1, 2-, 1, 3- and 1, 4-Cyclohexanedicarboxylates of Cd and Mn with chain and layered structures

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Electronic Supplementary Information

Table S1. Selected bond distances and angles for **I**

Bond	Distance (Å)	Bond	Amplitude
Cd(1)-O(1)	2.295(4)	O(1)-Cd(1)-O(1)#1	94.2(2)
Cd(1)-O(1)#1	2.295(4)	O(1)-Cd(1)-O(2)	55.22(14)
Cd(1)-O(2)	2.404(4)	O(1)-Cd(1)-O(2)#1	93.9(2)
Cd(1)-O(2)#1	2.404(4)	O(3)-Cd(1)-O(1)	105.2(2)
Cd(1)-O(3)	2.239(4)	O(3)#1-Cd(1)-O(1)	139.5(2)
Cd(1)-O(3)#1	2.239(4)	O(1)#1-Cd(1)-O(2)	93.9(2)
O(1)-C(1)	2.256(8)	O(1)#1-Cd(1)-O(2)#1	55.22(14)
O(2)-C(1)	1.260(7)	O(3)-Cd(1)-O(1)#1	139.5(2)
		O(3)#1-Cd(1)-O(1)#1	105.2(2)
		O(2)-Cd(1)-O(2)#1	136.6(2)
		O(3)-Cd(1)-O(2)	126.4(2)
		O(3)#1-Cd(1)-O(2)	87.8(2)
		O(3)-Cd(1)-O(2)#1	87.8(2)
		O(3)#1-Cd(1)-O(2)#1	126.4(2)
		O(3)#1-Cd(1)-O(3)	82.6(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+1/2

Table S2. Selected bond distances and angles for **II**

Bond	Distance (Å)	Bond	Amplitude
Cd(1)-O(1)	2.420(3)	O(1)-Cd(1)-O(2)	53.97(11)
Cd(1)-O(2)	2.345(3)	O(1)-Cd(1)-O(3)	112.91(12)
Cd(1)-O(3)	2.424(3)	O(1)-Cd(1)-O(4)	85.80(11)
Cd(1)-O(4)	2.624(3)	O(1)-Cd(1)-O(3)#1	92.13(11)
Cd(1)-O(3)#1	2.269(3)	O(2)-Cd(1)-O(3)	81.40(12)
Cd(1)#1-O(3)	2.269(3)	O(2)-Cd(1)-O(4)	139.74(11)
Cd(1)-N(1)	2.342(3)	O(2)-Cd(1)-O(3)#1	122.59(12)
Cd(1)-N(2)	2.359(3)	O(3)-Cd(1)-O(4)	121.05(9)
O(1)-C(11)	1.239(5)	O(3)-Cd(1)-O(3)#1	71.04(11)
O(2)-C(11)	1.249(5)	O(4)-Cd(1)-O(3)#1	52.09(9)
O(3)-C(18)	1.263(5)	N(1)-Cd(1)-O(1)	162.07(12)
C(18)-O(4)#1	1.243(5)	N(1)-Cd(1)-O(2)	123.37(11)
O(4)-C(18)#1	1.243(5)	N(1)-Cd(1)-O(3)	82.42(11)
		N(1)-Cd(1)-O(4)	94.23(10)
		N(1)-Cd(1)-O(3))#1	102.04(11)
		N(2)-Cd(1)-O(1)	91.99(12)
		N(2)-Cd(1)-O(2)	88.98(12)
		N(2)-Cd(1)-O(3)	139.14(11)
		N(2)-Cd(1)-O(4)	91.37(10)
		N(2)-Cd(1)-O(3))#1	142.74(11)
		N(1)-Cd(1)-N(2)	70.08(11)
		O(1)-C(11)-O(2)	120.7(4)
		O(4)#1-C(18)-O(3)	120.2(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+3/2,-z+1

Table S3. Selected bond distances and angles for **III**

Bond	Distance (Å)	Bond	Amplitude
Cd(1)-O(2)	2.325(2)	O(2)-Cd(1)-O(2)#1	180.0
Cd(1)-O(2)#1	2.325(2)	O(2)-Cd(1)-O(3)	97.62(9)
Cd(1)-O(3)	2.280(2)	O(2)-Cd(1)-O(3)#1	82.38(9)
Cd(1)-O(3)#1	2.280(2)	O(2)-Cd(1)-O(6)	90.26(8)
Cd(1)-O(6)	2.240(2)	O(2) -Cd(1)-O(6)#1	89.74(8)
Cd(1)-O(6)#1	2.240(2)	O(2) #1 -Cd(1)-O(3)	82.38(9)
Cd(2)-O(1)	2.339(2)	O(2)#1-Cd(1)-O(3)#1	97.62(9)
Cd(2)-O(2)#1	2.487(2)	O(2) #1-Cd(1)-O(6)	89.74(8)
Cd(2)-O(3)	2.602(3)	O(2)#1-Cd(1)-O(6)#1	90.26(8)
Cd(2)-O(4)	2.328(2)	O(3)-Cd(1)-O(3)#1	180.0
Cd(2)-O(5)	2.252(2)	O(3)-Cd(1)-O(6)	91.27(9)
Cd(2)-N(1)	2.379(2)	O(3)-Cd(1)-O(6)#1	88.73(9)
Cd(2)-N(2)	2.331(2)	O(3) #1-Cd(1)-O(6)	88.73(9)
O(1)-C(21)	1.243(4)	O(3)#1-Cd(1)-O(6)#1	91.27(9)
C(21)-O(2)#1	1.269(3)	O(6)-Cd(1)-O(6)#1	180.0
O(2)-C(21)#1	1.269(3)	O(1)-Cd(2)-O(2)#1	53.55(7)
O(3)-C(28)	1.234(4)	O(1)-Cd(2)-O(3)	93.48(9)
O(4)-C(28)	1.245(4)	O(1)-Cd(2)-O(4)	91.30(9)
O(5)-C(41)	1.245(4)	O(1)-Cd(2)-O(5)	159.70(8)
O(6)-C(41)	1.259(4)	O(2)#1-Cd(2)-O(3)	73.11(7)
		O(2)#1-Cd(2)-O(4)	112.54(8)
		O(2)#1-Cd(2)-O(5)	106.28(7)
		O(3)-Cd(2)-O(4)	51.39(8)
		O(3)-Cd(2)-O(5)	80.93(8)
		O(4)-Cd(2)-O(5)	100.09(8)
		N(1)-Cd(2)-O(1)	91.81(9)
		N(1)-Cd(2)-O(2)#1	86.18(8)
		N(1)-Cd(2)-O(3)	149.44(8)
		N(1)-Cd(2)-O(4)	158.49(9)
		N(1)-Cd(2)-O(5)	83.74(8)
		N(2)-Cd(2)-O(1)	93.47(8)
		N(2)-Cd(1)-O(2)#1	139.83(7)
		N(2)-Cd(2)-O(3)	138.36(8)
		N(2)-Cd(2)-O(4)	87.45(9)
		N(2)-Cd(2)-O(5)	103.70(8)
		N(1)-Cd(2)-N(2)	71.12(9)
		O(1)-C(21)-O(2)#1	120.2(3)
		O(3)-C(28)-O(4)	120.5(3)
		O(5)-C(41)-O(6)	126.1(3)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+1

