Supporting Materials

Syntheses, structures and luminescence of a series of coordination polymers constructed with 4-substituted 1,2,4-triazole and biscarboxylate co-ligands†

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Table S1 Selected bond lengths and angles for **1-8** (Å and ^{o}).

		1	
Cd(1)-O(1)	2.400(3)	Cd(1)-O(3B)	2.331(4)
Cd(1)-O(4B)	2.642(5)	Cd(1)-O(5)	2.254(3)
Cd(1)-O(6)	2.547(4)	Cd(1)-N(1)	2.337(3)
Cd(1)-N(4A)	2.316(3)	Cd(2)-O(1)	2.331(3)
Cd(2)-O(1D)	2.331(3)	Cd(2)-N(2)	2.339(3)
Cd(2)-N(2D)	2.339(3)	Cd(2)-N(5A)	2.316(3)
Cd(2)-N(5C)	2.316(3)		
O(3B)-Cd(1)-O(1)	148.89(15)	O(1)-Cd(1)-O(4B)	158.05(14)
O(5)-Cd(1)-O(1)	95.74(12)	O(1)-Cd(1)-O(6)	80.61(11)
N(1)-Cd(1)-O(1)	79.12(11)	N(4A)-Cd(1)-O(1)	83.73(11)
O(3B)-Cd(1)-O(4B)	52.22(17)	O(5)-Cd(1)-O(3B)	94.69(14)
O(3B)-Cd(1)-O(6)	82.04(16)	O(3B)-Cd(1)-N(1)	77.36(13)
N(4A)-Cd(1)-O(3B)	115.48(16)	O(5)-Cd(1)-O(4B)	85.07(14)
O(6)-Cd(1)-O(4B)	116.50(13)	N(1)-Cd(1)-O(4B)	110.51(14)
N(4A)-Cd(1)-O(4B)	77.08(13)	O(5)-Cd(1)-O(6)	54.02(13)
O(5)-Cd(1)-N(1)	150.31(14)	O(5)-Cd(1)-N(4A)	120.41(13)
N(1)-Cd(1)-O(6)	96.34(13)	N(4A)-Cd(1)-O(6)	162.47(12)
N(4A)-Cd(1)-N(1)	88.35(13)	O(1D)-Cd(2)-O(1)	180.0
N(2)-Cd(2)-N(2D)	180.00(17)	N(5A)-Cd(2)-N(5C)	180.00(12)
O(1)-Cd(2)-N(2)	82.99(12)	N(5A)-Cd(2)-O(1)	84.11(12)

N(5A)-Cd(2)-N(2)	92.28(13)		

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Cd(1)-O(1)	2.639(5)	Cd(1)-O(2)	2.241(5)
Cd(1)-O(4A)	2.245(5)	Cd(1)-O(5)	2.309(4)
Cd(1)-N(1)	2.270(5)	Cd(1)-N(5B)	2.382(5)
Cd(2)-O(1)	2.353(4)	Cd(2)-O(6D)	2.235(5)
Cd(2)-O(8C)	2.227(5)	Cd(2)-O(9)	2.283(4)
Cd(2)-N(2)	2.376(5)	Cd(2)-N(4B)	2.384(5)
O(2)-Cd(1)-O(1)	52.50(16)	O(4A)-Cd(1)-O(1)	138.87(17)
O(5)-Cd(1)-O(1)	111.69(15)	N(1)-Cd(1)-O(1)	84.49(16)
N(5B)-Cd(1)-O(1)	72.52(17)	O(2)-Cd(1)-O(4A)	90.73(19)
O(2)-Cd(1)-O(5)	96.44(18)	O(2)-Cd(1)-N(1)	133.34(19)
O(2)-Cd(1)-N(5B)	91.7(2)	O(4A)-Cd(1)-O(5)	87.46(17)
O(4A)-Cd(1)-N(1)	135.48(19)	O(4A)-Cd(1)-N(5B)	93.64(19)
N(1)-Cd(1)-O(5)	82.25(18)	O(5)-Cd(1)-N(5B)	171.79(19)
N(1)-Cd(1)-N(5B)	91.3(2)	O(6D)-Cd(2)-O(1)	167.47(19)
O(8C)-Cd(2)-O(1)	90.5(2)	O(9)-Cd(2)-O(1)	97.36(17)
O(1)-Cd(2)-N(2)	87.31(18)	O(1)-Cd(2)-N(4B)	78.06(17)
O(8C)-Cd(2)-O(6D)	93.0(2)	O(6D)-Cd(2)-O(9)	95.11(18)
O(6D)-Cd(2)-N(2)	81.45(19)	O(6D)-Cd(2)-N(4B)	96.08(19)
O(8C)-Cd(2)-O(9)	79.55(19)	O(8C)-Cd(2)-N(2)	80.24(19)
O(8C)-Cd(2)-N(4B)	164.4(2)	O(9)-Cd(2)-N(2)	159.29(18)
O(9)-Cd(2)-N(4B)	112.04(18)	N(2)-Cd(2)-N(4B)	88.65(18)

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Cd(1)-O(1)	2.354(4)	Cd(1)-O(8B)	2.250(4)
Cd(1)-O(10A)	2.222(4)	Cd(1)-O(13)	2.298(4)
Cd(1)-N(1)	2.337(5)	Cd(1)-N(4C)	2.371(5)
Cd(2)-O(2)	2.238(4)	Cd(2)-O(4D)	2.246(5)
Cd(2)-O(7)	2.333(4)	Cd(2)-N(2)	2.369(5)
Cd(2)-N(5C)	2.271(5)		
O(8B)-Cd(1)-O(1)	169.69(16)	O(10A)-Cd(1)-O(1)	90.92(18)
O(13)-Cd(1)-O(1)	93.47(15)	N(1)-Cd(1)-O(1)	79.08(16)
O(1)-Cd(1)-N(4C)	87.89(16)	O(10A)-Cd(1)-O(8B)	91.03(19)
O(8B)-Cd(1)-O(13)	96.84(16)	O(8B)-Cd(1)-N(1)	97.00(18)
O(8B)-Cd(1)-N(4C)	82.56(17)	O(10A)-Cd(1)-O(13)	79.10(16)
O(10A)-Cd(1)-N(1)	165.45(18)	O(10A)-Cd(1)-N(4C)	78.74(17)
O(13)-Cd(1)-N(1)	111.77(16)	O(13)-Cd(1)-N(4C)	157.81(16)
N(1)-Cd(1)-N(4C)	90.25(16)	O(2)-Cd(2)-O(4D)	91.53(17)
O(2)-Cd(2)-O(7)	90.07(16)	O(2)-Cd(2)-N(2)	92.09(17)
O(2)-Cd(2)-N(5C)	132.33(17)	O(4D)-Cd(2)-O(7)	88.31(16)
O(4D)-Cd(2)-N(2)	95.60(17)	O(4D)-Cd(2)-N(5C)	134.69(17)
O(7)-Cd(2)-N(2)	175.48(17)	N(5C)-Cd(2)-O(7)	81.92(16)
N(5C)-Cd(2)-N(2)	93.70(18)		

