Synthesis, Structure, Transformation Studies and Catalytic Properties of Open-Framework Cadmium Thiosulfate Compounds

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Table S1: Important bond distances and angles observed in $[Na_2(H_2O)_8][Cd(C_{10}H_8N_2)(S_2O_3)_2].2H_2O$, **I.**

Bond	Distance, Å	Bond	Distance, Å
Cd(1)-N(1)	2.263(7)	O(7)-Na(2)#1	2.396(10)
Cd(1)-N(2)	2.307(5)	O(8)-Na(2)#1	2.392(9)
Cd(1)-S(2B)	2.416(5)	O(6)-S(4)	1.450(5)
Cd(1)-S(1A)	2.480(3)	S(1B)-O(2B)	2.135(12)
Cd(1)-S(1B)	2.496(5)	O(1)-S(3)	1.456(5)
Cd(1)-S(2A)	2.527(3)	S(3)-O(3A)	1.417(9)
Na(1)-O(8)	2.391(10)	S(3)-O(3B)	1.439(8)
Na(1)-O(7)	2.393(10)	S(3)-O(2A)	1.485(10)
Na(1)-O(10)	2.399(10)	S(3)-O(2B)	1.510(8)
Na(1)-O(9)	2.425(10)	S(2A)-O(5A)	1.79(2)
Na(1)-O(12)	2.462(8)	S(2B)-O(5B)	2.008(12)
Na(1)-O(11)	2.471(11)	S(4)-O(4B)	1.421(7)
Na(2)-O(10)	2.366(9)	S(4)-O(4A)	1.448(9)
Na(2)-O(14)	2.368(11)	S(4)-O(5A)	1.486(9)
Na(2)-O(8)#2	2.392(9)	S(4)-O(5B)	1.508(8)
Na(2)-O(7)#2	2.396(10)	S(3)-S(1A)	1.984(3)
Na(2)-O(9)	2.403(9)	S(3)-S(1B)	2.028(5)
Na(2)-O(13)	2.417(10)	S(4)-S(2B)	1.934(5)
S(1A)-O(2A)	1.80(3)	S(4)-S(2A)	2.021(4)

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

Angle	Amplitude, deg	Angle	Amplitude, deg
N(1)-Cd(1)-N(2)	84.9(2)	O(3B)-S(3)-O(1)	115.2(6)
N(1)-Cd(1)-S(2B)	103.2(3)	O(3A)-S(3)-O(2A)	112.2(13)
N(2)-Cd(1)-S(2B)	124.2(2)	O(3B)-S(3)-O(2A)	67.5(11)
N(1)-Cd(1)-S(1A)	127.3(3)	O(1)-S(3)-O(2A)	91.0(12)
N(2)-Cd(1)-S(1A)	99.1(2)	O(3A)-S(3)-O(2B)	60.0(9)
S(2B)-Cd(1)-S(1A)	116.20(15)	O(3B)-S(3)-O(2B)	105.6(7)
N(1)-Cd(1)-S(1B)	107.0(3)	O(1)-S(3)-O(2B)	106.9(7)
N(2)-Cd(1)-S(1B)	125.3(2)	O(2A)-S(3)-O(2B)	161.9(11)
S(2B)-Cd(1)-S(1B)	105.13(16)	O(3A)-S(3)-S(1A)	127.0(8)
S(1A)-Cd(1)-S(1B)	31.78(14)	O(3B)-S(3)-S(1A)	109.9(5)
N(1)-Cd(1)-S(2A)	127.2(3)	O(1)-S(3)-S(1A)	109.6(3)
N(2)-Cd(1)-S(2A)	100.8(2)	O(2A)-S(3)-S(1A)	60.7(10)
S(2B)-Cd(1)-S(2A)	32.33(14)	O(2B)-S(3)-S(1A)	109.3(4)
S(1A)-Cd(1)-S(2A)	103.80(10)	O(3A)-S(3)-S(1B)	117.2(8)
S(1B)-Cd(1)-S(2A)	111.10(13)	O(3B)-S(3)-S(1B)	135.3(5)
O(8)-Na(1)-O(7)	86.6(3)	O(1)-S(3)-S(1B)	107.5(3)
O(8)-Na(1)-O(10)	94.4(3)	O(2A)-S(3)-S(1B)	100.1(10)
O(7)-Na(1)-O(10)	178.2(3)	O(2B)-S(3)-S(1B)	72.5(5)
O(8)-Na(1)-O(9)	167.8(3)	O(4B)-S(4)-O(4A)	43.7(8)
O(7)-Na(1)-O(9)	93.4(3)	O(4B)-S(4)-O(6)	113.3(5)
O(10)-Na(1)-O(9)	85.9(3)	O(4A)-S(4)-O(6)	123.8(8)
O(8)-Na(1)-O(12)	102.2(4)	O(4B)-S(4)-O(5A)	68.5(10)
O(7)-Na(1)-O(12)	95.1(4)	O(4A)-S(4)-O(5A)	111.1(11)
O(10)-Na(1)-O(12)	83.3(4)	O(6)-S(4)-O(5A)	88.2(9)

O(9)-Na(1)-O(12)	90.0(4)	O(4B)-S(4)-O(5B)	106.2(6)
O(8)-Na(1)-O(11)	81.9(5)	O(4A)-S(4)-O(5B)	62.6(8)
O(7)-Na(1)-O(11)	93.5(5)	O(6)-S(4)-O(5B)	109.5(6)
O(10)-Na(1)-O(11)	88.1(5)	O(5A)-S(4)-O(5B)	161.9(9)
O(9)-Na(1)-O(11)	85.9(5)	O(4B)-S(4)-S(2B)	132.1(4)
O(12)-Na(1)-O(11)	170.7(6)	O(4A)-S(4)-S(2B)	114.7(7)
O(10)-Na(2)-O(14)	82.1(4)	O(6)-S(4)-S(2B)	112.6(3)
O(10)-Na(2)-O(8)#2	94.3(3)	O(5A)-S(4)-S(2B)	100.0(8)
O(14)-Na(2)-O(8)#2	89.8(5)	O(5B)-S(4)-S(2B)	70.1(5)
O(10)-Na(2)-O(7)#2	170.3(3)	O(4B)-S(4)-S(2A)	110.6(5)
O(14)-Na(2)-O(7)#2	88.2(5)	O(4A)-S(4)-S(2A)	128.0(7)
O(8)#2-Na(2)-O(7)#2	86.5(4)	O(6)-S(4)-S(2A)	107.5(3)
O(10)-Na(2)-O(9)	87.1(4)	O(5A)-S(4)-S(2A)	59.3(8)
O(14)-Na(2)-O(9)	94.5(5)	O(5B)-S(4)-S(2A)	109.7(4)
O(8)#2-Na(2)-O(9)	175.6(3)	S(1B)-S(1A)-O(2A)	117.5(5)
O(7)#2-Na(2)-O(9)	92.8(3)	S(1B)-S(1A)-S(3)	71.9(3)
O(10)-Na(2)-O(13)	101.0(4)	O(2A)-S(1A)-S(3)	45.9(4)
O(14)-Na(2)-O(13)	170.3(5)	S(1A)-S(1B)-O(2B)	107.9(4)
O(8)#2-Na(2)-O(13)	80.8(4)	S(3)-S(1B)-O(2B)	42.4(2)
O(7)#2-Na(2)-O(13)	88.7(4)	S(2B)-S(2A)-O(5A)	111.6(5)
O(9)-Na(2)-O(13)	94.8(4)	O(5A)-S(2A)-S(4)	45.4(3)
O(3A)-S(3)-O(3B)	45.8(8)	S(2A)-S(2B)-O(5B)	116.5(5)
O(3A)-S(3)-O(1)	123.3(8)	S(4)-S(2B)-O(5B)	44.9(3)

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

Table S2: Important bond distances and angles observed in

$[Cd_2(C_{10}H_8N_2)_2(HS_2O_3)_2(S_2O_3)_2][(C_{10}H_9N_2)_2(C_{10}H_8N_2)_2].8H_2O$, **II.**

Bond	Distance, Å	Bond	Distance, Å
Cd(1)-N(1)	2.357(4)	S(1)-S(3)	2.029(2)
Cd(1)-N(1)#1	2.357(4)	S(2)-S(4)	2.030(3)
Cd(1)-S(1)	2.4801(16)	S(3)-O(3)	1.414(6)
Cd(1)-S(1)#1	2.4801(16)	S(3)-O(1)	1.441(5)
Cd(2)-N(2)	2.334(4)	S(3)-O(2)	1.491(7)
Cd(2)-N(2)#2	2.334(4)	S(4)-O(5)	1.354(6)
Cd(2)-S(2)#2	2.4922(17)	S(4)-O(6)	1.465(6)
Cd(2)-S(2)	2.4922(17)	S(4)-O(4)	1.619(9)

Angle	Amplitude, deg	Angle	Amplitude, deg
N(1)-Cd(1)-N(1)#1	94.0(2)	O(3)-S(3)-O(1)	114.6(5)
N(1)-Cd(1)-S(1)	112.58(13)	O(3)-S(3)-O(2)	109.9(5)
N(1)#1-Cd(1)-S(1)	91.91(12)	O(1)-S(3)-O(2)	110.8(4)
N(1)-Cd(1)-S(1)#1	91.91(12)	O(3)-S(3)-S(1)	107.5(3)
N(1)#1-Cd(1)-S(1)#1	112.58(13)	O(1)-S(3)-S(1)	106.2(2)
S(1)-Cd(1)-S(1)#1	144.37(10)	O(2)-S(3)-S(1)	107.5(3)
N(2)-Cd(2)-N(2)#2	94.5(2)	O(5)-S(4)-O(6)	117.8(5)
N(2)-Cd(2)-S(2)#2	110.86(12)	O(5)-S(4)-O(4)	104.5(6)
N(2)#2-Cd(2)-S(2)#2	94.57(12)	O(6)-S(4)-O(4)	110.7(5)
N(2)-Cd(2)-S(2)	94.57(12)	O(5)-S(4)-S(2)	111.2(3)
N(2)#2-Cd(2)-S(2)	110.86(12)	O(6)-S(4)-S(2)	105.1(3)
S(2)#2-Cd(2)-S(2)	142.55(10)	O(4)-S(4)-S(2)	107.1(5)

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

Table S3: Important bond distances and angles observed in $[Cd(C_{10}H_8N_2)(H_2O)_2(S_2O_3)].2H_2O$, **III.**

Bond	Distance, Å	Bond	Distance, Å
Cd(1)-N(1)	2.322(3)	S(1)-Cd(1)#2	2.6439(11)
Cd(1)-N(2)	2.325(3)	S(1)-S(2)	2.0160(13)
Cd(1)-O(1)	2.334(3)	O(3)-S(2)	1.461(3)
Cd(1)-O(2)	2.342(3)	O(4)-S(2)	1.450(4)
Cd(1)-O(3)	2.374(3)	O(5)-S(2)	1.423(4)
Cd(1)-S(1)#1	2.6439(11)		

Angle	Amplitude, deg	Angle	Amplitude, deg
N(1)-Cd(1)-N(2)	176.60(11)	N(2)-Cd(1)-S(1)#1	90.50(8)
N(1)-Cd(1)-O(1)	90.02(11)	O(1)-Cd(1)-S(1)#1	95.66(8)
N(2)-Cd(1)-O(1)	86.80(11)	O(2)-Cd(1)-S(1)#1	173.75(9)
N(1)-Cd(1)-O(2)	84.50(12)	O(3)-Cd(1)-S(1)#1	108.15(8)
N(2)-Cd(1)-O(2)	93.75(12)	O(3)-S(2)-S(1)	107.81(12)
O(1)-Cd(1)-O(2)	80.02(11)	O(4)-S(2)-S(1)	111.34(17)
N(1)-Cd(1)-O(3)	93.03(10)	O(4)-S(2)-O(3)	108.0(2)
N(2)-Cd(1)-O(3)	89.38(10)	O(5)-S(2)-S(1)	107.7(2)
O(1)-Cd(1)-O(3)	155.92(11)	O(5)-S(2)-O(4)	110.4(4)
O(2)-Cd(1)-O(3)	76.51(11)	O(5)-S(2)-O(3)	111.5(3)
N(1)-Cd(1)-S(1)#1	91.02(8)		

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

Table S4: Important bond distances and angles observed in $[Cd_2(C_{10}H_8N_2)_3(S_2O_3)_2]$, **IV.**

Bond	Distance, Å	Bond	Distance, Å
Cd(1)-O(1)#1	2.307(2)	Cd(2)-S(1)#4	2.5243(10)
Cd(1)-O(1)#2	2.307(2)	Cd(2)-S(1)	2.5243(9)
Cd(1)-N(1)#3	2.352(2)	O(1)-Cd(1)#2	2.307(2)
Cd(1)-N(1)	2.352(2)	S(1)-S(2)	2.0436(12)
Cd(1)-N(2)	2.392(2)	O(1)-S(2)	1.466(3)
Cd(1)-N(2)#3	2.392(2)	O(2)-S(2)	1.442(2)
Cd(2)-N(3)	2.312(2)	O(3)-S(2)	1.456(2)
Cd(2)-N(3)#4	2.312(2)		