Table S4. Selected bond distances and angles for **IV**

Bond	Distance (Å)	Bond	Amplitude
Mn(1)-O(1)	2.226(2)	O(1)-Mn(1)-O(1)#2	180.0
Mn(1)-O(1)#2	2.226(2)	O(1)-Mn(1)-O(3)	85.43(7)
Mn(1)-O(3)	2.145(2)	O(1)-Mn (1)-O(3)#2	94.57(7)
Mn(1)-O(3)#2	2.145(2)	O(1)-Mn (1)-O(5)	90.77(6)
Mn(1)-O(5)	2.1501(14)	O(1)-Mn (1)-O(5)#2	89.23(6)
Mn(1)-O(5)#2	2.1501(14)	O(1) #2-Mn (1)-O(3)	94.57(7)
Mn(2)-O(1)#2	2.371(2)	O(1)#2-Mn (1)-O(3)#2	85.43(7)
Mn(2)-O(2)#2	2.239(2)	O(1)#2-Mn (1)-O(5)	89.23(6)
O(4)-Mn(2)	2.155(2)	O(1)#2-Mn (1)-O(5)#2	90.77(6)
O(6)-Mn(2)	2.121(2)	O(3)-Mn (1)-O(3)#2	180.0
Mn(2)-N(1)	2.299(2)	O(3)-Mn (1)-O(5)	88.46(6)
Mn(2)-N(2)	2.247(2)	O(3)-Mn (1)-O(5)#2	91.54(6)
O(1)-C(21)	1.259(2)	O(3) #2-Mn (1)-O(5)	91.54(6)
C(21)-O(2)	1.259(2)	O(3)#2-Mn (1)-O(5)#2	88.46(6)
O(3)-C(28)	1.241(3)	O(5)-Mn(1)-O(5)#2	180.0
C(28)-O(4)#2	1.242(3)	O(1)#2-Mn(2)-O(2)#2	55.82(6)
O(5)-C(31)	1.255(2)	O(1)#2-Mn(2)-O(4)	106.73(6)
O(6)-C(31)	1.257(3)	O(1)#2-Mn (2)-O(6)	106.73(6)
		O(2)#2-Mn (2)-O(4)	92.35(7)
		O(2)#2-Mn (2)-O(6)	161.75(6)
		O(4)-Mn (2)-O(6)	98.86(7)
		N(1)-Mn (2)-O(1)#2	88.00(6)
		N(1)-Mn (2)-O(2)#2	89.12(7)
		N(1)-Mn (2)-O(4)	162.24(7)
		N(1)-Mn (2)-O(6)	84.58(6)
		N(2)-Mn (2)-O(1)#2	142.27(6)
		N(2)-Mn (1)-O(2)#2	90.81(7)
		N(2)-Mn (2)-O(4)	89.28(7)
		N(2)-Mn (2)-O(6)	103.62(6)
		N(1)-Mn (2)-N(2)	73.00(7)
		O(1)-C(21)-O(2)	119.4(2)
		O(3)-C(28)-O(4)#2	122.4(2)
		O(5)-C(31)-O(6)	124.6(2)

