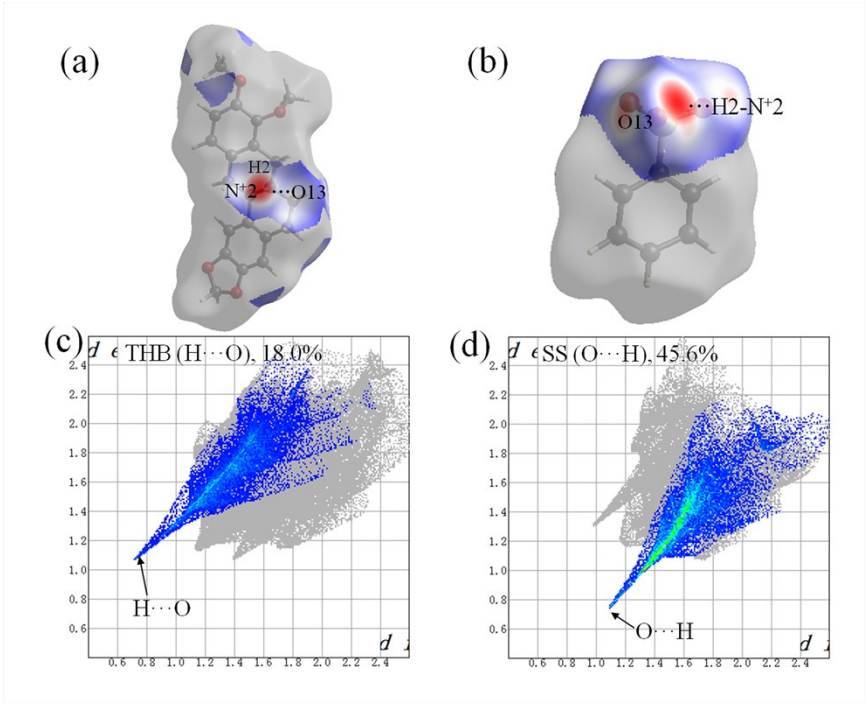

Fig. S1. Views of d_{norm} mapped on the Hirshfeld surfaces H···O contacts of THB (a) and O···H contacts of BS (b), and corresponding 2D fingerprint plots of H···O contacts of THB (c) and O···H contacts of BS (d).

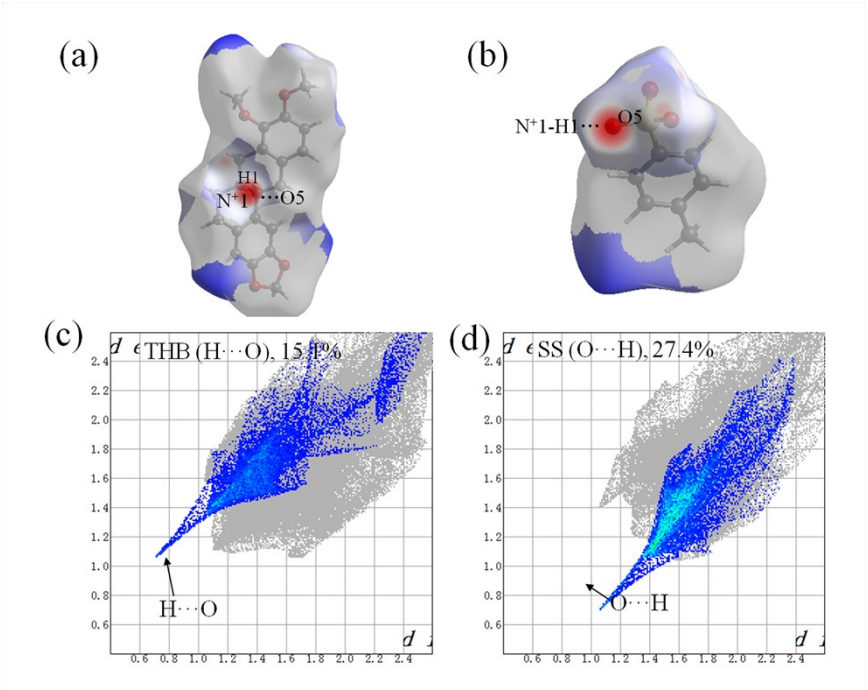

Fig. S2. Views of d_{norm} mapped on the Hirshfeld surfaces H···O contacts of THB (a) and O···H contacts of PTS (b), and corresponding 2D fingerprint plots of H···O contacts of THB (c) and O···H contacts of PTS (d).

