Supporting Information

Table. S1. Hydrogen bonding in compounds 1, 3 and 6

Compound 1		
C(12)-O(8a)	3.1512(5)	a: x,-1+y,z
C(11)-O(8a)	3.0860(5)	a: x,-1+y,z
C(9)-O(1a)	3.1594(5)	a: x, 1.5-y,0.5+z
C(10)-O(1a)	3.1382(5)	a: x, 1.5-y,0.5+z
C(30)-O(2)w	3.1424(5)	
C(21)-O(3)w	3.0972(5)	
C(38)-O(14)	3.0858(5)	
C(50)-O(4)w	3.1265(5)	
C(33)-O(43a)	3.1288(6)	a: x, 2.5-y,-0.5+z
C(107)-O(11a)	3.0401(6)	a: x, 2.5-y,-0.5+z
C(42)-O(7a)	3.1275(5)	a: x, 2.5-y,-0.5+z
C(43)-O(7a)	3.1808(9)	a: x, 2.5-y,-0.5+z
O(9)w-O(6a)w	2.7564(6)	a: 1-x, -0.5+y,0.5-z
O(6a)w-O(4a)w	2.6211(8)	a: 1-x, -0.5+y,0.5-z
O(6a)w-O(11a)w	3.0480(5)	a: 1-x, -0.5+y,0.5-z
O(11a)w-O(6a)	3.0389(5)	a: 1-x, -0.5+y,0.5-z
O(29)-O(1a)w	2.7562(6)	a: -x, 0.5+y,0.5-z
O(20)-O(5)w	2.8531(5)	
O(5)w-O(18a)	2.8671(9)	a: -x, 0.5+y,0.5-z
O(5)w-O(3a)w	2.6706(6)	a: -x, 0.5+y,0.5-z
O(3a)w-O(52a)	3.0152(6)	a: -x, 0.5+y,0.5-z
O(1a)w-O(3a)w	3.0363(9)	a: -x, 0.5+y,0.5-z
O(1a)w-O(2a)w	2.8168(4)	a: -x, 0.5+y,0.5-z
O(3a)w-O(2a)w	2.8406(7)	a: -x, 0.5+y,0.5-z
O(1a)w-O(12a)w	3.0724(6)	a: -x, 0.5+y,0.5-z
O(1a)w-O(10)w	2.8284(10)	a: -x, 0.5+y,0.5-z
O(4)-O(10)w	2.8137(7)	
O(10a)-O(10)w	2.8713(5)	a: x, 2.5-y,0.5+z
O(2a)w-O(12a)w	2.9100(7)	a: -x, 0.5+y,0.5-z
O(7a)w-O(12b)w	2.8812(4)	a: x, 2.5-y,0.5+z; b: -x, 0.5+y,0.5-z
O(7a)w-O(8a)w	2.6378(4)	a: x, 2.5-y,0.5+z
O(2a)w-O(8a)w	2.6207(4)	a: -x, 0.5+y,0.5-z
O(55a)-O(8b)w	2.9693(9)	a: -x, 0.5+y,0.5-z; b: x, 2.5-y,0.5+z
Compound 3		
C(18)-O(15)	3.1887(2)	
O(18)-C(29a)	3.1473(2)	a: -1-x,-1-y,1-z
O(29)-C(30a)	3.0247(2)	a: -1-x,-1-y,1-z
O(29)-C(31a)	3.1930(2)	a: -1-x,-1-y,1-z
O(15)-C(58a)	3.1714(3)	a: -1+x,-1+y, z
C(27)-O(34)	3.0517(3)	

O(33)-C(90a)	3.1761(2)	a: -x,-1-y, 1-z
O(61)-C(62a)	3.0841(2)	a: -x,-y, 1-z
O(21)-C(97a)	3.1903(2)	a: x, y, 1+z
O(28)-C(102a)	3.1390(3)	a: -x,1-y, 1-z
O(26)-C(8a)	3.1781(3)	a: 1+x,1+y, z
O(26)-C(9a)	3.0964(2)	a: 1+x,1+y, z
O(16)-C(9a)	3.1869(2)	a: 1+x,1+y, z
O(16)-C(10a)	2.9898(2)	a: 1+x,1+y, z
Compound 6		
O(15)-C(39a)	3.1018(2)	a: x, y, -1+z
O(15)-C(40a)	3.1494(3)	a: x, y, -1+z
O(58)-C(40a)	3.1472(2)	a: x, y, -1+z
O(6)-C(30a)	3.1393(3)	a: 1-x, 1-y, 1-z
O(4)-C(20a)	3.1150(2)	a: -x, 2-y, -z
O(37)-C(20)	3.1893(2)	
O(13)-C(20)	3.1784(3)	
O(13)-C(19)	3.1982(2)	
O(34)-C(28a)	3.1724(3)	a: -1+x, 1+y, -1+z
O(1)-C(13a)	3.0959(2)	a: -1+x, 1+y, z
O(26)-C(33a)	2.9349(3)	a: -1+x, 1+y, -1+z
O(21)-C(31a)	2.9909(2)	a: -1+x, 1+y, -1+z
O(10)-C(9a)	2.9385(2)	a: -x, 1-y, 1-z
O(38)-C(52a)	3.1681(3)	a: 1-x, 1-y, 1-z
O(23)-C(3)	3.1213(3)	
O(57)-N(7a)	3.0222(3)	a: x, 1+y, -1+z
O(17)-N(11a)	3.0841(2)	a: 1-x, 1-y, 1-z
O(37)-N(4)	2.8770(2)	
O(41)-N(6a)	2.7664(2)	a: 1-x, 1-y, 1-z
O(15)-N(10a)	2.9205(2)	a: -1+x, y, z
O(33)-N(2a)	2.9432(2)	a: -1+x, 1+y, z
π···π interactions in compound 6		
Cg(26)->Cg(38)	3.621(16)	
Cg(26): N(1)-->C(1)-->C(2)-->C(3)-->C(4)-->C(5) Cg(38): N(9)-->C(41)-->C(42)-->C(43)-->C(44)-->C(45) Calculated by Platon software.		

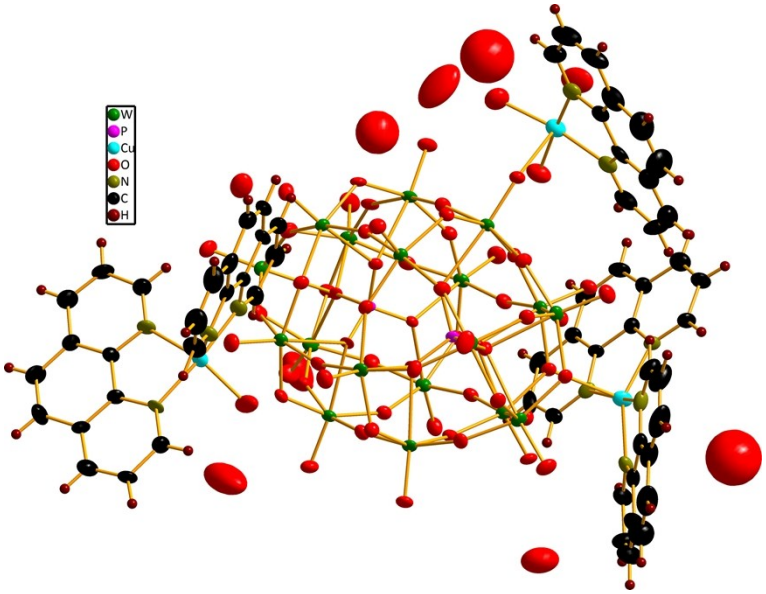


Fig. S1 ORTEP view of the asymmetric unit of compound **1**.

