Towards Rational Design of Zinc(II) and Cadmium(II) Sulfonate-Arsonates with Low Dimensional Aggregations

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Supporting Materials

Table S1. Selected bond lengths (Å) for **1-12**.

Compound **1**

Zn(1)-O(2)	2.178(2)	Zn(1)-O(3)#2	2.066(2)
Zn(1)-O(4)#2	2.337(3)	Zn(1)-O(7)	2.067(2)
Zn(1)-O(7)#1	2.064(2)	Zn(1)-O(1W)	2.033(3)
Zn(2)-O(1)#3	1.965(2)	Zn(2)-O(2)	2.081(2)
Zn(2)-O(3)#2	2.034(2)	Zn(2)-O(4)	2.187(3)
Zn(2)-O(7)#3	1.995(2)		
As(1)-O(1)	1.674(2)	As(1)-O(2)	1.699(2)
As(1)-O(3)	1.692(2)	S(1)-O(4)	1.484(3)
S(1)-O(5)	1.451(3)	S(1)-O(6)	1.427(3)

Compound **2**

Cd(1)-O(1)	2.338(5)	Cd(1)-O(2)#1	2.224(5)
Cd(1)-O(6)	2.323(6)	Cd(1)-O(8)#2	2.296(5)
Cd(1)-O(9)#1	2.293(5)	Cd(1)-O(1W)	2.334(6)
Cd(2)-O(1)	2.252(5)	Cd(2)-O(7)	2.301(5)
Cd(2)-O(7)#2	2.235(5)	Cd(2)-O(10)	2.286(6)
Cd(2)-O(1W)	2.616(7)	Cd(2)-O(2W)	2.298(6)
Cd(3)-O(3)#3	2.198(5)	Cd(3)-O(3)#4	2.218(5)
Cd(3)-O(4)#4	2.462(7)	Cd(3)-O(8)	2.328(5)
Cd(3)-O(9)	2.268(5)	Cd(3)-O(3W)	2.310(7)
As(1)-O(1)	1.688(5)	As(1)-O(2)	1.678(5)
As(1)-O(3)	1.682(5)	As(2)-O(7)	1.657(5)
As(2)-O(8)	1.697(5)	As(2)-O(9)	1.690(5)
S(1)-O(4)	1.455(7)	S(1)-O(5)	1.435(6)

S(1)-O(6)	1.468(6)	S(2)-O(10)	1.417(12)
S(2)-O(11)	1.50(2)	S(2)-O(12)	1.34(2)
S(2')-O(10)	1.522(8)	S(2')-O(11')	1.419(14)
S(2')-O(12')	1.427(12)		
Compound **3**			
Zn(1)-O(1)	1.991(4)	Zn(1)-O(6)	2.257(4)
Zn(1)-N(1)	2.157(4)	Zn(1)-N(2)	2.142(5)
Zn(1)-N(3)	2.168(5)	Zn(1)-N(4)	2.152(5)
Zn(2)-O(8)	2.021(4)	Zn(2)-O(12)	2.161(4)
Zn(2)-N(5)	2.204(5)	Zn(2)-N(6)	2.135(5)
Zn(2)-N(7)	2.141(5)	Zn(2)-N(8)	2.141(5)
As(1)-O(1)	1.659(4)	As(1)-O(2)	1.730(4)
As(1)-O(3)	1.663(4)	As(2)-O(7)	1.667(4)
As(2)-O(8)	1.662(4)	As(2)-O(9)	1.703(4)
S(1)-O(4)	1.433(5)	S(1)-O(5)	1.447(4)
S(1)-O(6)	1.453(4)	S(2)-O(10)	1.438(5)
S(2)-O(11)	1.429(5)	S(2)-O(12)	1.458(4)
Compound **4**			
Cd(1)-O(1)	2.218(6)	Cd(1)-O(4)	2.468(7)
Cd(1)-O(8)	2.183(7)	Cd(1)-O(11)	2.509(7)
Cd(1)-N(1)	2.346(7)	Cd(1)-N(2)	2.340(7)
Cd(2)-O(2)	2.166(7)	Cd(2)-O(5)	2.546(7)
Cd(2)-O(7)	2.227(6)	Cd(2)-O(10)	2.451(6)
Cd(2)-N(3)	2.339(8)	Cd(2)-N(4)	2.363(8)
As(1)-O(1)	1.663(6)	As(1)-O(2)	1.652(6)
As(1)-O(3)	1.707(6)	As(2)-O(7)	1.662(6)
As(2)-O(8)	1.646(6)	As(2)-O(9)	1.718(6)
S(1)-O(4)	1.474(7)	S(1)-O(5)	1.442(7)
S(1)-O(6)	1.443(7)	S(2)-O(10)	1.453(7)
S(2)-O(11)	1.441(7)	S(2)-O(12)	1.429(7)

Compound **5**			
Zn(1)-O(2)#1	1.9534(15)	Zn(1)-O(3)	1.9317(15)
Zn(1)-O(5)#1	2.2104(15)	Zn(1)-N(1)	2.1179(18)
Zn(1)-N(2)	2.1174(18)	As(1)-O(1)	1.7252(15)
As(1)-O(2)	1.6568(15)	As(1)-O(3)	1.6535(14)
S(1)-O(4)	1.4553(16)	S(1)-O(5)	1.4540(15)
S(1)-O(6)	1.4343(16)		
Compound **6**			
Cd(1)-O(1)	2.250(5)	Cd(1)-O(1)#1	2.270(5)
Cd(1)-O(6)	2.379(5)	Cd(1)-O(1W)	2.296(6)
Cd(1)-N(1)	2.364(7)	Cd(1)-N(2)	2.301(7)
Cd(2)-O(7)#2	2.216(5)	Cd(2)-O(9)	2.187(6)
Cd(2)-O(11)#2	2.469(6)	Cd(2)-O(11)	2.668(6)
Cd(2)-O(12)	2.737(6)	Cd(2)-N(3)	2.359(7)
Cd(2)-N(4)	2.353(8)		
As(1)-O(1)	1.665(5)	As(1)-O(2)	1.721(6)
As(1)-O(3)	1.652(5)	As(2)-O(7)	1.687(5)
As(2)-O(8)	1.722(5)	As(2)-O(9)	1.651(6)
S(1)-O(4)	1.432(6)	S(1)-O(5)	1.457(7)
S(1)-O(6)	1.467(6)	S(2)-O(10)	1.429(6)
S(2)-O(11)	1.473(6)	S(2)-O(12)	1.446(6)
Compound **7**			
Cd(1)-O(2)	2.192(6)	Cd(1)-O(3)#1	2.233(5)
Cd(1)-O(5)	2.574(6)	Cd(1)-O(6)#1	2.462(6)
Cd(1)-N(1)	2.335(7)	Cd(1)-N(2)	2.349(7)
As(1)-O(1)	1.719(5)	As(1)-O(2)	1.653(6)
As(1)-O(3)	1.665(6)	S(1)-O(4)	1.441(6)
S(1)-O(5)	1.451(6)	S(1)-O(6)	1.463(6)
Compound **8**			
Zn(1)-O(1)	1.992(2)	Zn(1)-O(3)#1	1.945(2)