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Cd(1)-O(1)	2.335(7)	Cd(1)-O(3A)	2.297(6)
Cd(1)-O(5)	2.238(5)	Cd(1)-O(9)	2.310(6)
Cd(1)-N(1)	2.363(2)	Cd(1)-N(4B)	2.423(3)
Cd(2)-O(2)	2.238(6)	Cd(2)-Cl(1)	2.6753(15)
Cd(2)-N(2)	2.3312(18)	Cd(2)-N(5B)	2.362(2)
Cd(2)-N(7)	2.364(2)	Cd(2)-N(8C)	2.370(2)
O(3A)-Cd(1)-O(1)	161.9(2)	O(5)-Cd(1)-O(1)	88.9(3)
O(9)-Cd(1)-O(1)	81.0(3)	O(1)-Cd(1)-N(1)	80.7(2)
O(1)-Cd(1)-N(4B)	86.0(2)	O(5)-Cd(1)-O(3A)	104.5(2)
O(3A)-Cd(1)-O(9)	84.3(3)	O(3A)-Cd(1)-N(1)	111.99(17)
O(3A)-Cd(1)-N(4B)	82.03(14)	O(5)-Cd(1)-O(9)	102.37(18)
O(5)-Cd(1)-N(1)	84.96(15)	O(5)-Cd(1)-N(4B)	171.36(15)
O(9)-Cd(1)-N(1)	160.16(19)	O(9)-Cd(1)-N(4B)	83.70(12)
N(1)-Cd(1)-N(4B)	87.36(9)	O(2)-Cd(2)-Cl(1)	160.16(15)
O(2)-Cd(2)-N(2)	113.59(15)	O(2)-Cd(2)-N(5B)	95.68(18)
O(2)-Cd(2)-N(7)	89.16(18)	O(2)-Cd(2)-N(8C)	78.43(16)
N(2)-Cd(2)-Cl(1)	85.15(6)	N(5B)-Cd(2)-Cl(1)	90.11(8)
N(7)-Cd(2)-Cl(1)	85.28(6)	N(8C)-Cd(2)-Cl(1)	82.91(7)
N(2)-Cd(2)-N(5B)	91.27(8)	N(2)-Cd(2)-N(7)	86.87(5)
N(2)-Cd(2)-N(8C)	167.98(9)	N(5B)-Cd(2)-N(7)	175.15(11)
N(5B)-Cd(2)-N(8C)	87.42(8)	N(7)-Cd(2)-N(8)#3	93.46(7)

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Cd(1)-O(1)	2.442(4)	Cd(1)-O(2)	2.484(4)
Cd(1)-O(4A)	2.300(3)	Cd(1)-O(8C)	2.384(3)
Cd(1)-O(9)	2.249(4)	Cd(1)-N(1)	2.480(4)
Cd(1)-N(4B)	2.345(4)	Cd(2)-O(5)	2.324(4)
Cd(2)-O(6)	2.466(4)	Cd(2)-O(7C)	2.305(3)
Cd(2)-O(8C)	2.472(3)	Cd(2)-O(10)	2.302(3)
Cd(2)-N(2)	2.353(4)	Cd(2)-N(5B)	2.330(3)
O(1)-Cd(1)-O(2)	51.72(12)	O(4A)-Cd(1)-O(1)	121.39(14)
O(8C)-Cd(1)-O(1)	152.94(12)	O(9)-Cd(1)-O(1)	80.72(18)
O(1)-Cd(1)-N(1)	77.88(14)	N(4B)-Cd(1)-O(1)	105.15(14)
O(4A)-Cd(1)-O(2)	81.00(13)	O(8C)-Cd(1)-O(2)	154.21(12)
O(9)-Cd(1)-O(2)	107.45(19)	N(1)-Cd(1)-O(2)	119.70(13)
N(4B)-Cd(1)-O(2)	78.71(13)	O(4A)-Cd(1)-O(8C)	82.30(13)
O(9)-Cd(1)-O(4A)	83.70(14)	O(4A)-Cd(1)-N(1)	159.04(13)
O(4A)-Cd(1)-N(4B)	95.38(13)	O(9)-Cd(1)-O(8C)	90.04(18)
O(8C)-Cd(1)-N(1)	77.13(12)	N(4B)-Cd(1)-O(8C)	83.45(12)
O(9)-Cd(1)-N(1)	92.25(16)	O(9)-Cd(1)-N(4B)	173.49(18)
N(4B)-Cd(1)-N(1)	86.32(14)	O(5)-Cd(2)-O(6)	53.75(12)
O(7C)-Cd(2)-O(5)	91.39(12)	O(5)-Cd(2)-O(8C)	143.26(12)
O(10)-Cd(2)-O(5)	102.73(15)	O(5)-Cd(2)-N(2)	86.93(15)
O(5)-Cd(2)-N(5B)	132.62(14)	O(7C)-Cd(2)-O(6)	142.29(12)
O(6)-Cd(2)-O(8C)	162.80(11)	O(10)-Cd(2)-O(6)	87.94(14)

N(2)-Cd(2)-O(6)	101.60(14)	N(5B)-Cd(2)-O(6)	81.09(13)
O(7C)-Cd(2)-O(8C)	54.26(11)	O(10)-Cd(2)-O(7C)	86.44(13)
O(7C)-Cd(2)-N(2)	88.81(14)	O(7C)-Cd(2)-N(5B)	135.75(12)
O(10)-Cd(2)-O(8C)	89.03(12)	N(2)-Cd(2)-O(8C)	80.43(13)
N(5B)-Cd(2)-O(8C)	81.86(12)	O(10)-Cd(2)-N(2)	169.32(13)
O(10)-Cd(2)-N(5B)	87.52(13)	N(5B)-Cd(2)-N(2)	89.23(13)

