

Electronic Supporting Information for:

[Zn(HPO₃)(C₁₁N₂O₂H₁₂)] and

[Zn₃(H₂O)(PO₄)(HPO₄)(C₆H₉N₃O₂)₂(C₆H₈N₃O₂)] :

Homochiral Zinc Phosphite/Phosphate Networks with Biofunctional Amino Acids

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Figure S5. The VCD (top) and IR (bottom) spectra of L-tryptophan in the solid state at room temperature.

Table S1. Selected bond lengths [Å], bond angles [°] and H-bonds for ZnHPO-CJ56.^a

Zn(1)-O(2)	1.935(4)	O(2)-Zn(1)-O(1)	117.46(15)	
Zn(1)-O(1)	1.939(3)	O(2)-Zn(1)-O(4)	109.26(14)	
Zn(1)-O(4)	1.952(3)	O(1)-Zn(1)-O(4)	110.83(15)	
Zn(1)-O(3)	1.993(3)	O(2)-Zn(1)-O(3)	107.23(15)	
P(1)-O(2)#1	1.517(4)	O(1)-Zn(1)-O(3)	103.02(15)	
P(1)-O(4)#2	1.523(4)	O(4)-Zn(1)-O(3)	108.51(14)	
P(1)-O(3)	1.527(3)	O(2)#1-P(1)-O(4)#2	112.71(19)	
O(1)-C(1)	1.284(6)	O(2)#1-P(1)-O (3)	113.6(2)	
O(2)-P(1)#2	1.517(4)	O(4)#2-P(1)-O (3)	110.4(2)	
O(4)-P(1)#1	1.523(4)	C(1)-O(1)-Zn (1)	118.7(4)	
O(5)-C(1)	1.217(9)	P(1)#2-O(2)-Zn (1)	133.7(2)	
C(1)-C(2)	1.535(6)	P(1)-O(3)-Zn(1)	127.67(19)	
C(2)-N(1)	1.496(7)	P(1)#1-O(4)-Zn (1)	128.21(19)	
C(2)-C(3)	1.539(7)	O(5)-C(1)-O (1)	126.6(4)	
C(3)-C(4)	1.506(8)	O(5)-C(1)-C (2)	119.1(4)	
C(4)-C(11)	1.365(8)	O(1)-C(1)-C (2)	114.3(6)	
C(4)-C(5)	1.434(7)	N(1)-C(2)-C (1)	106.3(4)	
C(5)-C(6)	1.411(8)	N(1)-C(2)-C (3)	110.0(4)	
C(5)-C(10)	1.425(9)	C(1)-C(2)-C (3)	112.7(4)	
C(6)-C(7)	1.380(9)	C(4)-C(3)-C (2)	114.8(5)	
C(7)-C(8)	1.396(11)	C(11)-C(4)-C (5)	106.9(5)	
C(8)-C(9)	1.374(11)	C(11)-C(4)-C (3)	129.8(5)	
C(9)-C(10)	1.398 (8)	C(5)-C(4)-C (3)	123.2(5)	
C(10)-N(2)	1.370(8)	N(2)-C(10)-C (9)	132.3(7)	
C(11)-N(2)	1.381(7)	N(2)-C(10)-C (5)	106.8(5)	
H-bonds				
D-H•••A	d (D-H)	d (H•••A)	d (D•••A)	<DHA
N(1)-H(2N)...O(5)#3	0.92(5)	2.03(5)	2.792(6)	140(4)
N(1)-H(2N)...O(2)#3	0.92(5)	2.58(5)	3.139(6)	120(4)
N(1)-H(1N)...O(4)#4	0.95(5)	2.09(5)	3.017(5)	165(4)
N(1)-H(1N)...O(3)#3	0.95(5)	2.47(5)	3.069(7)	121(4)
N(1)-H(1N)...O(3)#3	0.95(5)	2.47(5)	3.069(7)	121(4)

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

Table S2. Selected bond lengths [Å], bond angles [°] and H-bonds for ZnPO-CJ57.^a