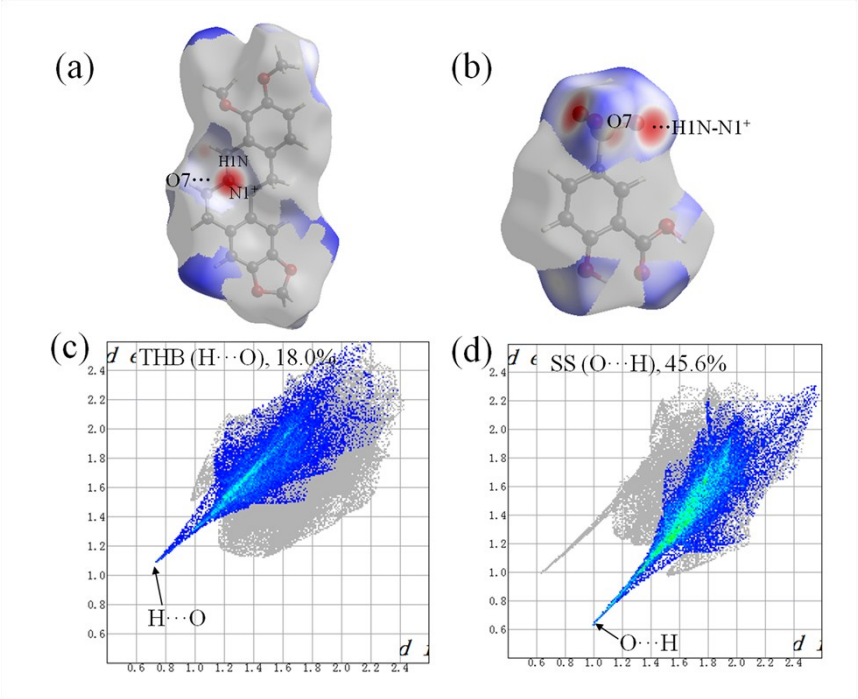

Fig. S3. Views of d_{norm} mapped on the Hirshfeld surfaces H···O contacts of THB (a) and O···H contacts of SS (b), and corresponding 2D fingerprint plots of H···O contacts of THB (c) and O···H contacts of SS (d).

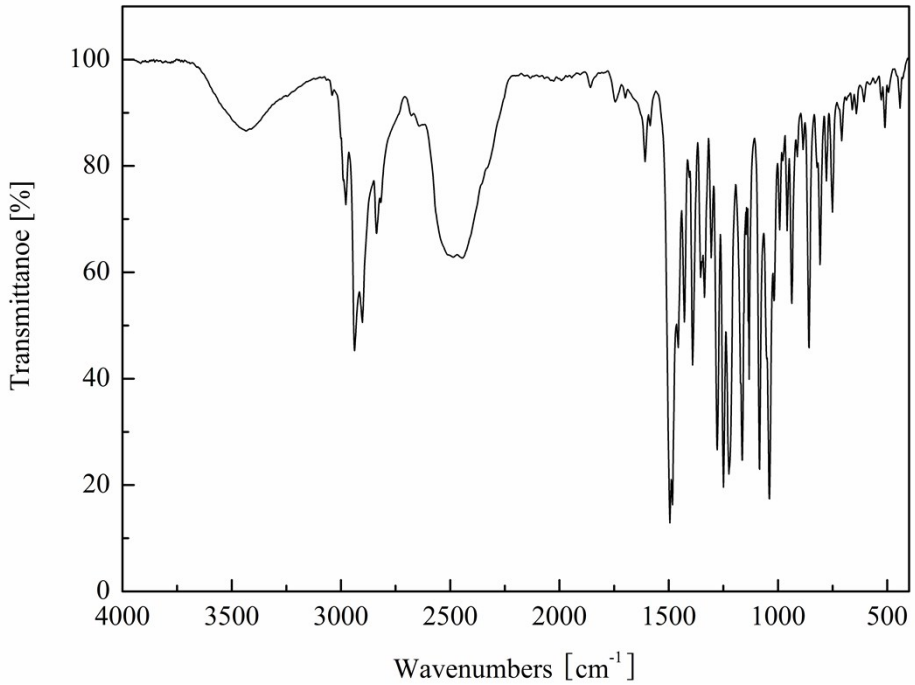

Fig. S4. IR spectra of compound THB-BS.