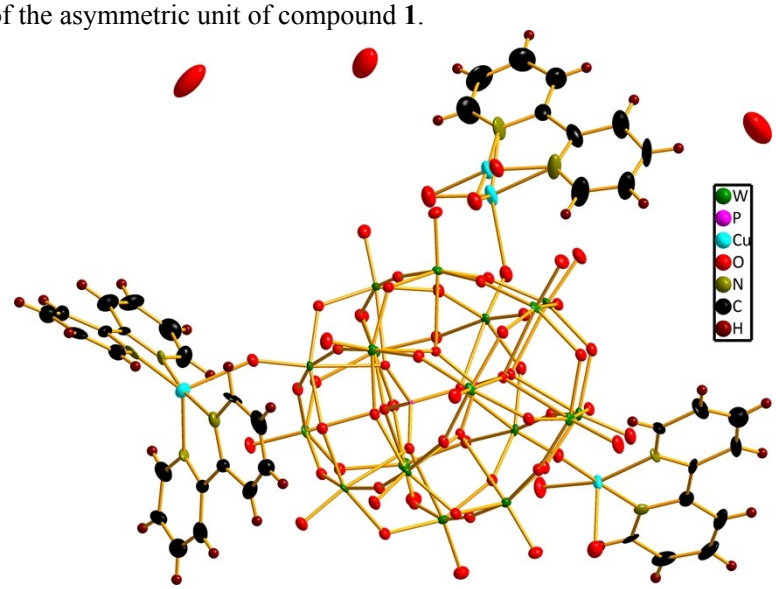


Fig. S2 ORTEP view of the asymmetric unit of compound **2**.

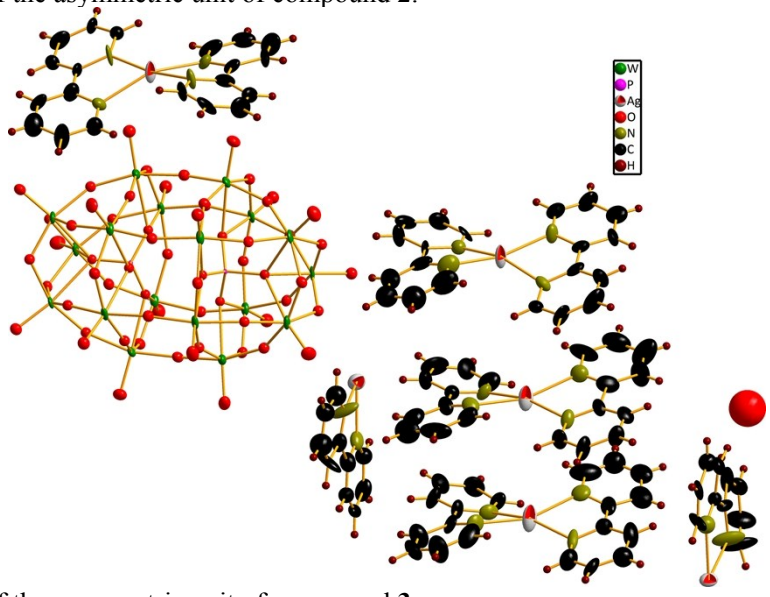


Fig. S3 ORTEP view of the asymmetric unit of compound **3**.

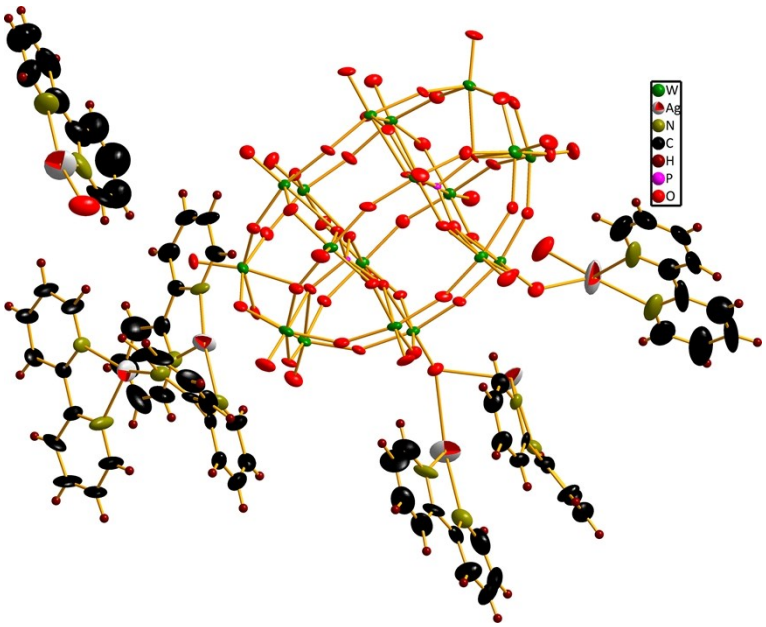


Fig. S4 ORTEP view of the asymmetric unit of compound **4**.

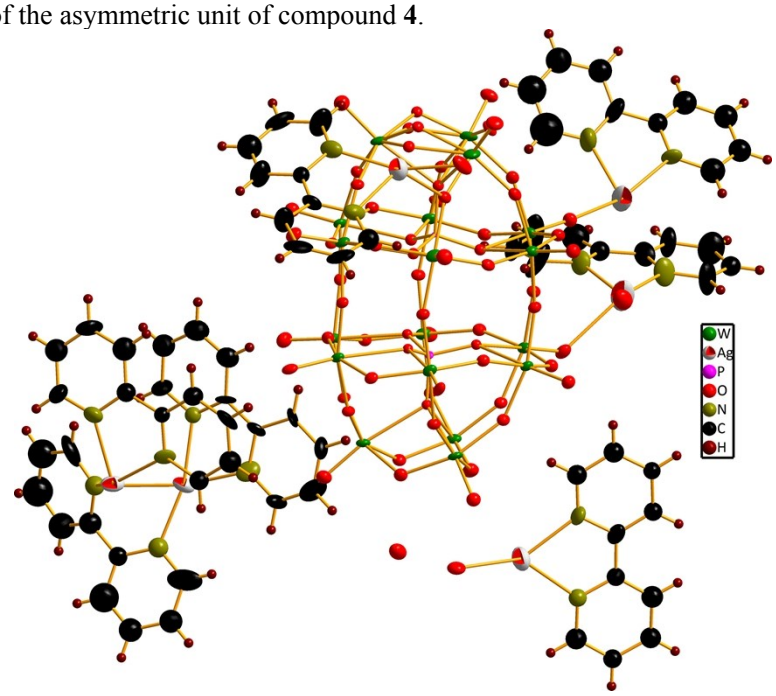


Fig. S5 ORTEP view of the asymmetric unit of compound **5**.

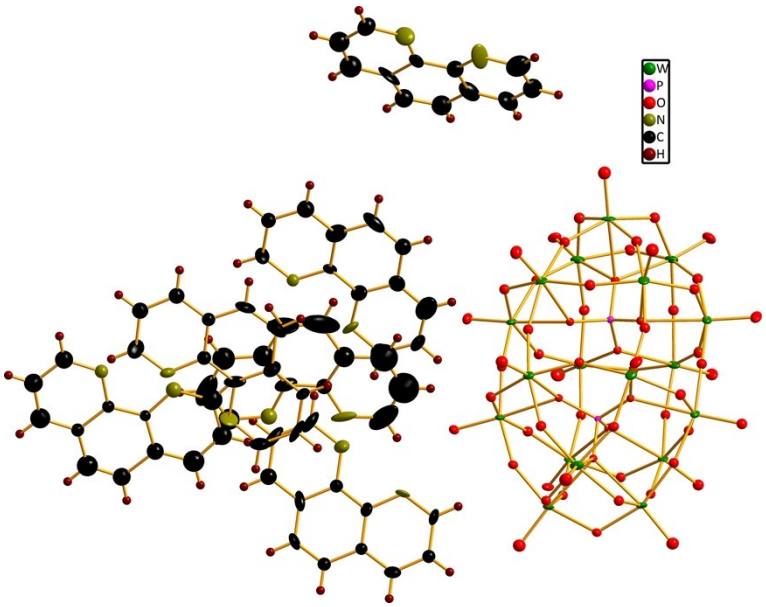


Fig. S6 ORTEP view of the asymmetric unit of compound **6**.

