# Solvent-cooperatively directed iodoargentate hybrids: structures and optical properties

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Supporting Information (SI)

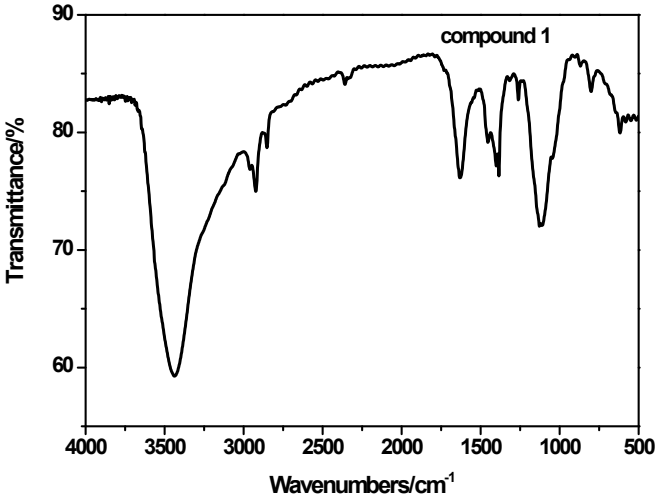
**Table. S1** Selected bond lengths (Å) and angles (°) for **1**-**7**.

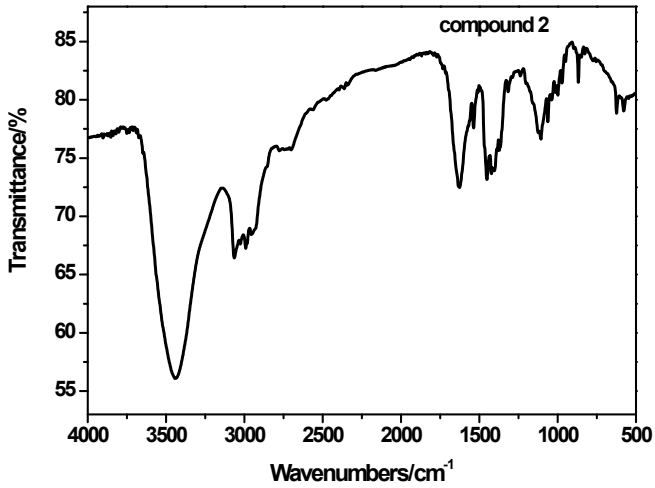
| | | | |
|---|---|---|---|
| Compound **1** | | | |
| Ag(1)-I(2) | 2.7733(9) | Ag(1)-I(3) | 2.9021(8) |
| Ag(1)-I(1) | 2.8413(8) | Ag(1)-I(5)#1 | 2.9211(9) |
| Ag(2)-I(6) | 2.7845(10) | Ag(2)-I(5) | 2.8570(9) |
| Ag(2)-I(4) | 2.8060(8) | Ag(2)-I(3) | 3.0573(9) |
| I(2)-Ag(1)-I(1) | 114.87(3) | I(2)-Ag(1)-I(5)#1 | 111.26(3) |
| I(2)-Ag(1)-I(3) | 107.15(3) | I(1)-Ag(1)-I(5)#1 | 103.46(3) |
| I(1)-Ag(1)-I(3) | 101.79(3) | I(3)-Ag(1)-I(5)#1 | 118.23(3) |
| I(6)-Ag(2)-I(4) | 106.28(3) | I(6)-Ag(2)-I(3) | 113.49(3) |
| I(6)-Ag(2)-I(5) | 118.22(3) | I(4)-Ag(2)-I(3) | 102.59(3) |
| I(4)-Ag(2)-I(5) | 122.30(3) | I(5)-Ag(2)-I(3) | 91.94(2) |
| Compound **2** | | | |
| Ag(1)-I(3) | 2.8173(7) | Ag(1)-I(2) | 2.9030(6) |
| Ag(1)-I(1) | 2.8451(6) | Ag(1)-I(2)#1 | 2.8730(6) |
| I(3)-Ag(1)-I(1) | 105.719(19) | I(3)-Ag(1)-I(2) | 114.134(19) |
| I(3)-Ag(1)-I(2)#1 | 116.62(2) | I(1)-Ag(1)-I(2) | 114.90(2) |
| I(1)-Ag(1)-I(2)#1 | 109.654(19) | I(2)#1-Ag(1)-I(2) | 95.976(17) |
| Compound **3** | | | |
| Ag(1)-I(5) | 2.7770(10) | Ag(1)-I(2) | 2.8834(11) |
| Ag(1)-I(4) | 2.8759(11) | Ag(1)-I(1) | 2.8970(11) |
| Ag(2)-I(3) | 2.7897(10) | Ag(2)-I(2) | 2.8628(11) |
| Ag(2)-I(7) | 2.8100(8) | Ag(2)-I(1) | 2.8834(10) |
| Ag(3)-I(6) | 2.7650(10) | Ag(3)-I(4) | 2.9246(12) |
| Ag(3)-I(1) | 2.9065(11) | Ag(3)-I(3) | 2.9578(11) |
| Ag(4)-I(8) | 2.7700(10) | Ag(4)-I(4) | 2.9449(12) |
| Ag(4)-I(3) | 2.8788(12) | Ag(4)-I(2) | 2.9963(12) |
| Ag(1)-Ag(2) | 3.2720(12) | Ag(1)-Ag(3) | 3.3462(12) |
| Ag(2)-Ag(3) | 3.0785(12) | Ag(2)-Ag(4) | 3.1904(12) |
| Ag(3)-Ag(4) | 3.2558(13) | | |
| I(5)-Ag(1)-I(4) | 111.72(3) | I(5)-Ag(1)-I(1) | 107.41(3) |
| I(5)-Ag(1)-I(2) | 116.68(4) | I(4)-Ag(1)-I(1) | 106.17(3) |
| I(4)-Ag(1)-I(2) | 108.76(3) | I(2)-Ag(1)-I(1) | 105.41(3) |
| I(3)-Ag(2)-I(7) | 111.70(3) | I(3)-Ag(2)-I(1) | 114.97(3) |
| I(3)-Ag(2)-I(2) | 111.06(3) | I(7)-Ag(2)-I(1) | 99.42(3) |
| I(7)-Ag(2)-I(2) | 112.84(3) | I(2)-Ag(2)-I(1) | 106.31(3) |