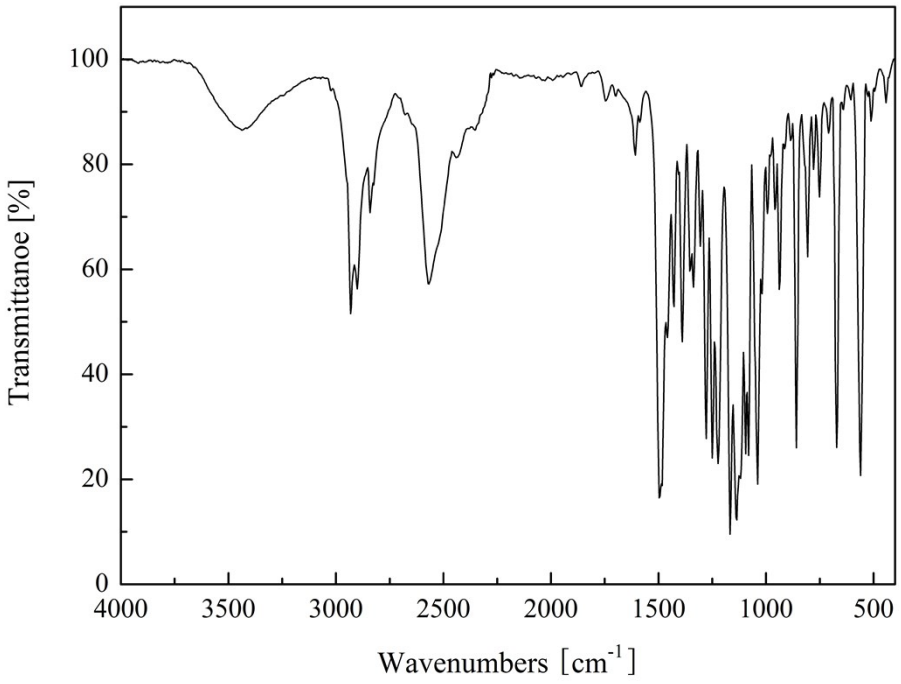

Fig. S5. IR spectra of compound THB-PTS.

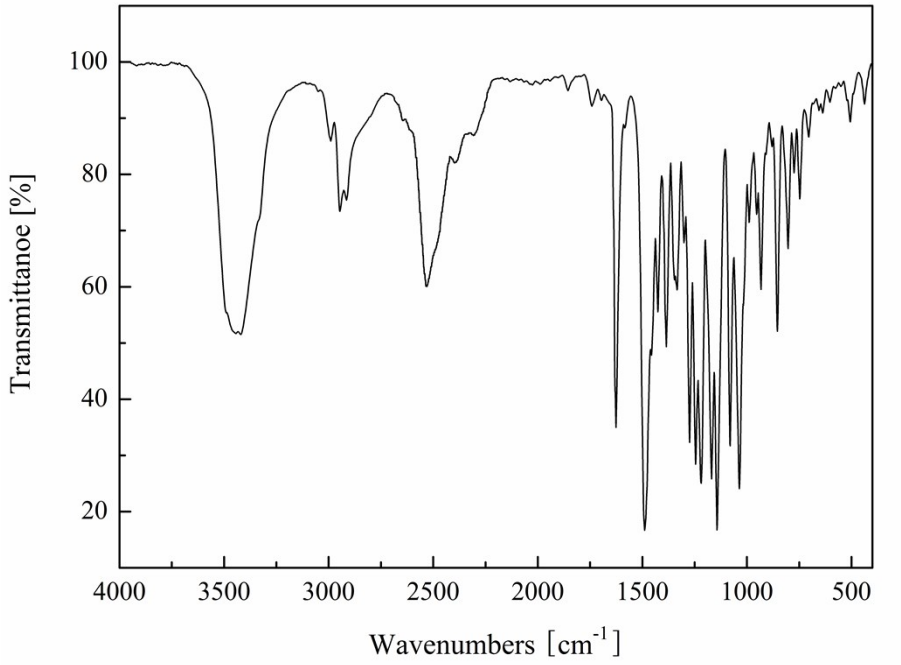

Fig. S6. IR spectra of compound THB-SS.