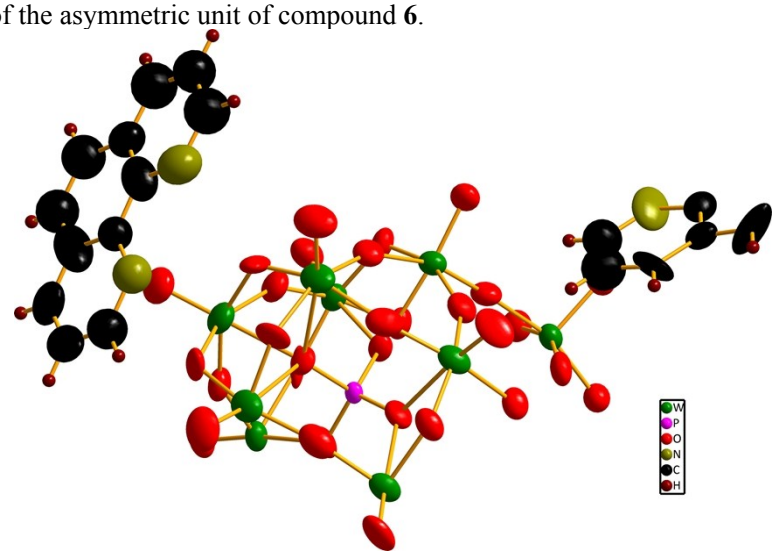
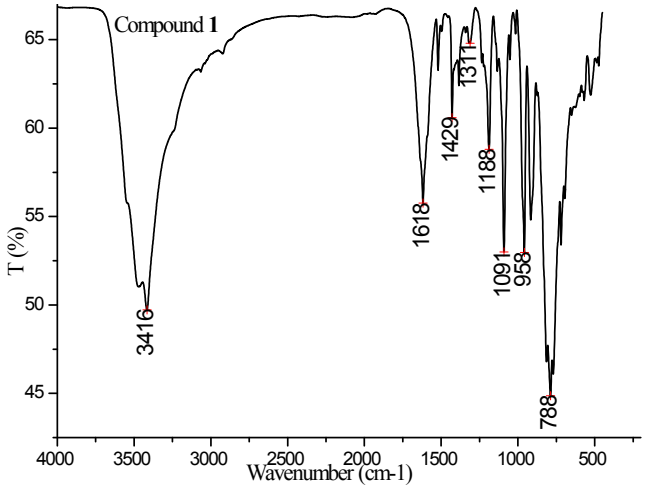
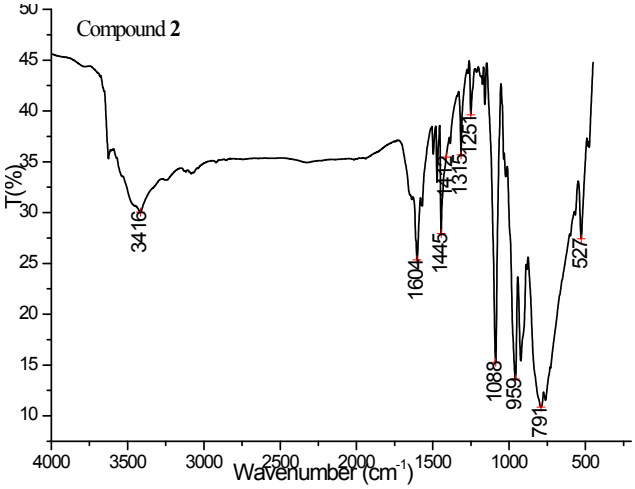
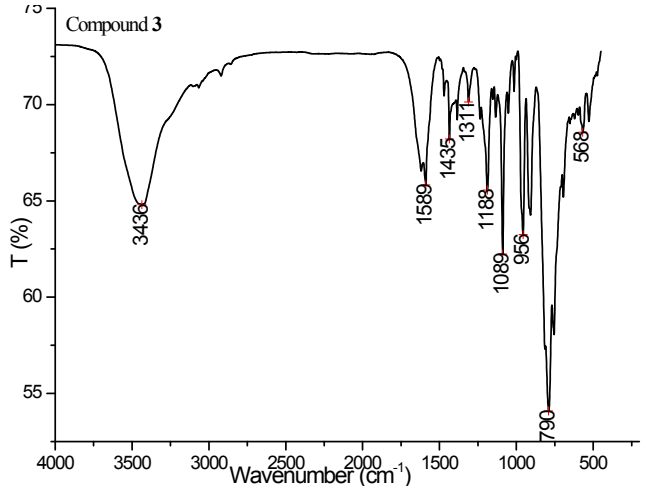
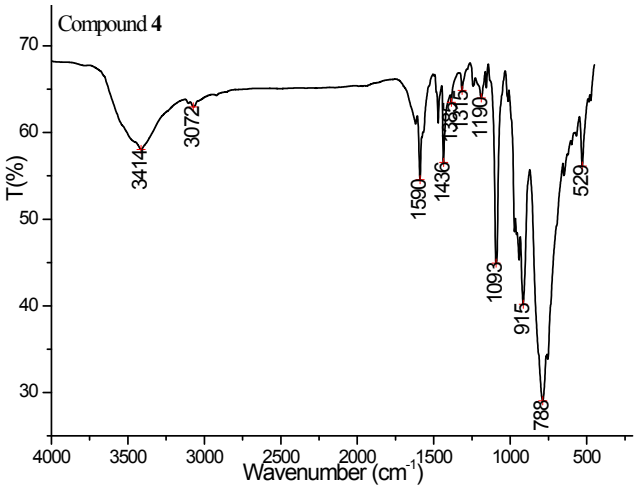


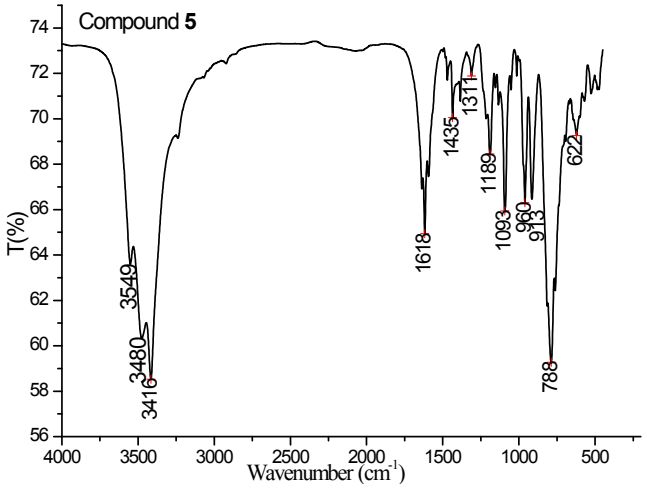
Fig. S7 ORTEP view of the asymmetric unit of compound 7.

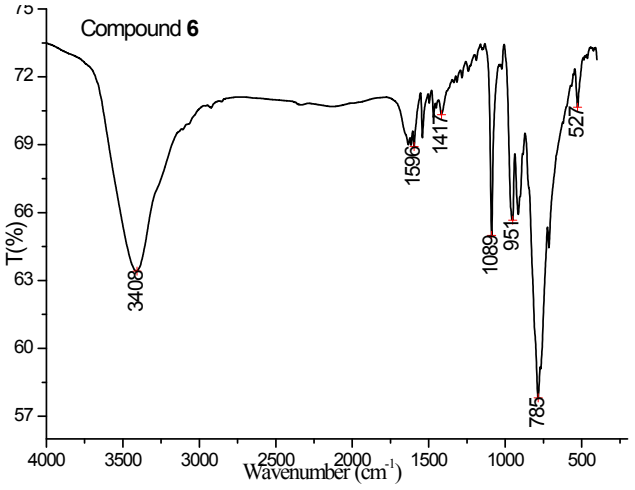

Compound 1
T (%)
Wavenumber (cm-1)
3416
1618
1429
1311
1188
1091
958
788


Compound 2
T(%)
Wavenumber (cm-1)
3416
1604
1445
1414
1315
1251
1088
959
791
527


Compound 3
T (%)
Wavenumber (cm-1)
3436
1589
1435
1311
1188
1089
956
790
568


Compound 4
T(%)
Wavenumber (cm-1)
3414
3072
1590
1436
1382
1315
1190
1093
915
788
529


Compound 5
T(%)
Wavenumber (cm-1)
3549
3480
3416
1618
1435
1311
1189
1093
960
913
788
622