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Cd(1)-O(1)	2.273(5)	Cd(1)-O(2)	2.501(6)
Cd(1)-O(4B)	2.341(5)	Cd(1)-O(7C)	2.343(5)
Cd(1)-O(8C)	2.529(5)	Cd(1)-N(1)	2.320(5)
Cd(1)-N(5A)	2.311(5)	Cd(2)-O(3B)	2.328(5)
Cd(2)-O(4B)	2.582(5)	Cd(2)-O(5)	2.399(5)
Cd(2)-O(6)	2.349(5)	Cd(2)-O(8C)	2.334(5)
Cd(2)-O(9)	2.298(5)	Cd(2)-N(2)	2.354(5)
O(1)-Cd(1)-O(2)	54.04(19)	O(1)-Cd(1)-O(4B)	101.65(19)
O(1)-Cd(1)-O(7C)	86.4(2)	O(1)-Cd(1)-O(8C)	139.77(19)
O(1)-Cd(1)-N(1)	138.9(2)	O(1)-Cd(1)-N(5A)	90.6(2)
O(4B)-Cd(1)-O(2)	104.20(18)	O(7C)-Cd(1)-O(2)	139.68(18)
O(2)-Cd(1)-O(8C)	165.80(18)	N(1)-Cd(1)-O(2)	85.92(19)
N(5A)-Cd(1)-O(2)	85.34(19)	O(4B)-Cd(1)-O(7C)	89.98(18)
O(4B)-Cd(1)-O(8C)	78.10(16)	N(1)-Cd(1)-O(4B)	77.39(19)
N(5A)-Cd(1)-O(4B)	167.36(19)	O(7C)-Cd(1)-O(8C)	53.47(16)
N(1)-Cd(1)-O(7C)	134.31(19)	N(5A)-Cd(1)-O(7C)	87.83(19)
N(1)-Cd(1)-O(8C)	80.89(18)	N(5A)-Cd(1)-O(8C)	90.64(17)
N(5A)-Cd(1)-N(1)	95.3(2)	O(3B)-Cd(2)-O(4B)	53.07(16)
O(3B)-Cd(2)-O(5)	85.24(18)	O(3B)-Cd(2)-O(6)	139.30(19)
O(3B)-Cd(2)-O(8C)	85.24(18)	O(9)-Cd(2)-O(3B)	89.4(2)
O(3B)-Cd(2)-N(2)	128.70(18)	O(5)-Cd(2)-O(4B)	136.44(16)
O(6)-Cd(2)-O(4B)	167.11(18)	O(8C)-Cd(2)-O(4B)	77.17(17)
O(9)-Cd(2)-O(4B)	94.06(18)	N(2)-Cd(2)-O(4B)	75.65(17)
O(6)-Cd(2)-O(5)	54.57(18)	O(8C)-Cd(2)-O(5)	88.59(18)
O(9)-Cd(2)-O(5)	97.92(19)	N(2)-Cd(2)-O(5)	144.43(19)
O(8C)-Cd(2)-O(6)	98.49(19)	O(9)-Cd(2)-O(6)	90.1(2)
O(6)-Cd(2)-N(2)	91.95(19)	O(9)-Cd(2)-O(8C)	171.23(19)
O(8C)-Cd(2)-N(2)	84.68(18)	O(9)-Cd(2)-N(2)	93.3(2)

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Zn(1)-O(1)	1.947(3)	Zn(1)-O(3)	1.934(3)
Zn(1)-N(1)	1.997(4)	Zn(1)-N(4A)	2.045(3)
O(3)-Zn(1)-O(1)	111.34(14)	O(1)-Zn(1)-N(1)	119.66(15)
O(1)-Zn(1)-N(4A)	96.57(14)	O(3)-Zn(1)-N(1)	114.84(14)
O(3)-Zn(1)-N(4A)	112.15(14)	N(1)-Zn(1)-N(4A)	99.81(15)

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Zn(1)-O(2)	2.002(3)	Zn(1)-O(3B)	2.164(4)
Zn(1)-O(4B)	2.223(5)	Zn(1)-N(1)	2.040(4)

Zn(1)-N(4A)	2.071(4)		
O(2)-Zn(1)-O(3B)	146.26(17)	O(2)-Zn(1)-O(4B)	97.71(14)
O(2)-Zn(1)-N(1)	104.19(14)	O(2)-Zn(1)-N(4A)	103.44(15)
O(3B)-Zn(1)-O(4B)	58.95(15)	N(1)-Zn(1)-O(3B)	91.94(15)
N(4A)-Zn(1)-O(3B)	100.21(16)	N(1)-Zn(1)-O(4B)	149.73(16)
N(4A)-Zn(1)-O(4B)	88.77(16)	N(1)-Zn(1)-N(4A)	105.85(16)

Symmetry transformations used to generate equivalent atoms: A x+1, y, z; B –x+1/2, y+1/2, -z+1/2; C –x-1/2, -y-1/2, -z; D -x+1/2, -y-1/2, -z for **1**; A -x-1/2, y-1/2, -z; B x, y, z-1; C -x, -y+1, -z+1; D x+1/2, -y+1/2, z for **2**; A -x, -y+1, -z+1; B x+1/2, -y+3/2, z; C x, y, z+1; D -x-1/2, y+1/2, -z for **3**; A -x+1/2, y-1/2, -z+3/2; B x, y, z+1; C -x+1, y, -z+3/2 for **4**; A -x+3/2, y-1/2, -z+1/2; B x, y, z-1; C -x+1/2, y-1/2, -z+1/2 for **5**; A x, y, z-1; B x+1, y, z; C -x+1, -y+1, -z for **6**; A –x, -y+3, -z for **7**; A x, y, z-1; B x+1, y, z for **8**.

Table S2 Hydrogen bonds for **2-8** (Å and ^{o}).

D-H···A	d(D-H)	d(H···A)	D(D···A)	<(DHA)
		1		
O(7)-H(1W)···O(2)^{i}	0.91(2)	2.21(2)	2.773(7)	119(2)
O(7)-H(2W)···O(5)	0.91(2)	2.41(2)	2.858(6)	110.2(19)
		2		
O(9)-H(1W)···O(3)^{i}	0.89(2)	2.00(3)	2.774(7)	146(5)
O(5)-H(2W)···O(7)^{ii}	0.90(2)	1.79(3)	2.645(7)	157(6)
		3		
O(13)-H(1W)···O(9)^{i}	0.892(19)	1.79(2)	2.661(6)	165(5)
O(13)-H(2W)···O(3)^{ii}	0.888(19)	2.02(3)	2.791(6)	144(4)
		4		
O(7)-H(7)···O(7)^{i}	0.90(2)	1.68(13)	2.450(14)	141(18)
O(9)-H(1W)···O(14)	0.90	2.24	3.054(5)	149.3
O(9)-H(2W)···O(8)	0.89	1.90	2.768(9)	162.1
O(10)-H(3W)···O(7)^{i}	0.92	1.95	2.853(8)	168.1
O(10)-H(4W)···O(6)	0.92	1.99	2.842(7)	152.9
O(11)-H(5W)···O(1)	0.86	2.37	3.058(8)	137.0
O(11)-H(6W)···O(6)^{ii}	0.86	2.35	2.824(6)	114.8
O(12)-H(7W)···O(4)^{iii}	0.89	1.93	2.773(7)	158.4
O(12)-H(8W)···O(13)	0.85	2.12	2.641	119.3
O(13)-H(9W)···O(14)^{iii}	0.91	2.10)	2.634(3)	116.9
O(13)-H(10W)···O(3)	0.91	2.02	2.740(7)	135.0

