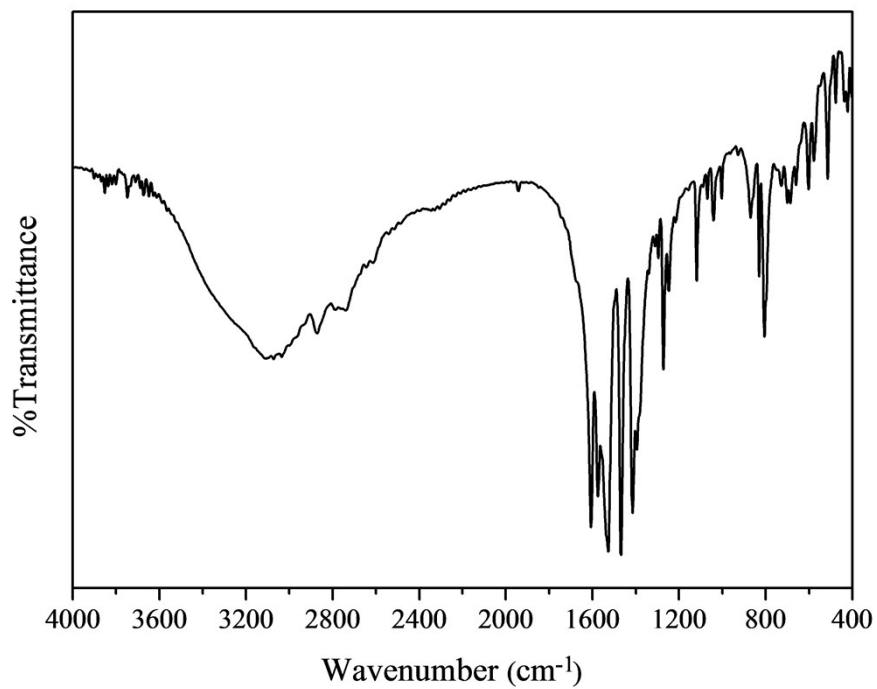


Figure S9. FT-IR spectrum of compound 3.

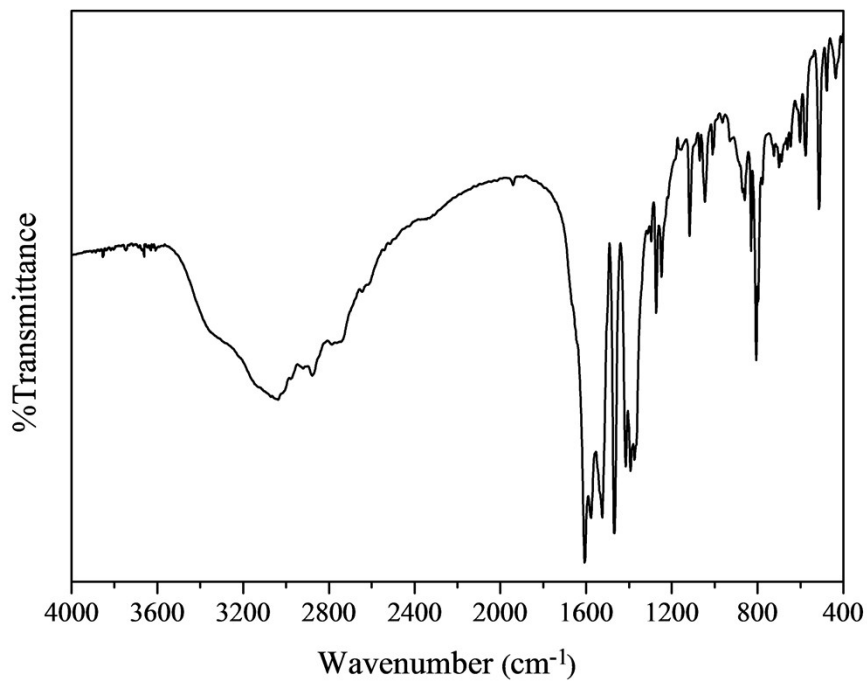


Figure S10. FT-IR spectrum of compound 4.