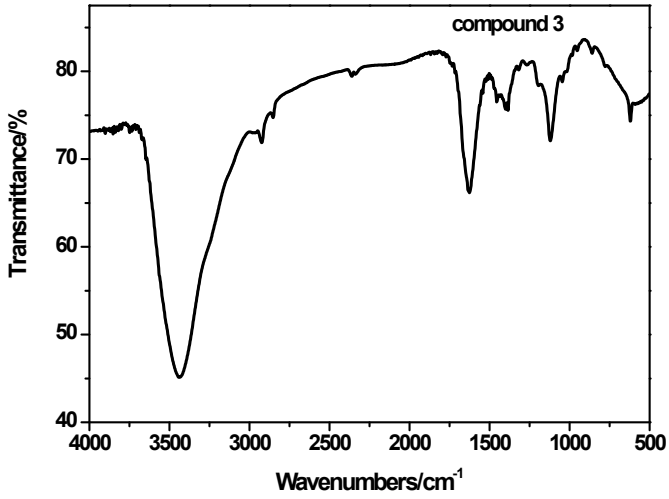
| | | | |
|---|---|---|---|
| I(6)-Ag(3)-I(1) | 123.65(4) | I(6)-Ag(3)-I(3) | 101.74(3) |
| I(6)-Ag(3)-I(4) | 108.06(3) | I(1)-Ag(3)-I(3) | 109.32(3) |
| I(1)-Ag(3)-I(4) | 104.66(3) | I(4)-Ag(3)-I(3) | 108.89(4) |
| I(8)-Ag(4)-I(3) | 117.68(4) | I(8)-Ag(4)-I(2) | 109.08(3) |
| I(8)-Ag(4)-I(4) | 109.64(3) | I(3)-Ag(4)-I(2) | 104.96(3) |
| I(3)-Ag(4)-I(4) | 110.52(4) | I(4)-Ag(4)-I(2) | 103.99(3) |
| Compound **4** | | | |
| Ag(1)-I(1)#1 | 2.8069(13) | Ag(1)-I(2)#2 | 2.8763(7) |
| Ag(1)-I(1) | 2.8514(13) | Ag(1)-I(2) | 2.8763(7) |
| I(1)#1-Ag(1)-I(1) | 109.96(4) | I(1)#1-Ag(1)-I(2) | 112.90(3) |
| I(1)#1-Ag(1)-I(2)#2 | 112.90(3) | I(1)-Ag(1)-I(2) | 105.76(3) |
| I(1)-Ag(1)-I(2)#2 | 105.76(3) | I(2)#2-Ag(1)-I(2) | 109.07(4) |
| Compound **5** | | | |
| Ag(1)-I(2) | 2.8242(9) | Ag(1)-I(3)#1 | 2.8460(9) |
| Ag(1)-I(1) | 2.8322(9) | Ag(1)-I(3) | 2.9095(10) |
| I(2)-Ag(1)-I(1) | 104.07(3) | I(2)-Ag(1)-I(3) | 108.64(3) |
| I(2)-Ag(1)-I(3)#1 | 115.37(3) | I(1)-Ag(1)-I(3) | 111.29(3) |
| I(1)-Ag(1)-I(3)#1 | 111.63(3) | I(3)#1-Ag(1)-I(3) | 105.92(3) |
| Compound **6** | | | |
| Ag(1)-I(1) | 2.9564(6) | Ag(1)-I(2) | 2.8338(6) |
| Ag(1)-I(6) | 2.8300(6) | Ag(1)-I(6)#1 | 2.8741(6) |
| Ag(2)-I(5)#1 | 2.8518(6) | Ag(2)-I(2) | 2.8185(6) |
| Ag(2)-I(1) | 2.9885(6) | Ag(2)-I(3) | 2.8220(6) |
| Ag(3)-I(1) | 2.9868(6) | Ag(3)-I(4) | 2.8358(6) |
| Ag(3)-I(3) | 2.8242(6) | Ag(3)-I(4)#1 | 2.8432(6) |
| Ag(4)-I(5) | 2.8223(6) | Ag(4)-I(3)#1 | 2.8909(6) |
| Ag(4)-I(4) | 2.8317(6) | Ag(4)-I(1) | 2.9269(6) |
| Ag(5)-I(6) | 2.8253(6) | Ag(5)-I(5) | 2.8508(6) |
| Ag(5)-I(2)#1 | 2.8485(6) | Ag(5)-I(1) | 2.9908(6) |
| Ag(1)-Ag(2) | 3.2039(7) | Ag(1)-Ag(5) | 3.2496(7) |
| Ag(2)-Ag(3) | 3.3540(7) | Ag(3)-Ag(4) | 3.1719(7) |
| Ag(4)-Ag(5) | 3.2238(7) | | |
| I(6)-Ag(1)-I(2) | 115.678(19) | I(6)-Ag(1)-I(1) | 111.367(18) |
| I(6)-Ag(1)-I(6)#1 | 109.548(19) | I(2)-Ag(1)-I(1) | 112.275(18) |
| I(2)-Ag(1)-I(6)#1 | 111.806(19) | I(6)#1-Ag(1)-I(1) | 94.139(16) |
| I(2)-Ag(2)-I(1) | 111.766(19) | I(2)-Ag(2)-I(3) | 114.149(18) |
| I(3)-Ag(2)-I(1) | 107.982(19) | I(2)-Ag(2)-I(5)#1 | 112.76(2) |
| I(5)#1-Ag(2)-I(1) | 94.949(16) | I(3)-Ag(2)-I(5)#1 | 113.55(2) |
| I(3)-Ag(3)-I(4) | 113.484(19) | I(3)-Ag(3)-I(1) | 107.968(19) |
| I(3)-Ag(3)-I(4)#1 | 113.04(2) | I(4)-Ag(3)-I(1) | 111.93(2) |
| I(4)-Ag(3)-I(4)#1 | 112.23(2) | I(4)#1-Ag(3)-I(1) | 96.961(16) |
| I(5)-Ag(4)-I(4) | 116.783(19) | I(5)-Ag(4)-I(1) | 113.215(19) |
| I(5)-Ag(4)-I(3)#1 | 108.821(19) | I(4)-Ag(4)-I(1) | 113.855(19) |
| I(4)-Ag(4)-I(3)#1 | 108.007(19) | I(3)#1-Ag(4)-I(1) | 93.308(16) |