Symmetry transformations used to generate equivalent atoms: #2 -x+2,-y,-z+2

Table S5. Selected bond distances and angles for **V**

Bond	Distance (Å)	Bond	Amplitude
Mn(1)-O(2)	2.211(4)	O(2)-Mn(1)-O(2)#1	178.9(2)
Mn(1)-O(2)#1	2.211(4)	O(2)-Mn(1)-O(3)	85.9(2)
Mn(1)-O(3)	2.155(4)	O(2)-Mn (1)-O(3)#1	94.8(2)
Mn(1)-O(3)#1	2.155(4)	O(2)-Mn (1)-O(6)	89.8(3)
Mn(1)-O(6)	2.141(6)	O(2)-Mn (1)-O(6)#1	89.4(3)
Mn(1)-O(6)#1	2.141(6)	O(2)#1-Mn (1)-O(3)	94.8(2)
Mn(2)-O(1)	2.424(4)	O(2)#1-Mn (1)-O(3)#1	85.9(2)
Mn(2)-O(2)	2.222(4)	O(2)#1-Mn (1)-O(6)	89.4(3)
Mn(2)-O(4)	2.107(4)	O(2)#1-Mn (1)-O(6)#1	89.8(3)
Mn(2)-O(5)	2.186(5)	O(3)-Mn (1)-O(3)#1	100.9(3)
Mn(2)-N(1)	2.255(5)	O(3)-Mn (1)-O(6)	86.8(2)
Mn(2)-N(2)	2.245(5)	O(3)-Mn (1)-O(6)#1	171.2(2)
O(1)-C(21)	1.252(6)	O(3) #1-Mn (1)-O(6)	171.2(2)
C(21)-O(2)	1.269(7)	O(3)#1-Mn (1)-O(6)#1	86.8(2)
O(3)-C(28)	1.244(6)	O(6)-Mn(1)-O(6)#1	85.8(4)
C(28)-O(4)	1.269(7)	O(1)-Mn(2)-O(2)	55.94(13)
O(5)-C(31)	1.205(7)	O(1)-Mn(2)-O(4)	86.0(2)
O(6)-C(31)	1.204(7)	O(1)-Mn (2)-O(5)	172.8(2)
		O(2)-Mn (2)-O(4)	93.8(2)
		O(2)-Mn (2)-O(5)	117.8(2)
		O(4)-Mn (2)-O(5)	91.3(2)
		N(1)-Mn (2)-O(1)	93.0(2)
		N(1)-Mn (2)-O(2)	94.8(2)
		N(1)-Mn (2)-O(4)	168.8(2)
		N(1)-Mn (2)-O(5)	90.9(2)
		N(2)-Mn (2)-O(1)	88.11(14)
		N(2)-Mn (1)-O(2)	142.2(2)
		N(2)-Mn (2)-O(4)	95.0(2)
		N(2)-Mn (2)-O(5)	98.7(2)
		N(1)-Mn (2)-N(2)	73.8(2)
		O(1)-C(21)-O(2)	119.6(5)
		O(3)-C(28)-O(4)	124.7(5)
		O(5)-C(31)-O(6)	123.3(7)

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2

Table S6. Selected bond distances and angles for **VI**

Bond	Distance (Å)	Bond	Amplitude
Cd(1)-O(1)	2.258(4)	O(1)-Cd(1)-O(2)	107.37(14)
Cd(1)-O(2)	2.286(4)	O(1)-Cd(1)-O(3)	78.61(14)
Cd(1)-O(3)	2.447(4)	O(1)-Cd(1)-O(3)#1	85.5(2)
Cd(1)-O(4)	2.607(4)	O(1)-Cd(1)-O(4)	89.2(2)
Cd(1)-O(5)	2.366(4)	O(1)-Cd(1)-O(5)	121.51(14)
Cd(1)-O(6)	2.428(4)	O(1)-Cd(1)-O(6)	155.84(14)
Cd(1)-O(3)#1	2.353(4)	O(2)-Cd(1)-O(3)	84.68(13)
O(3)-Cd(1)#1	2.353(4)	O(2)-Cd(1)-O(3)#1	150.72(14)
O(3)-C(1)	1.252(7)	O(2)-Cd(1)-O(4)	150.37(14)
C(1)-O(4)#1	1.261(7)	O(2)-Cd(1)-O(5)	78.4(2)
O(1)-C(8)	1.280(6)	O(2)-Cd(1)-O(6)	82.4(2)
C(8)-O(2)#4	1.247(7)	O(3)-Cd(1)-O(3)#1	71.9(2)
O(2)-C(8)#2	1.247(7)	O(3)-Cd(1)-O(4)	123.32(12)
		O(3)-Cd(1)-O(5)	156.80(14)
		O(3)-Cd(1)-O(6)	80.4(2)
		O(4)-Cd(1)-O(3)#1	51.87(13)
		O(4)-Cd(1)-O(5)	71.99(14)
		O(4)-Cd(1)-O(6)	92.3(2)
		O(5)-Cd(1)-O(3)#1	117.8(2)
		O(5)-Cd(1)-O(6)	81.7(2)
		O(6)-Cd(1)-O(3)#1	76.7(2)
		O(3)-C(1)-O(4)#1	120.5(5)
		O(1)-C(8)-O(2)#4	121.8(5)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z #4 -x+1/2,y,z-1/2