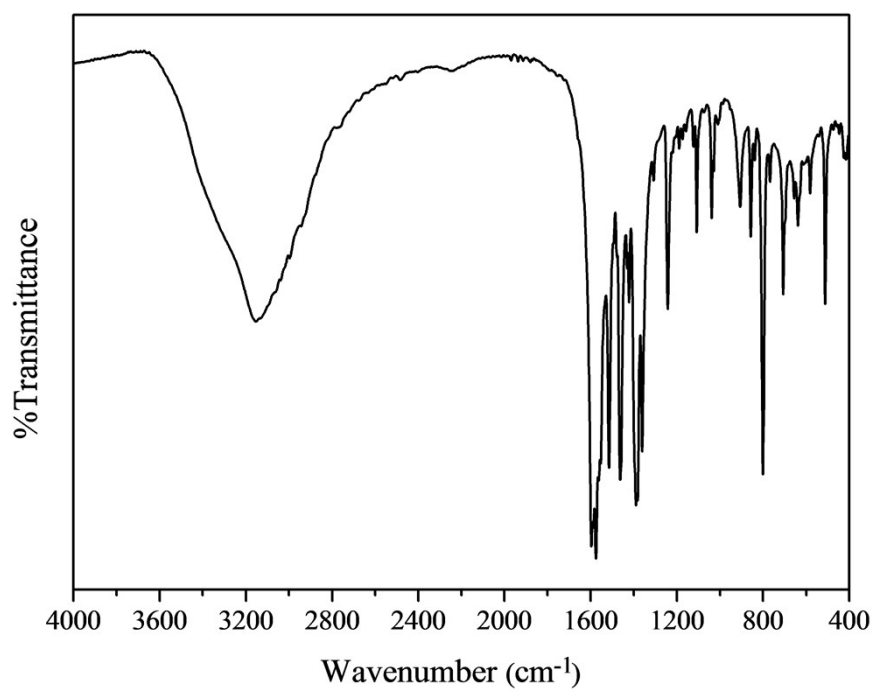


Figure S11. FT-IR spectrum of compound 5.

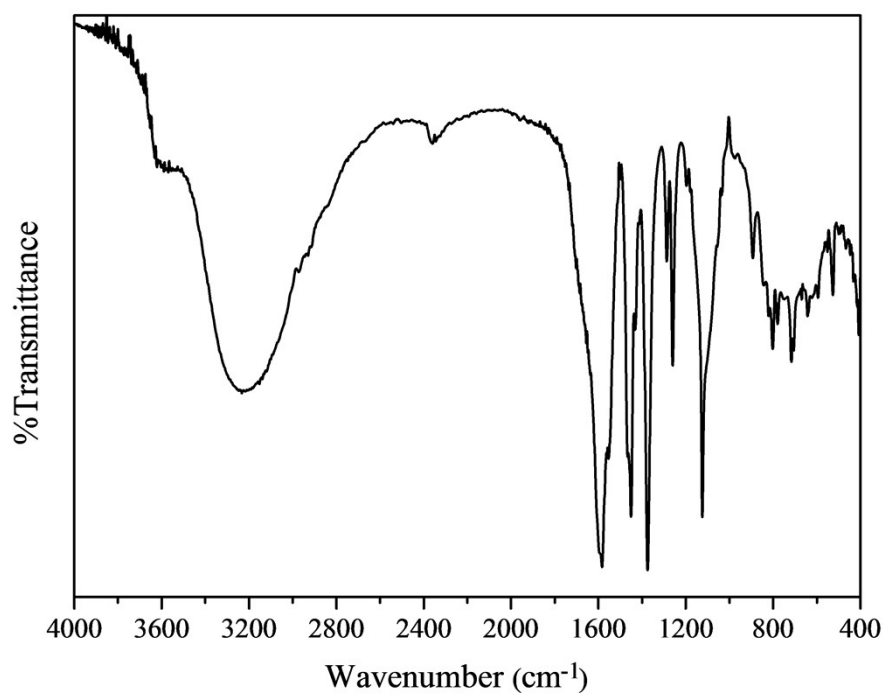


Figure S12. FT-IR spectrum of compound 6.