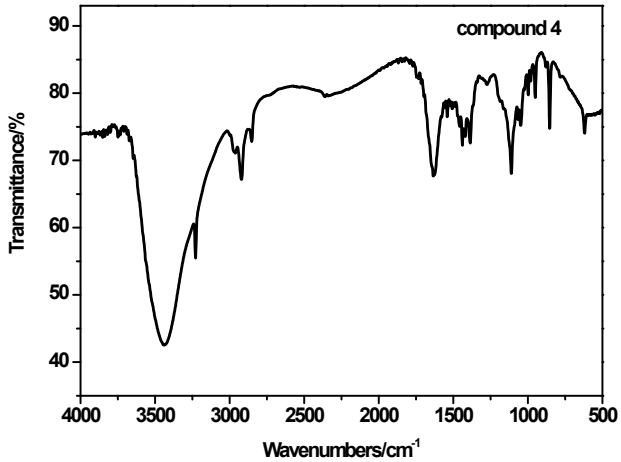
| | | | |
|---|---|---|---|
| I(6)-Ag(5)-I(2)#1 | 113.32(2) | I(6)-Ag(5)-I(1) | 110.499(19) |
| I(6)-Ag(5)-I(5) | 115.056(19) | I(2)#1-Ag(5)-I(1) | 96.732(16) |
| I(2)#1-Ag(5)-I(5) | 109.248(19) | I(5)-Ag(5)-I(1) | 110.503(19) |
| | | Compound **7** | |
| Ag(1)-I(3)#1 | 2.8175(4) | Ag(1)-I(3)#3 | 2.8468(4) |
| Ag(1)-I(2)#2 | 2.8284(4) | Ag(1)-I(1) | 2.9120(4) |
| Ag(2)-I(3) | 2.8311(4) | Ag(2)-I(1) | 2.8843(4) |
| Ag(2)-I(2) | 2.8794(4) | Ag(2)-I(1)#2 | 2.8971(4) |
| Ag(2)-Ag(2)#2 | 3.2572(6) | | |
| I(3)#1-Ag(1)-I(2)#2 | 113.505(12) | I(3)#1-Ag(1)-I(1) | 107.845(12) |
| I(3)#1-Ag(1)-I(3)#3 | 115.173(12) | I(2)#2-Ag(1)-I(1) | 104.974(12) |
| I(2)#2-Ag(1)-I(3)#3 | 107.096(12) | I(3)#3-Ag(1)-I(1) | 107.629(12) |
| I(3)-Ag(2)-I(2) | 106.877(12) | I(3)-Ag(2)-I(1)#2 | 116.618(12) |
| I(3)-Ag(2)-I(1) | 105.889(12) | I(2)-Ag(2)-I(1)#2 | 104.057(12) |
| I(2)-Ag(2)-I(1) | 112.022(12) | I(1)-Ag(2)-I(1)#2 | 111.418(11) |