Zn(1)-N(1)	2.218(3)	Zn(1)-N(2)	2.077(3)
Zn(1)-N(3)	2.158(3)		
As(1)-O(1)	1.657(2)	As(1)-O(2)	1.729(3)
As(1)-O(3)	1.652(2)	S(1)-O(4)	1.444(3)
S(1)-O(5)	1.420(3)	S(1)-O(6)	1.423(3)
Compound **9**			
Cd(1)-O(1)	2.1937(15)	Cd(1)-O(3)#1	2.2620(15)
Cd(1)-O(5)	2.4274(17)	Cd(1)-N(1)	2.3607(18)
Cd(1)-N(2)	2.3177(17)	Cd(1)-N(3)	2.3764(18)
As(1)-O(1)	1.6534(16)	As(1)-O(2)	1.7321(16)
As(1)-O(3)	1.6561(15)	S(1)-O(4)	1.4588(16)
S(1)-O(5)	1.4563(17)	S(1)-O(6)	1.4429(16)
Compound **10**			
Zn(1)-O(1)	1.950(2)	Zn(1)-O(2)#1	1.950(2)
Zn(1)-O(4)	2.128(2)	Zn(1)-N(1)	2.104(2)
Zn(1)-N(2)	2.152(2)		
As(1)-O(1)	1.650(2)	As(1)-O(2)	1.660(2)
As(1)-O(3)	1.721(2)	S(1)-O(4)	1.473(2)
S(1)-O(5)	1.438(2)	S(1)-O(6)	1.453(2)
Compound **11**			
Zn(1)-O(1)	1.999(2)	Zn(1)-O(5)	2.179(3)
Zn(1)-O(7)	1.980(2)	Zn(1)-N(1)	2.108(3)
Zn(1)-N(2)	2.089(3)	Zn(2)-O(3)	1.943(2)
Zn(2)-O(8)#1	1.977(2)	Zn(2)-O(12)#1	2.166(2)
Zn(2)-N(3)	2.139(3)	Zn(2)-N(4)	2.098(3)
As(1)-O(1)	1.673(2)	As(1)-O(2)	1.712(3)
As(1)-O(3)	1.658(2)	As(2)-O(7)	1.661(2)
As(2)-O(8)	1.662(2)	As(2)-O(9)	1.720(2)
S(1)-O(4)	1.450(3)	S(1)-O(5)	1.468(3)
S(1)-O(6)	1.440(3)	S(2)-O(10)	1.435(3)

S(2)-O(11)	1.439(3)	S(2)-O(12)	1.462(3)
Compound **12**			
Zn(1)-O(1)#1	1.981(4)	Zn(1)-O(3)	1.989(4)
Zn(1)-O(4)	2.052(4)	Zn(1)-N(1)	2.118(5)
Zn(1)-N(2)	2.151(6)	Zn(2)-O(8)	2.195(4)
Zn(2)-O(10)#2	1.946(4)	Zn(2)-O(11)	1.967(4)
Zn(2)-N(3)	2.088(6)	Zn(2)-N(4)	2.188(5)
As(1)-O(1)	1.671(4)	As(1)-O(2)	1.745(4)
As(1)-O(3)	1.661(5)	As(2)-O(10)	1.684(4)
As(2)-O(11)	1.663(4)	As(2)-O(12)	1.745(4)
S(1)-O(4)	1.473(5)	S(1)-O(5)	1.446(4)
S(1)-O(6)	1.453(5)	S(2)-O(7)	1.467(5)
S(2)-O(8)	1.467(5)	S(2)-O(9)	1.450(4)

Symmetry transformations used to generate equivalent atoms:

For **1**: #1 -x, -y, -z+1; #2 -x, y-1/2, -z+1/2; #3 x, -y+1/2, z-1/2.

For **2**: #1 x, -y+1/2, z-1/2; #2 -x, -y+1, -z+2; #3 -x, y+1/2, -z+5/2; #4 x, -y+1/2, z+1/2; #5 -x, -y+1, -z+3; #6 -x, y-1/2, -z+5/2.

For **5**: #1 -x+1/2, -y+1/2, -z.

For **6**: #1 -x+1, -y+1, -z; #2 -x+1, -y, -z+1.

For **7**: #1 -x+1, -y+2, -z+1.

For **8**: #1 -x+1, -y+2, -z+1.

For **9**: #1 -x+1, -y+2, -z+1.

For **10**: #1 -x+3/2, y-1/2, -z+3/2.

For **11**: #1 x, y+1, z.

For **12**: #1 -x+2, -y+1, -z; #2 -x+1, y-1/2, -z+1/2.

Table S2. Hydrogen bonds [Å and deg.] for compounds **3-12**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
Compound 3				
O(2)-H(2A)...O(7)	0.82	1.68	2.492(6)	167.6
O(9)-H(9A)...O(3)	0.82	1.76	2.569(5)	170.5
O(1W)-H(1WA)...O(5)	0.85	2.42	2.911(8)	117.8
O(1W)-H(1WB)...O(3)	0.85	2.01	2.863(7)	178.9
O(2W)-H(2WA)...O(2)	0.85	1.93	2.775(8)	179.4