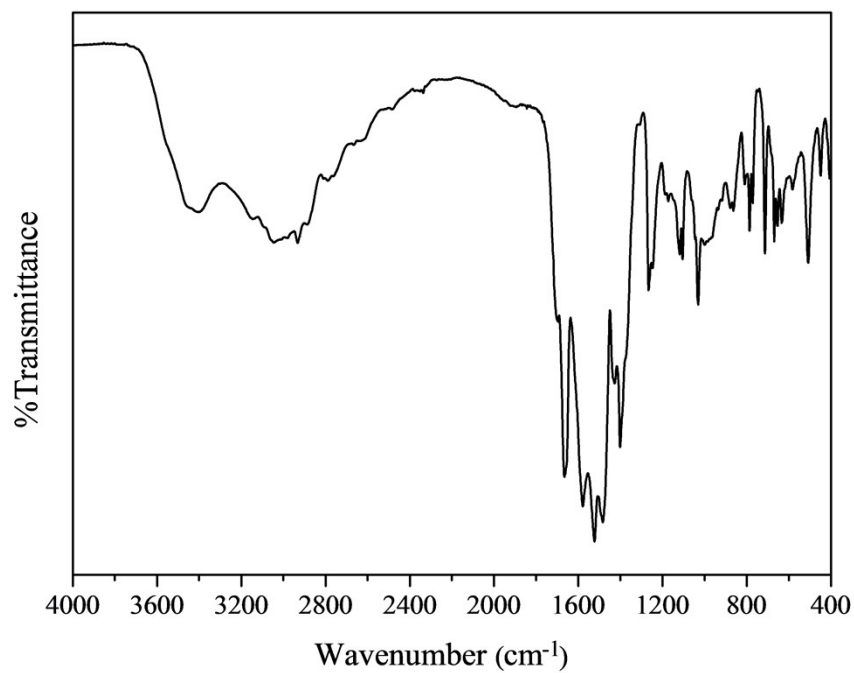


Figure S13. FT-IR spectrum of compound 7.

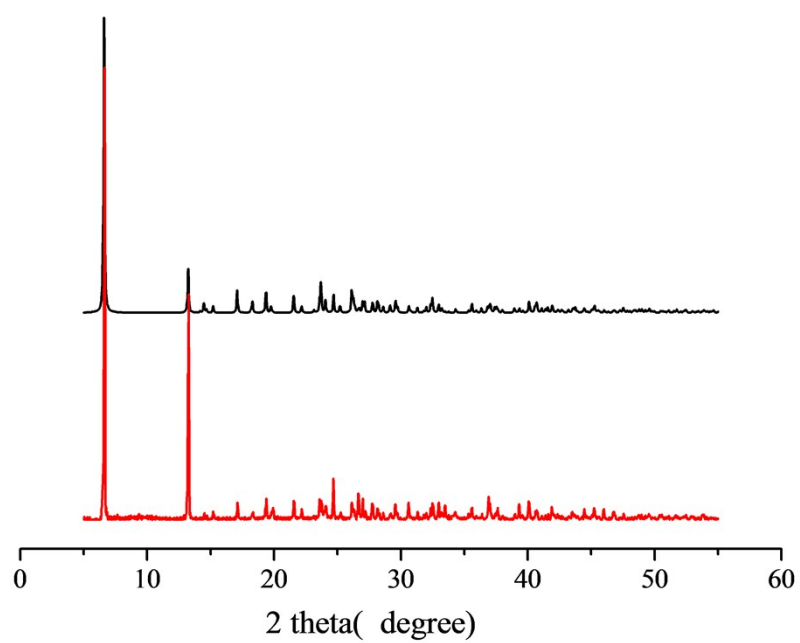


Figure S14 The simulated X-ray powder diffraction patterns (black) and the experimental one (red) of compound 1.