		5		
O(9)-H(1W)···O(8)^{i}	1.072(16)	2.491(13)	3.279(6)	129.5(12)
O(9)-H(2W)···O(6)^{ii}	0.85(2)	1.86(2)	2.668(5)	159(4)
O(10)-H(3W)···O(1)^{iii}	0.883(19)	1.80(2)	2.673(5)	168(5)
O(10)-H(4W)···O(17)	0.898(19)	1.88(2)	2.685(8)	148(3)
O(11)-H(5W)···O(12)^{iv}	0.89(2)	1.96(4)	2.800(8)	157(9)
O(11)-H(6W)···O(5)	0.87(2)	1.95(4)	2.764(6)	154(8)
O(12)-H(7W)···O(16)	0.898(18)	2.067(19)	2.880(10)	150(4)
O(12)-H(8W)···O(13)^{v}	0.90(2)	1.97(5)	2.762(8)	145(7)
		6		
O(9)-H(1W)···O(11)^{i}	0.87(2)	1.84(3)	2.701(10)	171(9)
O(9)-H(2W)···O(10)	0.89(2)	1.84(3)	2.727(8)	171(8)
O(10)-H(3W)···N(4)^{ii}	0.88(2)	2.17(6)	2.922(8)	142(8)
		7		
O(6)-H(1W)···O(4)^{i}	0.91(2)	1.78(3)	2.643(5)	158(6)
O(8)-H(2W)···N(5)^{ii}	0.89(2)	1.96(2)	2.831(5)	166(5)
		8		
O(5)-H(1W)···O(2)	0.893(19)	1.91(2)	2.783(5)	165(5)
O(5)-H(2W)···O(6)^{i}	0.899(19)	1.93(2)	2.820(6)	171(6)
O(6)-H(3W)···O(5)	0.89(2)	2.08(3)	2.953(7)	166(7)
O(6)-H(4W)···O(4)^{ii}	0.89(2)	1.90(3)	2.779(6)	167(6)

Symmetry transformations used to generate equivalent atoms: i -x+1,y,-z+1/2 for **1**; i -x, -y+1, -z ; ii -x, -y+1, -z+1 for **2**; i -x, -y+1, -z+1; ii -x, -y+1, -z for **3**; i -x, y, -z+3/2; ii -x+1/2, -y+1/2, -z+1; iii x, -y+1, z-1/2 for **4**; i -x+1/2, y-1/2, -z+1/2; ii x+1/2, -y+1/2, z+1/2; iii x-1/2, -y+1/2, z-1/2; iv x-1, y, z; v x+1/2, -y+1/2, z-1/2 for **5**; i -x+1, -y+1, -z+1; ii x+1, y, z-1 for **6**; i x, y-1, z; ii –x, -y+3, -z for **7**; i -x, -y+1, -z; ii x+1, y, z for **8**.

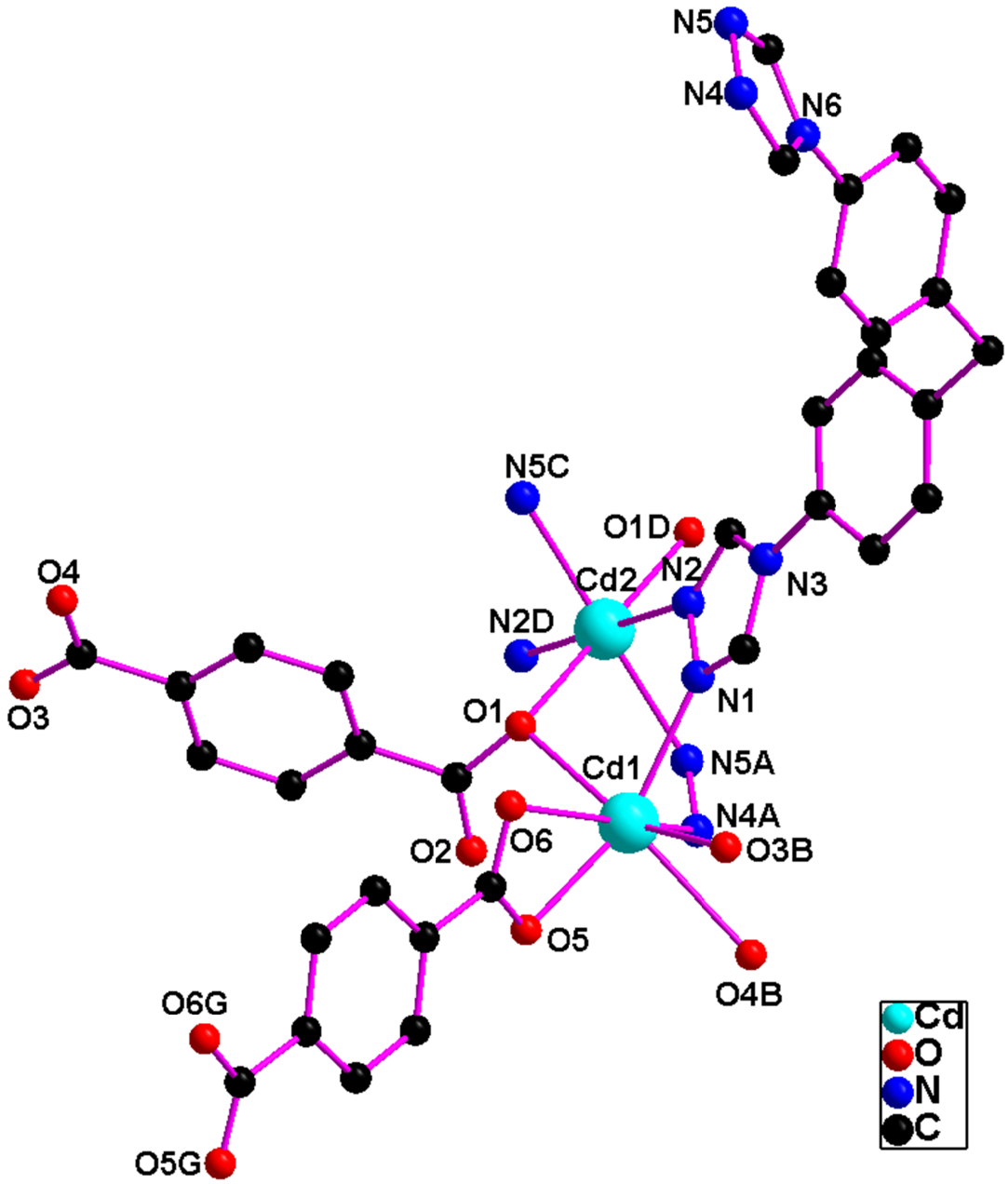

Fig. S1 The coordination environment of Cd(II) atoms in **1**. Symmetry transformations used to generate equivalent atoms: A x+1, y, z; B -x+1/2, y+1/2, -z+1/2; C -x-1/2, -y-1/2, -z; D -x+1/2, -y-1/2, -z; G -x+1/2, -y-1/2, -z+1.