Compound 6
T(%)
Wavenumber (cm-1)
3408
1596
1417
1089
951
785
527

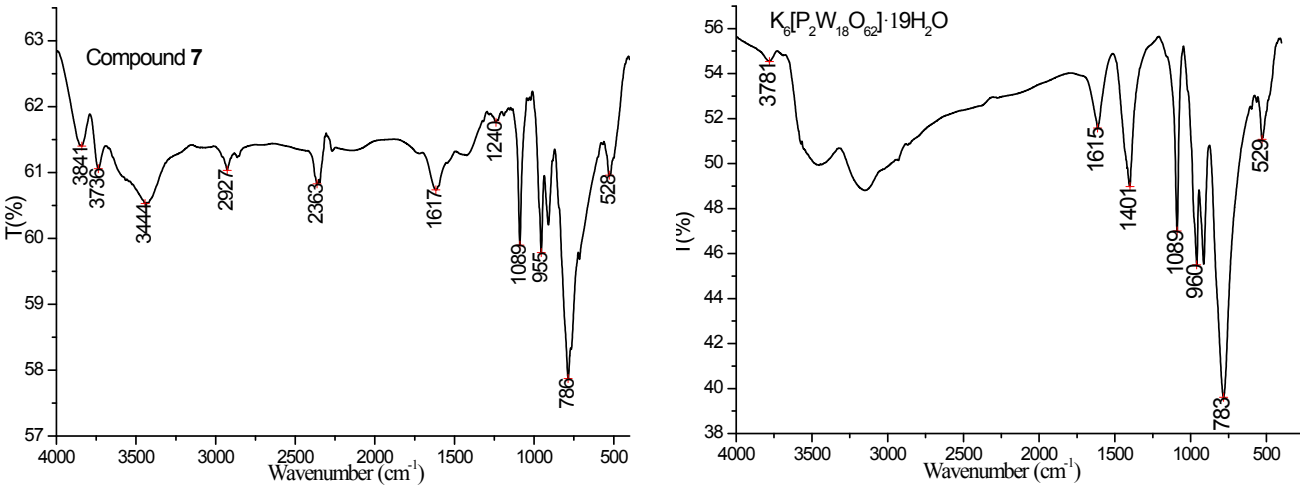
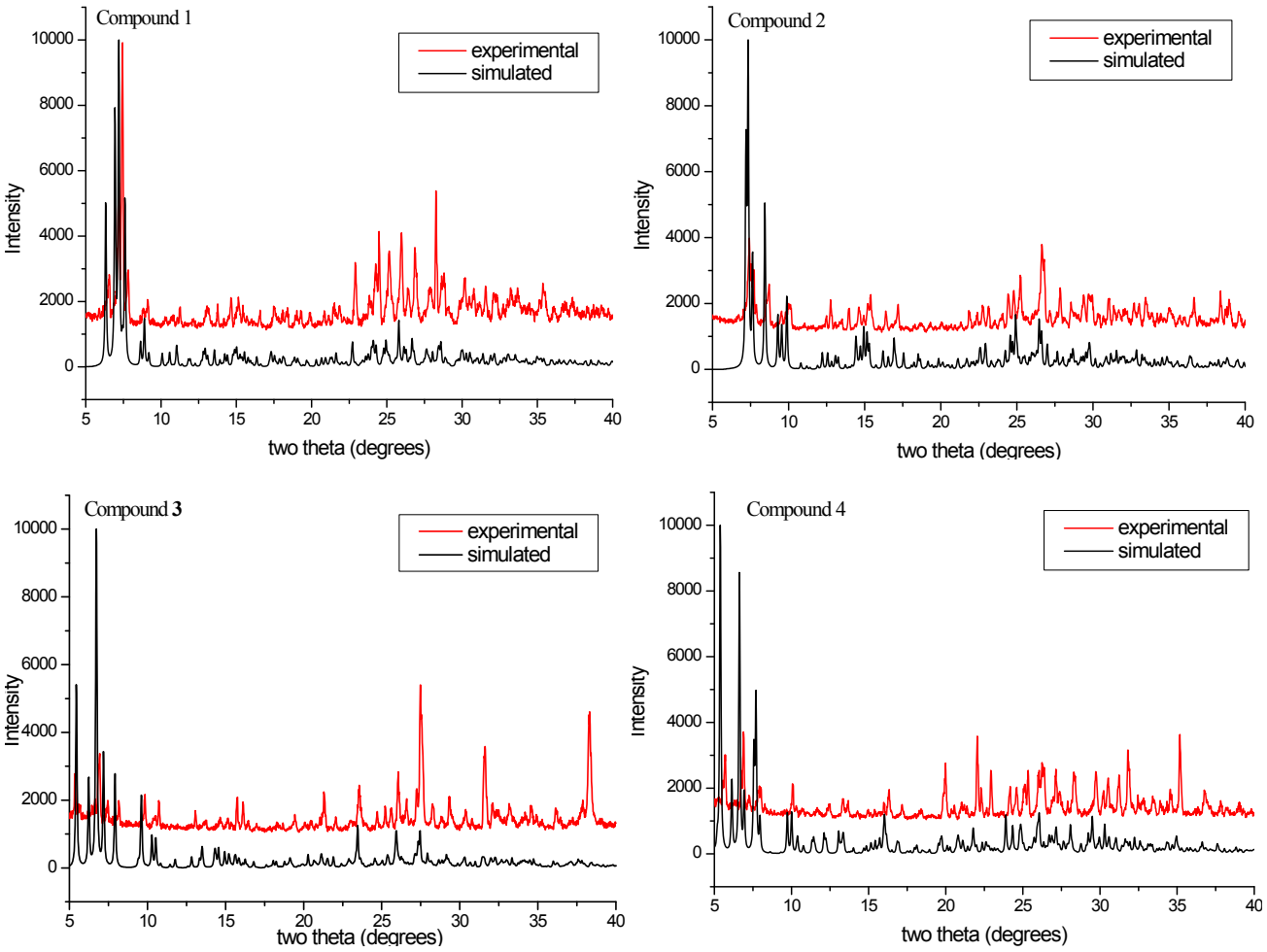


Fig. S8. IR spectra of compounds 1-7



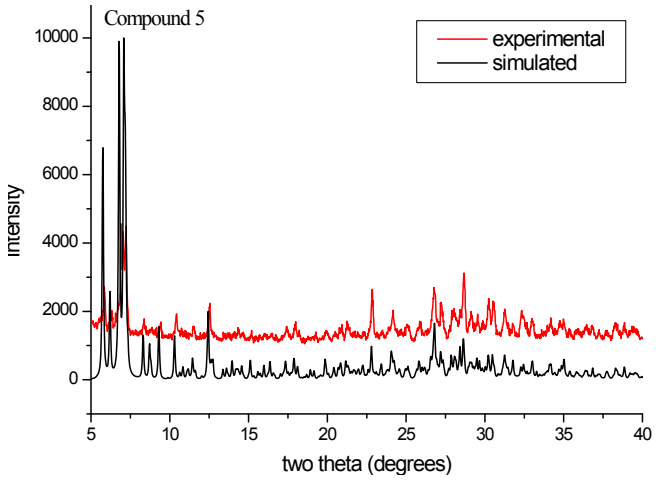
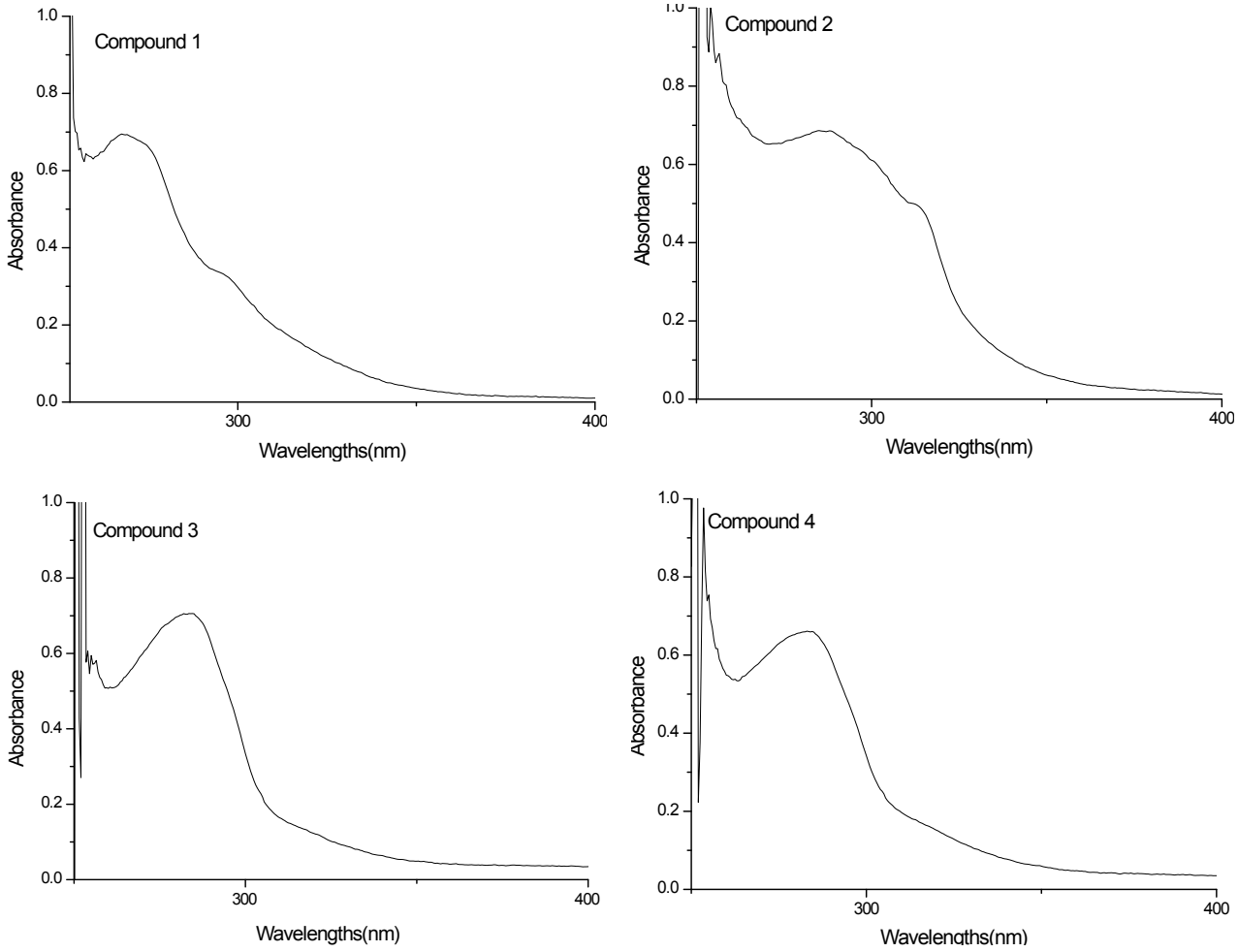