O(3W)-H(3WA)...O(7)	0.85	1.82	2.668(9)	178.3
O(3W)-H(3WB)...O(5W)	0.85	2.27	2.82(2)	122.1
O(4W)-H(4WA)...O(2W)	0.85	2.23	2.836(12)	127.8
O(4W)-H(4WB)...O(3W)	0.85	1.89	2.742(13)	177.3
O(6W)-H(6WA)...O(7W)	0.85	2.14	2.65(2)	118.5
O(8W)-H(8WA)...O(7W)	0.85	1.86	2.71(2)	178.9
Compound 4				
O(3)-H(3A)...O(7)#1	0.82	1.77	2.553(9)	158.9
O(9)-H(9A)...O(1)#2	0.82	1.80	2.591(8)	160.8
Compound 5				
O(1)-H(1A)...O(4)#1	0.82	1.87	2.678(2)	170.9
Compound 6				
O(2)-H(2A)...O(3)#1	0.82	1.81	2.630(9)	179.8
O(8)-H(8B)...O(7)#2	0.82	1.76	2.557(7)	165.2
O(1W)-H(1WA)...O(3)#3	0.85	1.84	2.648(8)	158.6
O(1W)-H(1WB)...O(5)	0.85	2.25	2.691(9)	112.1
Compound 7				
O(1)-H(1A)...O(3)#1	0.82	1.80	2.579(8)	158.6
O(1W)-H(1WA)...O(2)	0.85	2.12	2.969(15)	175.8
Compound 9				
O(2)-H(2A)...O(4)	0.82	1.91	2.711(2)	163.6
O(1W)-H(1WB)...O(3)	0.85	1.98	2.835(2)	179.8
Compound 11				
O(2)-H(2A)...O(1W)	0.82	1.77	2.583(4)	172.0
O(9)-H(9B)...O(1)	0.82	1.81	2.627(3)	173.7
O(1W)-H(1WA)...O(4W)	0.85	1.91	2.704(5)	155.7
O(1W)-H(1WB)...O(10)#1	0.85	1.90	2.747(5)	177.1
O(3W)-H(3WA)...O(2W)#2	0.85	1.97	2.774(5)	158.5
O(3W)-H(3WB)...O(11)	0.85	1.98	2.835(4)	179.5
O(4W)-H(4WB)...O(6)#3	0.85	2.40	2.829(5)	111.7
O(4W)-H(4WA)...O(3W)	0.85	1.88	2.673(5)	154.3
Compound 12				
O(2)-H(2A)...O(6)#2	0.82	1.95	2.768(7)	174.6
O(12)-H(12)...O(10)#1	0.82	2.23	2.801(6)	126.9
O(2W)-H(2WA)...O(5)	0.85	2.05	2.899(10)	177.4

O(2W)-H(2WB)...O(1W)	0.85	2.28	2.836(15)	123.0

Symmetry transformations used to generate equivalent atoms:

For **4**: #1 x+1, y, z; #2 x-1, y, z.

For **5**: #1 -x+1/2, y-1/2, -z+1/2.

For **6**: #1 -x, -y+1, -z; #2 -x+2, -y, -z+1; #3 x+1, y, z.

For **7**: #1 -x, -y+2, -z+1.

For **11**: #1 x, y+1, z; #2 –x-1, -y, z-1/2; #3 –x-1, -y+1, z-1/2.

For **12**: #1 -x+1, -y+1/2, -z+1/2. #2 –x+2, -y+2, -z.

Table S3. π…π interactions between the aromatic rings for compounds **3**-**12**

Compound	Aromatic rings involved	Dihedral angle (^{o})	Distance (Å)
3	[C(1), C(2), C(3), C(4), C(5), C(6)]…[C(43), C(44), C(45), C(46), C(47), N(7)]#1	18.4	3.837
	[C(7), C(8), C(9), C(10), C(11), C(12)]…[C(13), C(14), C(15), C(16), C(17), N(1)]#2	9.8	3.692
	[C(13), C(14), C(15), C(16), C(17), N(1)]…[C(18), C(19), C(20), C(21), C(22), N(2)]#2	3.0	3.923
	[C(43), C(44), C(45), C(46), C(47), N(7)]…[C(48), C(49), C(50), C(51), C(52), N(8)]#1	6.5	3.758
4	[C(13), C(14), C(15), C(16), C(17), N(1)]…[C(28), C(29), C(30), C(31), C(32), N(4)]#1	7.4	4.000
	[C(18), C(19), C(20), C(21), C(22), N(2)]…[C(28), C(29), C(30), C(31), C(32), N(4)]#2	4.3	3.934
	[C(28), C(29), C(30), C(31), C(32), N(4)]…[C(13), C(14), C(15), C(16), C(17), N(1)]#3	7.4	4.000
	[C(28), C(29), C(30), C(31), C(32), N(4)]…[C(18), C(19), C(20), C(21), C(22), N(2)]#4	4.3	3.934
5	[C(10), C(11), C(12), C(13), C(17), C(18)]…[C(10), C(11), C(12), C(13), C(17), C(18)]#1	0	3.594
	[C(13), C(14), C(15), C(16), C(17), N(1)]…[C(13), C(14), C(15), C(16), C(17), N(1)]#2	0	3.605
6	[C(16), C(17), C(18), C(19), C(23), C(24)]…[C(16), C(17), C(18), C(19), C(23), C(24)]#1	0	3.810
	[C(19), C(20), C(21), C(22), C(23), N(2)]…[C(19), C(20), C(21), C(22), C(23), N(2)]#2	0	3.759
	[C(25), C(26), C(27), C(28), C(30), N(3)]…[C(25), C(26), C(27), C(28), C(30), N(3)]#3	0	3.455
	[C(28), C(29), C(30), C(31), C(35), C(36)]…[C(28), C(29), C(30), C(31), C(35), C(36)]#4	1.4	3.567

7	[C(10), C(11), C(12), C(13), C(17), C(18)]…[C(10), C(11), C(12), C(13), C(17), C(18)]#1	0	3.626
	[C(13), C(14), C(15), C(16), C(17), N(2)]…[C(13), C(14), C(15), C(16), C(17), N(2)]#2	0	3.741
8	[C(1), C(2), C(3), C(4), C(5), C(6)]…[C(7), C(8), C(9), C(10), C(11), N(1)]#1	22	3.950
	[C(7), C(8), C(9), C(10), C(11), N(1)]…[C(17), C(18), C(19), C(20), C(21), N(3)]#2	6.5	3.526
9	[C(1), C(2), C(3), C(4), C(5), C(6)]…[C(1), C(2), C(3), C(4), C(5), C(6)]#1	0	4.320
	[C(7), C(8), C(9), C(10), C(11), N(1)]…[C(12), C(13), C(14), C(15), C(16), N(2)]#2	7.1	4.214
	[C(7), C(8), C(9), C(10), C(11), N(1)]…[C(17), C(18), C(19), C(20), C(21), N(3)]#3	3.7	3.545
	[C(17), C(18), C(19), C(20), C(21), N(3)]…[C(7), C(8), C(9), C(10), C(11), N(1)]#4	3.7	3.545
10	[C(1), C(2), C(3), C(4), C(5), C(6)]…[C(1), C(2), C(3), C(4), C(5), C(6)]#1	0	3.570
	[C(7), C(8), C(9), C(10), C(11), N(1)]…[C(12), C(13), C(14), C(15), C(16), N(2)]#2	2.4	3.611
	[C(12), C(13), C(14), C(15), C(16), N(2)]…[C(12), C(13), C(14), C(15), C(16), N(2)]#3	0	3.541
11	[C(1), C(2), C(3), C(4), C(5), C(6)]…[C(18), C(19), C(20), C(21), C(22), N(2)]#1	8.5	3.615
	[C(1), C(2), C(3), C(4), C(5), C(6)]…[C(23), C(24), C(25), C(26), C(27), N(3)]#2	10.9	3.734
	[C(18), C(19), C(20), C(21), C(22), N(2)]…[C(23), C(24), C(25), C(26), C(27), N(3)]#3	4.1	4.344
12	[C(19), C(20), C(21), C(22), C(23), N(2)]…[C(28), C(29), C(30), C(31), C(35), C(36)]#1	1.4	3.621

Symmetry transformations used to generate equivalent atoms:

For **3**: #1 2-x, 2-y, 1-z; #2 1-x, 2-y, 2-z.