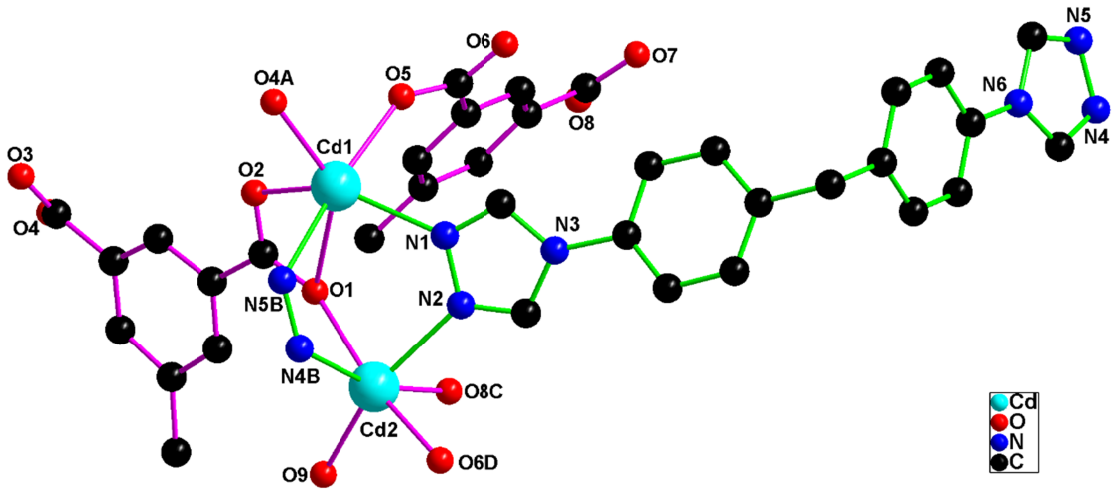

Fig. S2 The coordination environment of Cd(II) atoms in **2**. Symmetry transformations used to generate equivalent atoms: A -x-1/2, y-1/2, -z; B x, y, z-1; C -x, -y+1, -z+1; D x+1/2, -y+1/2, z.

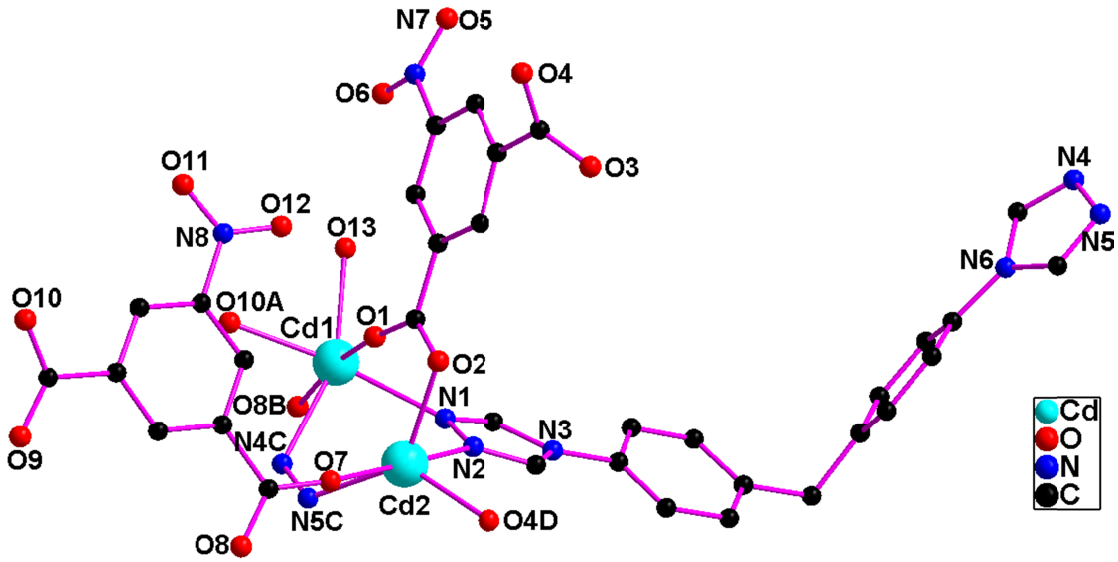

Fig. S3 The coordination environment of Cd(II) atoms in **3**. Symmetry transformations used to generate equivalent atoms: A -x, -y+1, -z+1; B x+1/2, -y+3/2, z; C x, y, z+1; D -x-1/2, y+1/2, -z.

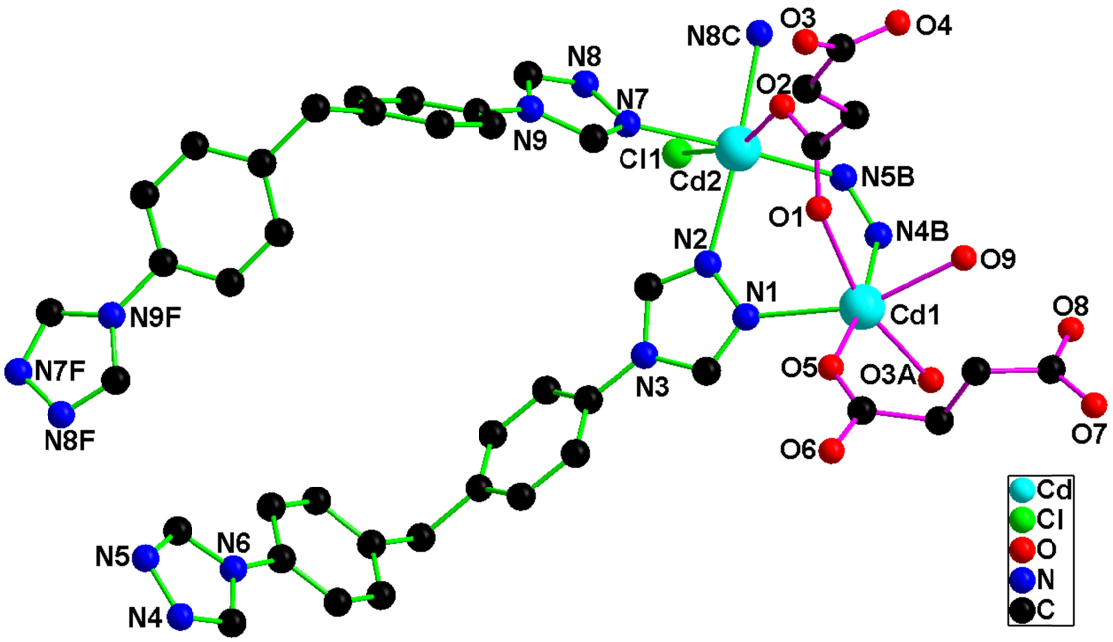

Fig. S4 The coordination environment of Cd(II) atoms in **4**. Symmetry transformations used to generate equivalent atoms: A -x+1/2, y-1/2, -z+3/2; B x, y, z+1; C -x+1, y, -z+3/2; F -x+1, y, -z+1/2.