Angle	Amplitude, deg	Angle	Amplitude, deg
O(1)#1-Cd(1)-O(1)#2	177.26(12)	N(2)-Cd(1)-N(2)#3	80.69(12)
O(1)#1-Cd(1)-N(1)#3	98.74(9)	N(3)-Cd(2)-N(3)#4	107.15(13)
O(1)#2-Cd(1)-N(1)#3	79.39(8)	N(3)-Cd(2)-S(1)#4	110.65(7)
O(1)#1-Cd(1)-N(1)	79.39(8)	N(3)#4-Cd(2)-S(1)#4	112.28(7)
O(1)#2-Cd(1)-N(1)	98.74(9)	N(3)-Cd(2)-S(1)	112.28(7)
N(1)#3-Cd(1)-N(1)	95.08(12)	N(3)#4-Cd(2)-S(1)	110.65(7)
O(1)#1-Cd(1)-N(2)	92.10(9)	S(1)#4-Cd(2)-S(1)	103.92(4)
O(1)#2-Cd(1)-N(2)	89.99(9)	O(2)-S(2)-O(3)	112.87(15)
N(1)#3-Cd(1)-N(2)	167.50(8)	O(2)-S(2)-O(1)	112.03(16)
N(1)-Cd(1)-N(2)	93.02(9)	O(3)-S(2)-O(1)	109.77(14)
O(1)#1-Cd(1)-N(2)#3	89.99(9)	O(2)-S(2)-S(1)	108.17(12)
O(1)#2-Cd(1)-N(2)#3	92.10(9)	O(3)-S(2)-S(1)	105.61(10)
N(1)#3-Cd(1)-N(2)#3	93.02(9)	O(1)-S(2)-S(1)	108.05(11)
N(1)-Cd(1)-N(2)#3	167.50(8)		

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2, -y+3/2, z-1/2; #2 -x+1/2, -y+3/2, -z+1; #3 -x+1, y, -z+1/2; #4 -x+1, y, -z+3/2.

Table S5: Important bond distances and angles observed in $[Cd_4(C_{10}H_8N_2)_5(S_2O_3)_4]$, **V.**

Bond	Distance, Å	Bond	Distance, Å
Cd(1)-N(1)	2.280(3)	S(1)-S(2)	2.0745(12)
Cd(1)-N(2)	2.361(3)	S(4)-S(3)	2.0459(13)
Cd(1)-S(3)	2.4398(11)	S(2)-O(1)	1.458(3)
Cd(1)-S(1)	2.5422(10)	S(2)-O(3)	1.434(3)
Cd(2)-N(3)	2.299(3)	S(2)-O(4)	1.444(2)
Cd(2)-N(4)	2.305(2)	S(4)-O(2)#1	1.464(3)
Cd(2)-O(1)	2.318(3)	S(4)-O(5)	1.422(3)
Cd(2)-O(2)	2.334(3)	S(4)-O(6)	1.438(3)
Cd(2)-N(5)	2.361(3)	O(2)-S(4)#2	1.464(3)

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

Angle	Amplitude, deg	Angle	Amplitude, deg
N(1)-Cd(1)-N(2)	91.04(10)	N(4)-Cd(2)-S(1)	91.89(7)
N(1)-Cd(1)-S(3)	121.66(8)	O(1)-Cd(2)-S(1)	61.73(7)
N(2)-Cd(1)-S(3)	107.88(8)	O(2)-Cd(2)-S(1)	136.26(6)
N(1)-Cd(1)-S(1)	113.54(8)	N(5)-Cd(2)-S(1)	90.21(7)
N(2)-Cd(1)-S(1)	93.97(7)	O(3)-S(2)-O(4)	113.38(16)
S(3)-Cd(1)-S(1)	119.21(3)	O(3)-S(2)-O(1)	111.87(17)
N(3)-Cd(2)-N(4)	173.59(10)	O(4)-S(2)-O(1)	112.52(17)
N(3)-Cd(2)-O(1)	89.89(10)	O(3)-S(2)-S(1)	109.42(13)
N(4)-Cd(2)-O(1)	95.48(10)	O(4)-S(2)-S(1)	105.30(11)
N(3)-Cd(2)-O(2)	93.15(9)	O(1)-S(2)-S(1)	103.63(11)
N(4)-Cd(2)-O(2)	84.88(9)	O(5)-S(4)-O(6)	113.2(2)
O(1)-Cd(2)-O(2)	75.15(9)	O(5)-S(4)-O(2)#1	111.89(19)
N(3)-Cd(2)-N(5)	88.90(9)	O(6)-S(4)-O(2)#1	108.94(18)
N(4)-Cd(2)-N(5)	88.01(9)	O(5)-S(4)-S(3)	108.25(14)
O(1)-Cd(2)-N(5)	151.78(9)	O(6)-S(4)-S(3)	109.04(14)
O(2)-Cd(2)-N(5)	133.07(9)	O(2)#1-S(4)-S(3)	105.13(11)
N(3)-Cd(2)-S(1)	93.74(8)		

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

Table S6: Important bond distances and angles observed in $[Cd_2(C_{10}H_8N_2)_2(H_2O)_3(SO_4)_2].2H_2O$, **VI.**

Bond	Distance, Å	Bond	Distance, Å
Cd(1)-N(1)	2.273(5)	Cd(2)-O(7)	2.355(7)
Cd(1)-N(2)	2.289(5)	Cd(2)-O(8)	2.383(7)
Cd(2)-N(3)#1	2.295(5)	O(6)-Cd(2)#7	2.329(5)
Cd(2)-N(4)#2	2.320(5)	S(1)-O(2)	1.486(7)
N(3)-Cd(2)#5	2.295(5)	S(1)-O(5)	1.449(6)
N(4)-Cd(2)#2	2.320(5)	S(1)-O(9)	1.427(8)
Cd(1)-O(1)	2.356(6)	S(1)-O(10)	1.433(6)
Cd(1)-O(2)	2.364(7)	S(2)-O(3)	1.510(5)
Cd(1)-O(3)	2.407(5)	S(2)-O(4)#4	1.466(6)
Cd(1)-O(4)	2.509(5)	S(2)-O(6)	1.483(5)
Cd(2)-O(5)	2.279(6)	S(2)-O(11)	1.454(5)
Cd(2)-O(6)#3	2.329(5)	O(4)-S(2)#6	1.466(6)

Angle	Amplitude, deg	Angle	Amplitude, deg
N(1)-Cd(1)-N(2)	173.8(2)	O(5)-Cd(2)-O(7)	83.3(3)
N(1)-Cd(1)-O(1)	102.47(19)	N(3)#1-Cd(2)-O(7)	84.2(2)
N(2)-Cd(1)-O(1)	82.9(2)	N(4)#2-Cd(2)-O(7)	89.4(2)
N(1)-Cd(1)-O(2)	90.3(2)	O(6)#3-Cd(2)-O(7)	175.8(2)
N(2)-Cd(1)-O(2)	87.1(2)	O(5)-Cd(2)-O(8)	174.6(4)
O(1)-Cd(1)-O(2)	142.6(2)	N(3)#1-Cd(2)-O(8)	87.8(2)
N(1)-Cd(1)-O(3)	88.79(18)	N(4)#2-Cd(2)-O(8)	91.2(2)
N(2)-Cd(1)-O(3)	88.57(18)	O(6)#3-Cd(2)-O(8)	86.7(3)
O(1)-Cd(1)-O(3)	85.00(19)	O(7)-Cd(2)-O(8)	91.3(3)
O(2)-Cd(1)-O(3)	130.8(2)	O(9)-S(1)-O(10)	114.2(5)
N(1)-Cd(1)-O(4)	86.14(18)	O(9)-S(1)-O(5)	110.8(4)
N(2)-Cd(1)-O(4)	98.4(2)	O(10)-S(1)-O(5)	111.5(4)
O(1)-Cd(1)-O(4)	74.71(18)	O(9)-S(1)-O(2)	103.1(6)
O(2)-Cd(1)-O(4)	71.2(2)	O(10)-S(1)-O(2)	107.2(4)
O(3)-Cd(1)-O(4)	157.45(18)	O(5)-S(1)-O(2)	109.5(5)
O(5)-Cd(2)-N(3)#1	92.4(2)	O(11)-S(2)-O(4)#4	111.1(4)
O(5)-Cd(2)-N(4)#2	88.0(2)	O(11)-S(2)-O(6)	110.7(4
N(3)#1-Cd(2)-N(4)#2	173.6(2)	O(4)#4-S(2)-O(6)	107.5(3)
O(5)-Cd(2)-O(6)#3	98.7(3)	O(11)-S(2)-O(3)	110.7(4)
N(3)#1-Cd(2)-O(6)#3	92.0(2)	O(4)#4-S(2)-O(3)	109.8(3)
N(4)#2-Cd(2)-O(6)#3	94.3(2)	O(6)-S(2)-O(3)	107.0(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x, y+1, -z; #2 -x+1, y, -z+1; #3 x, y+1, z; #4 -x+1/2, y-1/2, -z; #5 -x, y-1, -z;
#6 -x+1/2, y+1/2, -z; #7 x, y-1, z.

Table S7: Important bond distances and angles observed in $[Cd(C_{10}H_8N_2)(SO_4)]$, **VII.**

Bond	Distance, Å	Bond	Distance, Å
Cd(1)-O(1)#1	2.289(5)	Cd(1)-N(2)	2.394(8)
Cd(1)-O(1)	2.289(5)	O(1)-S(1)	1.440(4)
Cd(1)-O(1)#2	2.289(5)	S(1)-O(1)#6	1.440(4)
Cd(1)-O(1)#3	2.289(5)	S(1)-O(1)#7	1.440(4)
Cd(1)-N(1)	2.350(8)	S(1)-O(1)#8	1.440(4)

Angle	Amplitude, deg	Angle	Amplitude, deg
O(1)#1-Cd(1)-O(1)	83.5(6)	O(1)-Cd(1)-N(2)	80.40(9)
O(1)#1-Cd(1)-O(1)#2	160.80(18)	O(1)#2-Cd(1)-N(2)	80.40(9)
O(1)-Cd(1)-O(1)#2	93.3(6)	O(1)#3-Cd(1)-N(2)	80.40(9)
O(1)#1-Cd(1)-O(1)#3	93.3(6)	N(1)-Cd(1)-N(2)	180.000(1)
O(1)-Cd(1)-O(1)#3	160.80(18)	O(1)#6-S(1)-O(1)#7	110.52(16)
O(1)#2-Cd(1)-O(1)#3	83.5(6)	O(1)#6-S(1)-O(1)	107.4(3)
O(1)#1-Cd(1)-N(1)	99.60(9)	O(1)#7-S(1)-O(1)	110.52(16)
O(1)-Cd(1)-N(1)	99.60(9)	O(1)#6-S(1)-O(1)#8	110.52(16)
O(1)#2-Cd(1)-N(1)	99.60(9)	O(1)#7-S(1)-O(1)#8	107.4(3)
O(1)#3-Cd(1)-N(1)	99.60(9)	O(1)-S(1)-O(1)#8	110.52(16)
O(1)#1-Cd(1)-N(2)	80.40(9)		

Symmetry transformations used to generate equivalent atoms:
#1 y+1/2, x-1/2, z; #2 -y+1/2, -x+1/2, z; #3 -x+1, -y, z; #6 -x+1, -y-1, z; #7 y+1, -x, -z+1;
#8 -y, x-1, -z+1.

Table S8: Important hydrogen bond interactions observed in $[Na_2(H_2O)_8][Cd(C_{10}H_8N_2)(S_2O_3)_2].2H_2O$, **I;** $[Cd_2(C_{10}H_8N_2)_2(HS_2O_3)_2(S_2O_3)_2][(C_{10}H_9N_2)_2(C_{10}H_8N_2)_2].8H_2O$, **II;** and $[Cd(C_{10}H_8N_2)(H_2O)_2(S_2O_3)].2H_2O$, **III.**

D - H…A	D - H (Å)	H…A (Å)	D…A (Å)	D-H…A (°)
Compound **I**				
C(4) – H(4)…O(2B)	0.93	2.56	3.394(14)	150
C(7) – H(7)…O(3B)	0.93	2.17	2.961(16)	142
Compound **II**				
N(4) – H(4B)…N(5)	0.86	1.88	2.736(8)	175
C(4) – H(4)…O(5)	0.93	2.35	3.239(10)	160
C(9C) – H(9)…O(2)	0.93	2.43	3.293(10)	155
C(15) – H(15)…O(4)	0.93	2.55	3.453(14)	164
C(17) – H(17)…O(2)	0.93	2.46	3.353(9)	162
C(18) – H(18)…O(200)	0.93	2.55	3.444(8)	161
C(21) – H(21)…O(1)	0.93	2.42	3.291(9)	157
C(30) – H(30)…O(5)	0.93	2.40	3.324(10)	173
Compound **III**				
O(1) – H(1A)…O(3)	0.94	1.92	2.852(4)	170
O(1) – H(1B)…O(4) intra	0.95	1.75	2.678(5)	166
O(2) – H(2B)…O(100)	0.95	1.76	2.704(7)	172
O(100) – H(101)…O(200)	0.81	2.12	2.811(10)	143

Table S9. Experimental conditions employed for the study of the transformation reactions.