For **4**: #1 0.5-x, -0.5+y, 0.5-z; #2 1.5-x, -0.5+y, 0.5-z; #3 0.5-x, 0.5+y, 0.5-z; #4 1.5-x, 0.5+y, 0.5-z. For **5**: #1 1-x, y, -0.5-z; #2 1-x, -y, -z.

For **6**: #1 1-x, -y, -z; #2 2-x, -y, -z; #3 1-x, 1-y, 1-z; #4 –x, 1-y, 1-z.

For **7**: #1 2-x, 1-y, 1-z; #2 1-x, 1-y, 1-z.

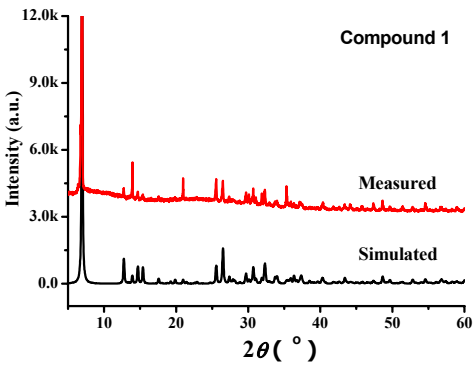
For **8**: #1 1-x, 1-y, 1-z; #2 -1+x, y, z.

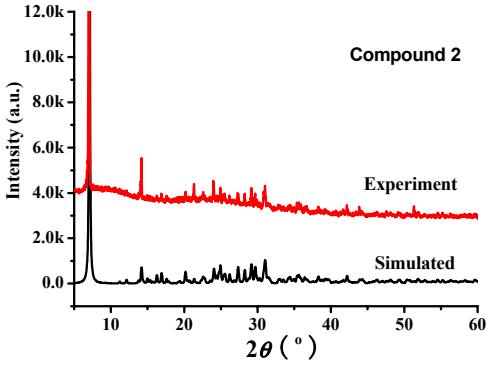
For **9**: #1 2-x, 3-y, 1-z; #2 1-x, 2-y, -z; #3 1+x, y, z; #4 -1+x, y, z.

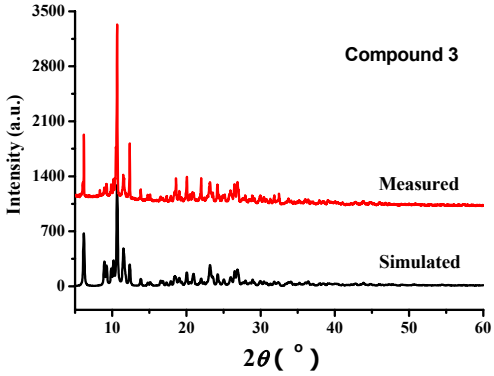
For **10**: #1 2-x, 2-y, 1-z; #2 1-x, 1-y, 1-z; #3 1-x, 2-y, 1-z.

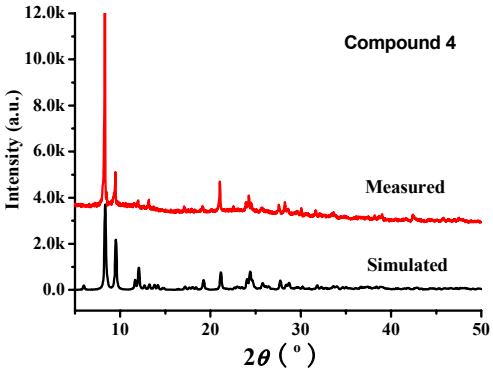
For **11**: #1 0.5+x, 1.5-y, z; #2 x, 1+y, z; #3 -0.5+x, 1.5-y, z.

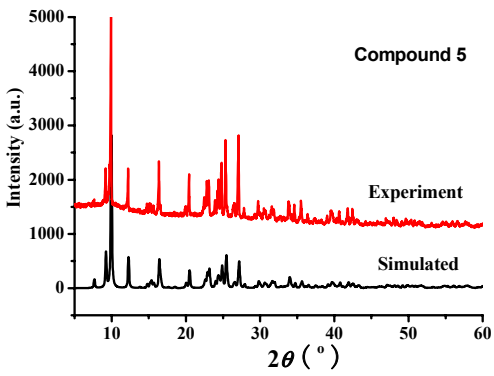
For **12**: #1 x, 1+y, z.

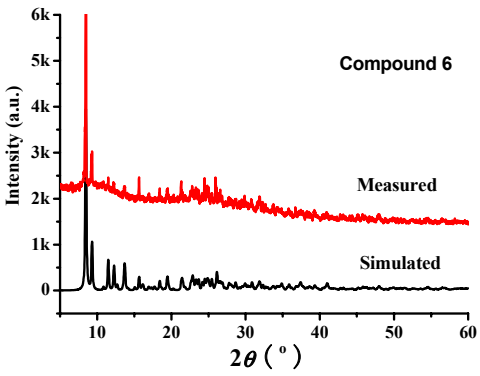

Compound 1
Measured
Simulated
Intensity (a.u.)
12.0k
9.0k
6.0k
3.0k
0.0
10
20
30
40
50
60
2θ(°)

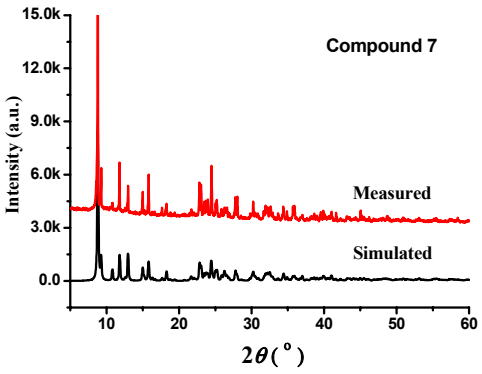

Compound 2
Experiment
Simulated
Intensity (a.u.)
12.0k
10.0k
8.0k
6.0k
4.0k
2.0k
0.0
10
20
30
40
50
60
2θ(°)

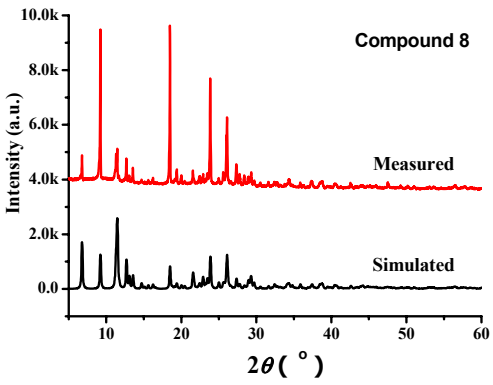

Compound 3
Measured
Simulated
Intensity (a.u.)
3500
2800
2100
1400
700
0
10
20
30
40
50
60
2θ(°)