Zn(1)-O(8)	1.904(4)	O(9)-Zn(1)-N (2)	110.17(19)
Zn(1)-O(11)	1.939(4)	O(7)-Zn(2)-O (1 0)	107.60(19)
Zn(1)-O(9)	1.954(4)	O(7)-Zn(2)-O (1 4)	113.74(17)
Zn(1)-N(2)	2.036(5)	O(10)-Zn(2)-O (1 4)	110.57(17)
Zn(2)-O(7)	1.923(4)	O(7)-Zn(2)-N (5)	121.90(19)
Zn(2)-O(10)	1.957(4)	O(10)-Zn(2)-N (5)	102.59(19)
Zn(2)-O(14)	1.957(4)	O(14)-Zn(2)-N (5)	99.68(19)
Zn(2)-N(5)	2.016(5)	O(1W)-Zn(3)-O (1 3)	117.6(2)
Zn(3)-O(1W)	1.933(5)	O(1W)-Zn(3)-N (8)	112.9(2)
Zn(3)-O(13)	1.932(4)	O(13)-Zn(3)-N (8)	119.2(2)
Zn(3)-N(8)	1.988(5)	O(1W)-Zn(3)-N (7)	100.2(2)
Zn(3)-N(7)	2.088(5)	O(13)-Zn(3)-N (7)	105.6(2)
P(1)-O(10)	1.510(4)	N(8)-Zn(3)-N (7)	96.1(2)
P(1)-O(7)#1	1.510(4)	O(10)-P(1)-O (7) # 1	113.5(3)
P(1)-O(9)	1.531(4)	O(10)-P(1)-O (9)	111.5(2)
P(1)-O(12)	1.592(4)	O(7)#1-P(1)-O (9)	111.2(2)
P(2)-O(8)#2	1.512(4)	O(10)-P(1)-O (1 2)	105.8(2)
P(2)-O(11)	1.526(4)	O(7)#1-P(1)-O (1 2)	108.7(2)
P(2)-O(14)	1.534(4)	O(9)-P(1)-O (1 2)	105.7(2)
P(2)-O(13)	1.555(4)	O(8)#2-P(2)-O (1 1)	111.6(3)
O(8)-Zn(1)-O(11)	108.07(19)	O(8)#2-P(2)-O (1 4)	110.2(3)
O(8)-Zn(1)-O(9)	114.91(18)	O(11)-P(2)-O (1 4)	111.9(2)
O(11)-Zn(1)-O(9)	107.33(18)	P(1)#2-O(7)-Zn(2)	135.9(3)
O(8)-Zn(1)-N(2)	115.6(2)	P(2)#1-O(8)-Zn(1)	137.6(3)
O(11)-Zn(1)-N(2)	99.3(2)	P(1)-O(9)-Zn(1)	129.6(3)

H-bonds

D-H...A	d (D-H)	d (H...A)	d (D...A)	<DHA
O(12)-H(1)...O(6)#3	0.97(2)	1.77(2)	2.722(6)	169(5)
N(9)-H(3A)...O(1)#4	0.86	1.83	2.682(7)	169.5
N(3)-H(4B)...O(5)#1	0.89	1.93	2.824(6)	176.8
N(3)-H(4C)...O(6)#3	0.89	2.10	2.878(6)	145.0
N(3)-H(4D)...O(9)#1	0.89	2.04	2.849(6)	149.9
N(6)-H(7A)...O(12)#5	0.86	2.36	2.938(8)	125.3
N(7)-H(9A)...O(3)	0.90	2.21	2.671(8)	111.2
N(4)-H(10A)...O(4)#1	0.89	2.04	2.871(7)	155.3
N(4)-H(10B)...O(2)#6	0.89	2.00	2.863(6)	162.2
N(4)-H(10B)...O(13)	0.89	2.59	3.036(6)	111.8
N(4)-H(10C)...O(14)	0.89	1.94	2.804(7)	164.4
N(1)-H(11)...O(1)#7	0.86	1.99	2.731(7)	143.2
O(1W)-H(2)...O(5)#6	0.958(18)	1.68(2)	2.611(6)	164(5)
O(1W)-H(2)...O(2)#6	0.958(18)	2.44(4)	2.940(6)	112(2)
O(1W)-H(3)...O(13)#2	0.931(17)	1.78(3)	2.547(6)	137(5)

^a Symmetry transformations used to generate equivalent atoms: #1 $x, y, z-1$ #2 $x, y, z+1$ #3 $x-1, y, z+1$ #4 $x-1/2, -y+3/2, -z+1$ #5 $x+1/2, -y+3/2, -z+1$ #6 $-x+1, -y+2, z$ #7 $-x+2, -y+2, z+1$ #8 $x+1, y, z-1$.