Transformation of I

S. No	Composition	Temp (°C)	Time (h)	Product
1	**I** + H_2O	30	6	**I**
2	**I** + H_2O	30	12	**I** + **III**
3	**I** + H_2O	30	24	**I** + **III**
4	**I** + H_2O	30	36	**I** + **III**
5	**I** + H_2O	30	48	**I** + **III**
6	**I** + H_2O	30	60	**III**
7	**I** + H_2O	45	6	**I** + **III**
8	**I** + H_2O	45	12	**III**
9	**I** + H_2O	45	24	**III**
10	**I** + H_2O	45	36	**III**
11	**I** + H_2O	45	48	**III**
12	**I** + H_2O	45	60	**III**
13	**I** + H_2O	60	6	**III**
14	**I** + H_2O	60	12	**III** + **V**
15	**I** + H_2O	60	24	**III** + **V**
16	**I** + H_2O	60	36	**III** + **V**
17	**I** + H_2O	60	48	**V**
18	**I** + H_2O	60	60	**V**
19	0.25**I** + 55H_2O + 22EtOH	30	6	**I** + **III**
20	0.25**I** + 55H_2O + 22EtOH	30	12	**I** + **III**
21	0.25**I** + 55H_2O + 22EtOH	30	24	**III**
22	0.25**I** + 55H_2O + 22EtOH	30	36	**III**
23	0.25**I** + 55H_2O + 22EtOH	30	48	**III**
24	0.25**I** + 55H_2O + 22EtOH	30	60	**III**
25	0.25**I** + 55H_2O + 22EtOH	45	6	**III**
26	0.25**I** + 55H_2O + 22EtOH	45	12	**III**
27	0.25**I** + 55H_2O + 22EtOH	45	24	**III**
28	0.25**I** + 55H_2O + 22EtOH	45	36	**III** + **V**
29	0.25**I** + 55H_2O + 22EtOH	45	48	**V**
30	0.25**I** + 55H_2O + 22EtOH	45	60	**V**
31	0.25**I** + 55H_2O + 22EtOH	60	6	**V**

32	0.25**I** + 55H_2O + 22EtOH	60	12	**V**
33	0.25**I** + 55H_2O + 22EtOH	60	24	**V**
34	0.25**I** + 55H_2O + 22EtOH	60	36	**V** + **VI**
35	0.25**I** + 55H_2O + 22EtOH	60	48	**V** + **VI**
36	0.25**I** + 55H_2O + 22EtOH	60	60	**V** + **VI**

Table S10. Experimental conditions employed for the study of the transformation reactions.

Transformation of III

S. No	Composition	Temp (°C)	Time (h)	Product
1	**III** + H_2O	30	6	**III**
2	**III** + H_2O	30	12	**III**
3	**III** + H_2O	30	24	**III**
4	**III** + H_2O	30	36	**III**
5	**III** + H_2O	30	48	**III**
6	**III** + H_2O	30	60	**III**
7	**III** + H_2O	45	6	**III**
8	**III** + H_2O	45	12	**III**
9	**III** + H_2O	45	24	**III**
10	**III** + H_2O	45	36	**III**
11	**III** + H_2O	45	48	**III** + **V**
12	**III** + H_2O	45	60	**III** + **V**
13	**III** + H_2O	60	6	**III**
14	**III** + H_2O	60	12	**III** + **V**
15	**III** + H_2O	60	24	**III** + **V**
16	**III** + H_2O	60	36	**V**
17	**III** + H_2O	60	48	**V**
18	**III** + H_2O	60	60	**V**
19	0.33**III** + 55H_2O + 22EtOH	30	6	**III**
20	0.33**III** + 55H_2O + 22EtOH	30	12	**III**
21	0.33**III** + 55H_2O + 22EtOH	30	24	**III**
22	0.33**III** + 55H_2O + 22EtOH	30	36	**III**
23	0.33**III** + 55H_2O + 22EtOH	30	48	**III**
24	0.33**III** + 55H_2O + 22EtOH	30	60	**III**
25	0.33**III** + 55H_2O + 22EtOH	45	6	**III**
26	0.33**III** + 55H_2O + 22EtOH	45	12	**III** + **V**
27	0.33**III** + 55H_2O + 22EtOH	45	24	**III** + **V**
28	0.33**III** + 55H_2O + 22EtOH	45	36	**V**
29	0.33**III** + 55H_2O + 22EtOH	45	48	**V**
30	0.33**III** + 55H_2O + 22EtOH	45	60	**V**

31	0.33**III** + 55H_2O + 22EtOH	60	6	**V**
32	0.33**III** + 55H_2O + 22EtOH	60	12	**V**
33	0.33**III** + 55H_2O + 22EtOH	60	24	**V + VI**
34	0.33**III** + 55H_2O + 22EtOH	60	36	**V + VI**
35	0.33**III** + 55H_2O + 22EtOH	60	48	**V + VI**
36	0.33**III** + 55H_2O + 22EtOH	60	60	**V + VI**
37	1 **III** + 0.5 *bpy* +110 H_2O	30	60	**III**
38	1 **III** + 0.25 *bpy* +110 H_2O	30	60	**III**
39	1 **III** + 0.5 *bpy* +110 H_2O	45	4	**III**
40	1 **III** + 0.5 *bpy* +110 H_2O	45	8	**III + IV**
41	1 **III** + 0.5 *bpy* +110 H_2O	45	12	**III + IV**
42	1 **III** + 0.5 *bpy* +110 H_2O	45	20	**IV**
43	1 **III** + 0.25 *bpy* +110 H_2O	45	4	**III**
44	1 **III** + 0.25 *bpy* +110 H_2O	45	8	**III + IV + V**
45	1 **III** + 0.25 *bpy* +110 H_2O	45	12	**III + IV + V**
46	1 **III** + 0.25 *bpy* +110 H_2O	45	20	**III + IV + V**
47	1 **III** + 0.5 *bpy* +110 H_2O	60	4	**III + IV + V**
48	1 **III** + 0.5 *bpy* +110 H_2O	60	8	**III + IV + V**
49	1 **III** + 0.5 *bpy* +110 H_2O	60	12	**III + IV**
50	1 **III** + 0.5 *bpy* +110 H_2O	60	20	**III + IV**
51	1 **III** + 0.25 *bpy* +110 H_2O	60	4	**III + IV + V**
52	1 **III** + 0.25 *bpy* +110 H_2O	60	8	**III + IV + V**
53	1 **III** + 0.25 *bpy* +110 H_2O	60	12	**V**
54	1 **III** + 0.25 *bpy* +110 H_2O	60	20	**V**
55	**III** + EtOH	110	12	**CdS**
56	**III** + EtOH	110	24	**VII + CdS**
57	**III** + EtOH	110	36	**VII + CdS**
58	**III** + EtOH	110	48	**VII + CdS**

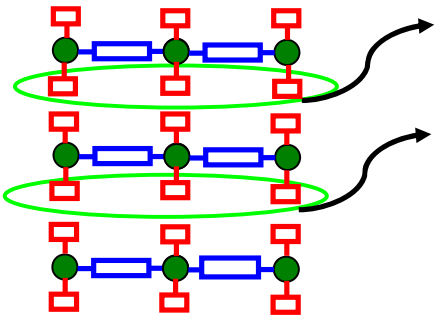
Table S11: The interpretation of the thermal studies (TGA) of compounds **I-VII**

Compounds	**Initial wt loss (%), (Temp range)**	**2nd wt loss (%), (Temp range)**	**Observed & calculated wt loss (%)**	**Calcined product (ICDD No:)**
I	15 % (30-100 ^{o}C) Loss of water	33 %(150-400 ^{o}C) Loss of water, *bpy* and part of the sulfur	48 % (obs), 51 % (cal)	$CdSO_4$ and Na_2SO_4 (14-0352 and 25-1111)
II	76 % (30-400 ^{o}C), Loss of water and *bpy*		76 % (obs), 76 % (cal)	$CdSO_4$ (14-0352)
III	8 % (30-100 ^{o}C) Loss of lattice water	49 % (150-400 ^{o}C) Loss of coordinated water and *bpy*	57 % (obs), 61 % (cal)	$CdSO_4$ and $Cd_3O_2SO_4$ (14-0352 and 32-0140)
IV	64 % (200-420 ^{o}C), Loss of *bpy*		64 % (obs), 63 % (cal)	$CdSO_4$ and $Cd_3O_2SO_4$ (14-0352 and 32-0140)
V	59 % (230-450 ^{o}C), Loss of *bpy*		59 % (obs), 60 % (cal)	$CdSO_4$ and $Cd_3O_2SO_4$ (14-0352 and 32-0140)
VI	12 % (30-125 ^{o}C) Loss of water	38 % (290-450 ^{o}C) Loss of water and *bpy*	50 % (obs), 49 % (cal)	$CdSO_4$ (86-1558)
VII	43 % (350-475 ^{o}C), Loss of *bpy*		43 % (obs), 43 % (cal)	$CdSO_4$ (86-1558)

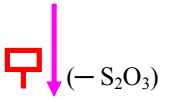
Table S12. The product obtained from the cyanosilylation reaction catalyzed by compound **III-VII**

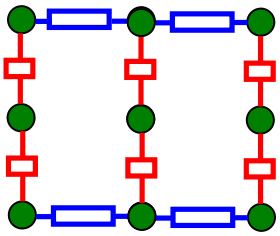
Catalyst (compound)	**Yield (%)**
III	**98**
IV	**40**
V	**40**
VI	**63**
VII	**60**

Scheme 1. Schematic showing a possible pathway for the transformation of **I** to **III** and **V** by the rearrangement of thiosulfate and *bpy* unit in a plane. Green spheres represent the Cd centers, red boxes represent the thiosulfate units and blue boxes represent the *bpy* units

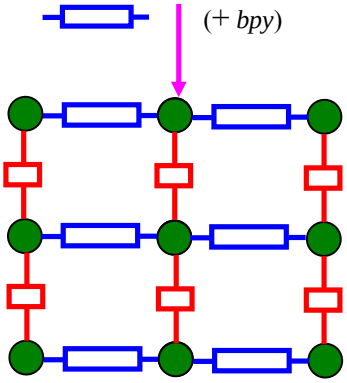


$[Na_2(H_2O)_8][Cd(C_{10}H_8N_2)(S_2O_3)_2].2H_2O$ (1D chain of **I**)





$[Cd(C_{10}H_8N_2)(H_2O)_2(S_2O_3)].2H_2O$ (2D layer of **III**)