Compound 4
Measured
Simulated
Intensity (a.u.)
12.0k
10.0k
8.0k
6.0k
4.0k
2.0k
0.0
10
20
30
40
50
2θ(°)


Compound 5
Experiment
Simulated
Intensity (a.u.)
5000
4000
3000
2000
1000
0
10
20
30
40
50
60
2θ(°)


Compound 6
Measured
Simulated
Intensity (a.u.)
6k
5k
4k
3k
2k
1k
0
10
20
30
40
50
60
2θ(°)


Compound 7
Measured
Simulated
Intensity (a.u.)
15.0k
12.0k
9.0k
6.0k
3.0k
0.0
10
20
30
40
50
60
2θ(°)


Compound 8
Measured
Simulated
Intensity (a.u.)
10.0k
8.0k
6.0k
4.0k
2.0k
0.0
10
20
30
40
50
60
2θ(°)

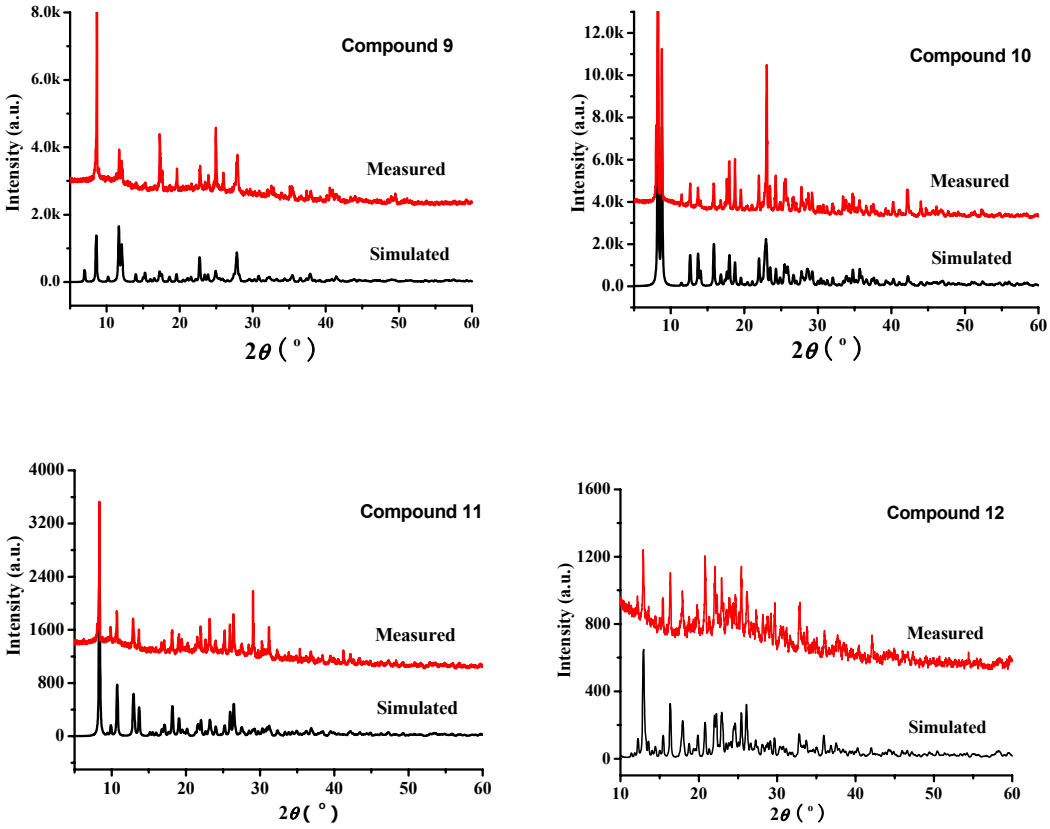
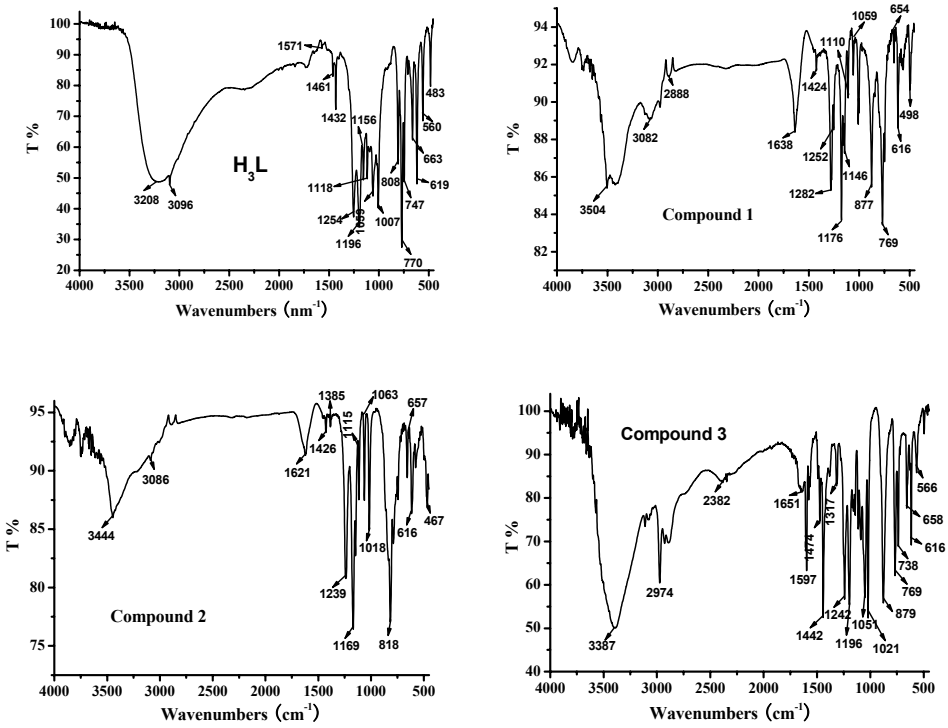