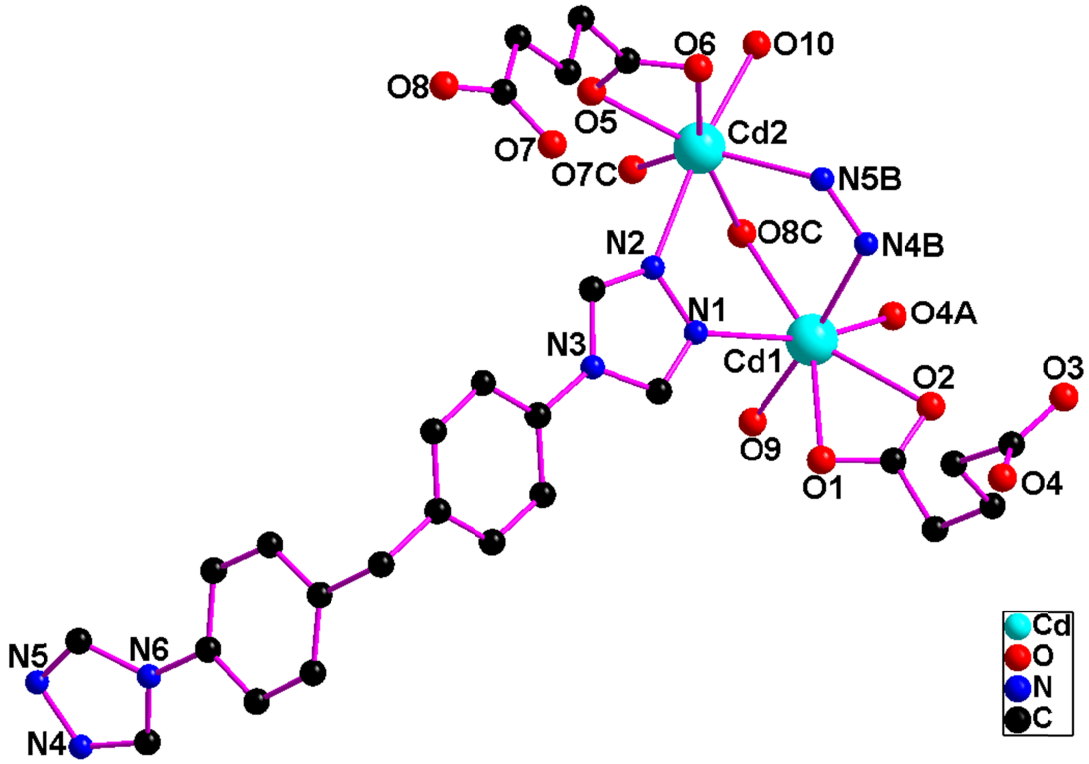

Fig. S5 The coordination environment of Cd(II) atom in **5**. Symmetry transformations used to generate equivalent atoms: A -x+3/2, y-1/2, -z+1/2; B x, y, z-1; C -x+1/2, y-1/2, -z+1/2.

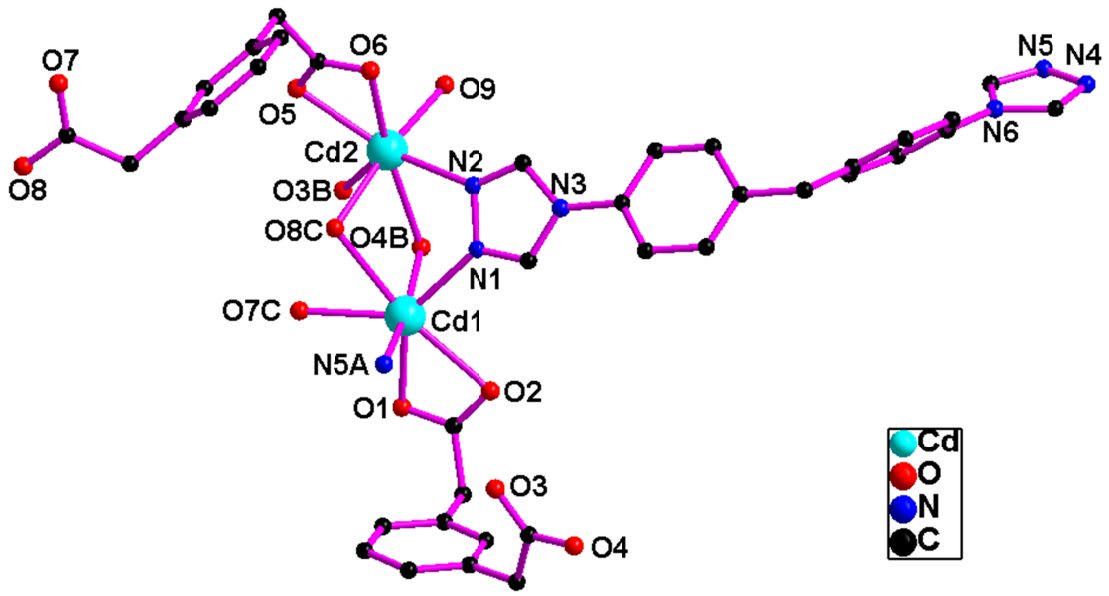

Fig. S6 The coordination environment of Cd(II) atom in **6**. Symmetry transformations used to generate equivalent atoms: A x, y, z-1; B x+1, y, z; C -x+1, -y+1, -z.

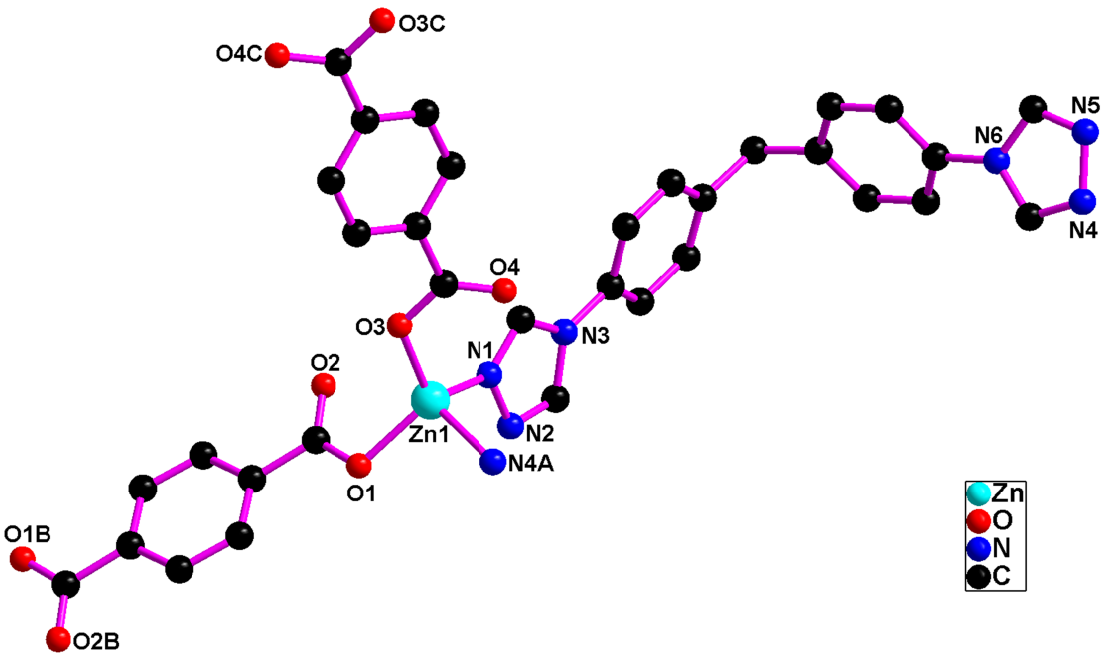

Fig. S7 The coordination environment of Zn(II) atom in **7**. Symmetry transformations used to generate equivalent atoms: A -x, -y+3, -z; B -x, -y+1, -z+1; C -x+1, -y+2, -z+1.