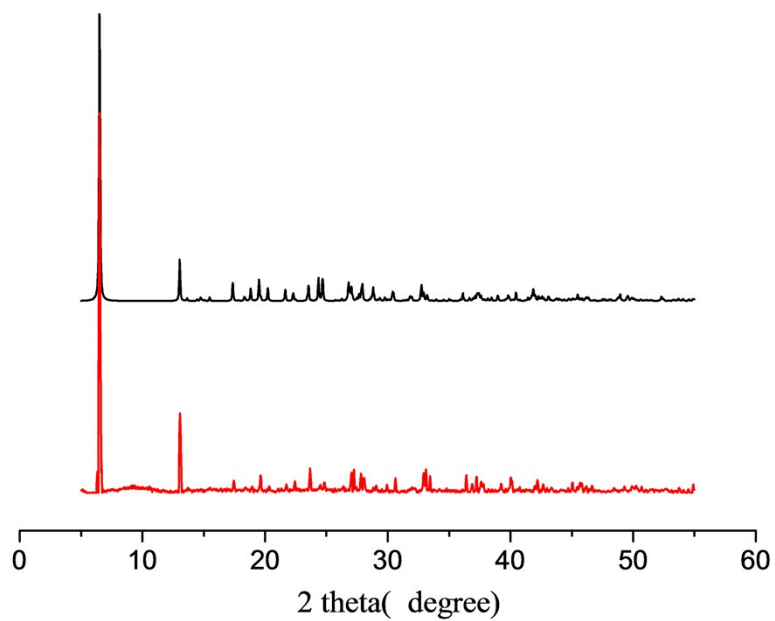


Figure S15 The simulated X-ray powder diffraction patterns (black) and the experimental one (red) of compound **2**.

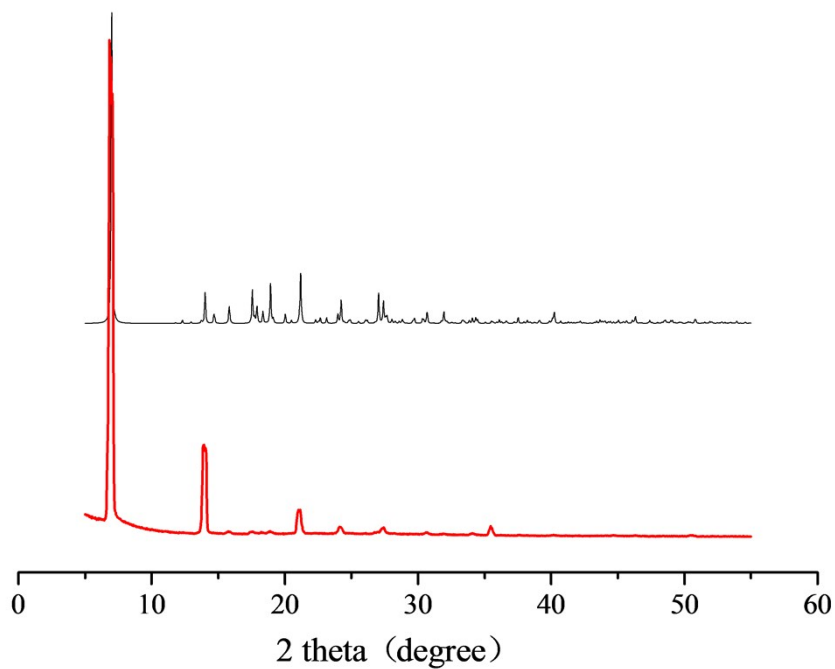


Figure S16 The simulated X-ray powder diffraction patterns (black) and the experimental one (red) of compound **3**.

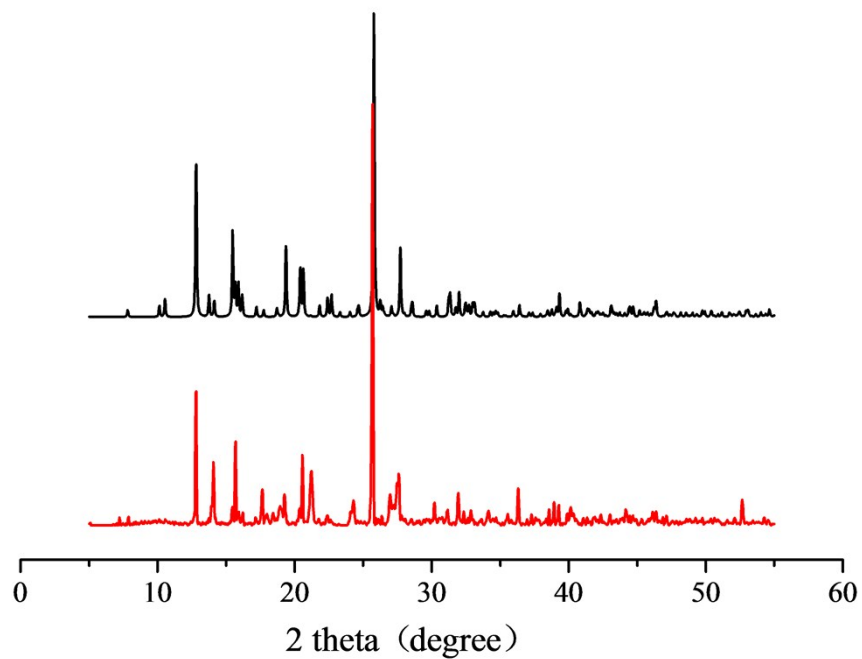


Figure S17 The simulated X-ray powder diffraction patterns (black) and the experimental one (red) of compound 4.