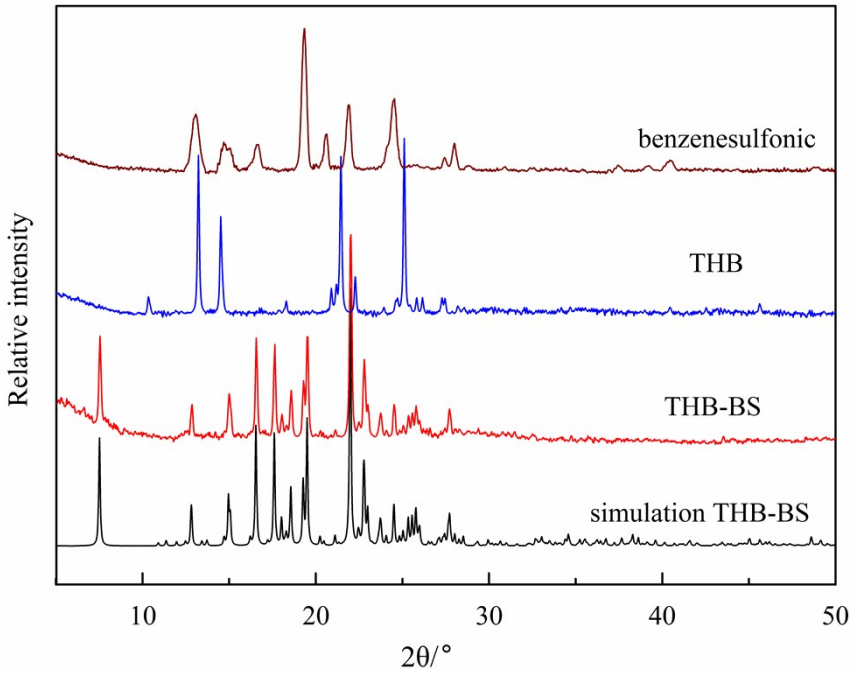

Fig. S7. Comparison of XRD patterns: experimental XRD patterns of benzenesulfonic acid, THB and THB-BS, and the simulated patterns of THB-BS.

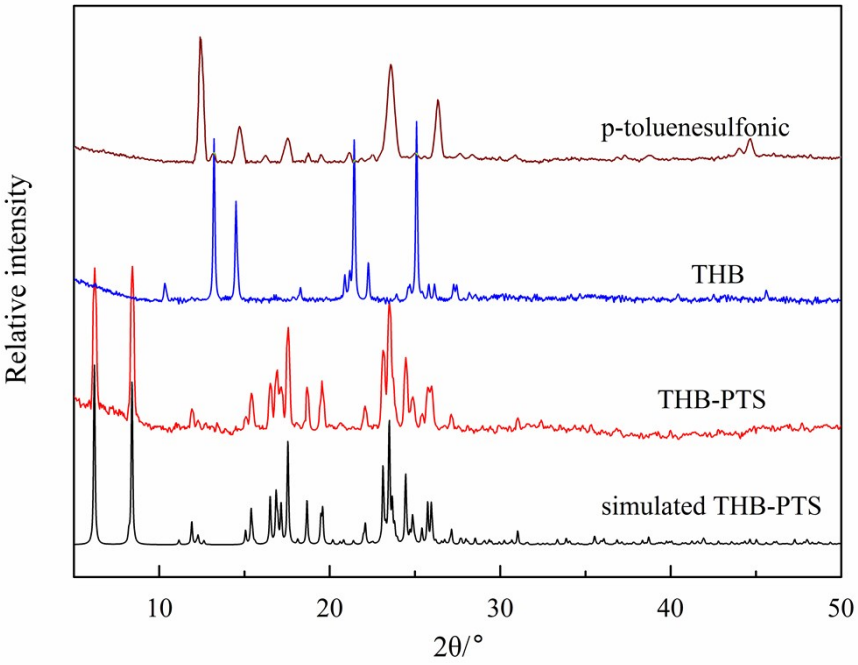

Fig. S8 Comparison of XRD patterns: experimental XRD patterns of p-toluenesulfonic acid, THB and THB-PTS, and the simulated patterns of THB-PTS.