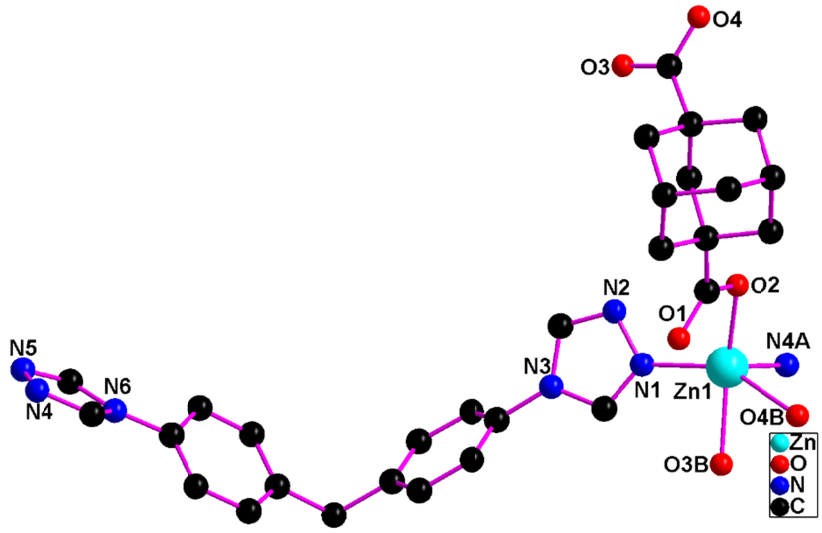

Fig. S8 The coordination environment of Zn(II) atom in **8**. Symmetry transformations used to generate equivalent atoms: A x, y, z-1; B x+1, y, z.

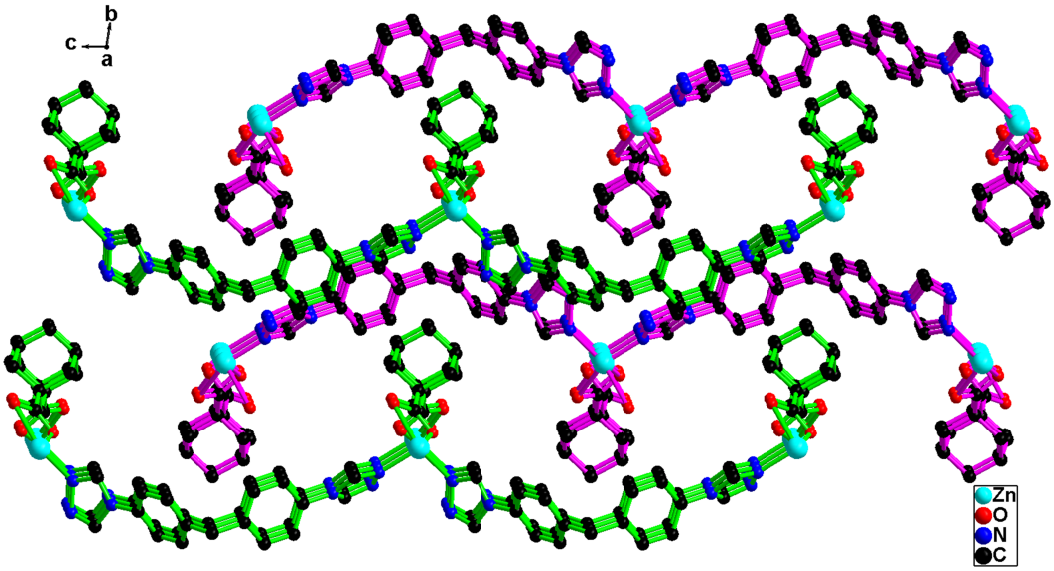

Fig. S9 The pack plot in **8**.

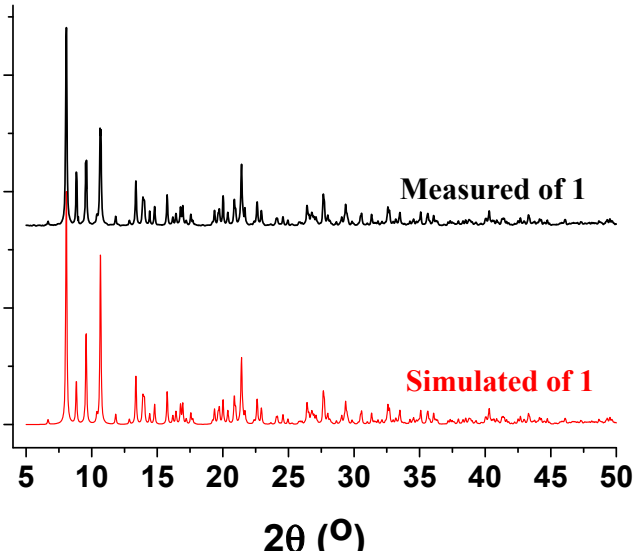

Fig. S10 PXRD patterns of the measured and simulated diagram from single crystal data of **1**.

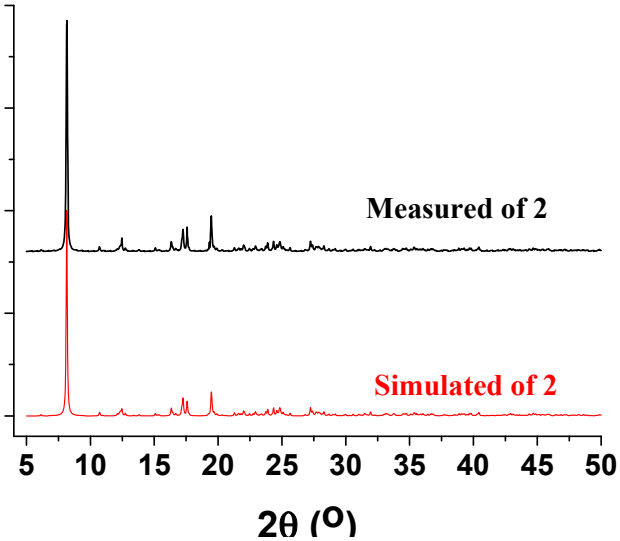

Fig. S11 PXRD patterns of the measured and simulated diagram from single crystal data of **2**.