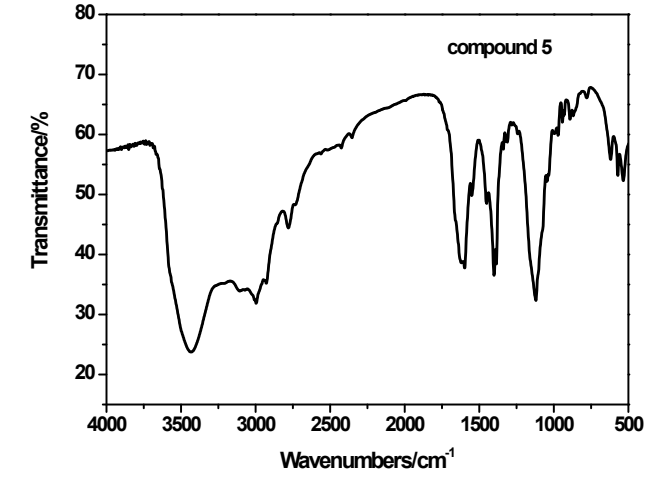
Symmetry code: for **1**: #1 -x+1, -y+1, -z+1; for **2**: #1 -x+1,-y+1,-z; for **3**: #1 x+0, -y+0, -z+1/2; #2 -x+1, -y+1/2, z+0; #3 -x+3/2, -y+1/2, -z+1/2; #4 -x+3/2, y+0, -z+0; for **4**: #1 x+1/2, y, -z+1/2; #2 -x+1, y+1/2, -z+1; #3 x-1/2, y, -z+1/2; #4 -x+1, -y, -z+1; #5 x, -y+3/2, z; for **5**: -x, -y, -z; for **6**: #1 x, -y+1/2, z-1/2; #2 x, -y+1/2, z+1/2; #3 -x+1, -y+1, -z+2; for **7**: #1 x, y+1, z; #2 -x+1, -y+2, -z+1; #3 -x+1, y+1/2, -z+3/2; #4 x, y-1, z; #5 -x+1, y-1/2, -z+3/2.