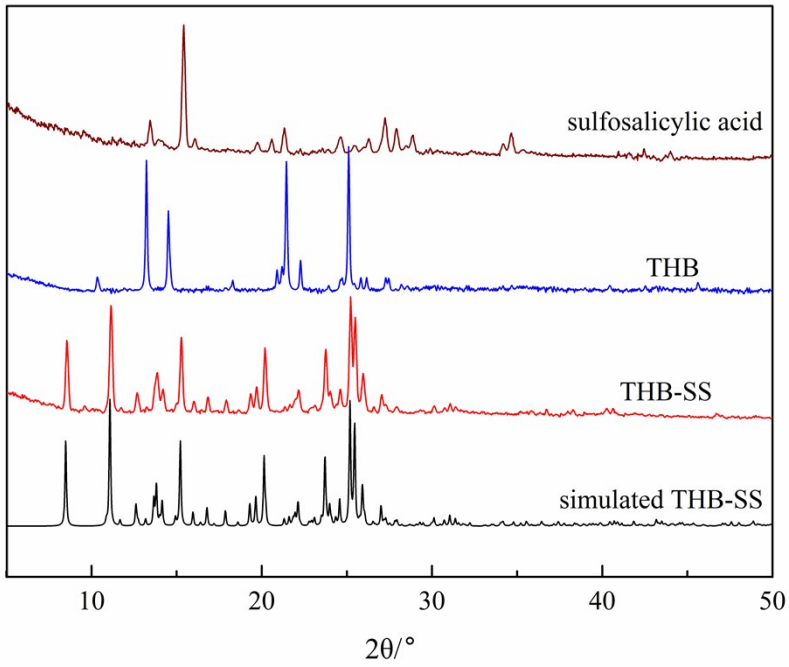

Fig. S9 Comparison of XRD patterns: experimental XRD patterns of sulfosalicylic acid, THB and THB-SS, and the simulated patterns of THB-SS.

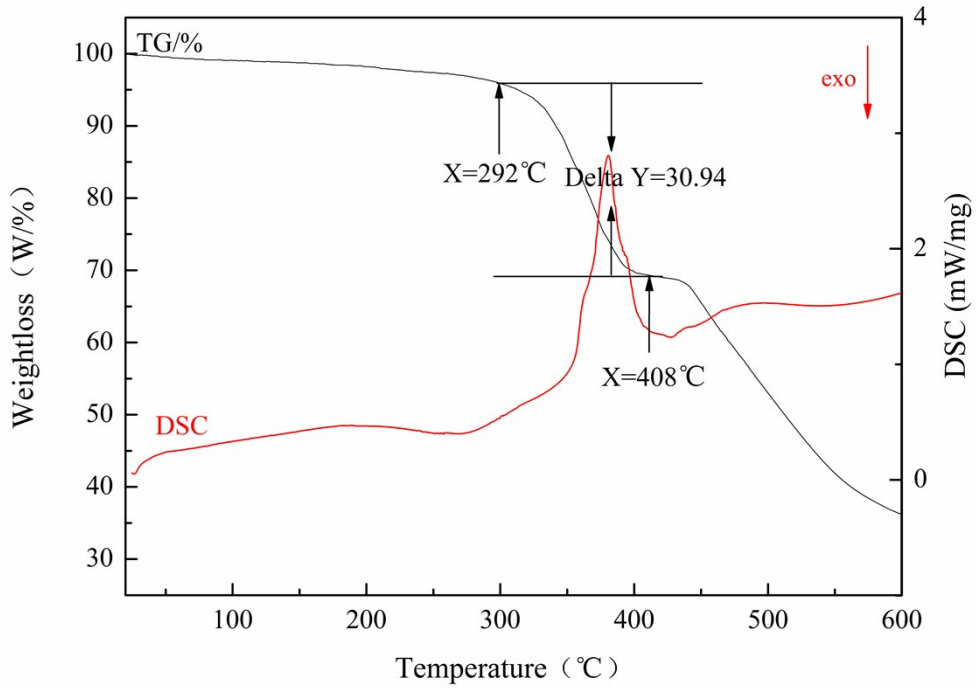

Fig. S10. TG-DSC curve of THB-BS.