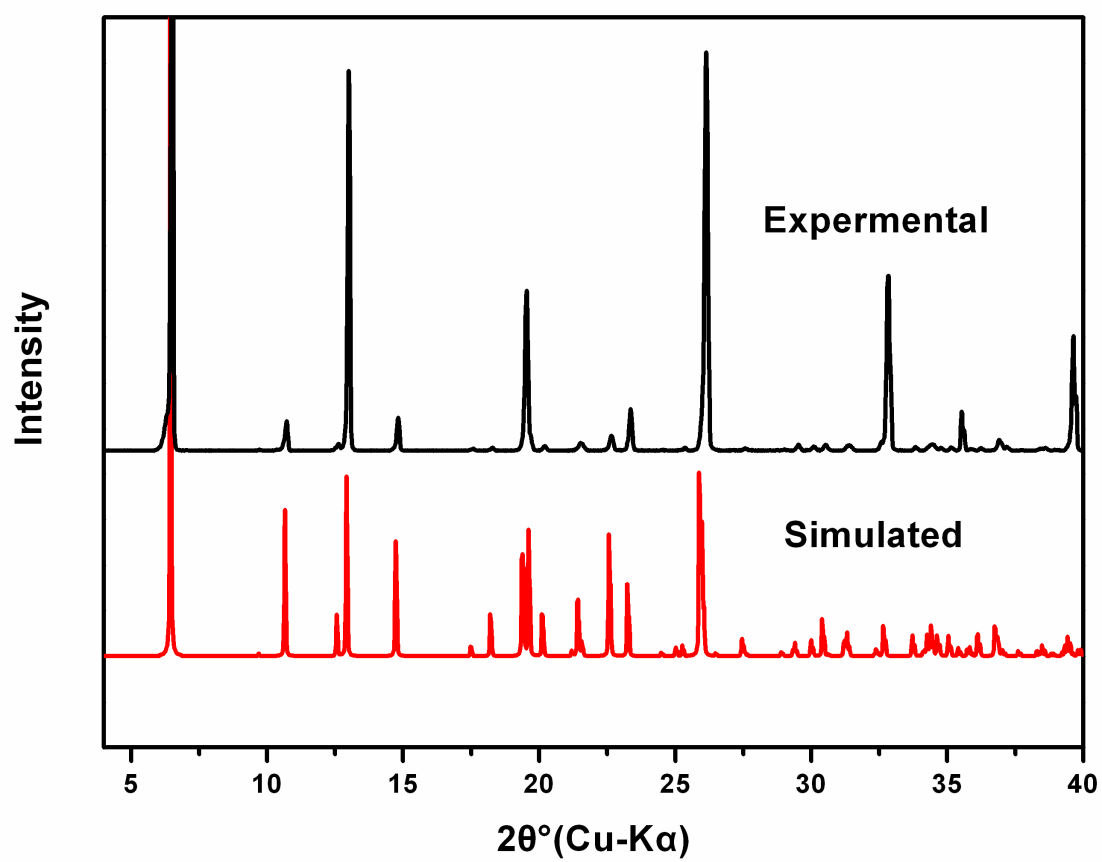


Figure S1(a)