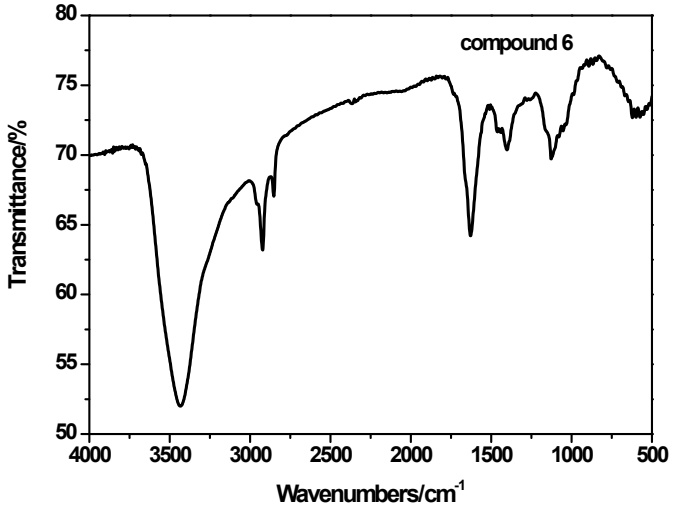



compound 2
Transmittance/%
85
80
75
70
65
60
55
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers/cm-1


compound 3
Transmittance/%
80
70
60
50
40
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers/cm-1


compound 4
Transmittance/%
90
80
70
60
50
40
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers/cm-1