Table S7. Selected bond distances and angles for **VII**

Bond	Distance (Å)	Bond	Amplitude
Cd(1)-O(1)	2.339(4)	O(1)-Cd(1)-O(2)	51.66(14)
Cd(1)-O(2)	2.600(5)	O(1)-Cd(1)-O(3)	82.7(2)
Cd(1)-O(3)	2.329(5)	O(1)-Cd(1)-O(4)	131.8(2)
Cd(1)-O(4)	2.384(4)	O(1)-Cd(1)-O(7)	108.5(2)
Cd(1)-O(7)	2.351(4)	O(2)-Cd(1)-O(3)	125.9(2)
Cd(1)-N(1)	2.390(5)	O(2)-Cd(1)-O(4)	174.5(2)
Cd(1)-N(2)	2.362(4)	O(2)-Cd(1)-O(7)	72.9(2)
Cd(2)-O(2)	2.278(4)	O(3)-Cd(1)-O(4)	54.5(2)
Cd(2)-O(5)	2.702(5)	O(3)-Cd(1)-O(7)	101.6(2)
Cd(2)-O(6)	2.233(5)	O(4)-Cd(1)-O(7)	101.6(2)
Cd(2)-O(7)	2.695(4)	N(1)-Cd(1)-O(1)	83.0(2)
Cd(2)-O(8)	2.298(5)	N(1)-Cd(1)-O(2)	94.9(2)
Cd(2)-N(3)	2.403(4)	N(1)-Cd(1)-O(3)	108.1(2)
Cd(2)-N(4)	2.405(4)	N(1)-Cd(1)-O(4)	90.0(2)
O(1)-C(41)	1.222(7)	N(1)-Cd(1)-O(7)	149.3(2)
O(2)-C(41)	1.270(7)	N(2)-Cd(1)-O(1)	129.6(2)
O(3)-C(48)	1.241(8)	N(2)-Cd(1)-O(2)	88.25(14)
O(4)-C(48)	1.245(8)	N(2)-Cd(1)-O(2)	145.4(2)
O(5)-C(51)	1.198(8)	N(2)-Cd(1)-O(4)	91.0(2)
O(6)-C(51)	1.245(7)	N(2)-Cd(1)-O(7)	81.2(2)
O(7)-C(58)	1.233(7)	N(1)-Cd(1)-N(2)	70.13(14)
O(8)-C(58)	1.251(7)	O(2)-Cd(2)-O(5)	95.4(2)
		O(2)-Cd(2)-O(6)	107.2(2)
		O(2)-Cd(2)-O(7)	72.2(1)
		O(2)-Cd(2)-O(8)	106.0(2)
		O(5)-Cd(2)-O(6)	49.9(3)
		O(5)-Cd(2)-O(7)	123.1(2)
		O(5)-Cd(2)-O(8)	84.4(2)
		O(6)-Cd(2)-O(7)	173.1(1)
		O(6)-Cd(2)-O(8)	124.9(2)
		O(7)-Cd(2)-O(8)	49.9(1)
		N(3)-Cd(2)-O(2)	83.6(2)
		N(3)-Cd(2)-O(5)	135.6(4)
		N(3)-Cd(2)-O(6)	87.9(2)
		N(3)-Cd(2)-O(7)	98.3(2)
		N(3)-Cd(2)-O(8)	83.6(2)
		N(4)-Cd(2)-O(2)	145.9(2)
		N(4)-Cd(2)-O(5)	118.4(2)
		N(4)-Cd(2)-O(6)	92.6(2)
		N(4)-Cd(2)-O(7)	91.3(3)
		N(4)-Cd(2)-O(8)	83.2(2)
		N(3)-Cd(2)-N(4)	69.4(2)

Table S8. Selected bond distances and angles for **VIII**

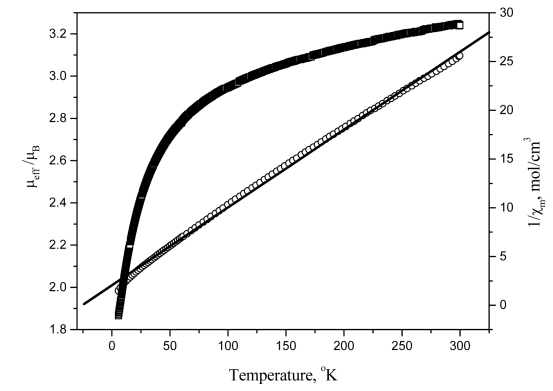
Bond	Distance (Å)	Bond	Amplitude
Mn(1)-O(1)	2.256(4)	O(1)-Mn(1)-O(2)	57.5(2)
Mn(1)-O(2)	2.264(4)	O(1)-Mn (1)-O(3)	92.7(2)
Mn(1)-O(3)	2.097(4)	O(1)-Mn (1)-O(5)	151.7(2)
Mn(1)-O(5)	2.161(4)	O(2)-Mn (1)-O(3)	102.5(2)
Mn(1)-N(1)	2.244(5)	O(2)-Mn (1)-O(5)	94.5(2)
Mn(1)-N(2)	2.265(5)	O(3)-Mn (1)-O(5)	90.0(2)
C(21)-O(1)	1.245(7)	N(1)-Mn(1)-O(1)	99.7(2)
C(21)-O(2)	1.256(7)	N(1)-Mn(1)-O(2)	152.4(2)
C(28)-O(3)	1.245(8)	N(1)-Mn(1)-O(3)	93.3(2)
C(28)-O(4)	1.247(8)	N(1)-Mn(1)-O(5)	108.2(2)
		N(2)-Mn(1)-O(1)	92.1(2)
		N(2)-Mn(1)-O(2)	90.7(2)
		N(2)-Mn(1)-O(3)	166.5(2)
		N(2)-Mn(1)-O(5)	91.8(2)
		N(1)-Mn(1)-N(2)	73.4(2)
		O(1)-C(21)-O(2)	120.8(6)
		O(3)-C(28)-O(4)	125.4(6)