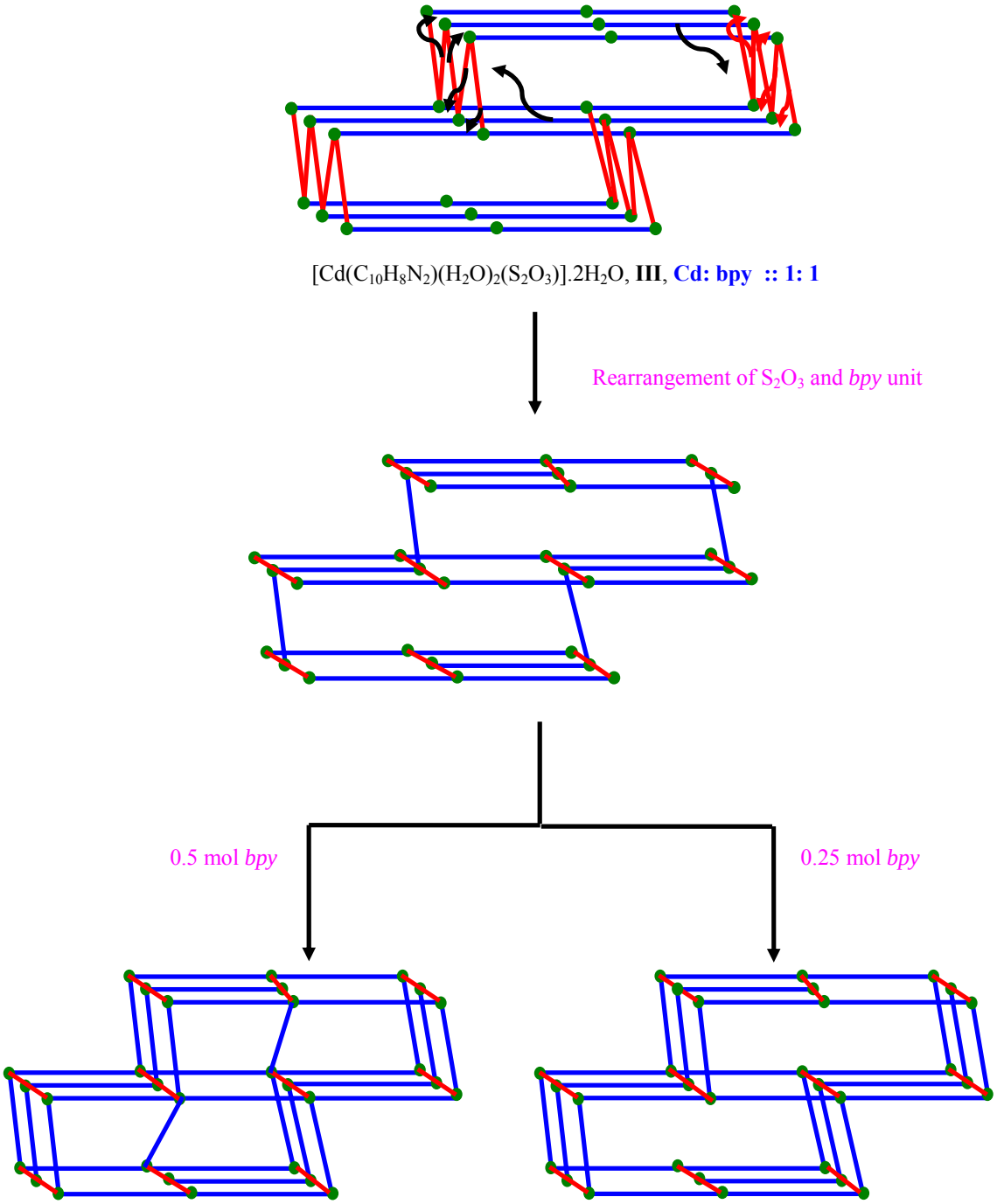


$Cd_4(C_{10}H_8N_2)_5(S_2O_3)_4]$ (2D layer of **V**)

$$[Na_2(H_2O)_8][Cd(C_{10}H_8N_2)(S_2O_3)_2].2H_2O + H_2O \xrightarrow[-[Na_2(H_2O)_8]]{-S_2O_3} [Cd(C_{10}H_8N_2)(H_2O)_2(S_2O_3)].2H_2O$$

$$[Cd(C_{10}H_8N_2)(H_2O)_2(S_2O_3)].2H_2O + C_{10}H_8N_2 \rightarrow [Cd_4(C_{10}H_8N_2)_5(S_2O_3)_4]$$

Scheme 2. Schematic showing a possible pathway for the transformation of **III** to **IV** and **V** by the rearrangement of thiosulfate and *bpy* unit. Green spheres represent the Cd centers, red lines represent the thiosulfate units and blue lines represent the *bpy* units.



$[Cd(C_{10}H_8N_2)(H_2O)_2(S_2O_3)].2H_2O$, **III**, **Cd: bpy :: 1: 1**

$[Cd_2(C_{10}H_8N_2)_3(S_2O_3)_2]$, **IV**, **Cd: bpy :: 1: 1.5**

$[Cd_4(C_{10}H_8N_2)_5(S_2O_3)_4]$, **V**, **Cd: bpy :: 1: 1.25**

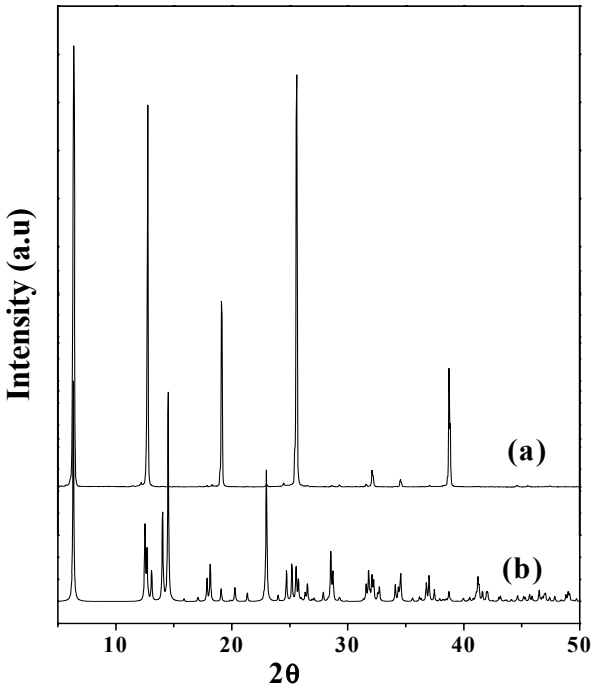


Fig. S1: Powder XRD (CuKα) pattern of **I**, (a) experimental and (b) simulated.

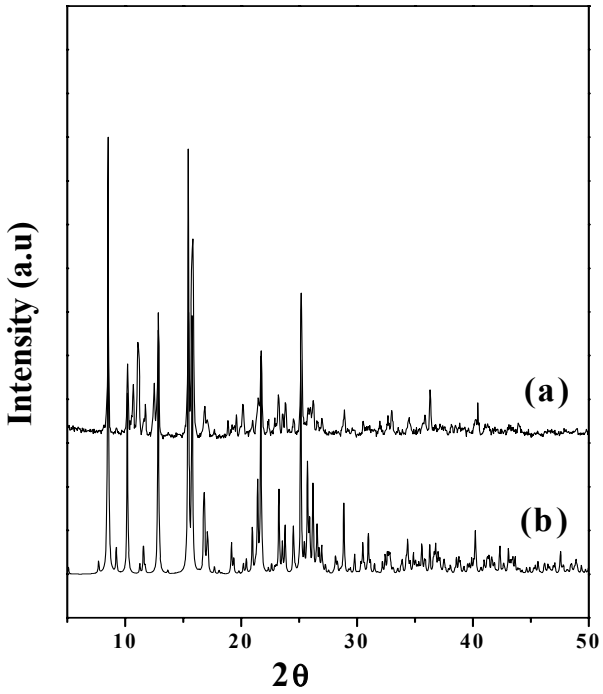


Fig. S2: Powder XRD (CuKα) pattern of **II**, (a) experimental and (b) simulated.

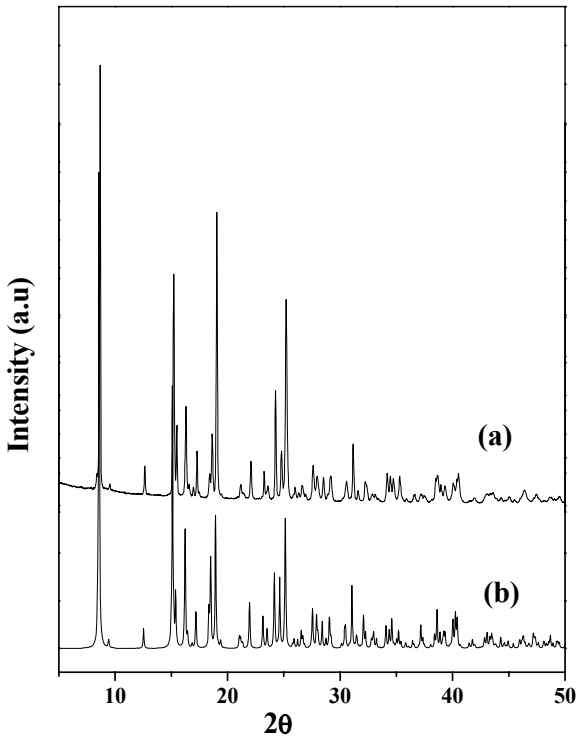


Fig. S3: Powder XRD (CuKα) pattern of **III**, (a) experimental and (b) simulated

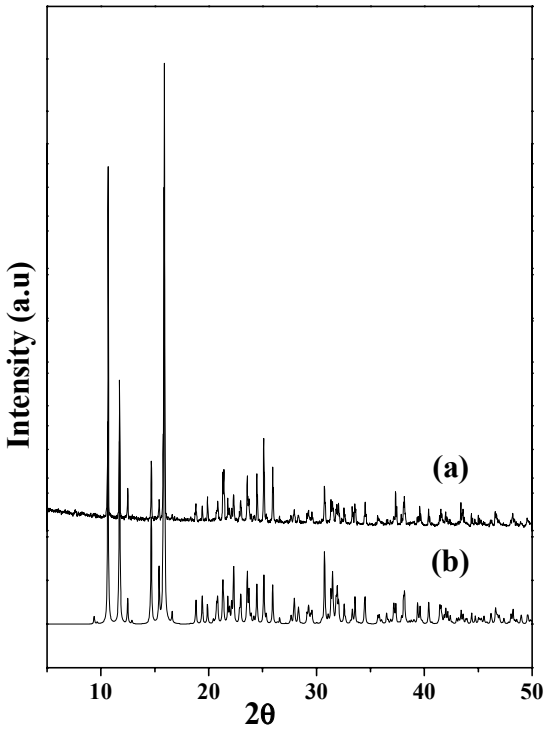


Fig. S4: Powder XRD (CuKα) pattern of **IV**, (a) experimental and (b) simulated.

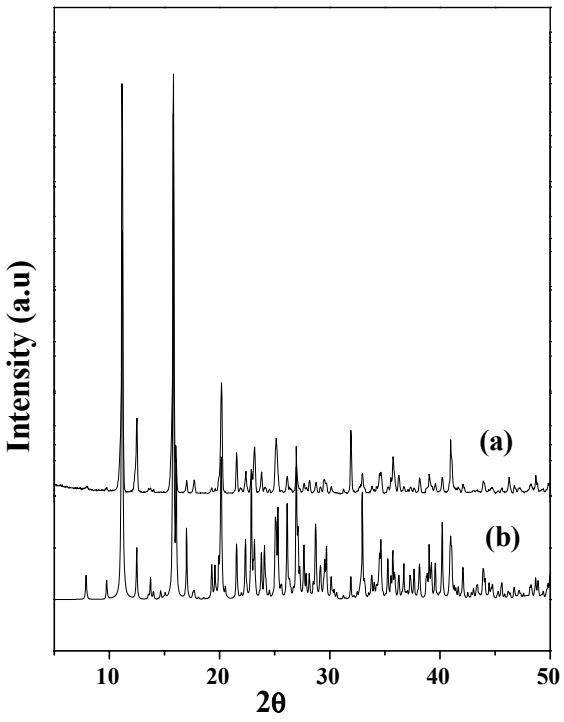


Fig. S5: Powder XRD (CuKα) pattern of **V**, (a) experimental and (b) simulated.

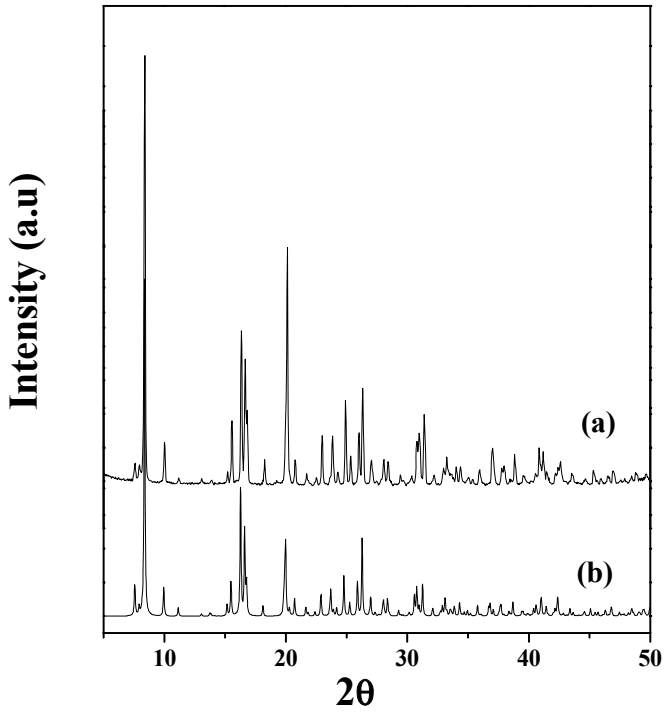


Fig. S6: Powder XRD (CuKα) pattern of **VI**, (a) experimental and (b) simulated.