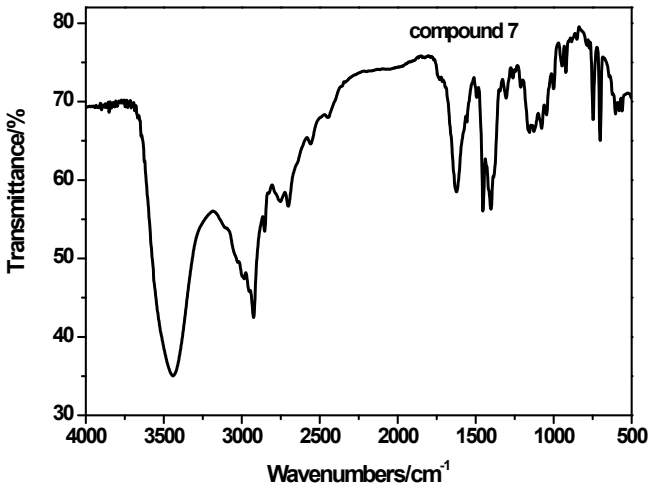
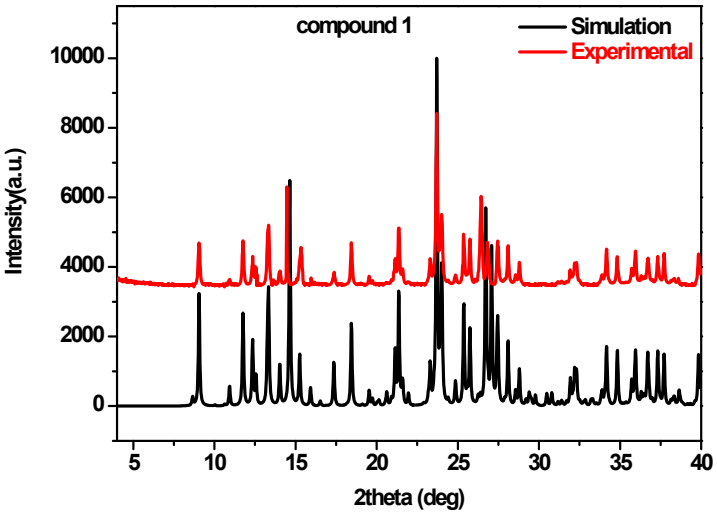
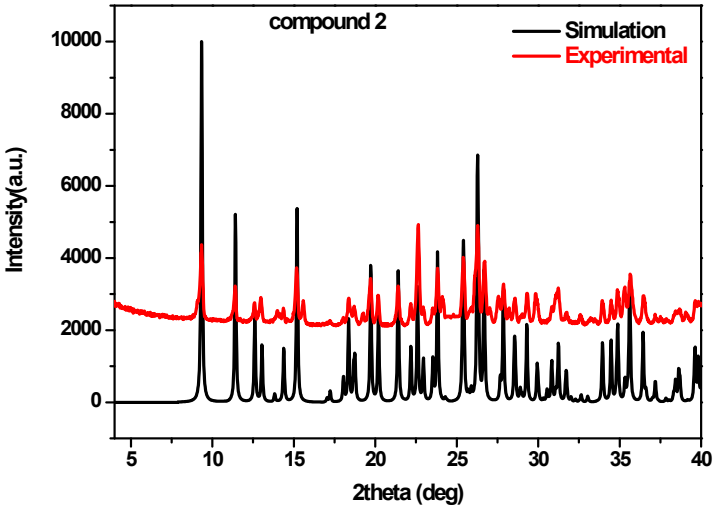
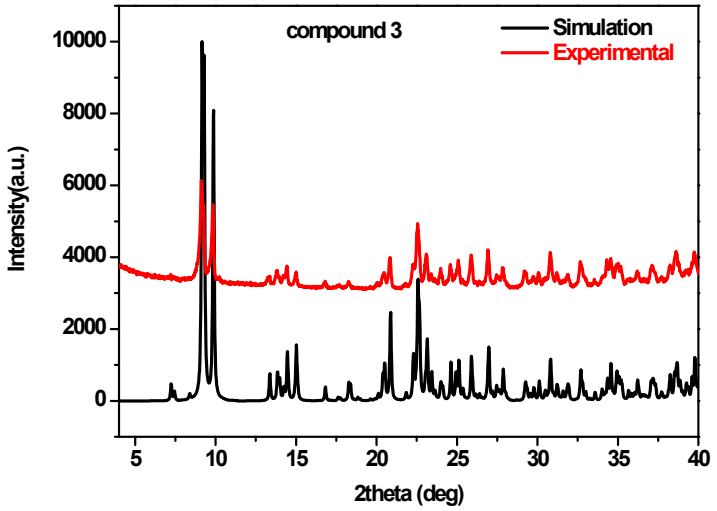
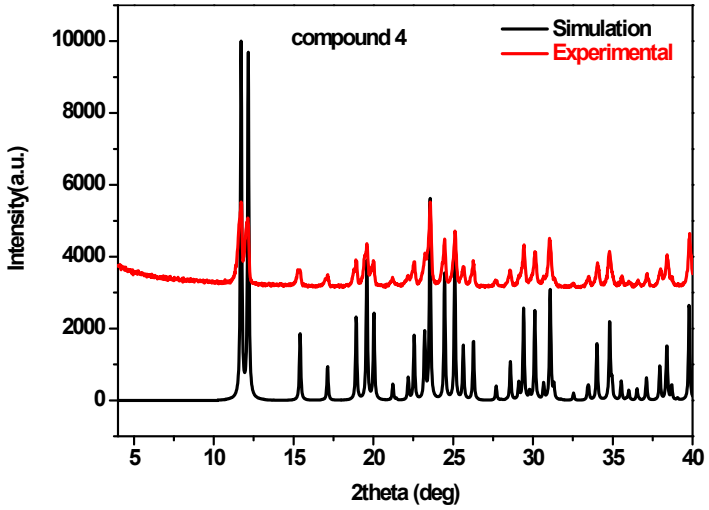