Figure S1. Simulated and measured XRD powder patterns for compounds **1-12.**



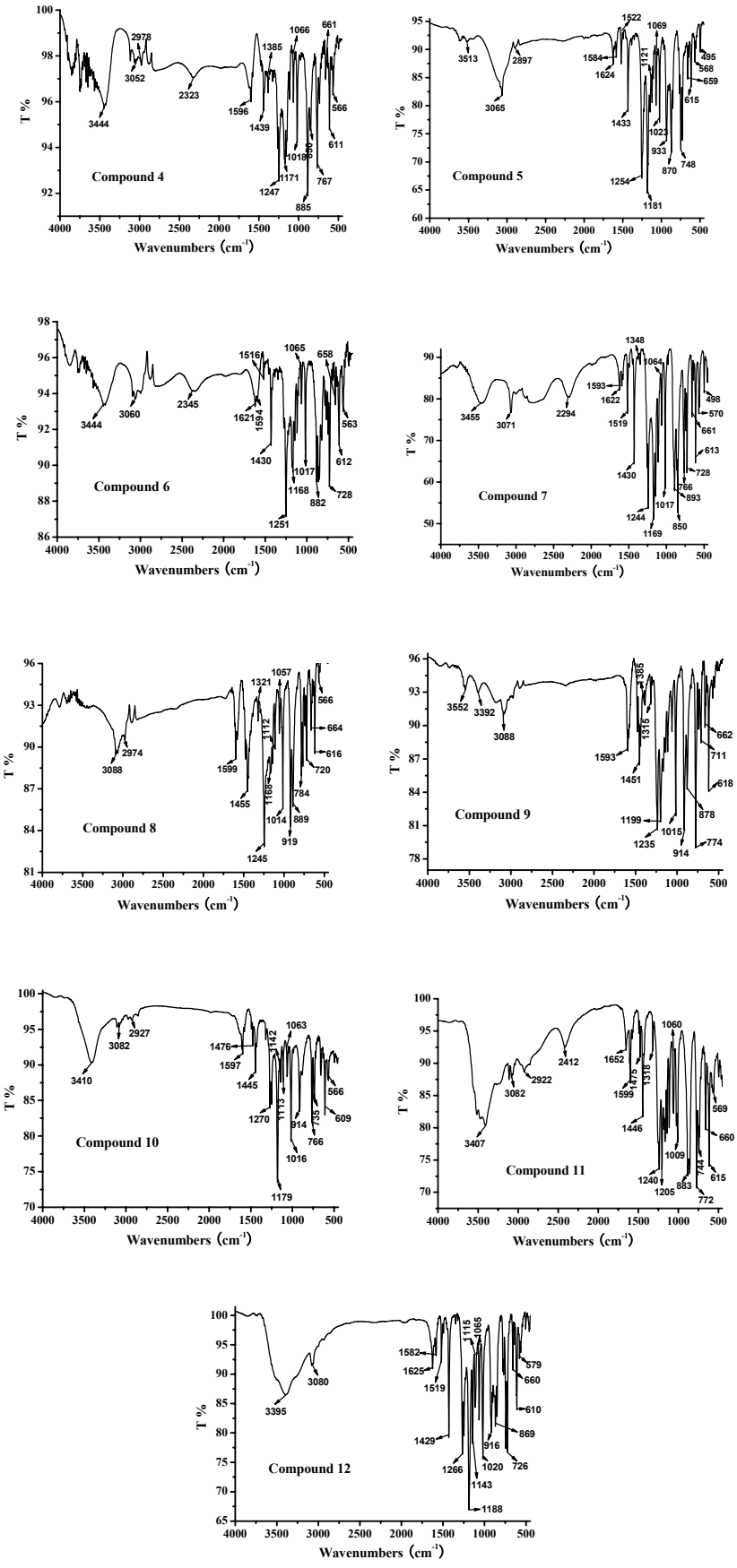
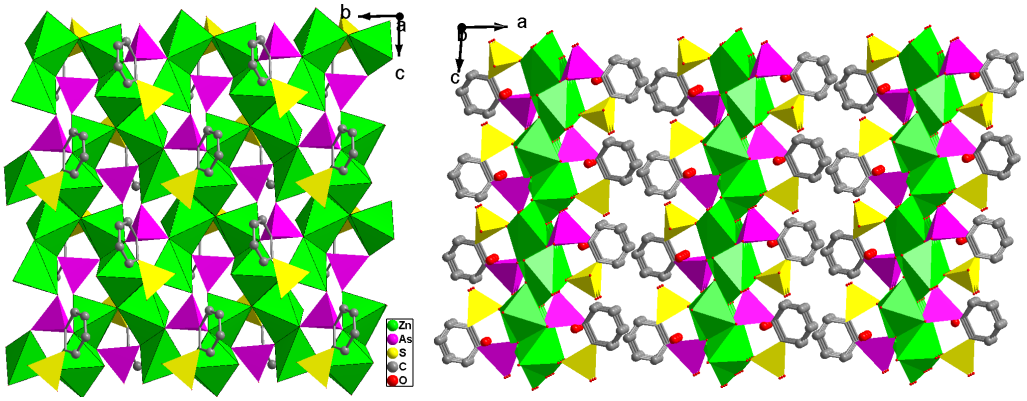


Figure S2. The IR spectra of ligand **H_3L** and compounds **1-12**. Their IR data (KBr, cm^{-1}) are