Fig. S9 X-ray powder diffraction patterns of compounds 1-5.



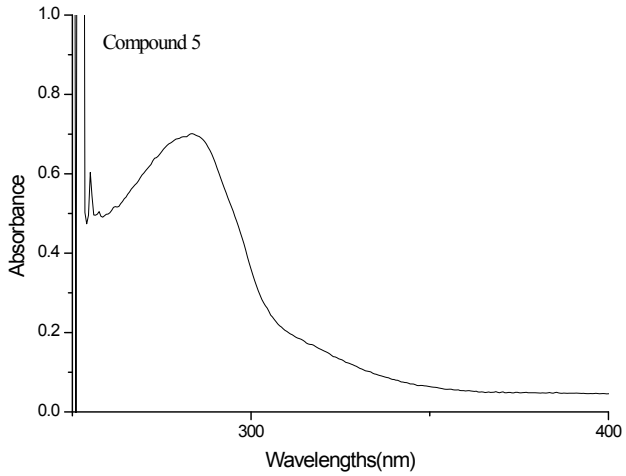
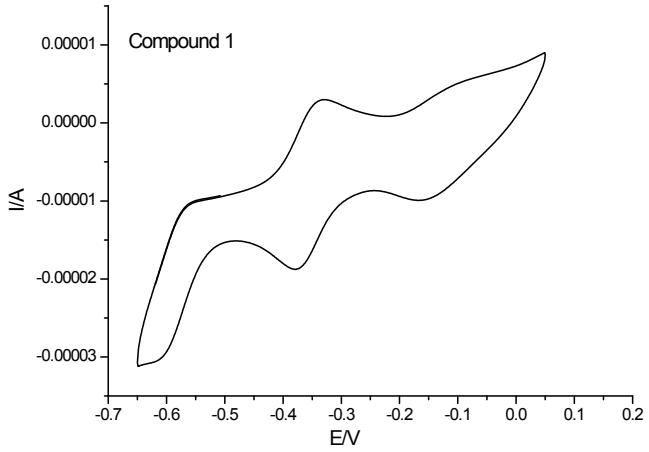
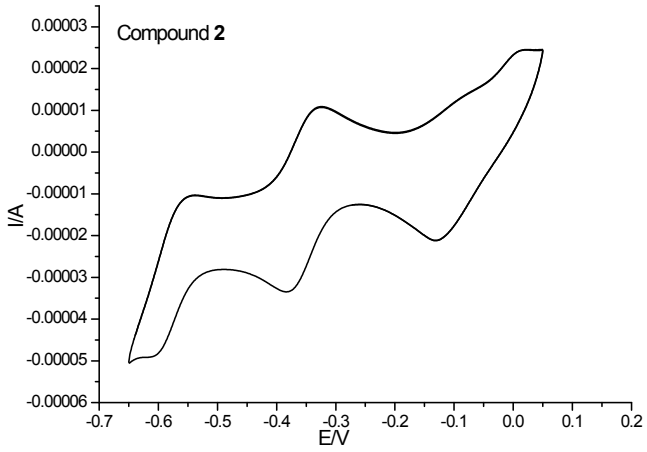
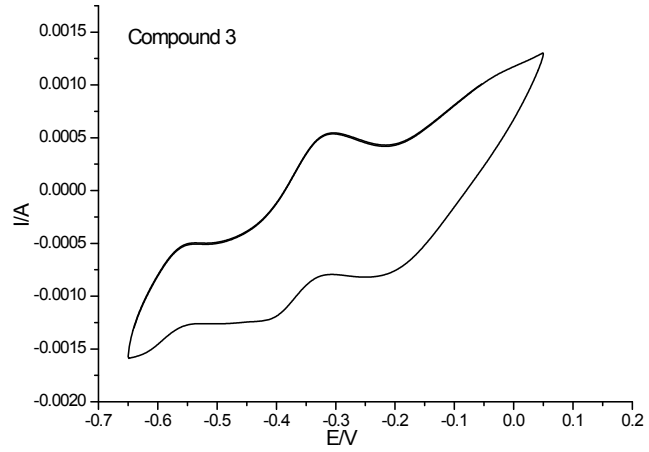
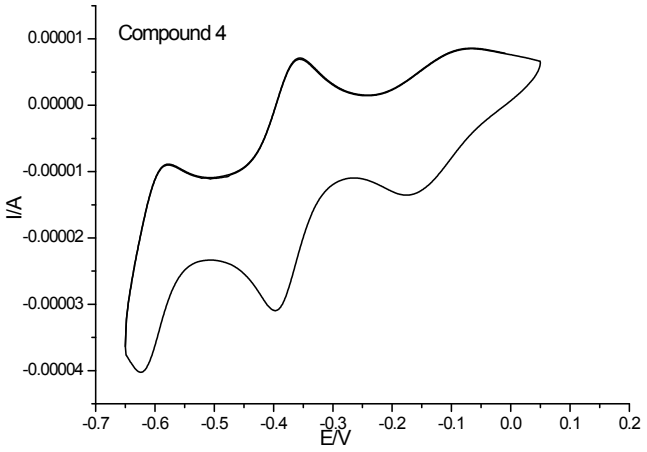