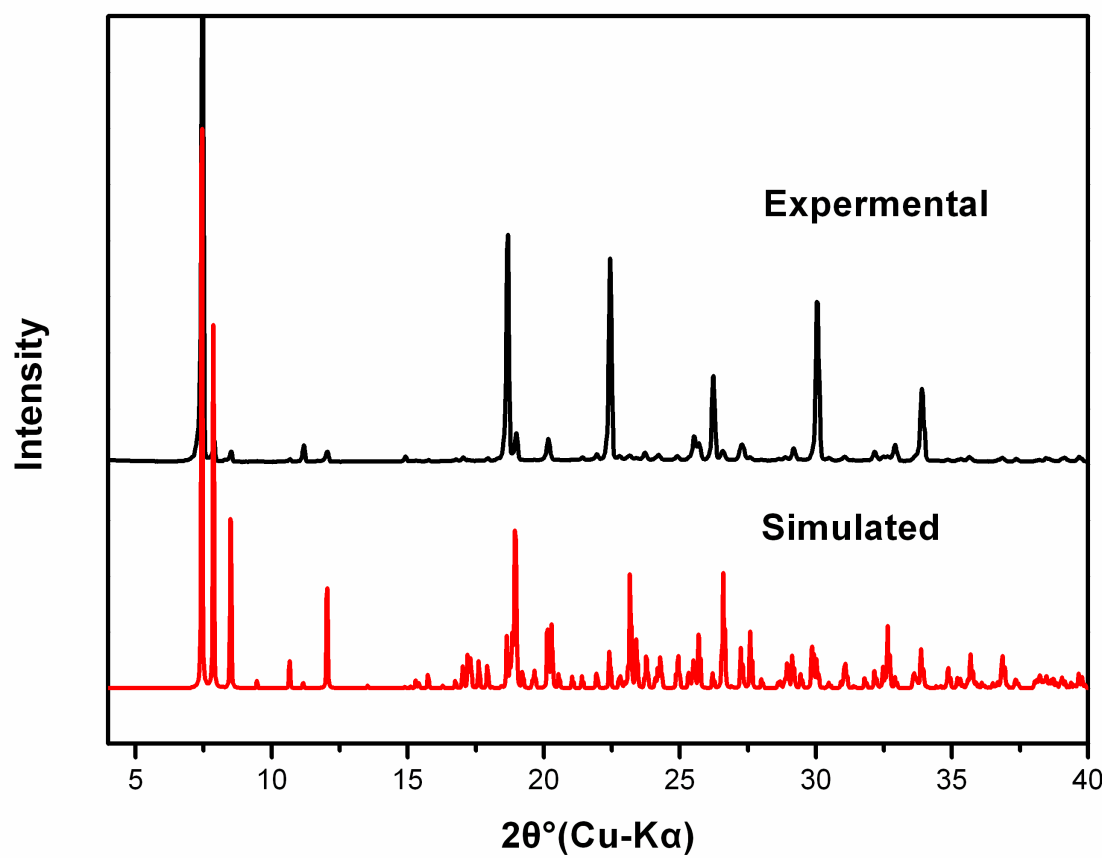


Figure S1(b)

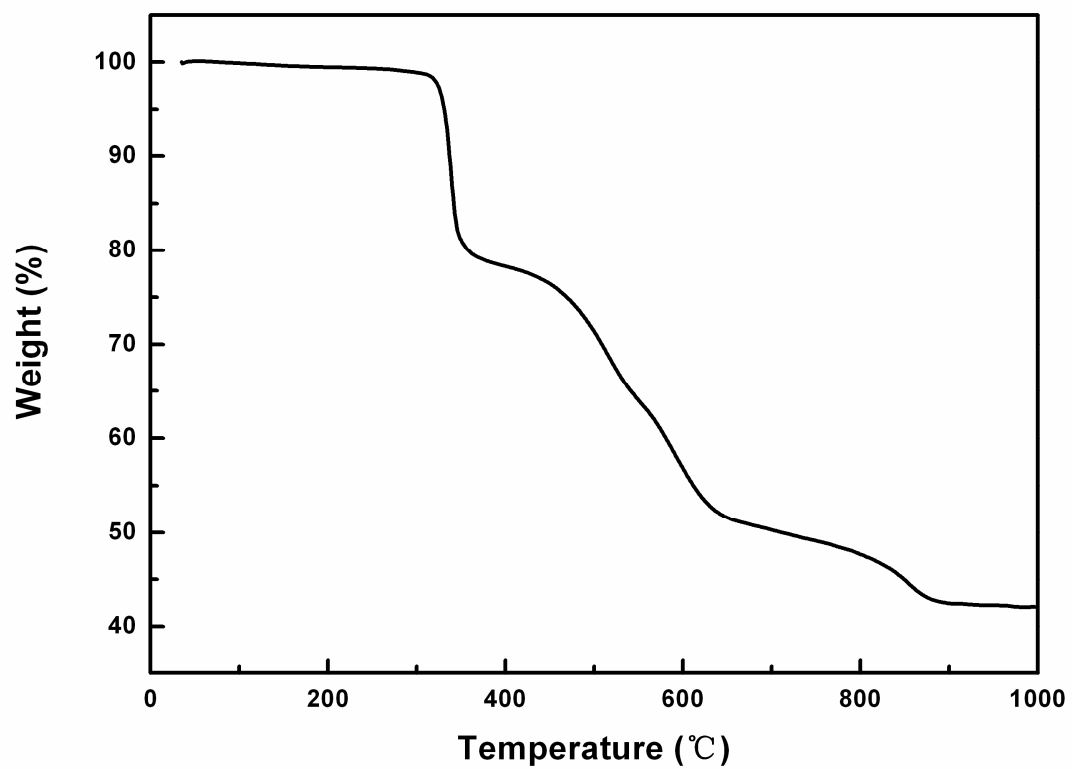


Figure S2(a)