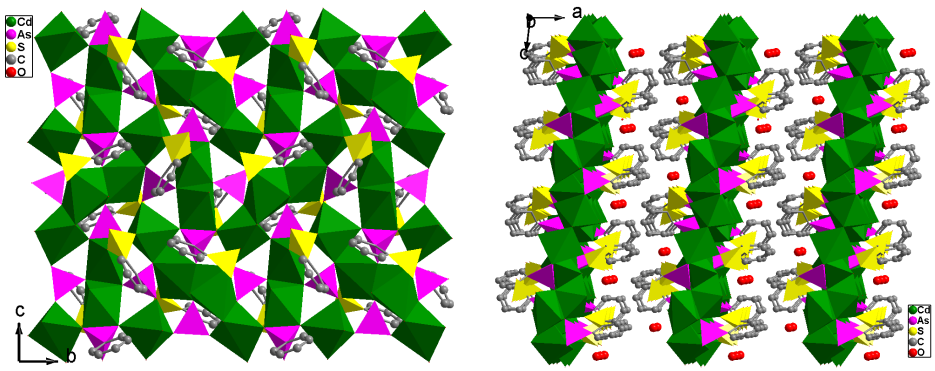
shown as follows: For **1**: 3504 (s), 3082 (w), 2888 (w), 1638 (m), 1424 (w), 1282 (s), 1252 (m), 1176 (vs), 1146 (m), 1110 (m), 1059 (m), 1010 (m), 877 (s), 769 (vs), 747 (m), 654 (w), 616 (m), 568 (w), 498 (m). For **2**: 3444 (m), 3086 (w), 1621 (m), 1426 (w), 1385 (w), 1239 (s), 1169 (vs), 1147 (m), 1115 (m), 1063 (m), 1018 (s), 818 (vs), 789 (m), 745 (w), 657 (m), 616 (m), 577 (w), 467 (w). For **3**: 3387 (vs), 3111 (w), 2974 (m), 2382 (w), 1651 (w), 1606 (w), 1597 (s), 1577 (w), 1567 (w), 1491 (w), 1474 (m), 1442 (vs), 1383 (w), 1317 (m), 1242 (s), 1196 (s), 1158 (w), 1142 (w), 1113 (m), 1090 (m), 1051 (s), 1021 (vs), 879 (vs), 769 (s), 738 (m), 658 (m), 616 (m), 566 (m), 497 (w). For **4**: 3444 (m), 3116 (w), 3052 (w), 2978 (w), 2323 (w), 1596 (m), 1439 (m), 1385 (m), 1327 (w), 1263 (m), 1247 (s), 1171 (s), 1153 (m), 1114 (m), 1066 (m), 1018 (s), 885 (vs), 850 (m), 767 (vs), 738 (m), 661 (m), 611 (m), 566 (m), 497 (w). For **5**: 3513 (w), 3065 (m), 2897 (w), 1624 (m), 1584 (w), 1522 (m), 1493 (w), 1433 (m), 1385 (w), 1349 (w), 1254 (vs), 1181 (vs), 1146 (w), 1121 (w), 1105 (w), 1069 (m), 1023 (m), 933 (s), 870 (s), 852 (w), 764 (w), 748 (s), 729 (m), 659 (m), 644 (w), 615 (m), 568 (w), 555 (w), 495 (m). For **6**: 3444 (w), 3060 (w), 2345 (w), 1621 (w), 1594 (w), 1516 (w), 1430 (m), 1346 (w), 1276 (w), 1251 (vs), 1168 (m), 1142 (w), 1116 (m), 1065 (m), 1017 (s), 882 (s), 861 (s), 848 (s), 820 (w), 781 (w), 766 (m), 742 (m), 728 (s), 658 (m), 612 (m), 563 (m). For **7**: 3455 (w), 3071 (m), 2771 (w), 2294 (w), 1622 (w), 1593 (w), 1579 (w), 1519 (m), 1495 (w), 1452 (w), 1430 (s), 1348 (w), 1257 (m), 1244 (vs), 1169 (vs), 1144 (m), 1112 (m), 1104 (w), 1064 (m), 1017 (s), 979 (w), 893 (s), 865 (w), 850 (vs), 766 (s), 742 (m), 728 (s), 661 (m), 640 (w), 613 (s), 570 (m), 561 (m), 498 (m), 455 (w). For **8**: 3088 (m), 2974 (w), 2888 (w), 1599 (m), 1579 (w), 1478 (w), 1455 (s), 1321 (w), 1245 (vs), 1168 (w), 1140 (w), 1112 (m), 1057 (m), 1014 (s), 919 (s), 889 (s), 784 (m), 766 (m), 741 (m), 720 (m), 664 (m), 616 (m), 566 (w). For **9**: 3552 (w), 3392 (w), 3088 (w), 2332 (w), 1593 (m), 1581 (w), 1477 (m), 1451 (m), 1441 (w), 1385 (w), 1315 (m), 1235 (s), 1199 (s), 1166 (w), 1142 (w), 1112 (m), 1061 (m), 1015 (s), 970 (w), 914 (s), 878 (m), 774 (vs), 740 (m), 711 (m), 662 (m), 637 (w), 618 (s), 568 (w), 549 (w). For **10**: 3410 (m), 3082 (w), 2927 (w), 1597 (m), 1499 (w), 1476 (w), 1445 (m), 1319 (w), 1270 (m), 1250 (m), 1179 (vs), 1142 (m), 1112 (m), 1063 (m), 1043 (w), 1016 (s), 914 (m), 889 (w), 880 (w), 766 (s), 735 (m), 660 (m), 609 (m), 566 (w), 495 (w). For **11**: 3407 (m), 3113 (w), 3082 (w), 2922 (w), 2412 (w), 1652 (w), 1599 (m), 1576 (w), 1492 (w), 1475 (m), 1446 (m), 1318 (m), 1240 (s), 1205 (s), 1166 (m), 1142 (m), 1114 (m), 1114 (m), 1060 (m), 1024 (w), 1009 (s), 883 (s), 858 (s), 772 (vs), 744 (m), 660 (m), 615 (s), 569 (w), 496 (w). For **12**: 3395 (m), 3080

(w), 1625 (m), 1583 (w), 1519 (m), 1495 (w), 1429 (s), 1346 (w), 1266 (s), 1249 (m), 1188 (vs), 1143 (m), 1115 (m), 1065 (m), 1020 (s), 916 (m), 869 (m), 849 (m), 778 (m), 769 (m), 743 (s), 726 (s), 660 (m), 643 (w), 610 (m), 579 (m), 564 (w), 505 (w), 462 (w).



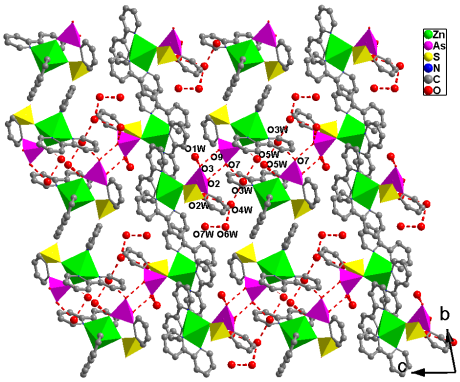
(a) (b)

Figure S3. (a) A metal sulfonate-arsonate layer in **1**. (b) View of the 3D supra-molecular structure of compound **1**. The CSO_3, $CAsO_3$ tetrahedra and ZnO_x (x = 5, 6) polyhedra are shaded in yellow, purple, and bright green, respectively.

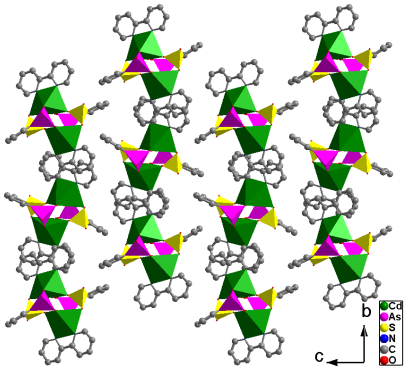


(a) (b)

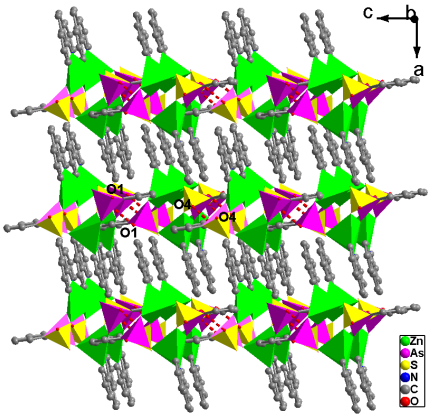
Figure S4. (a) A metal sulfonate-arsonate layer in **2**. (b) View of the 3D supra-molecular structure of compound **2**. The CdO_6 octahedra, CSO_3 and $CAsO_3$ tetrahedra are shaded in green, yellow and pink, respectively.