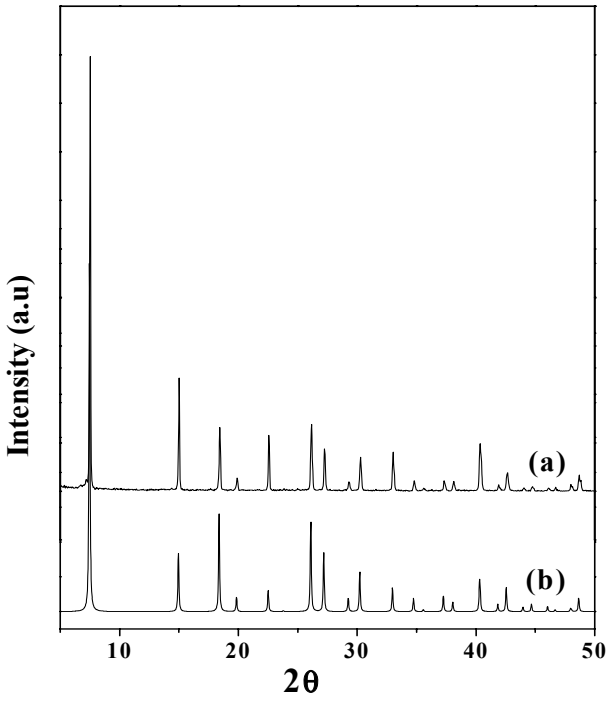


Fig. S7: Powder XRD (CuKα) pattern of **VII**, (a) experimental and (b) simulated.

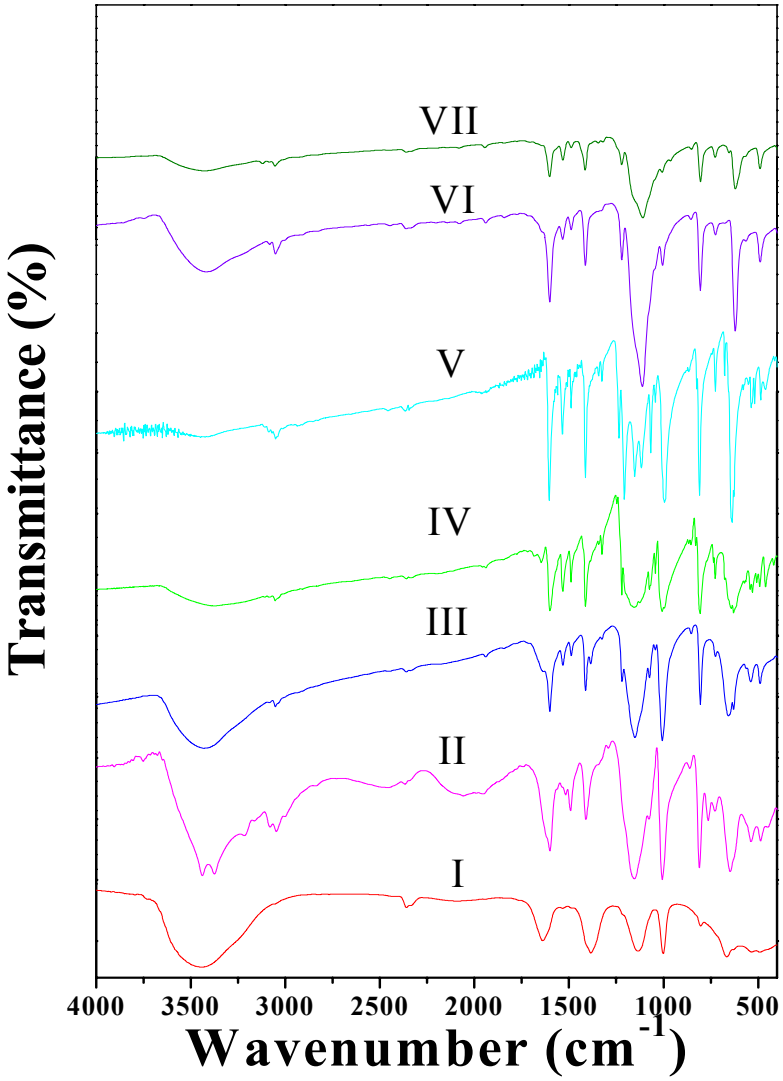


Fig. S8: IR spectra of **I- VII.**

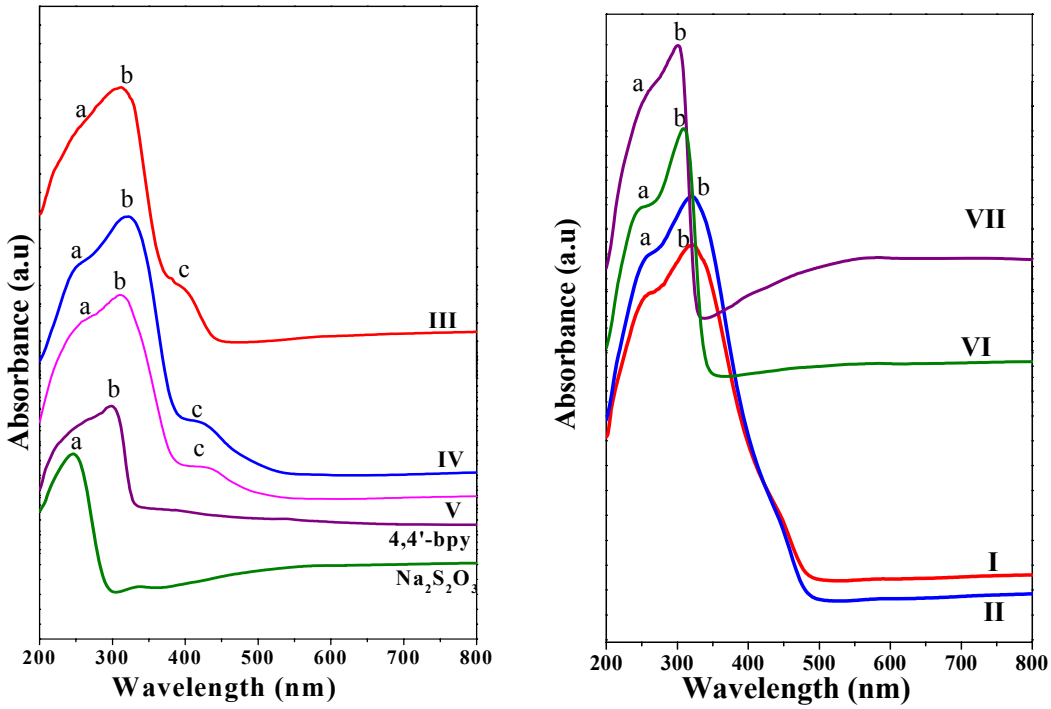


Fig. S9: The solid state UV-visible absorbance spectra of $Na_2S_2O_3$, 4,4'-bipyridine and compounds **I-VII**. Compounds **III**, **IV** and **V** exhibit three peaks while compounds **I**, **II**, **VI** and **VII** exhibit two peaks. a → centered at ~255 nm, which could be due to the charge transfer from the thiosulfate and the sulfate to the metal. b → centered at ~300-320 nm, which could be due to the intra-ligand (4,4'-bpy) electron transfer. c → centered at ~400-410 nm, which could be due to the charge transfer from the bipyridine to the metal.

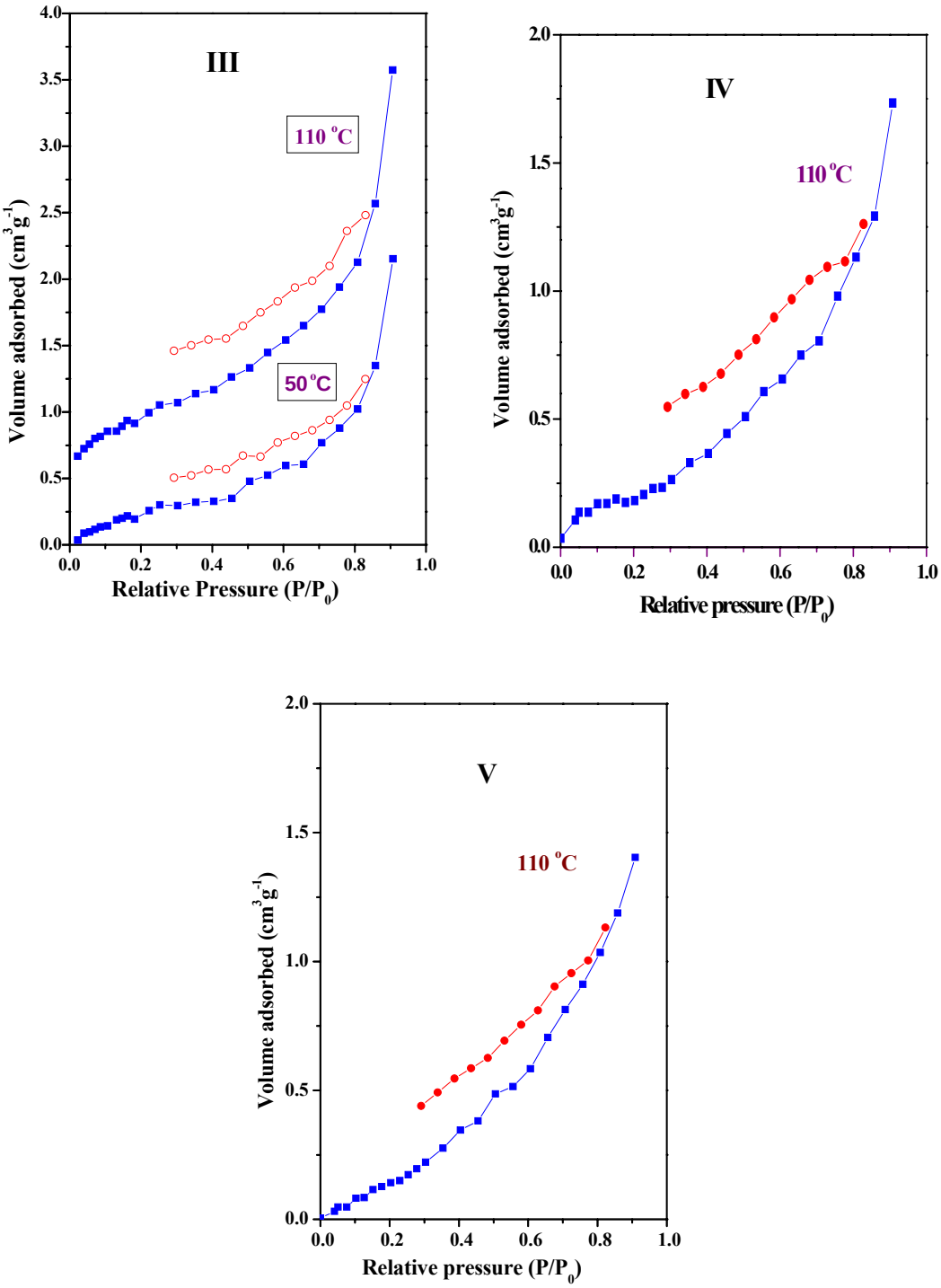


Fig. S10. The N_2 adsorption-desorption isotherm of the thiosulfate compounds III, IV and V. Blue lines correspond to adsorption and red lines correpond to desorption isotherm.