Table S9. Selected bond distances and angles for **IX**

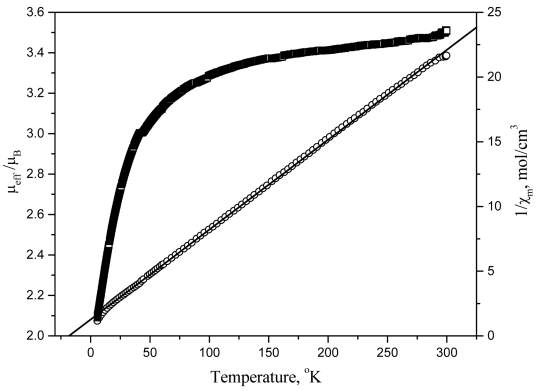
Bond	Distance (Å)	Bond	Amplitude
O(1)-Cd(1)	2.250(7	O(1)-Cd(1)-O(1)#2	105.3(2)
Cd(1)-O(1)#2	2.404(7)	O(1)-Cd(1)-O(2)#1	97.5(3)
Cd(1)-O(2)#1	2.227(7)	O(1)-Cd(1)-O(3)#2	163.3(3)
Cd(1)-O(3)#2	2.413(6)	O(1)-Cd(1)-O(3)#5	86.2(3)
Cd(1)-O(3)#5	2.271(7)	O(1)-Cd(1)-O(4)#6	104.8(3)
Cd(1)-O(4)#6	2.298(7)	O(1)#2-Cd(1)-O(2)#1	82.0(2)
C(7)-O(1)	1.261(12)	O(1)#2-Cd(1)-O(3)#2	91.4(2)
C(7)-O(2)	1.246(11)	O(1)#2-Cd(1)-O(3)#5	162.6(3)
C(8)-O(3)	1.293(12)	O(1)#2-Cd(1)-O(4)#6	71.2(2)
C(8)-O(4)	1.248(12)	O(2)#1-Cd(1)-O(3)#2	85.0(3)
		O(2)#1-Cd(1)-O(3)#5	110.0(3)
		O(2)#1-Cd(1)-O(4)#6	148.7(3)
		O(3)#2-Cd(1)-O(3)#5	77.5(3)
		O(3)#2-Cd(1)-O(4) #6	79.9(3)
		O(3)#5-Cd(1)-O(4) #6	93.3(3)
		O(1)-C(7)-O(2)	124.0(10)
		O(3)-C(8)-O(4)	119.8(9)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,y+1/2,-z+3/2 #2 -x+1/2,y-1/2,-z+3/2 #5 x,-y+1,z+1/2 #6 x,-y,z+1/2

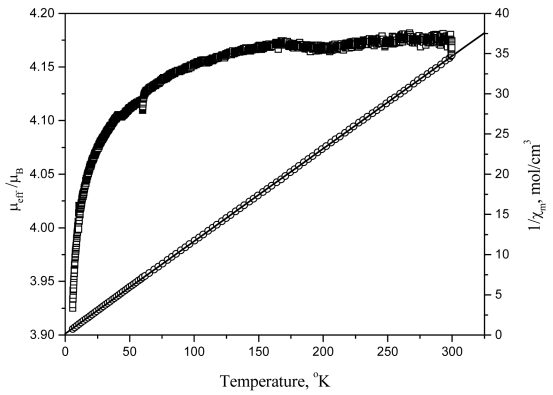
Fig S1: Plots of experimental μ_{eff} vs T (□) and $1/\chi_m$ vs T (○) of (a) **IV** (b) **V** and (c) **VIII**. The solid line shows the Curie-Weiss fitting.



(a)



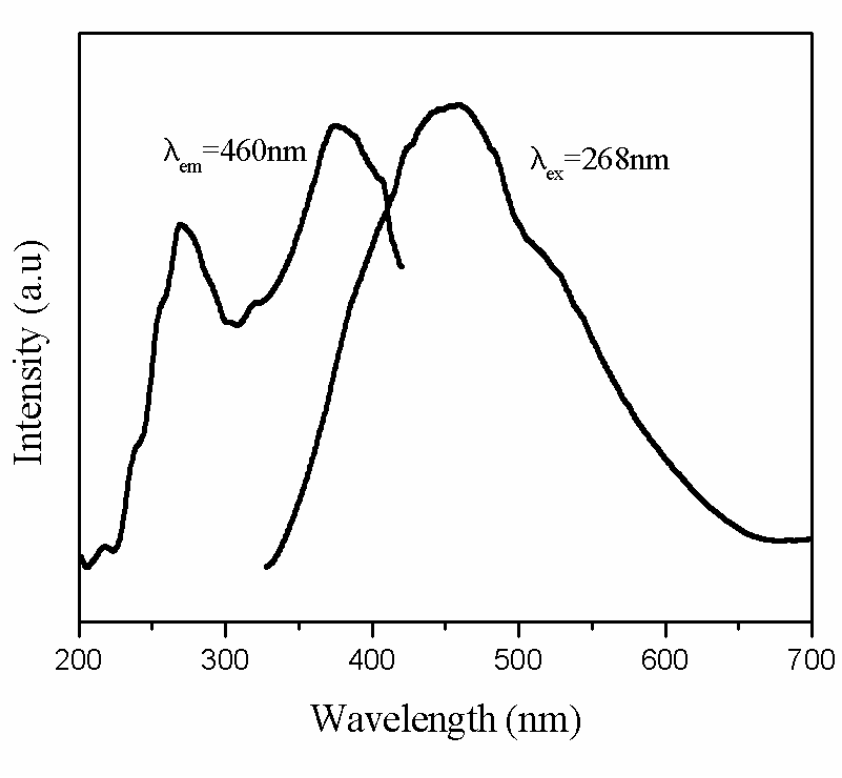
(b)