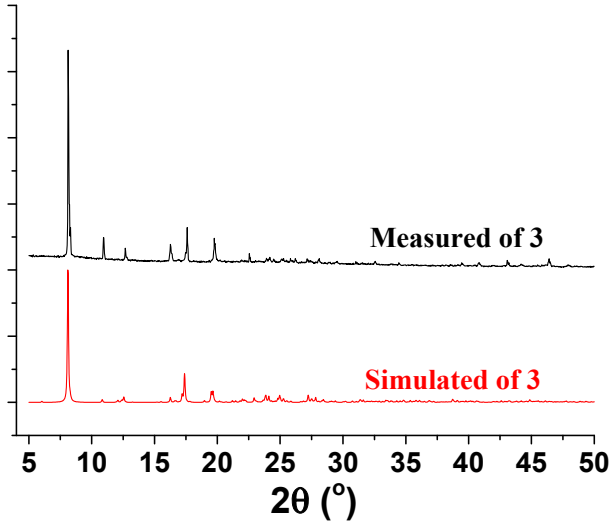

Fig. S12 PXRD patterns of the measured and simulated diagram from single crystal data of **3**.

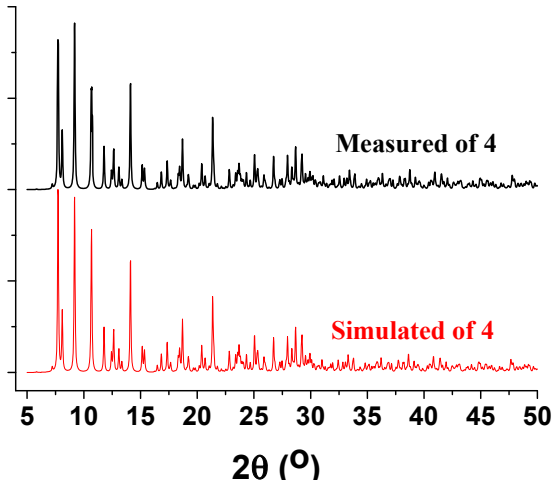

Fig. S13 PXRD patterns of the measured and simulated diagram from single crystal data of **4**.

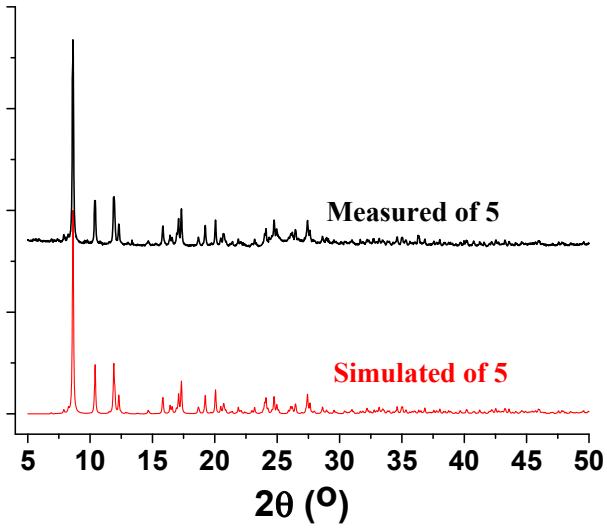

Fig. S14 PXRD patterns of the measured and simulated diagram from single crystal data of **5**.

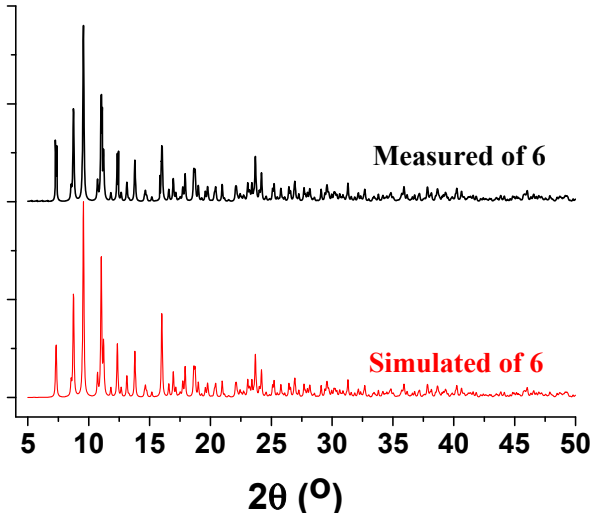

Fig. S15 PXRD patterns of the measured and simulated diagram from single crystal data of **6**.

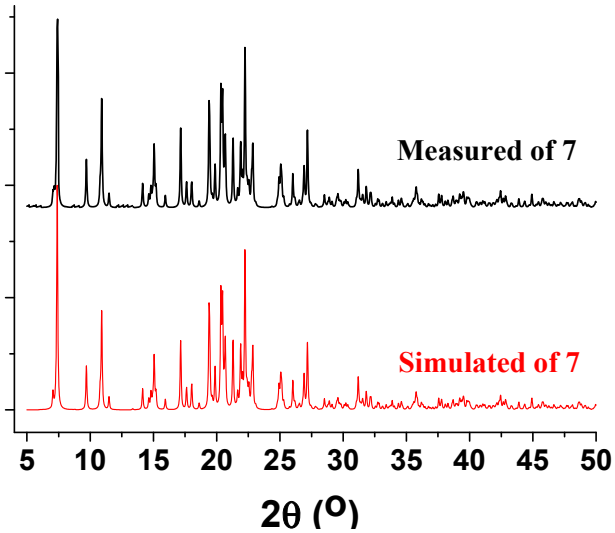

Fig. S16 PXRD patterns of the measured and simulated diagram from single crystal data of **7**.

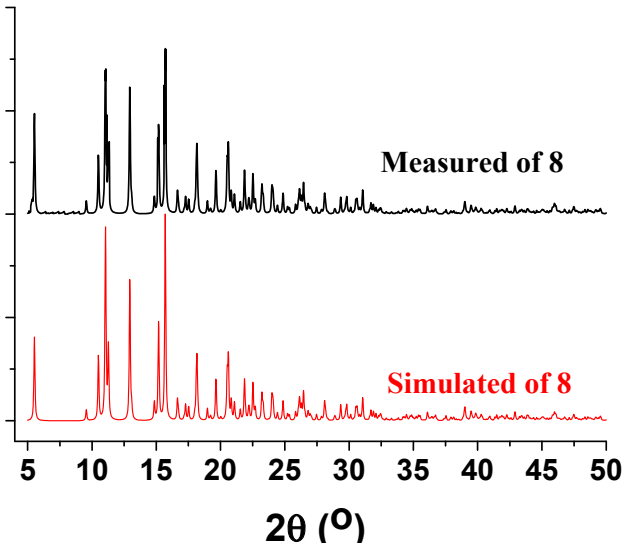

Fig. S17 PXRD patterns of the measured and simulated diagram from single crystal data of **8**.