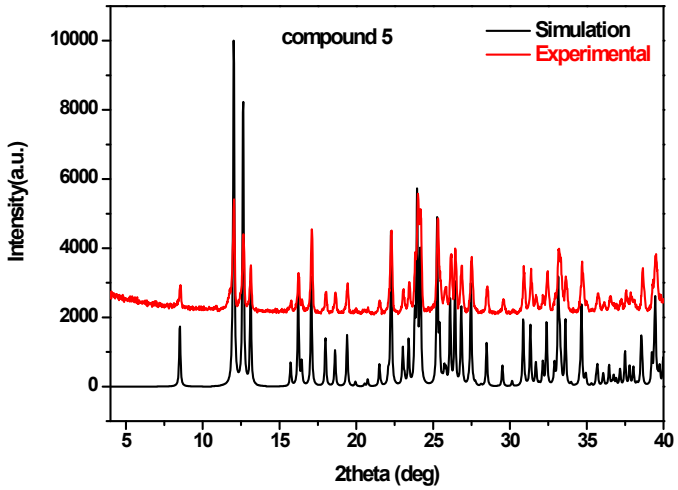

**Figure. S1** IR spectra for **1** -7

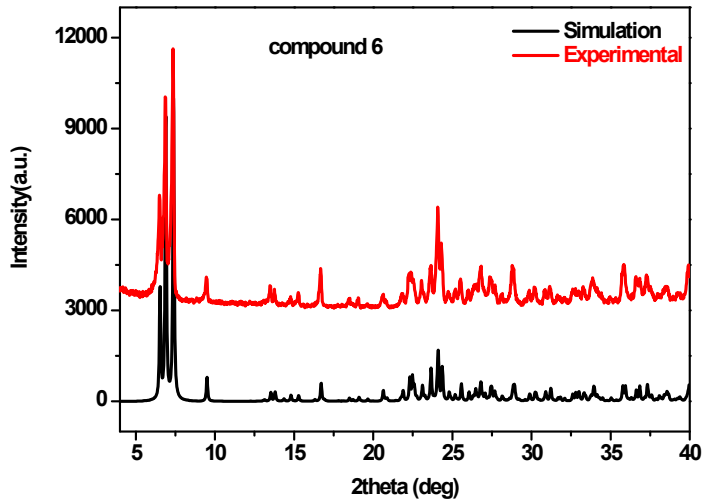

compound 1
Simulation
Experimental
Intensity(a.u.)
2theta (deg)
0
2000
4000
6000
8000
10000
5
10
15
20
25
30
35
40