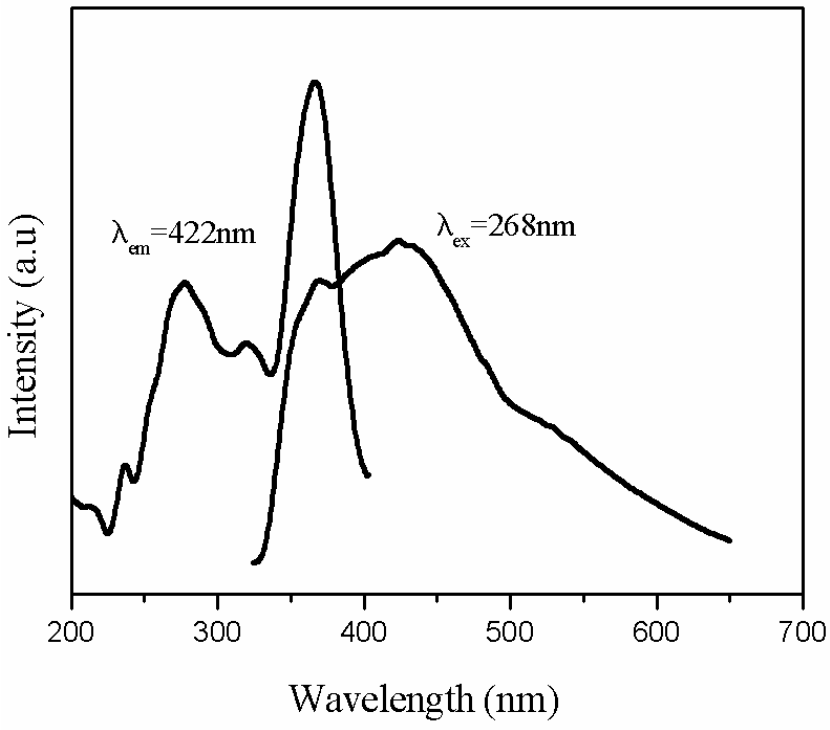
(c)

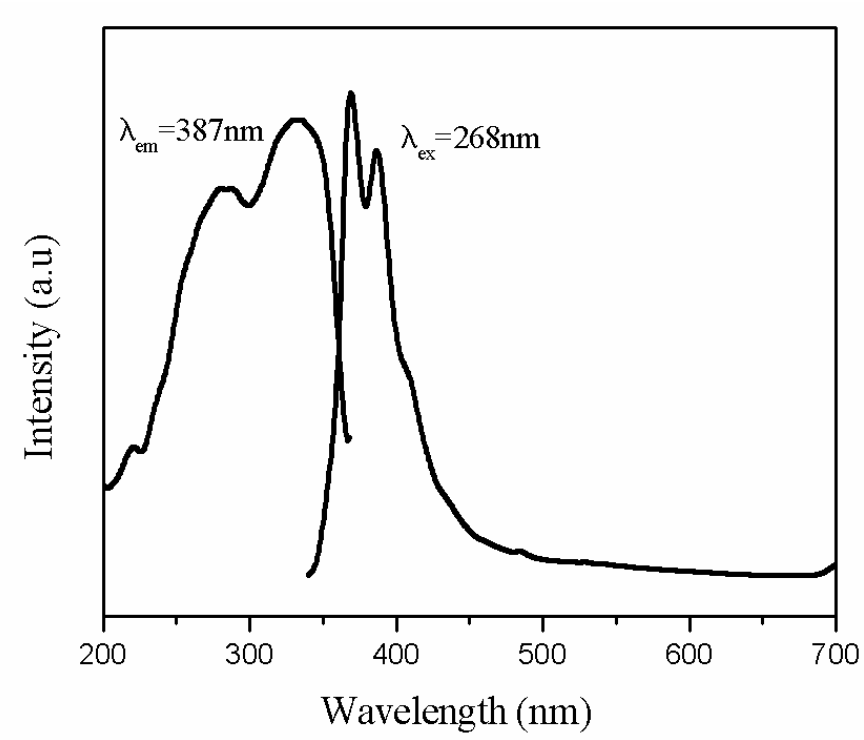
Fig. S2: Photoluminescence spectra of (a) **I**, (b) **II**, (c) **III**, (d) **IV**, (e) **V**, (f) **VI**, (g) **VII**, (h) **VIII** and (i) **IX**

(a)

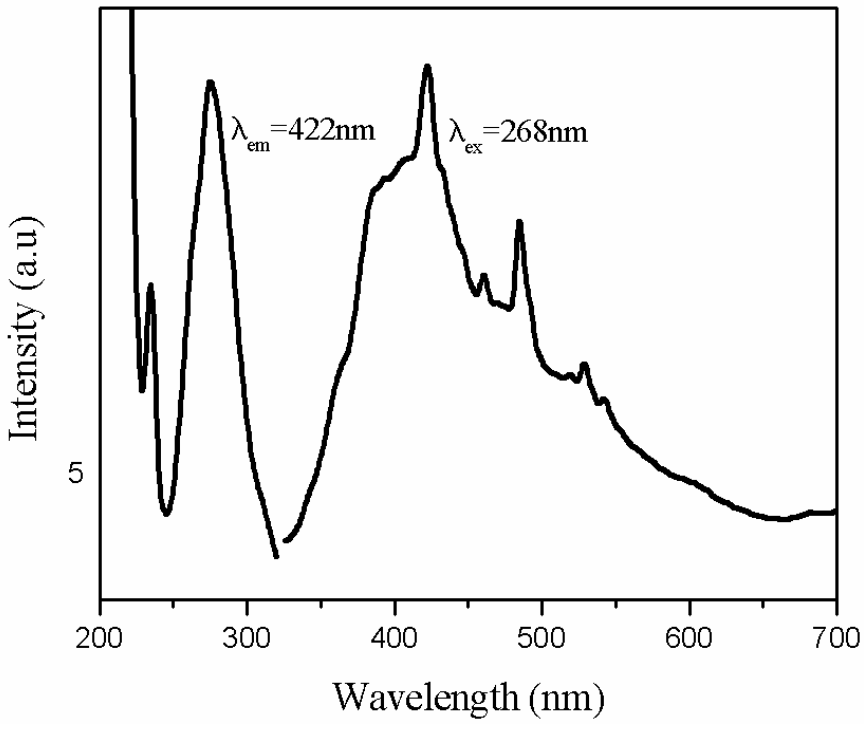


(b)