Fig. S10. UV-Vis spectrum for compound 1-5









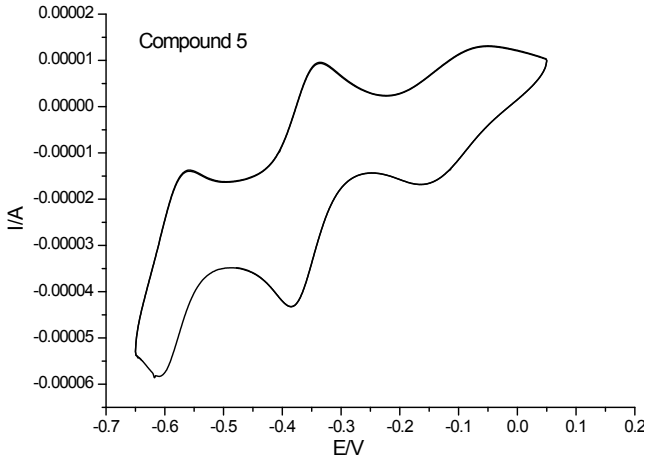
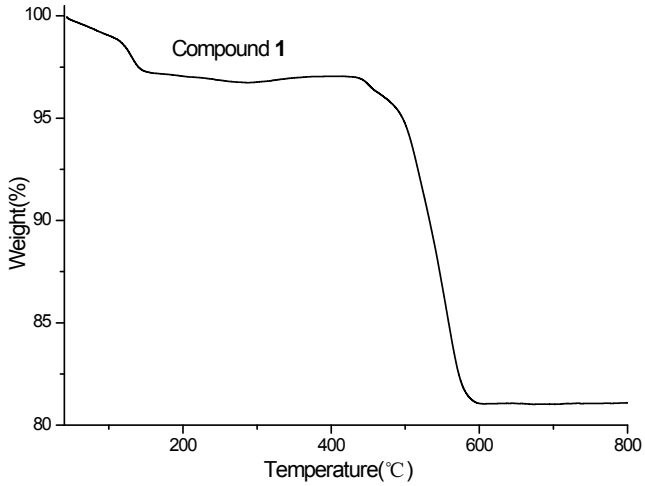
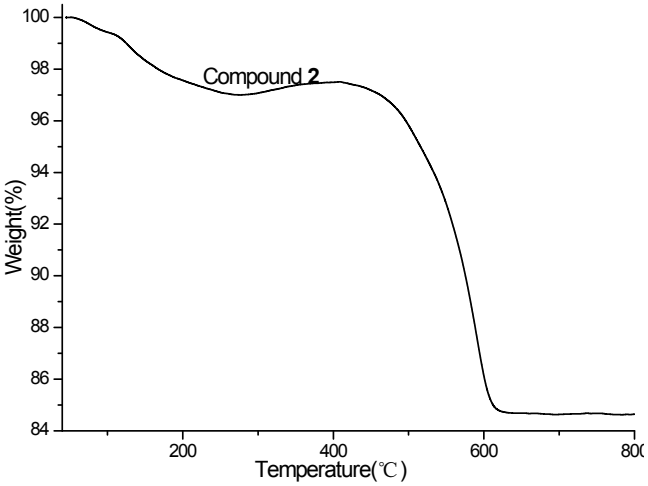
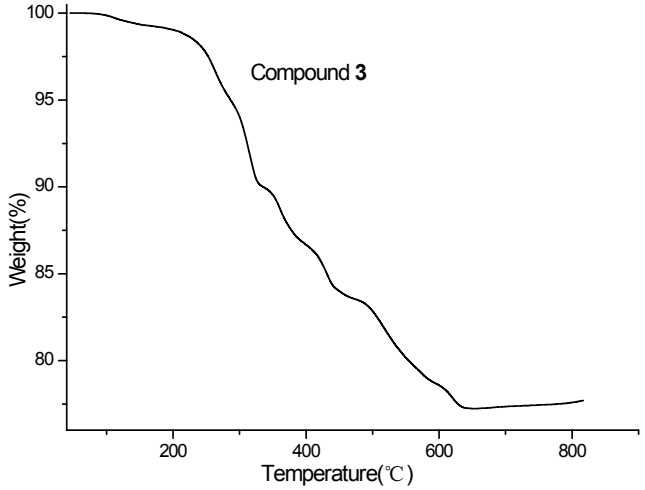
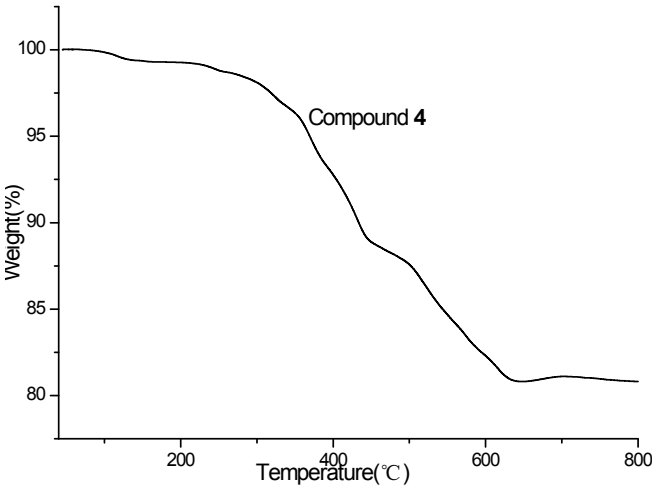


Fig. S11. The cyclic voltammograms of compound 1-5









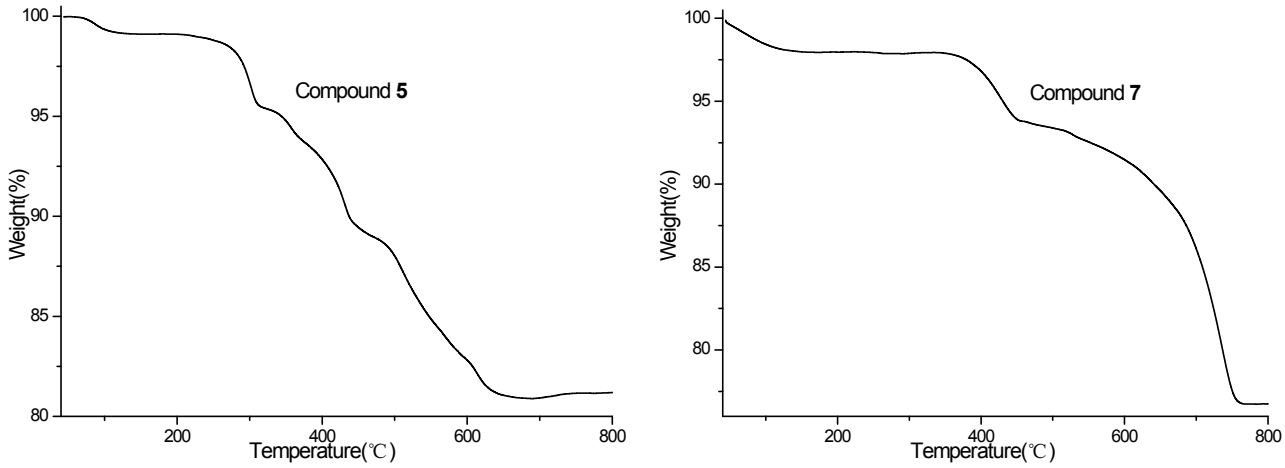


Fig. S12. The TG curves of compound **1**-**5** and compound **7**.