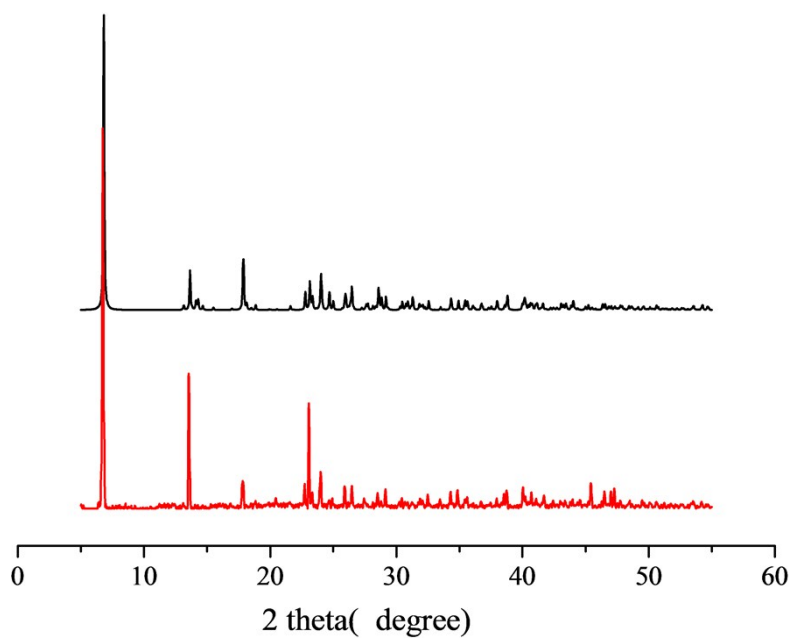


Figure S18 The simulated X-ray powder diffraction patterns (black) and the experimental one (red) of compound 5.

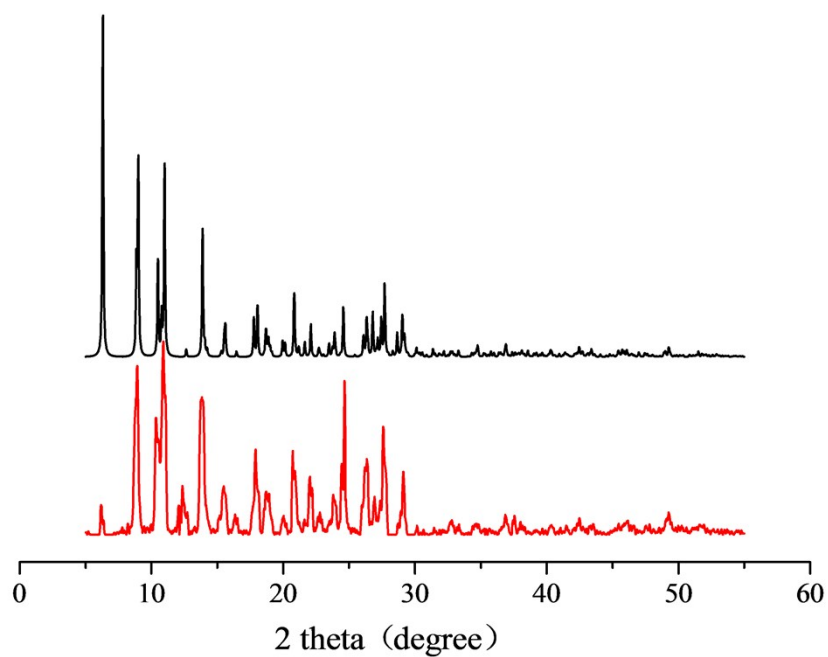


Figure S19 The simulated X-ray powder diffraction patterns (black) and the experimental one (red) of compound 6.