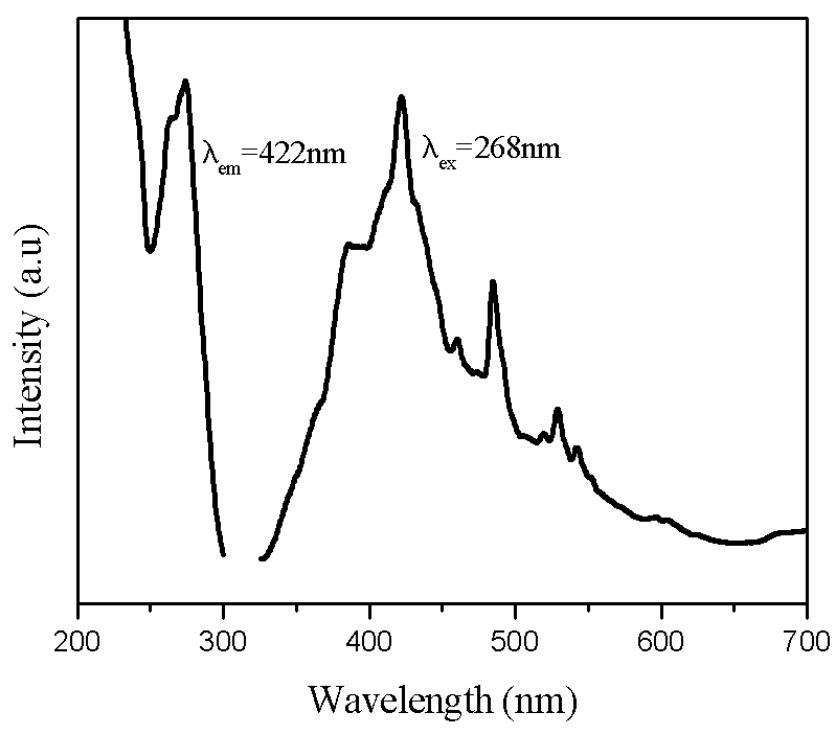



λem=387nm
λex=268nm
Intensity (a.u)
200
300
400
500
600
700
Wavelength (nm)

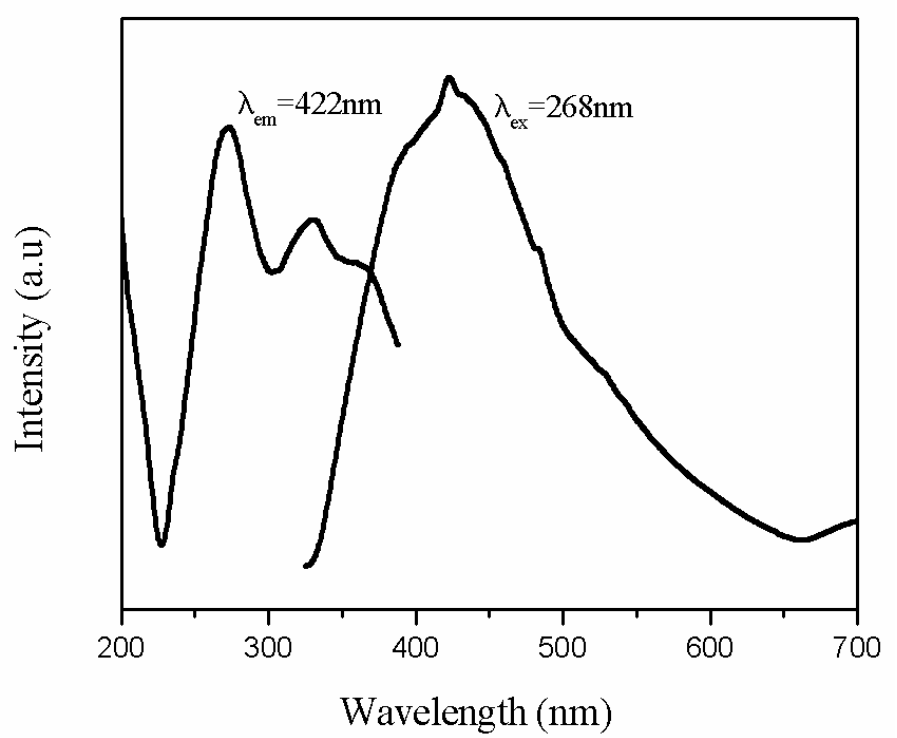
(c)


λem=422nm
λex=268nm
Intensity (a.u)
5
200
300
400
500
600
700
Wavelength (nm)

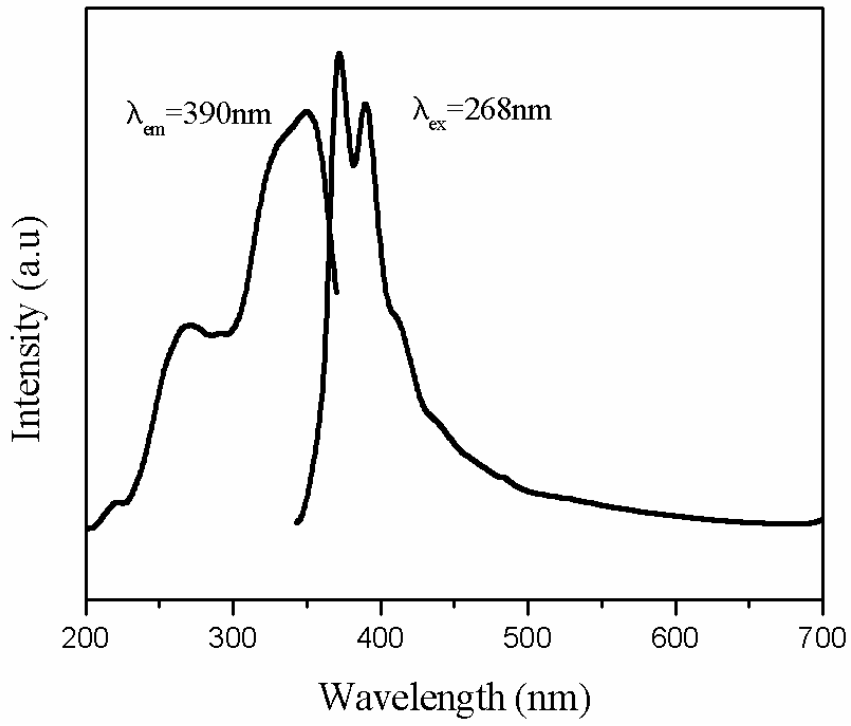
(d)