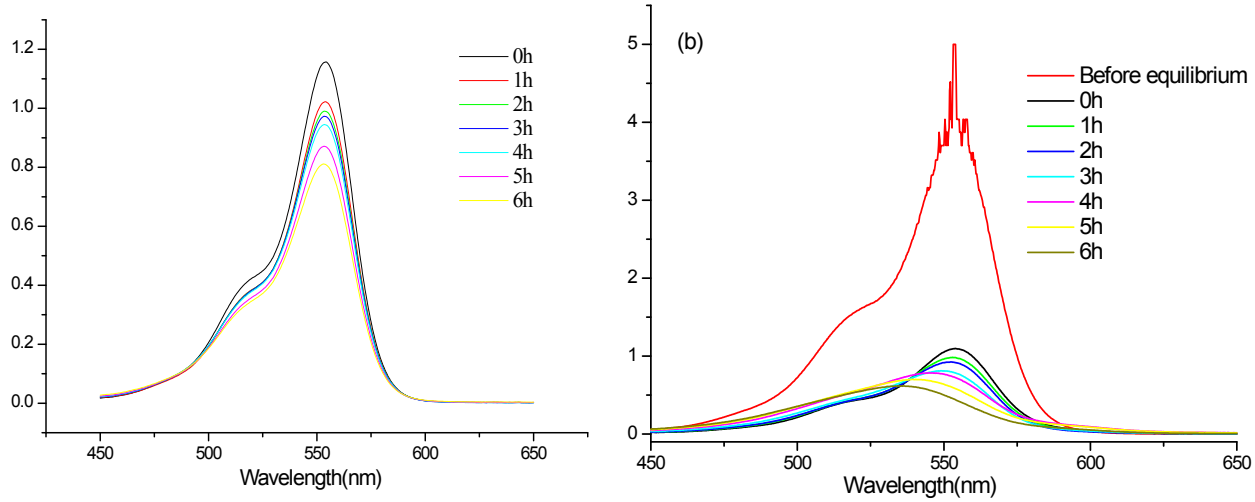
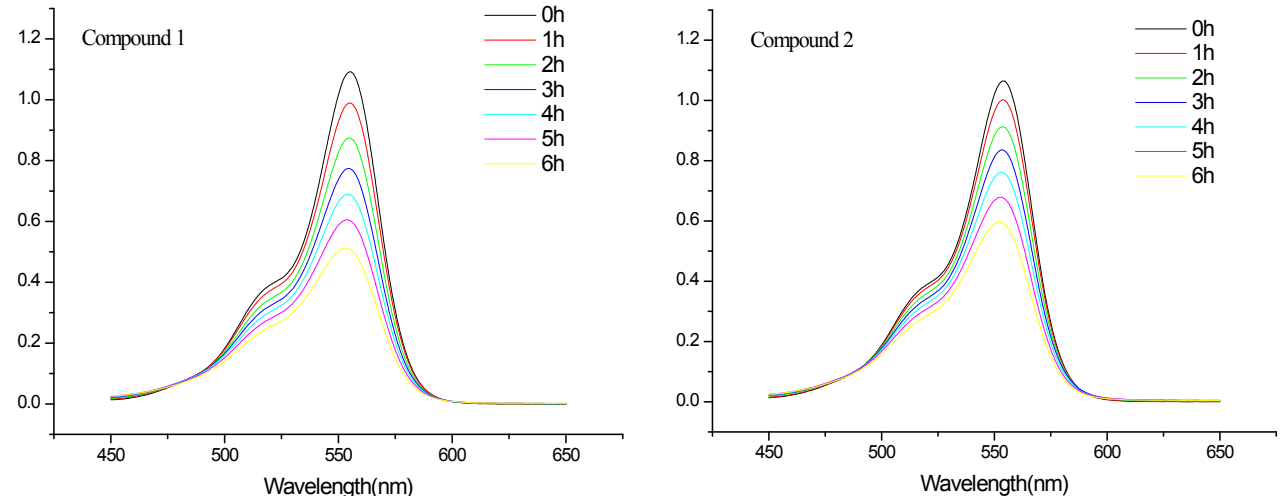


Fig. S13 (a) UV-Vis absorption spectra of the RhB solutions degraded without photocatalysts under UV irradiation at different time intervals. (b) UV-Vis absorption spectra of the RhB solutions degraded with $K_6[P_2W_{18}O_{62}]\cdot 19H_2O$ as the photocatalyst. However, in contrast to compounds **1**-**7**, $K_6[P_2W_{18}O_{62}]\cdot 19H_2O$ is easy to be dissolved in the RhB solution and the solution was magnetically stirred in the dark for about 24h to achieve the adsorption equilibrium.



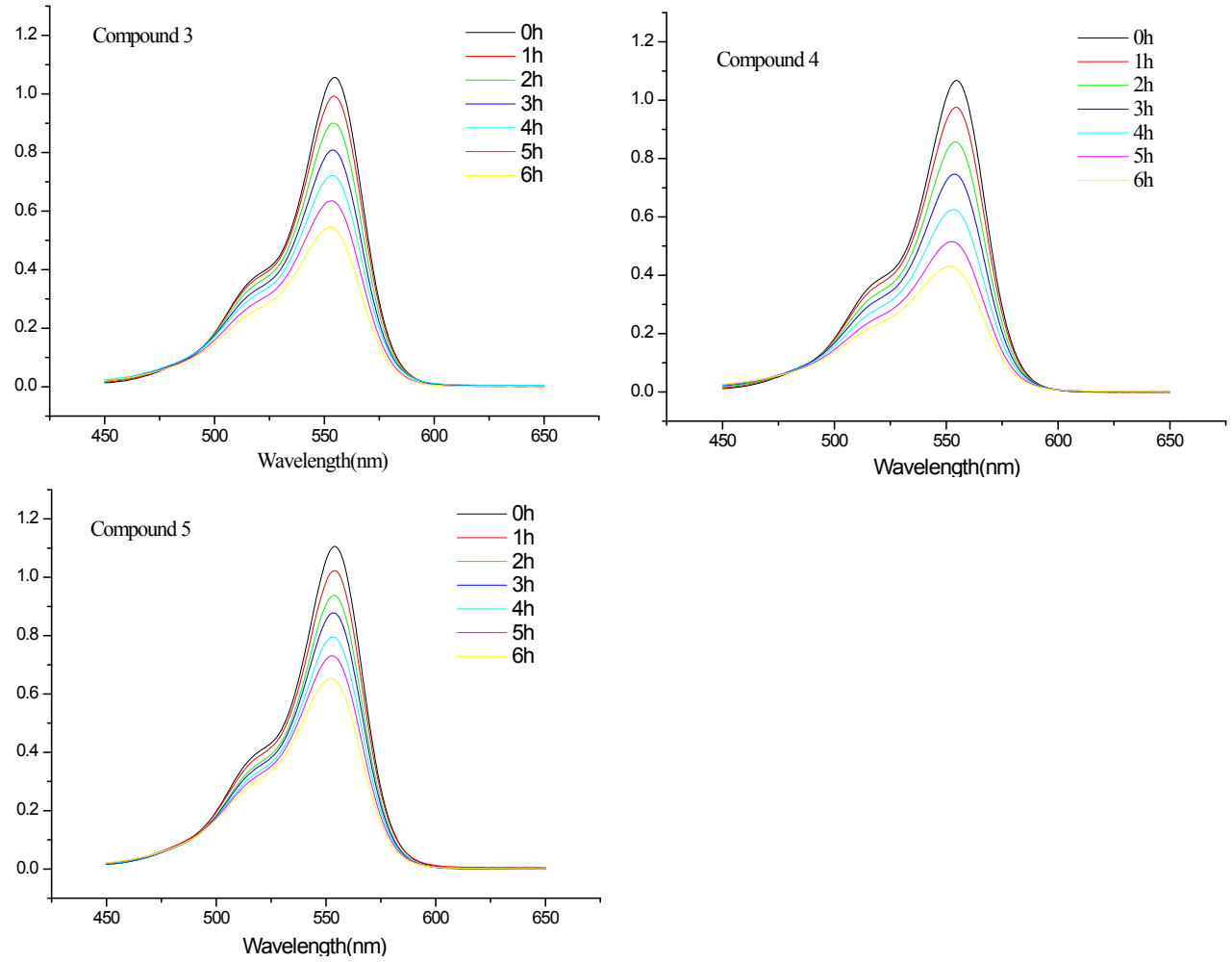


Fig. S14 UV-Vis absorption spectra of the RhB solutions degraded with compounds **1**–**5**.

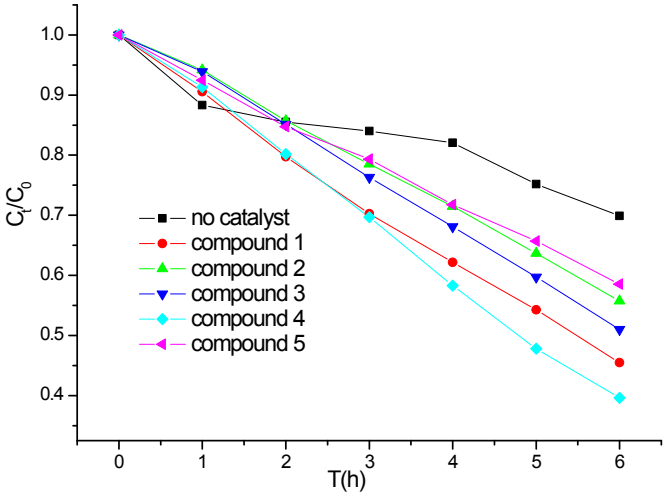


Fig. S15 Changes in the C_t/C_0 plots of RhB solutions versus reaction time for compounds **1**-**5**.