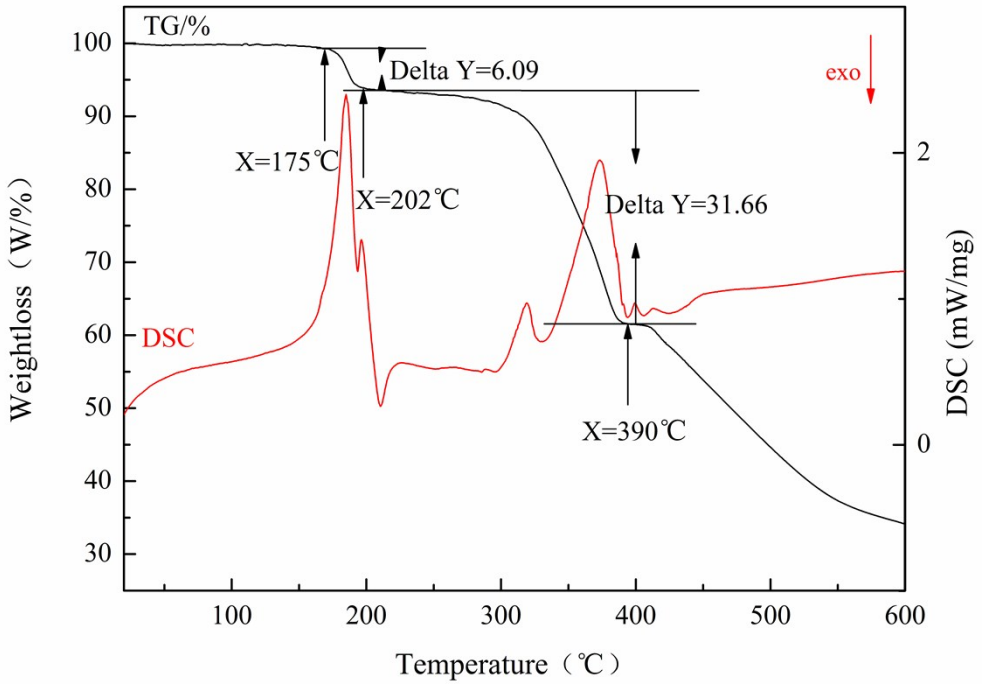

Fig. S11. TG-DSC curve of THB-PTS.

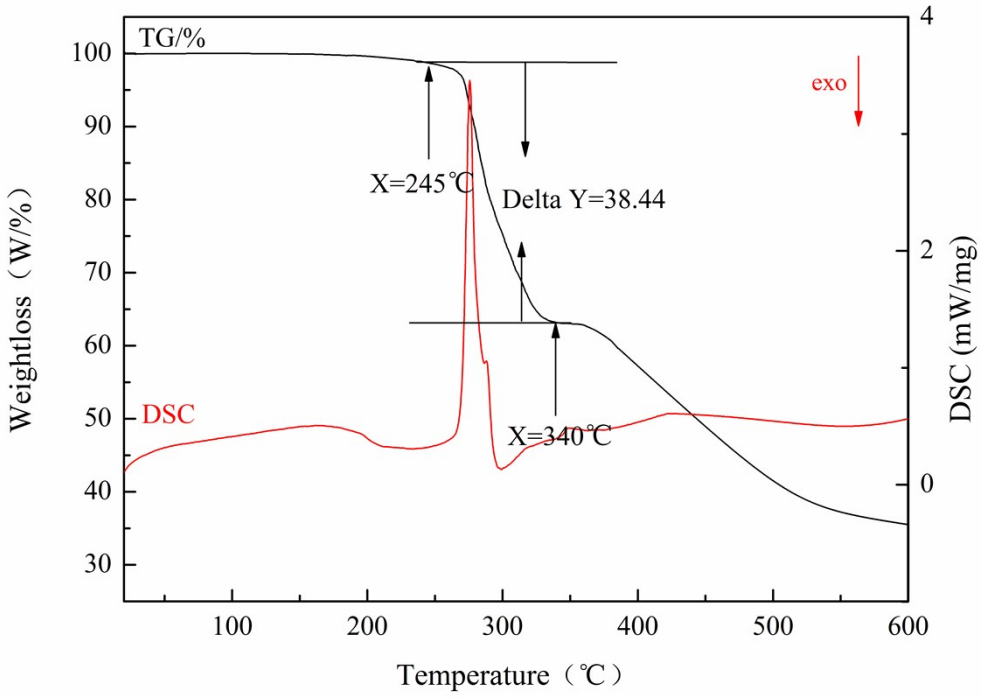

Fig. S12. TG-DSC curve of THB-SS.