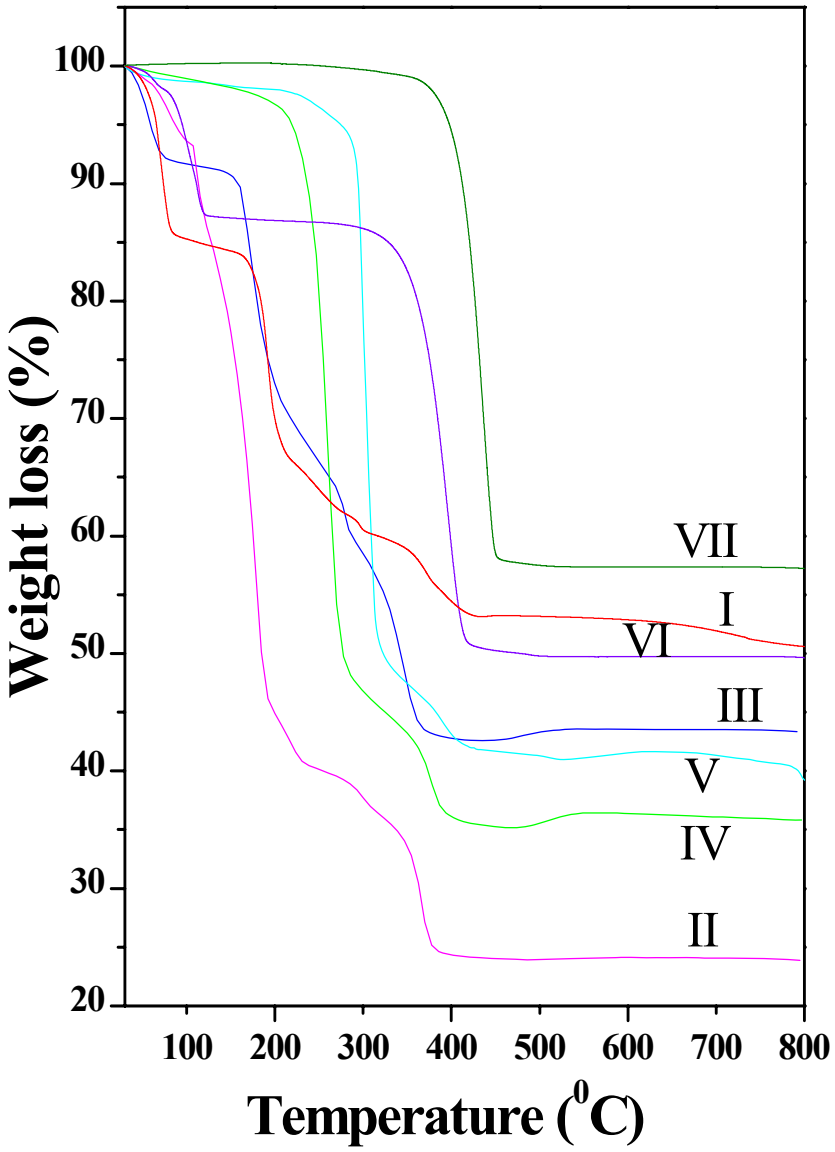
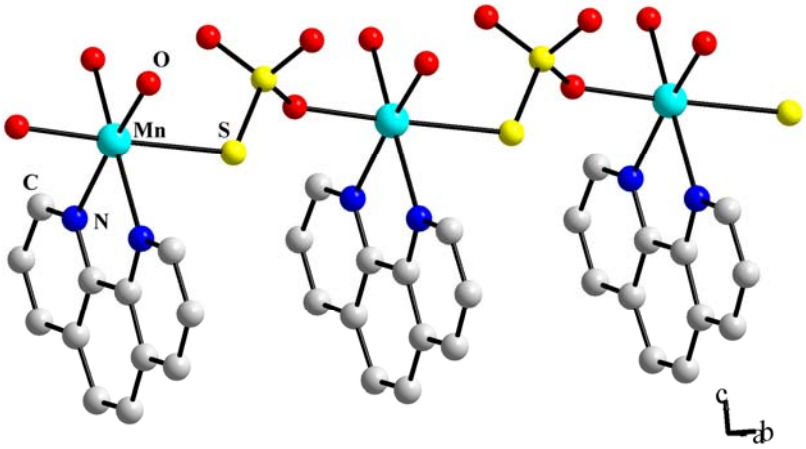
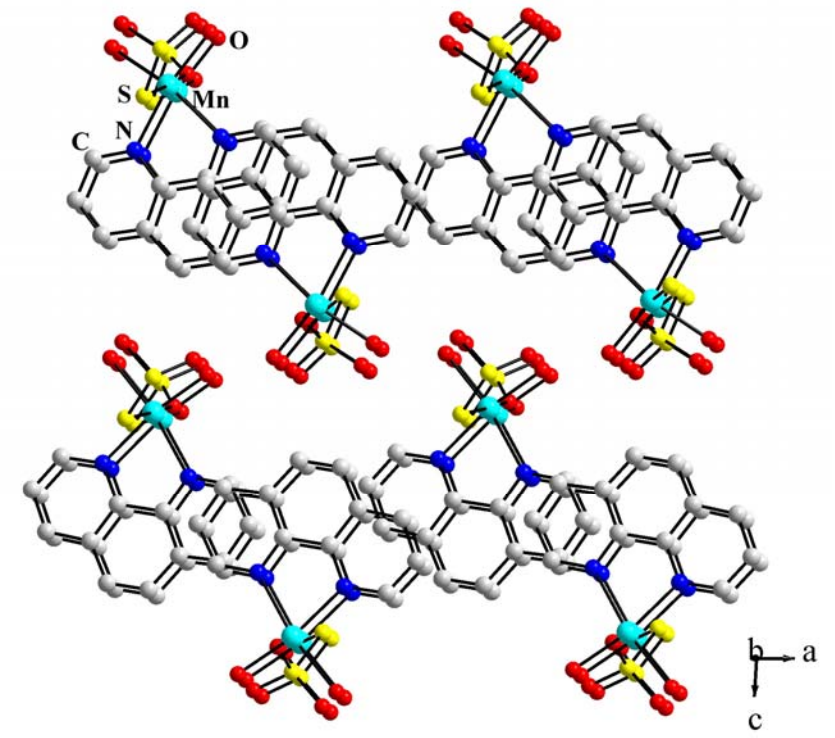


Fig. S11: TGA studies (in oxygen atmosphere) of **I-V.**



(a)



(b)

Fig. S12: (a) One-dimensional manganese thiosulfate chain in $[Mn(S_2O_3)_2(C_{12}H_8N_2)(H_2O)_2]$.

(b) Packing diagram of $[Mn(S_2O_3)_2(C_{12}H_8N_2)(H_2O)_2]$. Note that the 1,10-phenanthroline offers the π··· π interactions in the compound.

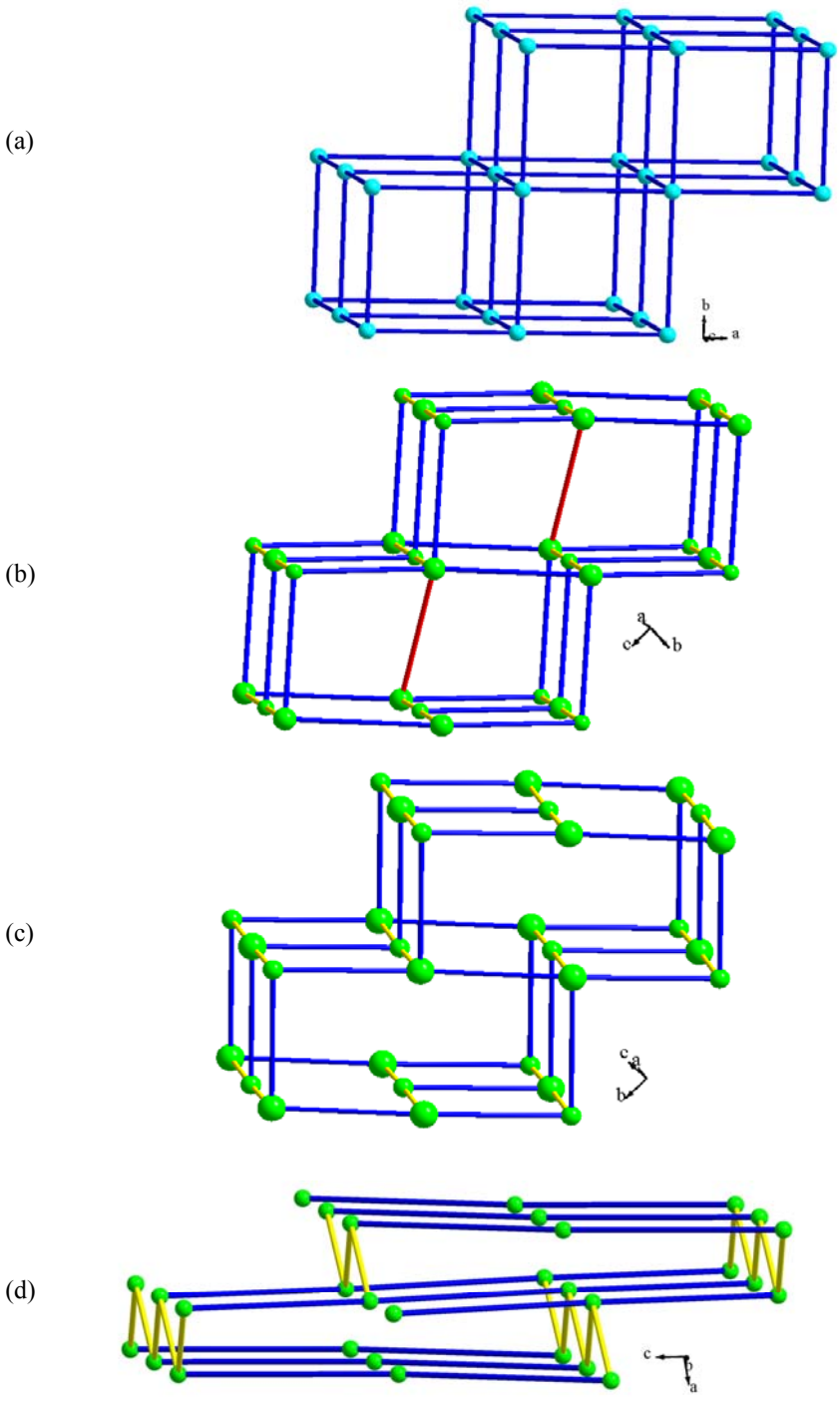


Fig. S13. The schematic diagram of (a) **pcu** net (b) structure **IV** (c) structure **V** (d) structure **III**.

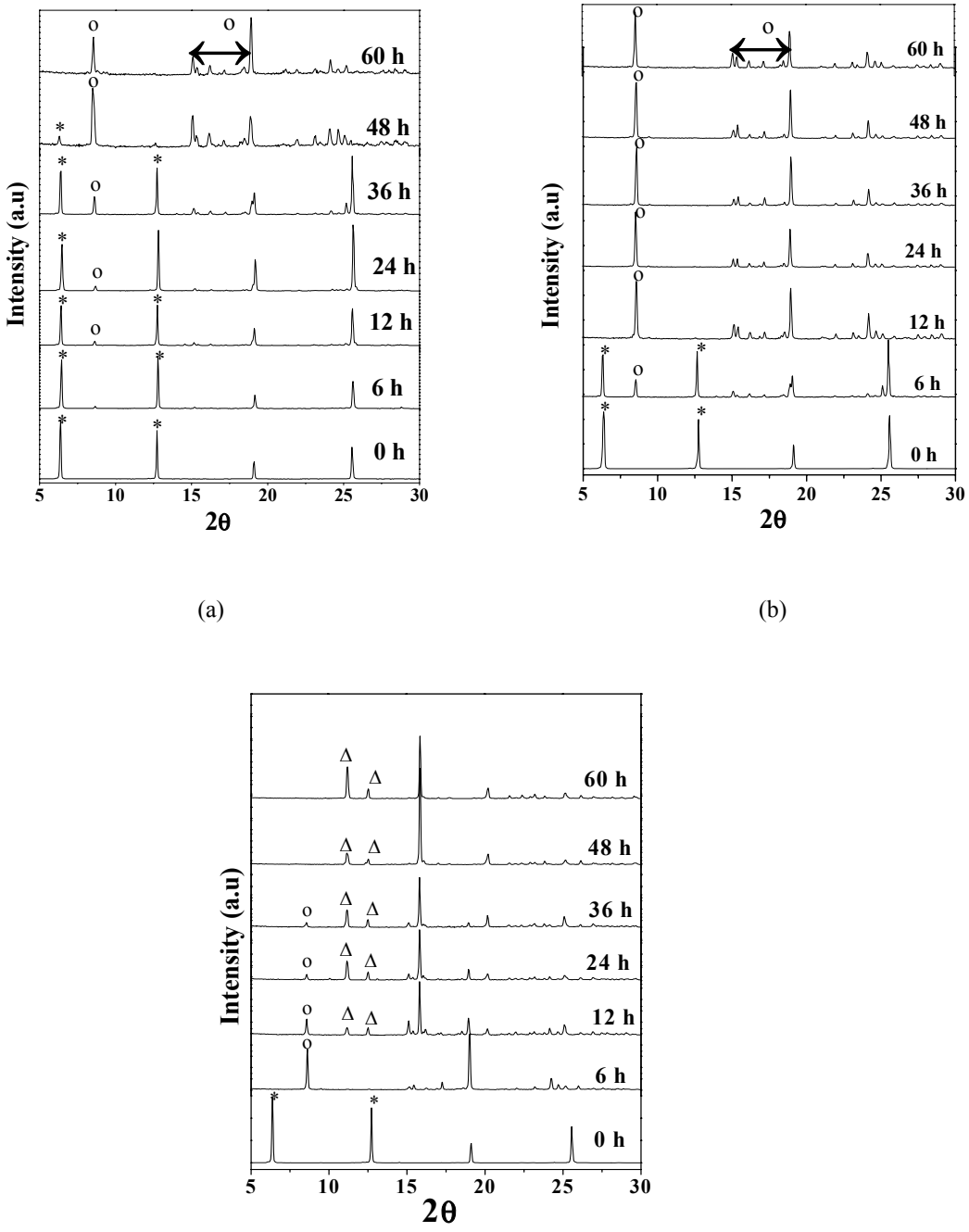


Fig. S14: The PXRD pattern of the transformation reaction of **I** in water medium (a) at 30 ^{o}C (b) at 45 ^{o}C (c) at 60 ^{o}C. (∗ = **I**, o = **III** and ∆ = **V**).