λem=422nm
λex=268nm
Intensity (a.u)
200
300
400
500
600
700
Wavelength (nm)

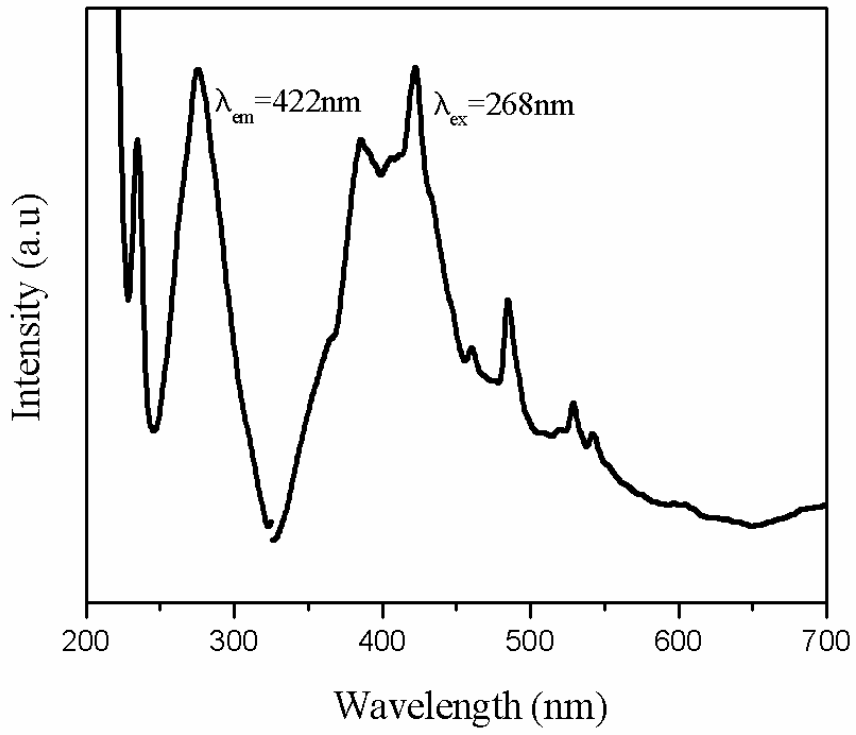
(e)


λem=422nm
λex=268nm
Intensity (a.u)
200
300
400
500
600
700
Wavelength (nm)

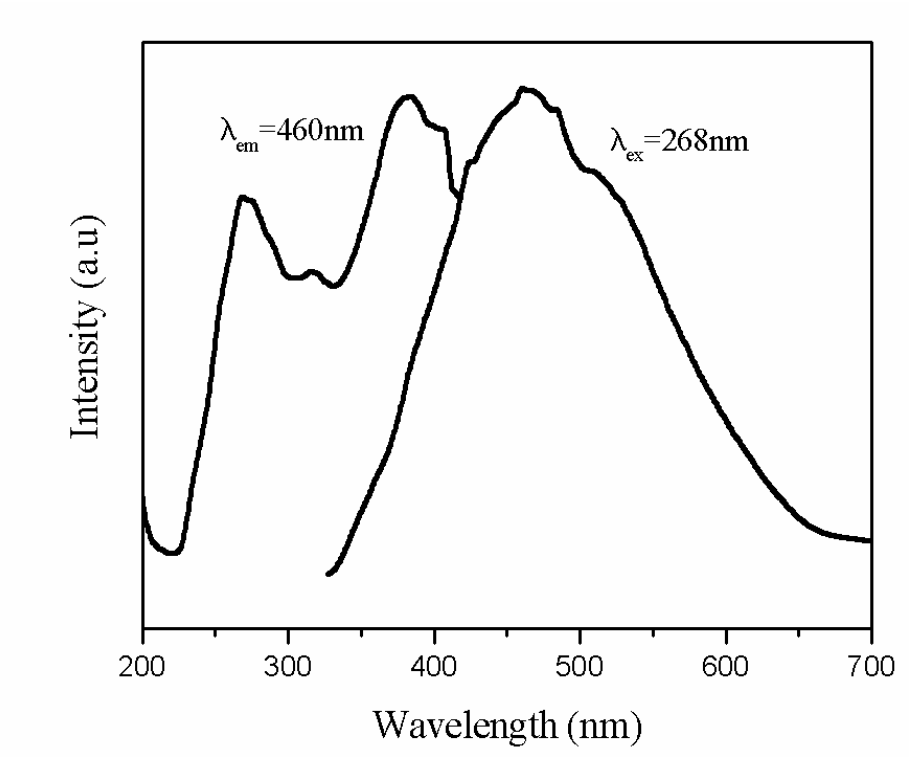
(f)


λem=390nm
λex=268nm
Intensity (a.u)
200
300
400
500
600
700
Wavelength (nm)

(g)


λem=422nm
λex=268nm
Intensity (a.u)
200
300
400
500
600
700
Wavelength (nm)

(h)


λem=460nm
λex=268nm
Intensity (a.u)
200
300
400
500
600
700
Wavelength (nm)

(i)