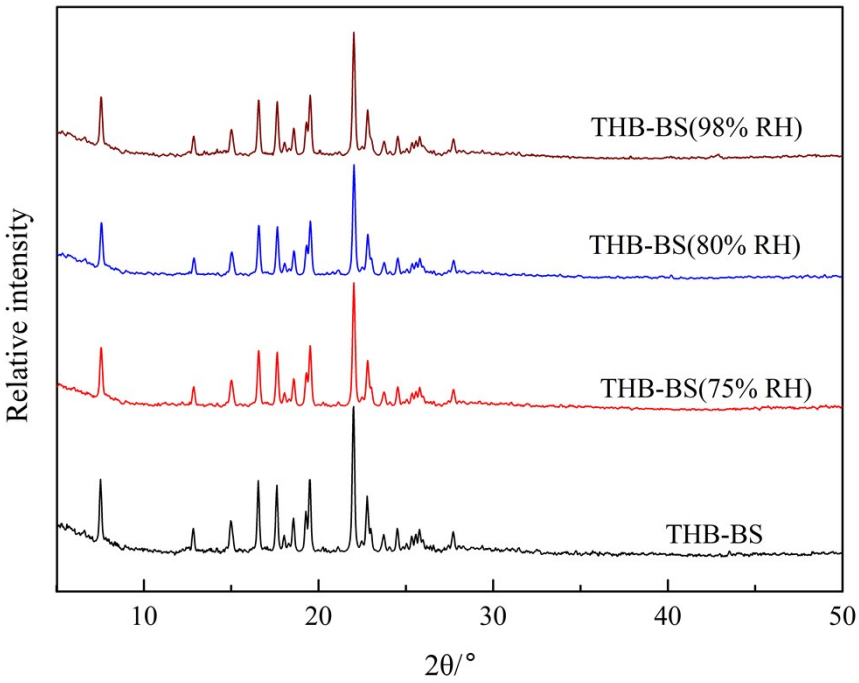

Fig. S13. The XRD plots for THB-BS pre and post hygroscopic measurements

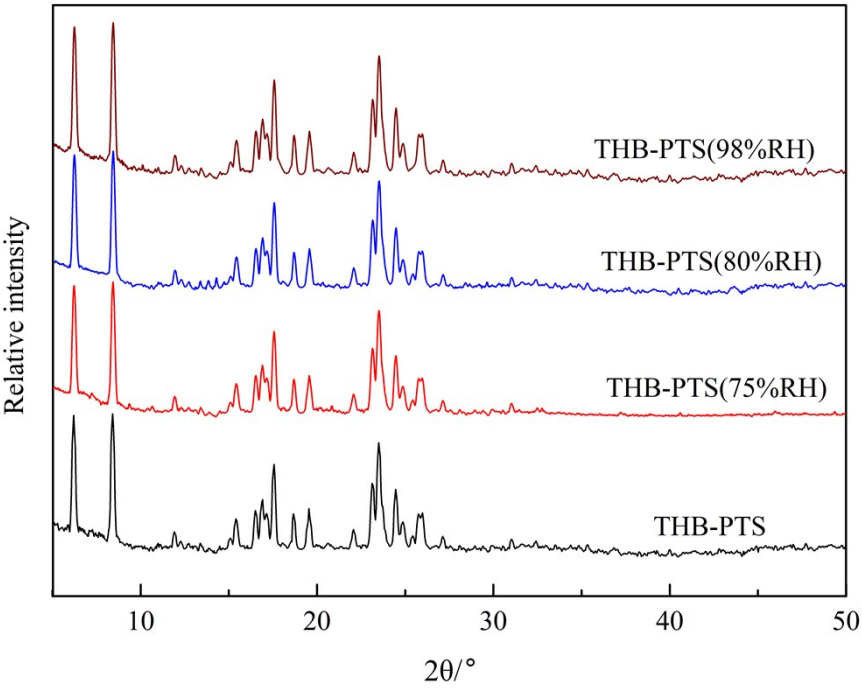

Fig. S14. The XRD plots for THB-PTS pre and post hygroscopic measurements

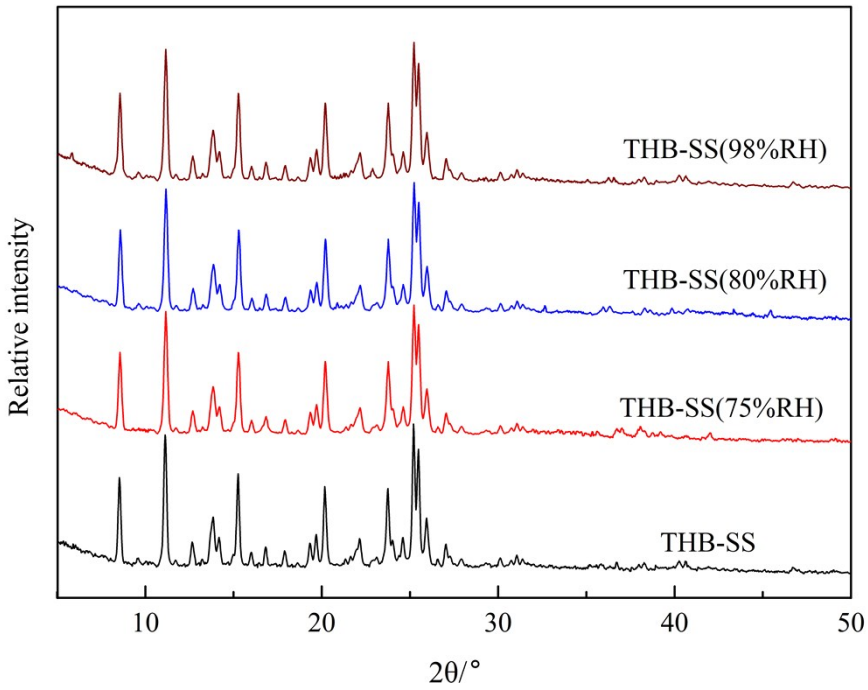

Fig. S15. The XRD plots for THB-SS pre and post hygroscopic measurements

Table S1 Hydrogen bond lengths/Å and angles/° for THB-BS.