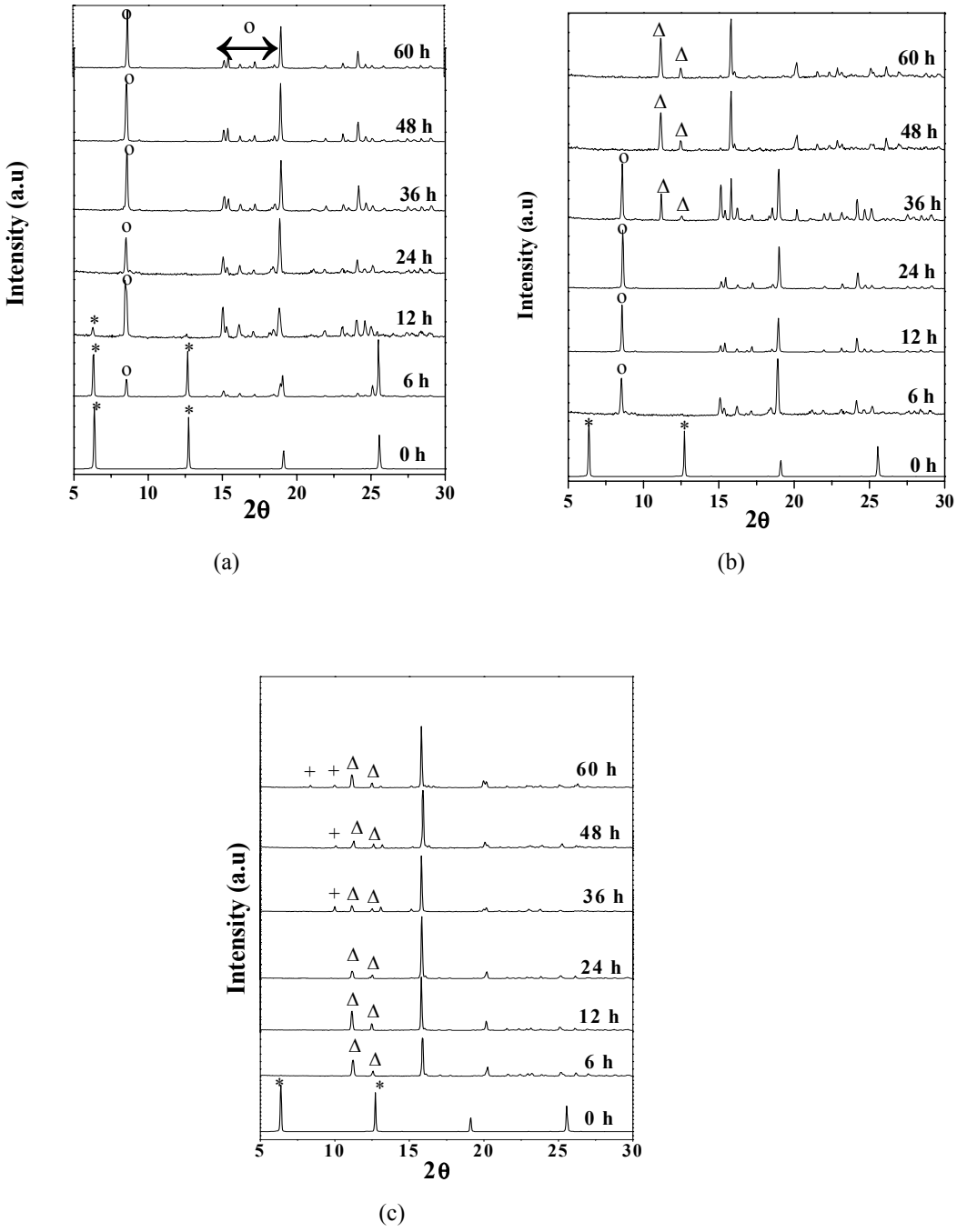


Fig. S15: The PXRD pattern of the transformation reaction of **I** in water-ethanol mixture (a) at 30 ^{o}C (b) at 45 ^{o}C (c) at 60 ^{o}C. (∗ = **I**, o = **III,** ∆ = **V** and + = **VI**).

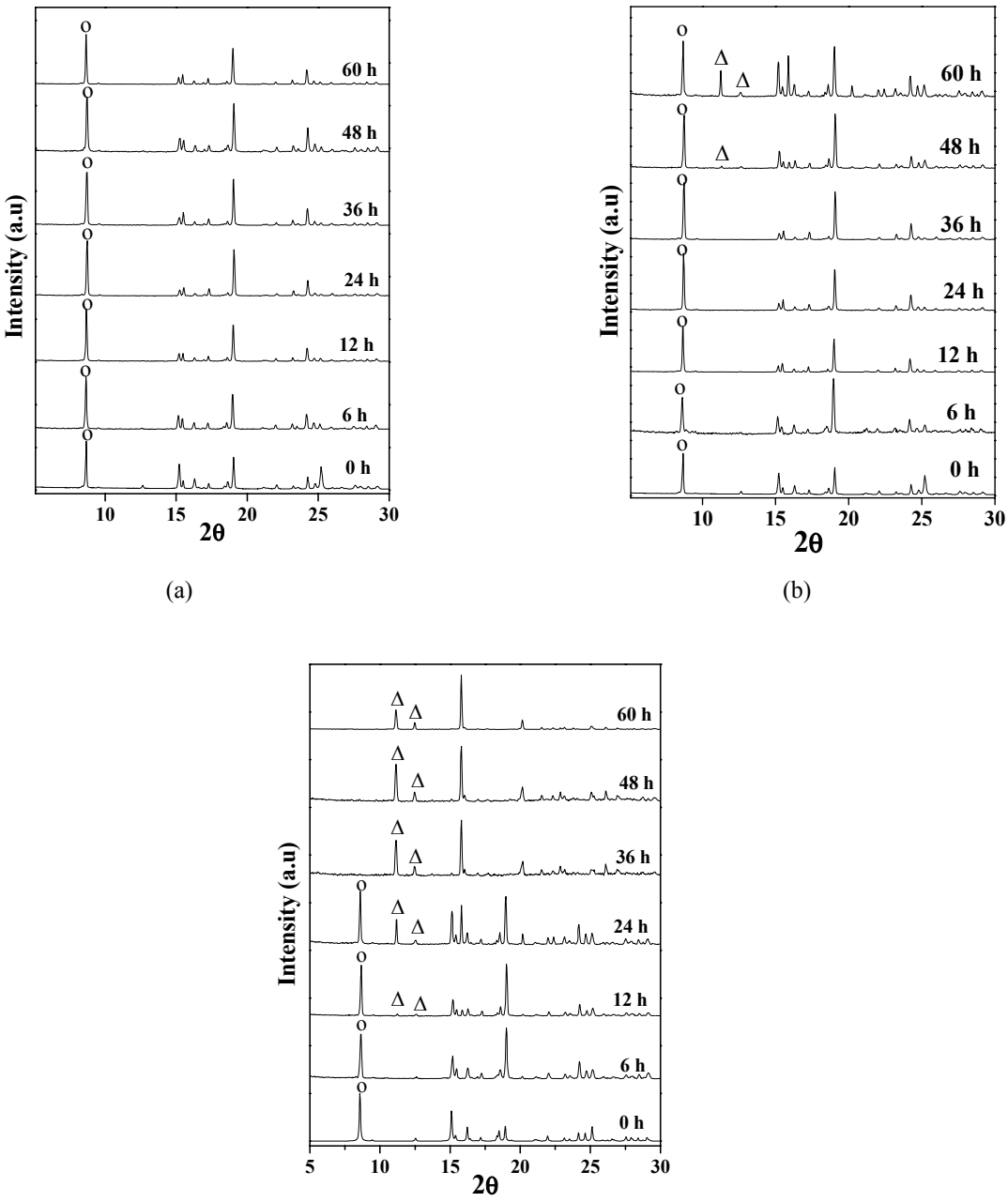


Fig. S16: The PXRD pattern of the transformation reaction of **III** in water medium (a) at 30 ^{o}C (b) at 45 ^{o}C (c) at 60 ^{o}C. (o = **III** and Δ = **V**).

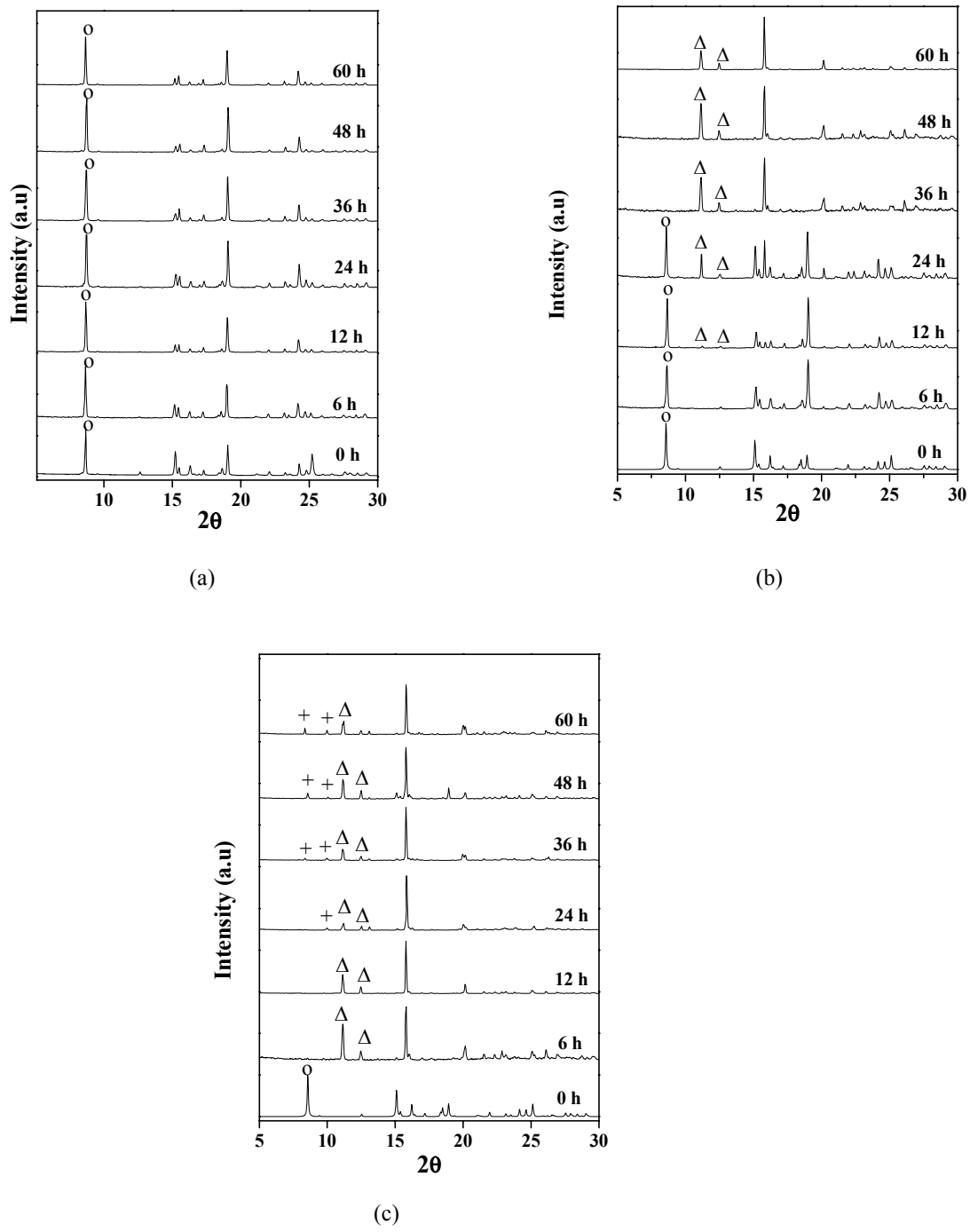


Fig. S17: The PXRD pattern of the transformation reaction of **III** in water-ethanol mixture (a) at 30 ^{o}C (b) at 45 ^{o}C (c) at 60 ^{o}C. (o = **III,** Δ = **V** and + = **VI**).