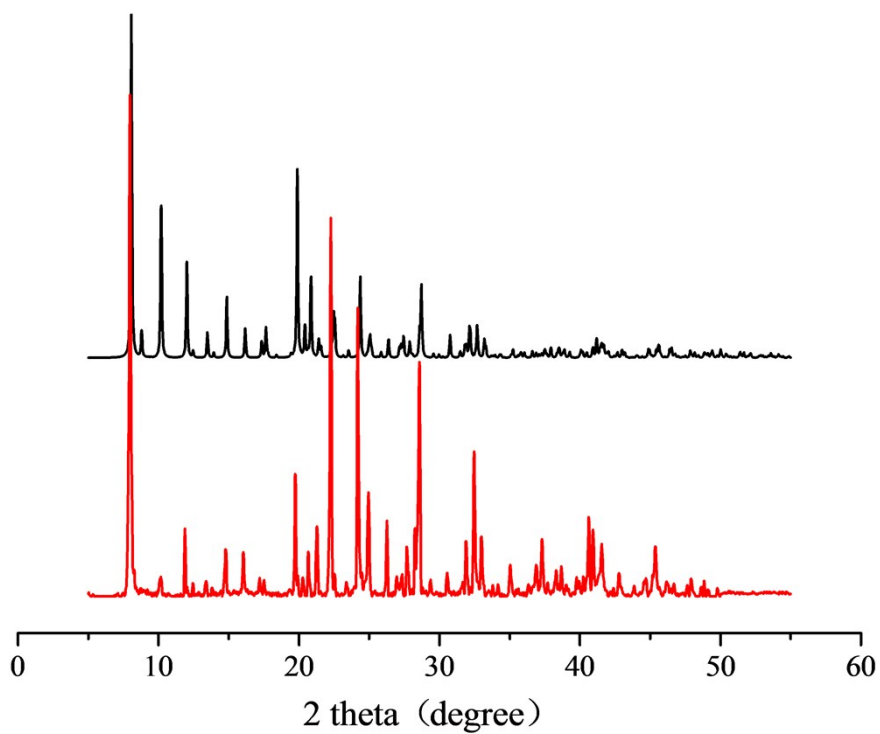


Figure S20 The simulated X-ray powder diffraction patterns (black) and the experimental one (red) of compound 7.

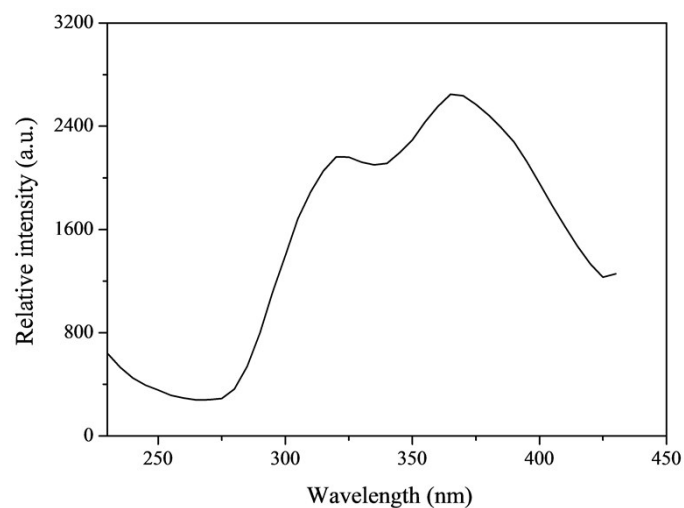


Figure S21 Excitation spectrum of compound **1** in the solid state at room temperature.

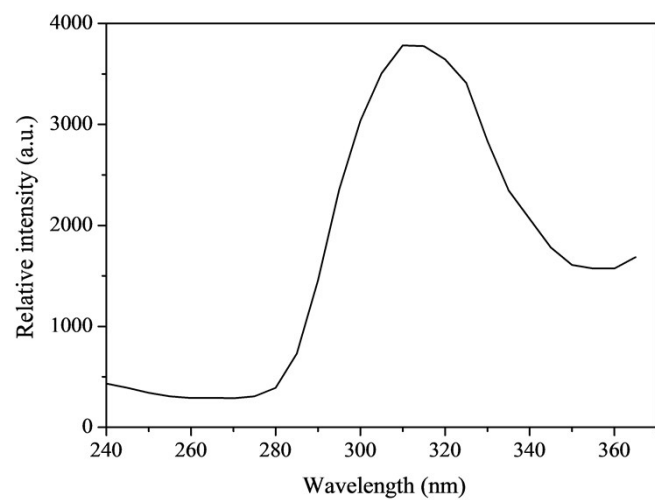


Figure S22 Excitation spectrum of compound **2** in the solid state at room temperature.