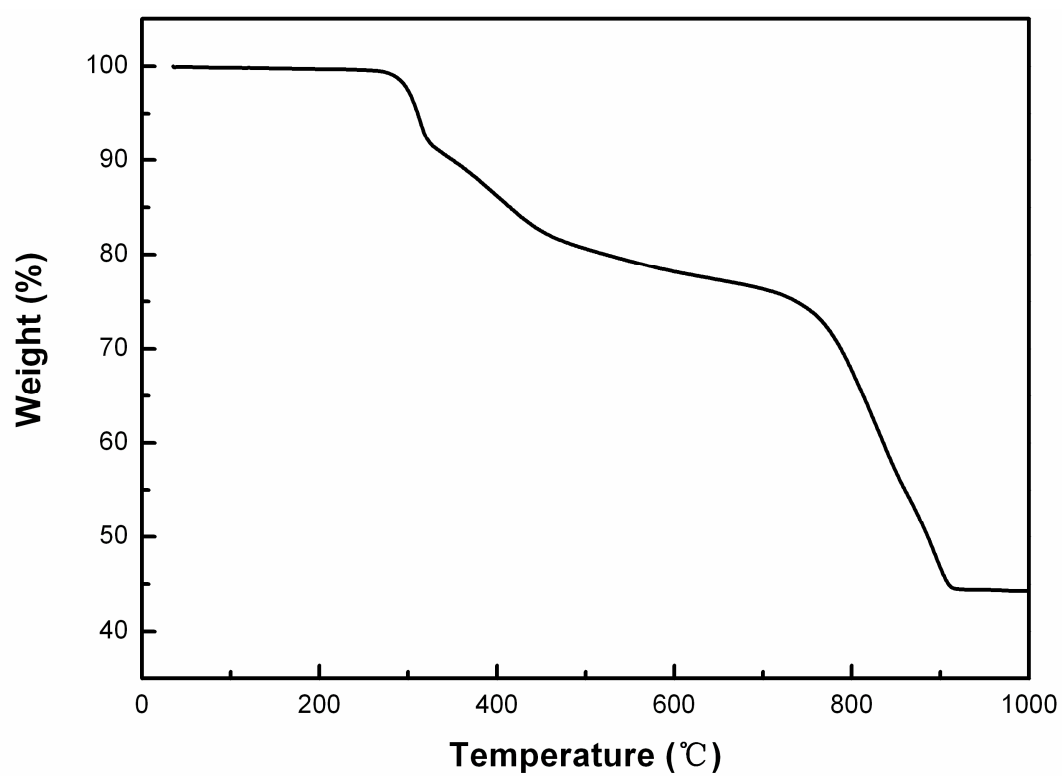


Figure S2 (b)