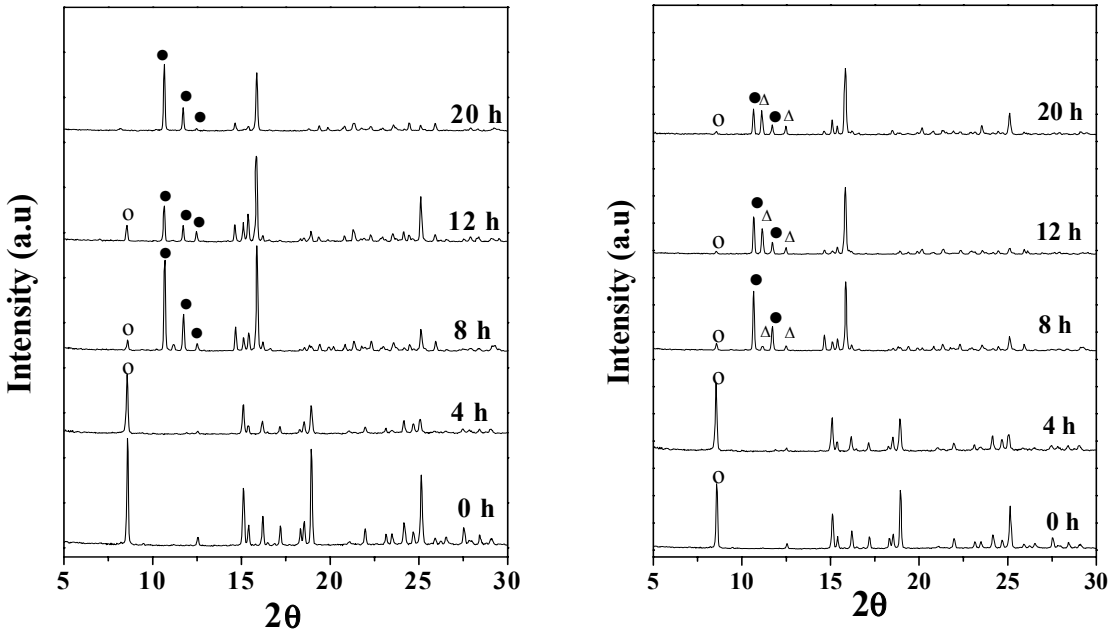


Fig. S18: The PXRD pattern of the transformation reaction for compound **III** at 45 ^{0}C

(a) The compound **III** heated with *bpy* with mole ratio; 1: 0.50

(b) The compound **III** heated with *bpy* with mole ratio; 1: 0.25. (o = **III,** ● = **IV** and Δ = **V**)**.**

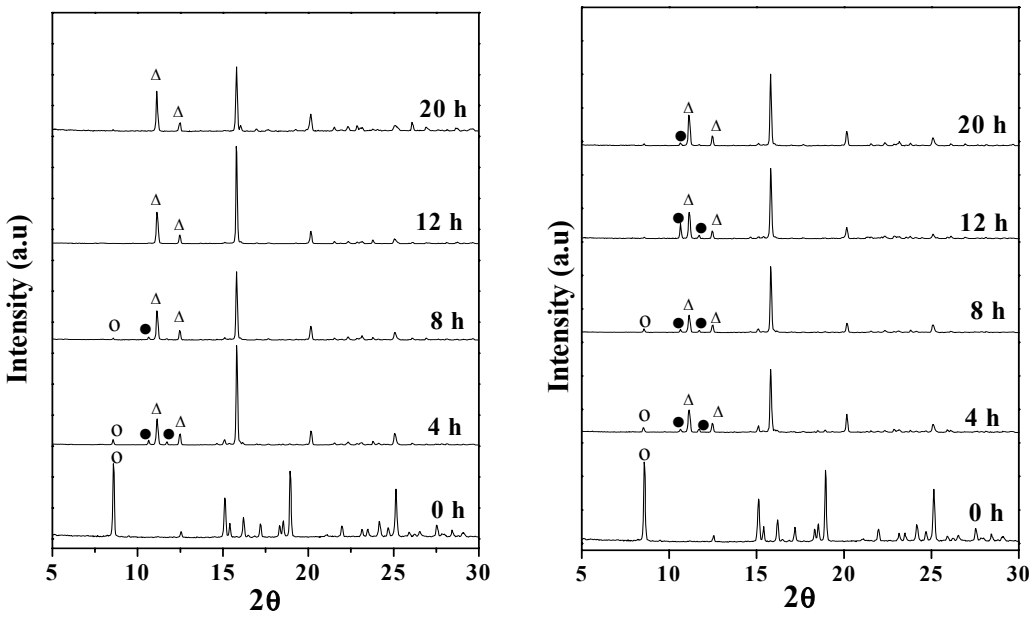


Fig. S19: The PXRD pattern of the transformation reaction for compound **III** at 60 ^{0}C

(a)The compound **III** heated with *bpy* with mole ratio; 1: 0.25

(b)The compound **III** heated with *bpy* with mole ratio; 1: 0.50. (o = **III,** ● = **IV** and ∆ = **V**).

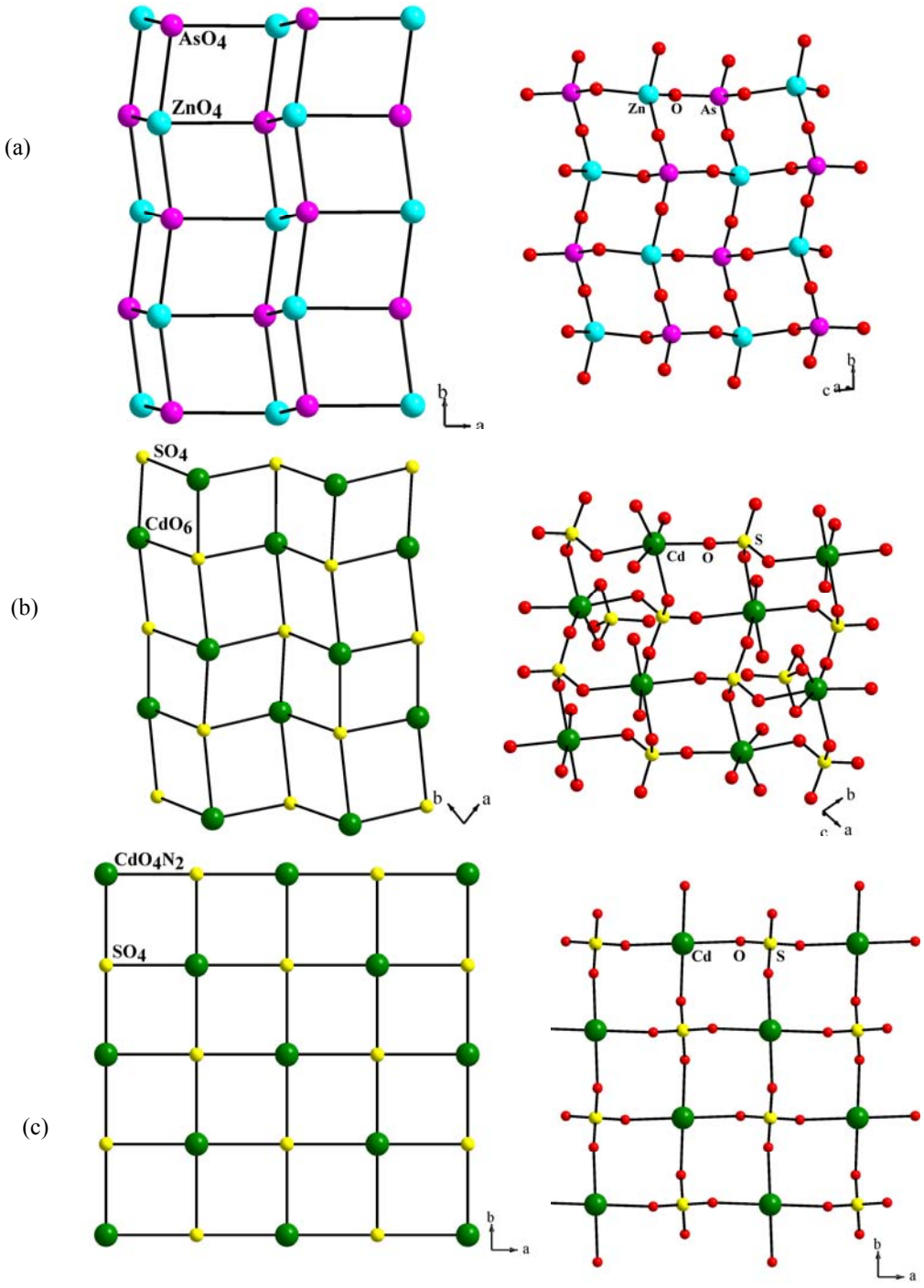
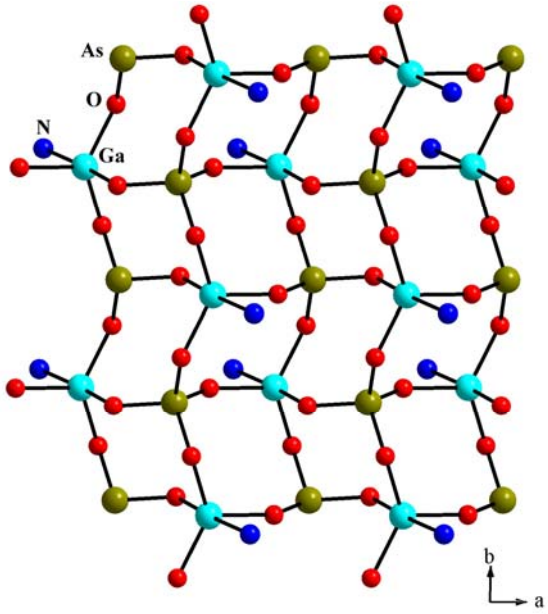


Fig. S20: (a) Four-connected layer in zinc-arsenate. Cyan spheres represent the zinc atoms and purple spheres represent the arsenic atoms. (b) Four-connected layer in cadmium-sulfate (c) Four-connected layer in **VII**. Green spheres represent the cadmium atoms and yellow spheres represent the sulfur atoms in both the figures.

(a)



(b)

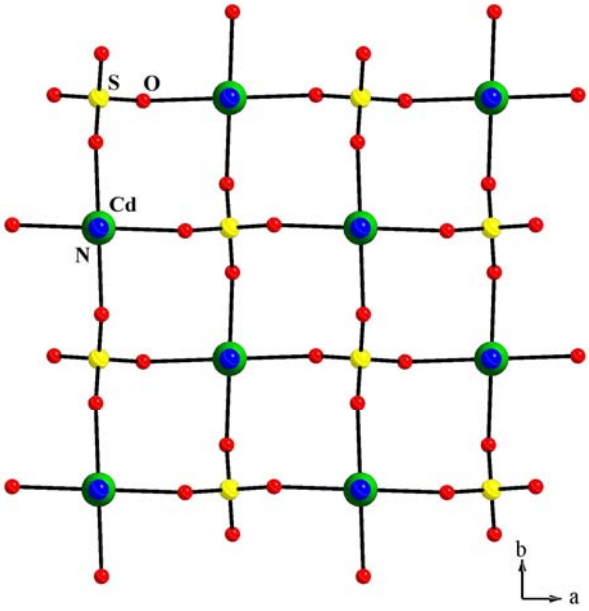


Fig. S21: Fully four-connected inorganic layer of (a) gallium-phosphate and (b) structure **VII.**

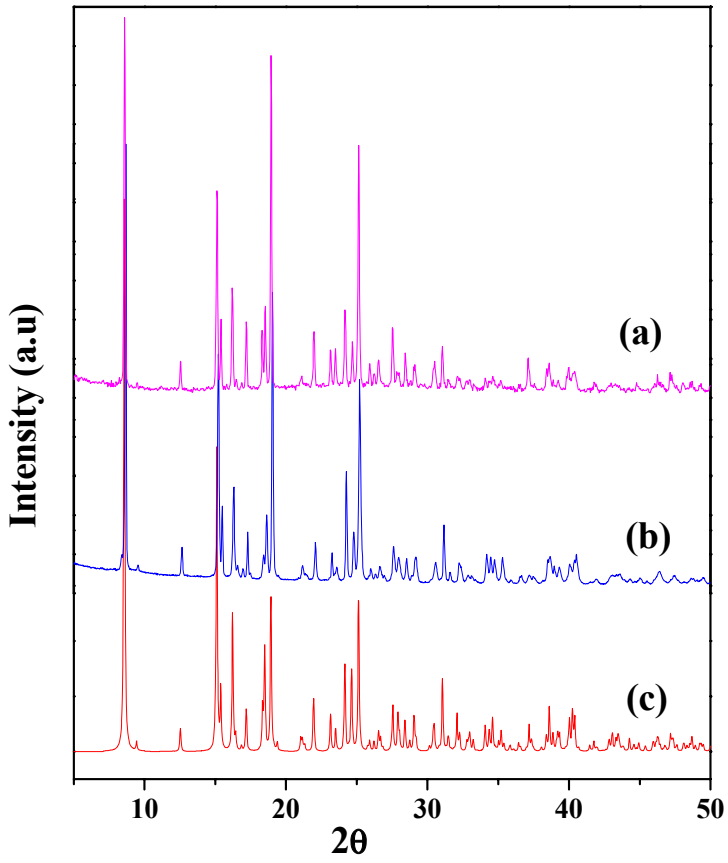


Fig. S22: Powder XRD (CuKα) pattern of **III**, (a) after catalytic reaction, (b) as synthesized and (c) simulated.