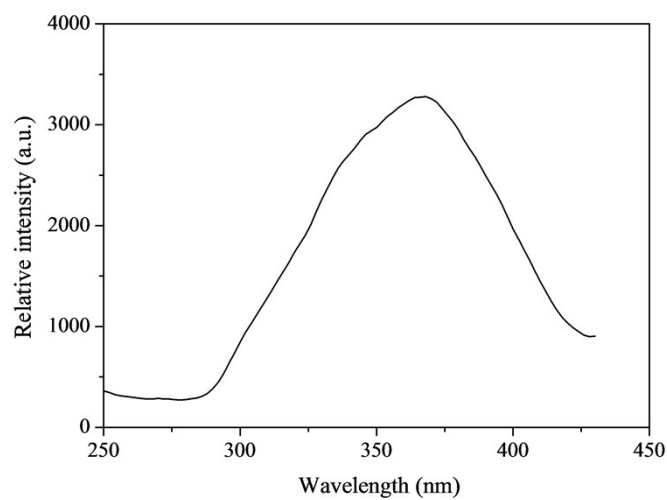


Figure S23 Excitation spectrum of compound **3** in the solid state at room temperature.

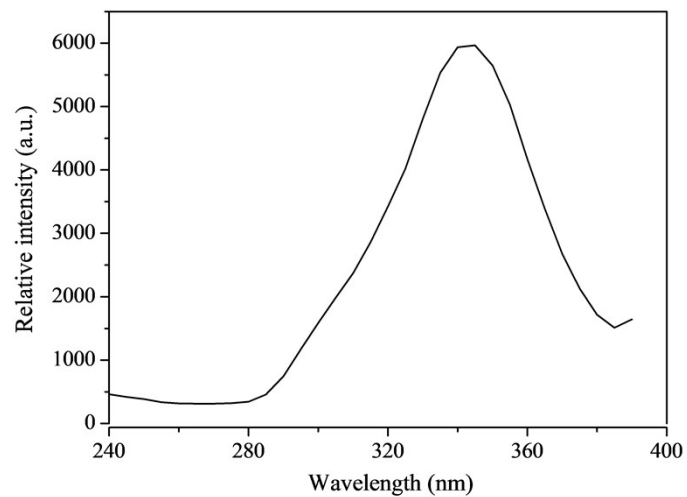


Figure S24 Excitation spectrum of compound **4** in the solid state at room temperature.

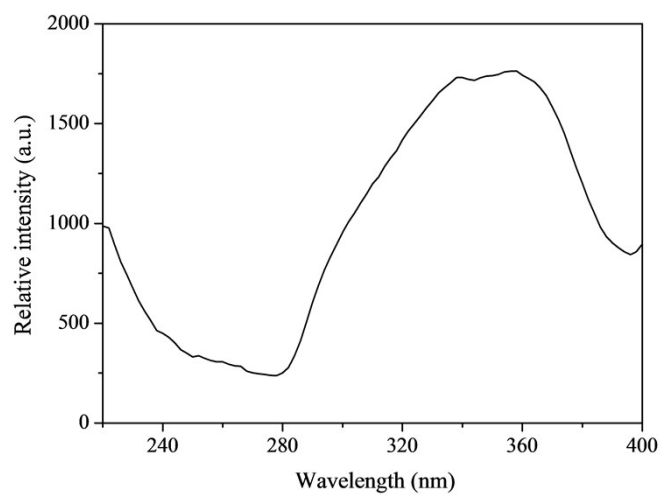


Figure S25 Excitation spectrum of compound **5** in the solid state at room temperature.