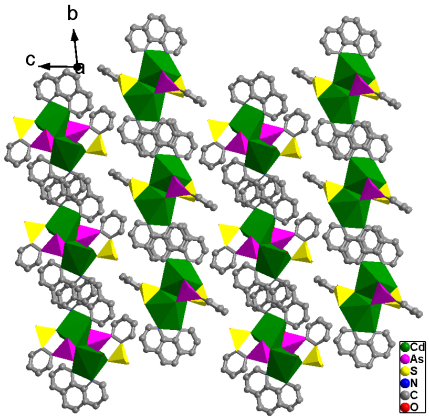
Compound **3**



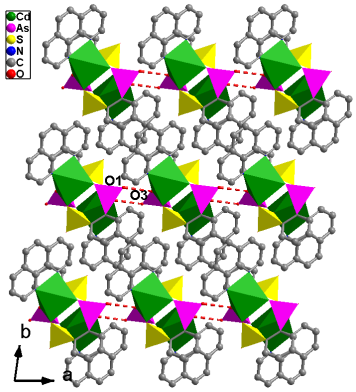
Compound **4**



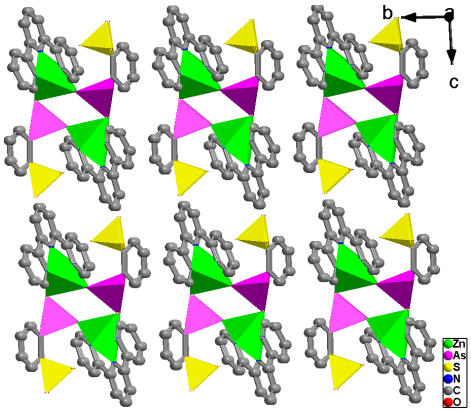
Compound **5**



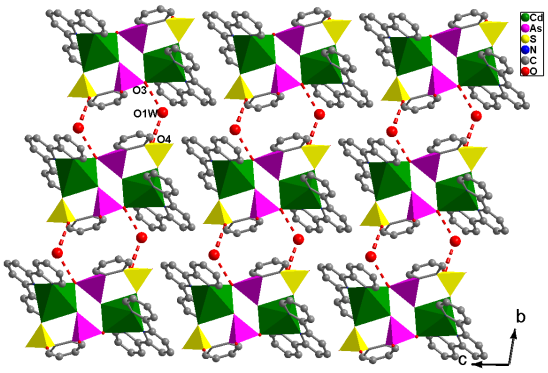
Compound **6**

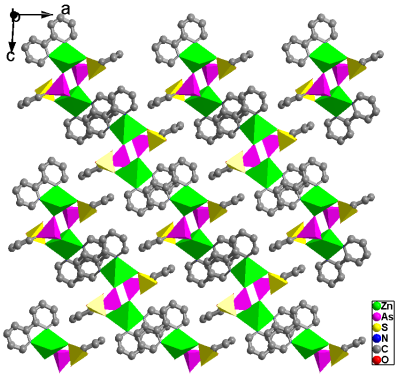


Compound **7**



Compound **8**





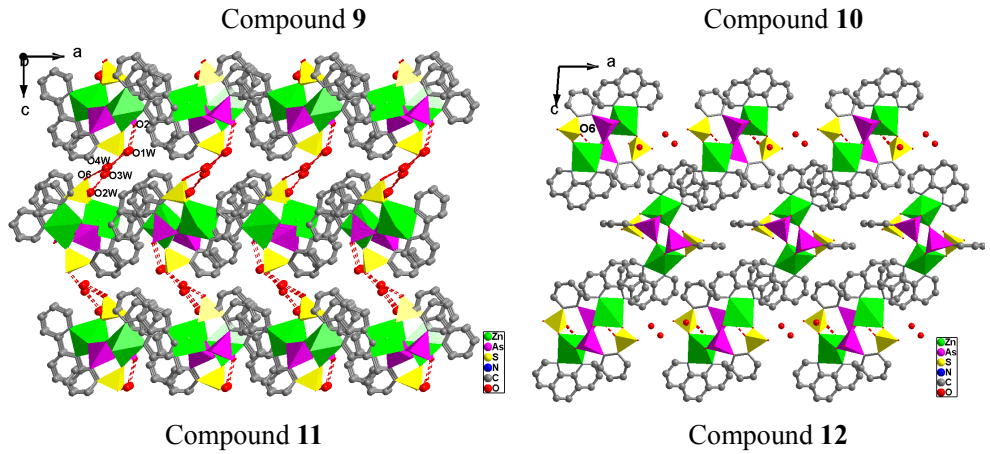


Figure S5. View of the 3D supra-molecular structures of compounds **3-12**. Hydrogen bonds are drawn as dashed lines. The CSO_3, $CAsO_3$ tetrahedra and ZnO_xN_y (CdO_xN_y) polyhedra are shaded in yellow, purple, and bright green (green), respectively.

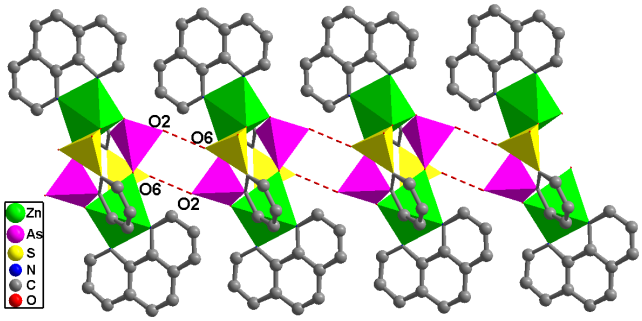
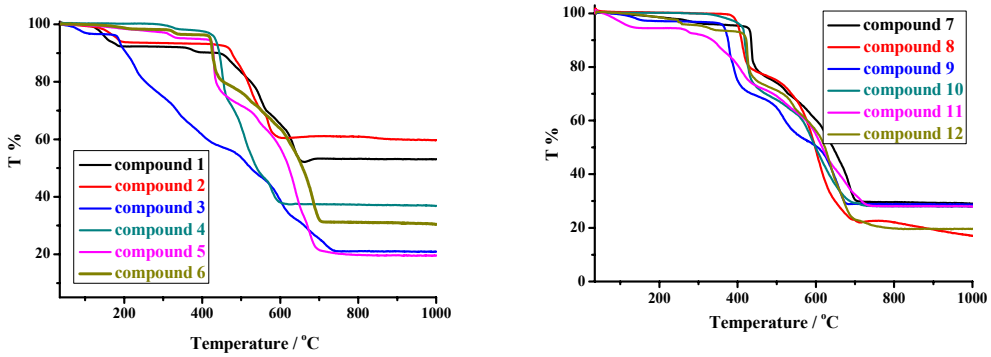


Figure S6. View of a hydrogen-bonded 1D chain in compound **12**.



(a) (b)

Figure S7. TGA curves for compounds **1-12**.