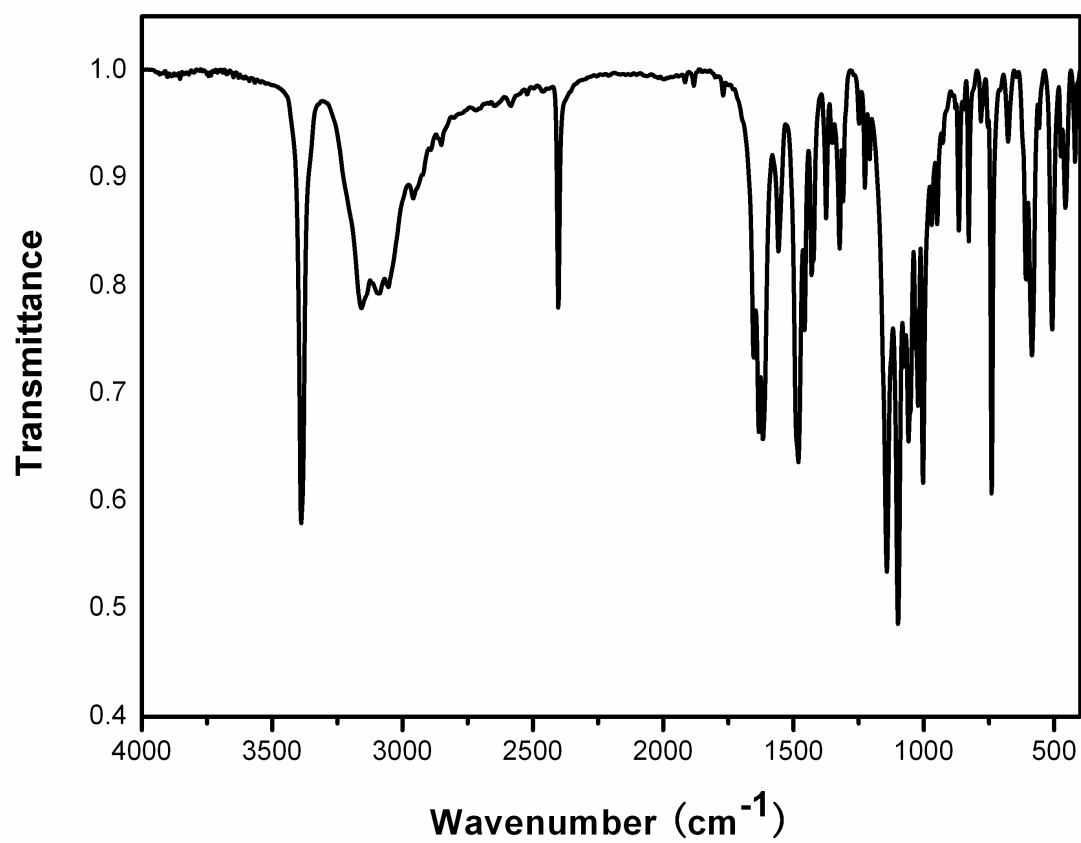


Figure S3

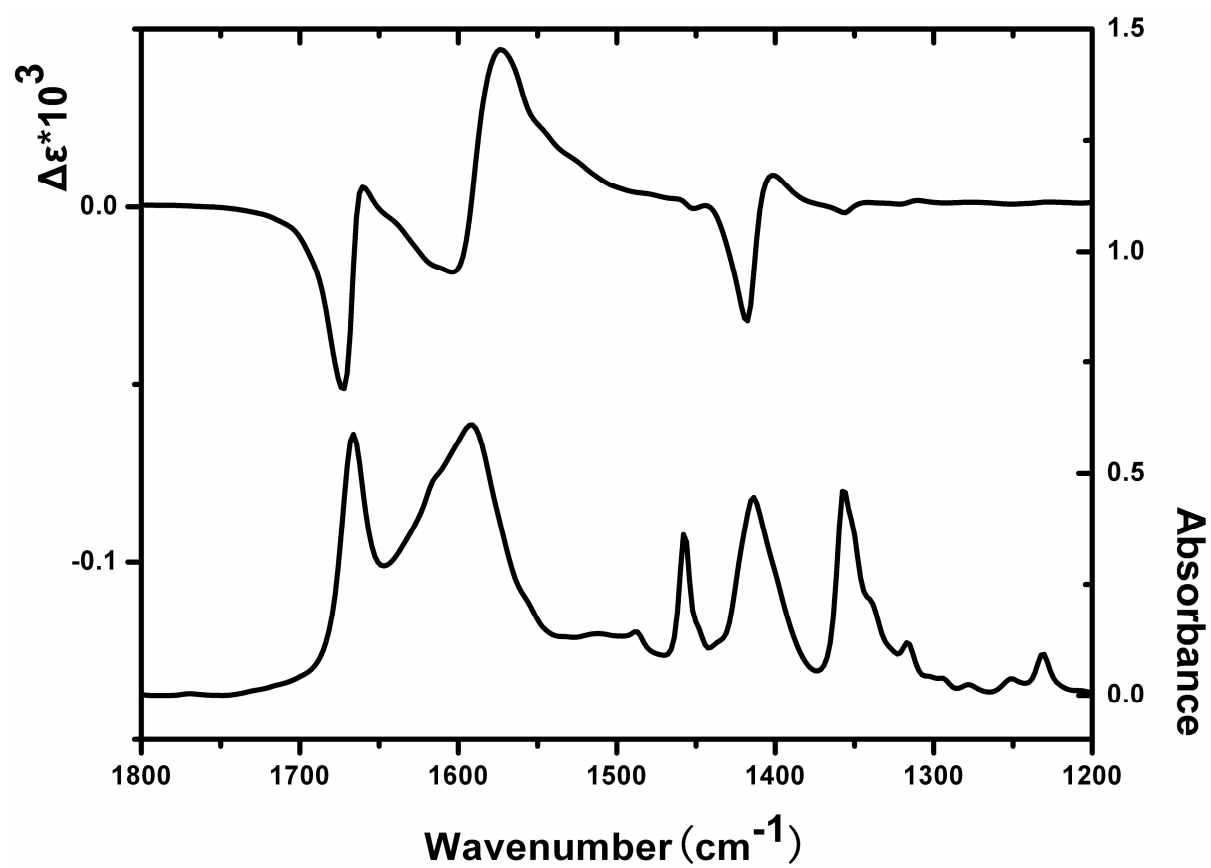