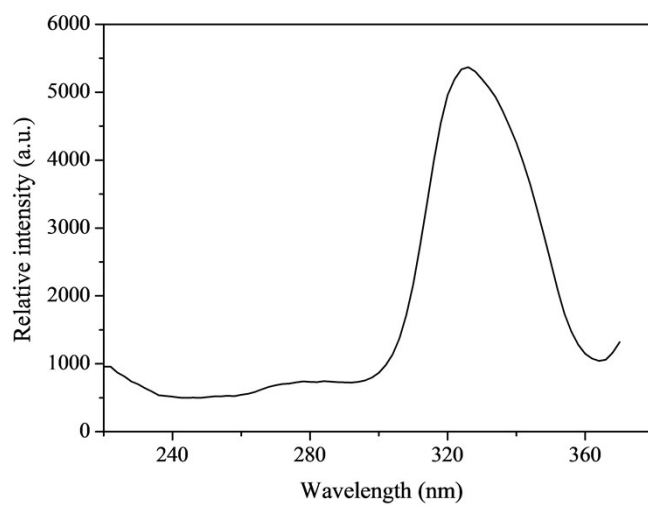


Figure S26 Excitation spectrum of compound **6** in the solid state at room temperature.

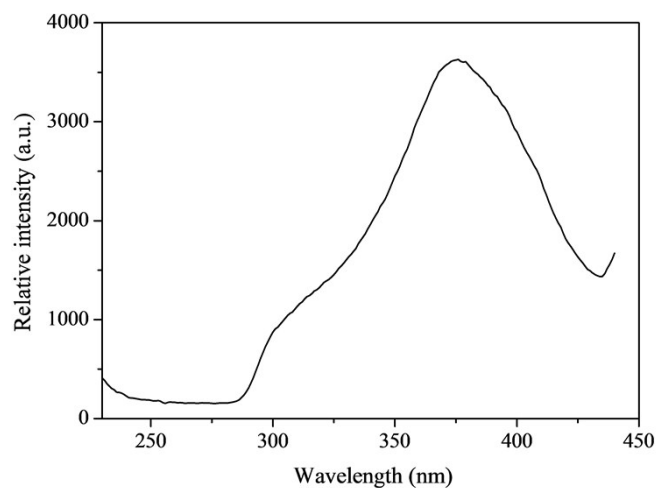


Figure S27 Excitation spectrum of compound **7** in the solid state at room temperature.

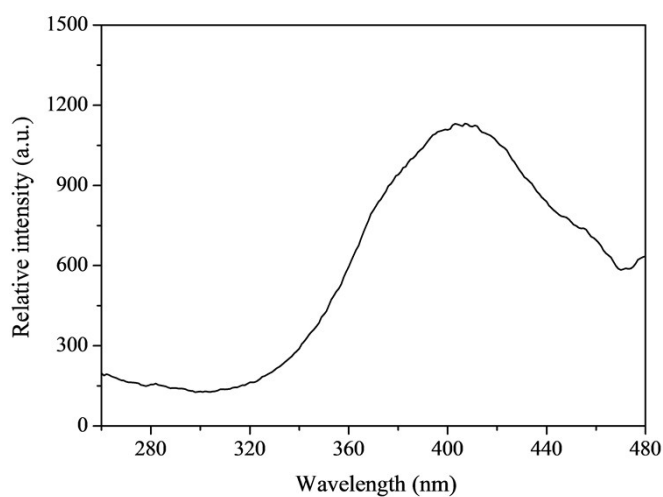


Figure S28 Excitation spectrum of free ligand H₃pPyMIDC in the solid state at room temperature.

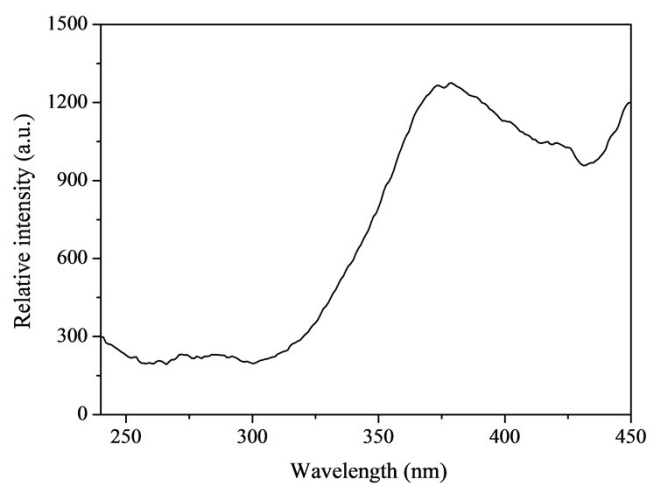


Figure S29 Excitation spectrum of free ligand H₃mPyMIDC in the solid state at room temperature.