compound 2
Simulation
Experimental
Intensity(a.u.)
2theta (deg)
0
2000
4000
6000
8000
10000
5
10
15
20
25
30
35
40


compound 3
Simulation
Experimental
Intensity(a.u.)
2theta (deg)
0
2000
4000
6000
8000
10000
5
10
15
20
25
30
35
40


compound 4
Simulation
Experimental
Intensity(a.u.)
2theta (deg)
0
2000
4000
6000
8000
10000
5
10
15
20
25
30
35
40


compound 5
Simulation
Experimental
Intensity(a.u.)
2theta (deg)
0
2000
4000
6000
8000
10000
5
10
15
20
25
30
35
40


compound 6
Simulation
Experimental
Intensity(a.u.)
2theta (deg)
0
3000
6000
9000
12000
5
10
15
20
25
30
35
40

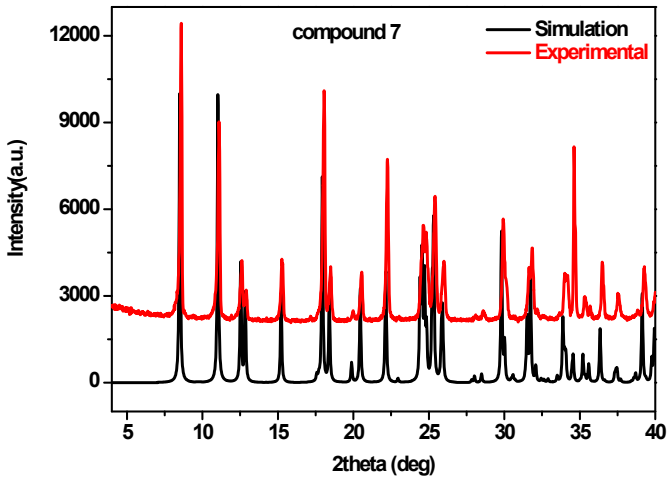



**Fig. S2** Experimental XRD patterns of compound **1**-**7** exposed in air (red) and simulation patterns of compound **1** - **7** (black).

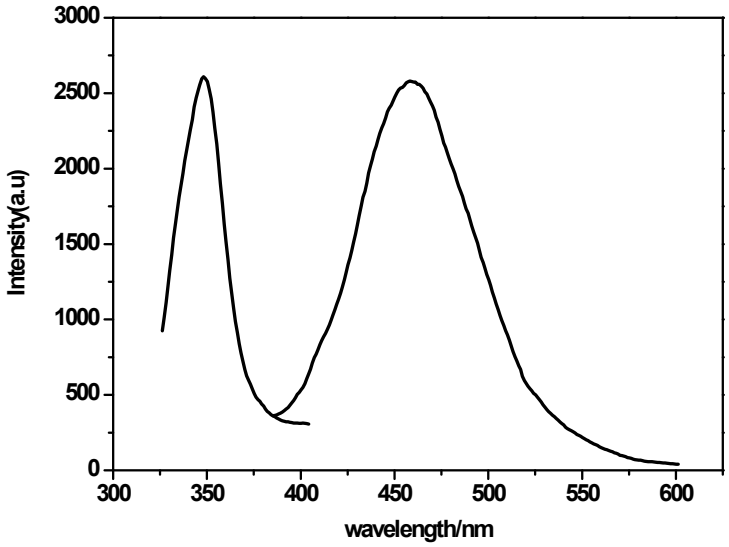



**Fig. S3** Excitation spectra (left) at 348 nm and emission spectra (right) at 462 nm of compound **4**.