Figure S4

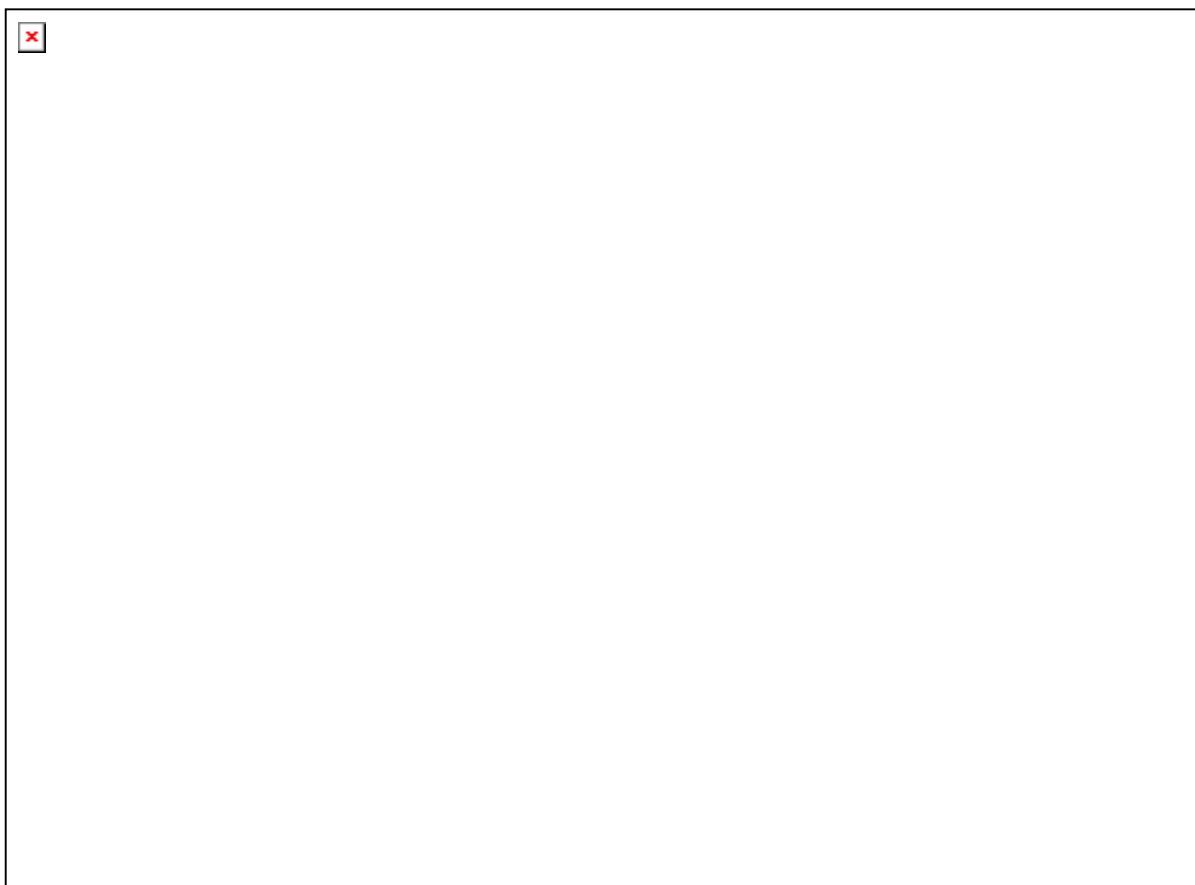


Figure S5