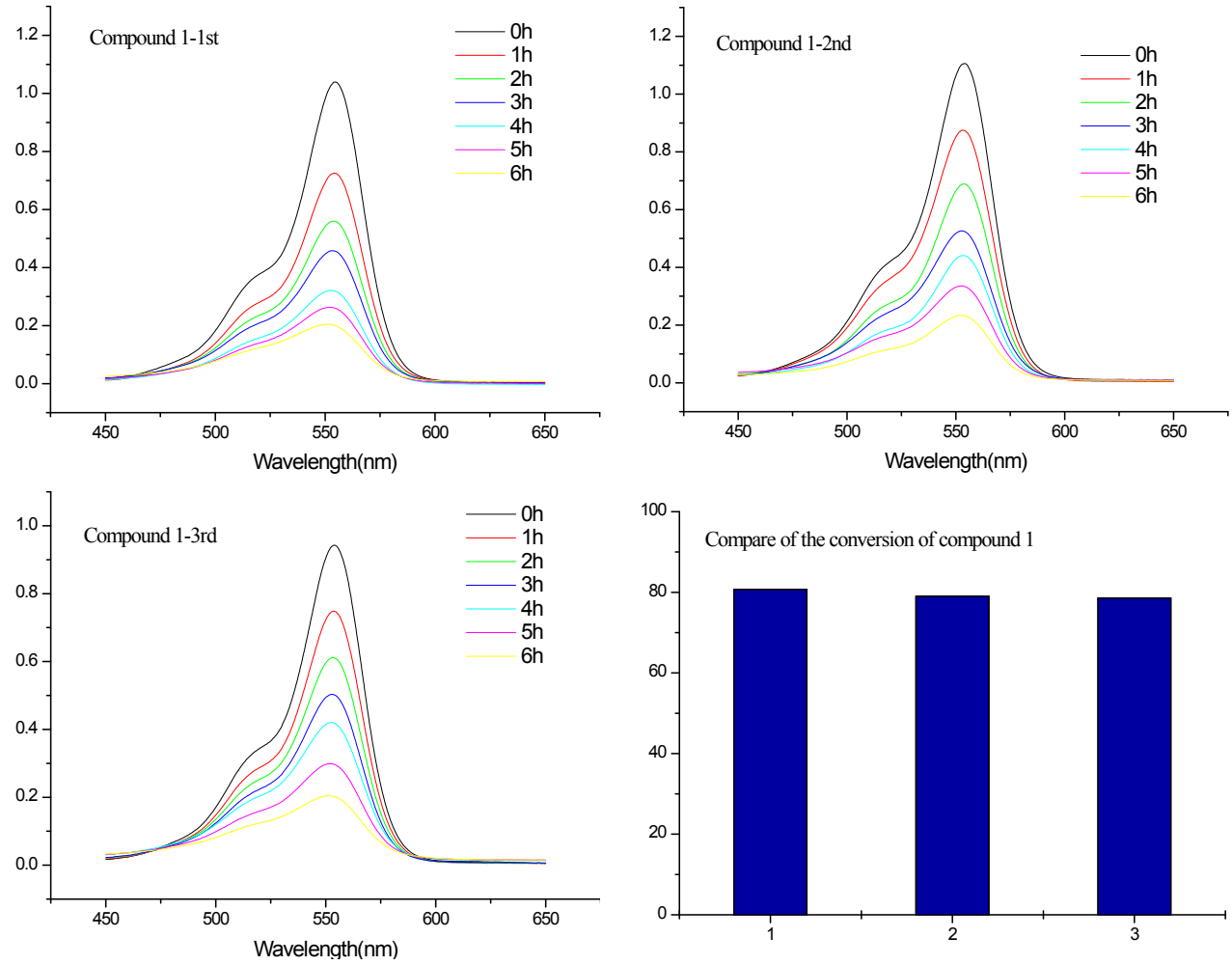


Fig. S16 The reproducible ability of compound **1** for photodegradation of RhB for 3 cycles.

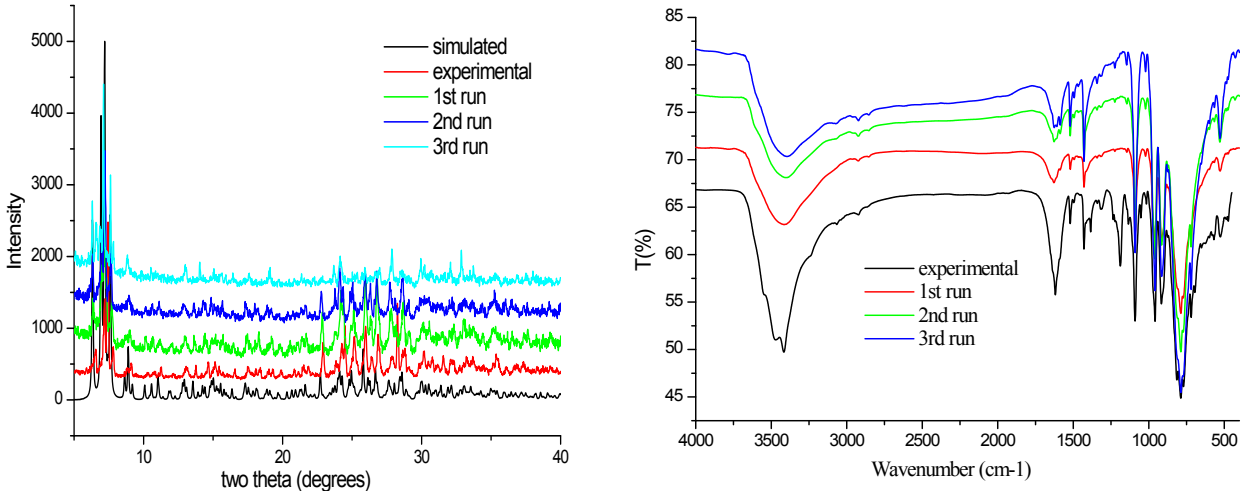


Fig. S17 X-ray powder diffraction patterns and IR spectra of compound **1** after three cycles of photodegradation of RhB.

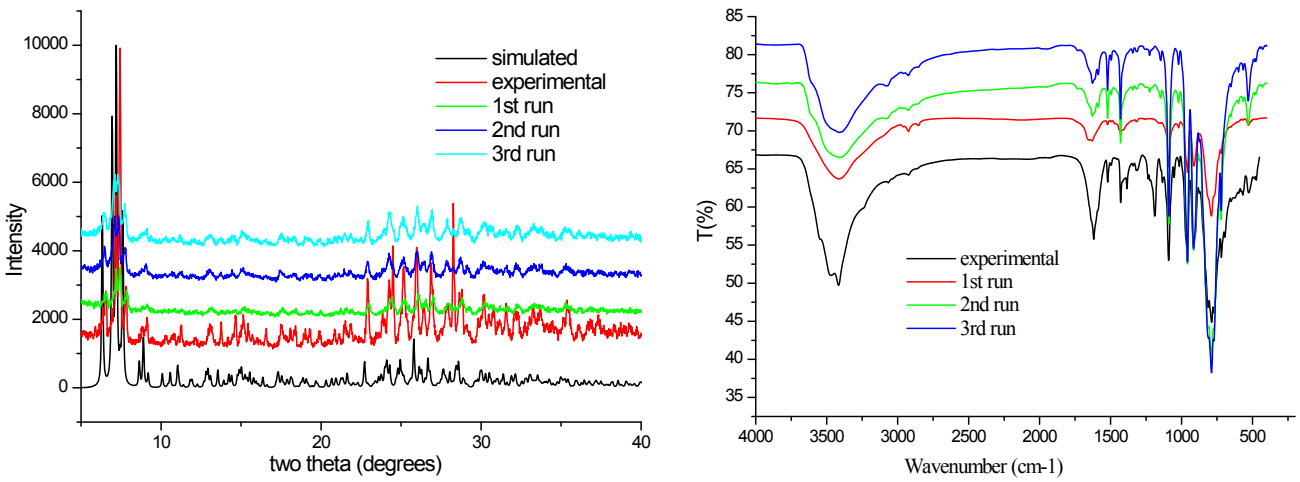


Fig. S18 X-ray powder diffraction patterns and IR spectra of compound 1 after three cycles of epoxidation of styrene to styrene oxide.