D-H···A	d(D-H)	d(H···A	d(D···A	∠DHA
N^+1-H1···O9	0.98	1.81	2.765(19)	164.7
N^+2-H2···O13$^{\#1}$	0.98	1.86	2.752(18)	148.8
C7-H7A···O2$^{\#2}$	0.97	2.55	3.34(3)	138.5
C8-H8A···O11$^{\#3}$	0.97	2.23	3.15(2)	158.1
C15-H15A···O13	0.97	2.34	3.26(2)	157.8
C20-H20C···O6$^{\#3}$	0.96	2.58	3.41(3)	145.6
C27-H27A···O12$^{\#1}$	0.97	2.51	3.20(2)	127.8
C27-H27A···O6$^{\#4}$	0.97	2.49	3.29(3)	140.3
C28-H28A···O14	0.97	2.40	3.24(2)	145.1
C36-H36···O14	0.98	2.55	3.40(2)	145.7
C39-H3A···O8	0.96	2.51	3.08(3)	118.2
C42-H42···O12	0.93	2.47	2.89(3)	106.9
C43-H43···O14$^{\#5}$	0.93	2.43	3.24(3)	144.9
C44-H44···O12$^{\#5}$	0.93	2.41	3.22(3)	144.9
C52-H52···O9	0.93	2.57	2.93(3)	104.3

Symmetry codes: #1 -x+2,y+1/2,-z+1; #2 x-1,y,z; #3 -x+2,y+1/2,-z; #4 -x+1,y-1/2,-z.

Table S2 Hydrogen bond lengths/Å and angles/° for THB-PTS.

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠DHA
N^+1-H1···S1	0.98	2.71	3.554(2)	145.2
N^+1-H1···O5	0.98	1.80	2.776(2)	173.3
C5-H5···O1$^{\#1}$	0.98	2.51	3.344(3)	143.1
C7-H7A···O2	0.97	2.48	3.185(3)	129.0

C13-H13A···O1$^{\#1}$	0.97	2.60	3.461(3)	147.3
C14-H14···O1$^{\#2}$	0.93	2.65	3.552(3)	164.0
C18-H18···O1$^{\#3}$	0.93	2.61	3.513(4)	162.7
C20-H20B···O1$^{\#2}$	0.96	2.63	3.418(4)	139.1
C25-H25A···O5$^{\#4}$	0.97	2.59	3.214(4)	122.1
C26-H26C···O3	0.96	2.58	3.093(4)	113.6

Symmetry codes: #1 -x+1,-y+1,-z+1; #2 x-1,y,z; #3 -x+2,-y,-z; #4 -x+2,-y+1,-z; #5 -x+1,-y,-z+1

Table S3 Hydrogen bond lengths/Å and angles/° for THB-SS.

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠DHA
C4-H4···O7	0.93	2.64	3.406(4)	140.4
C8-H8B···O6$^{\#1}$	0.97	2.41	3.212(4)	139.9
C15-H15A···O5$^{\#2}$	0.97	2.38	3.324(4)	163
C19-H19A···O8$^{\#3}$	0.96	2.63	3.452(6)	143.4
C19-H19C···O4	0.96	2.39	2.899(6)	112.4
C20-H20B···O9$^{\#4}$	0.96	2.57	3.169(5)	120.3
N1^{+}-H1N···O7$^{\#1}$	0.98	1.85	2.826(4)	170.7
N1^{+}-H1N···S1$^{\#1}$	0.98	2.76	3.593(3)	143.8
O8-H8···O9	0.82	1.87	2.598(4)	146.5
O10-H10···O6$^{\#5}$	0.82	1.78	2.573(3)	162.8
O10-H10···S1$^{\#5}$	0.82	2.96	3.664(2)	145.9

Symmetry codes: #1 x,-y+1/2,z+1/2; #2 x-1,-y+1/2,z-1/2; #3 -x+1,y+1/2,-z+3/2; #4 -x,y+1/2,-z+3/2; #5 x-1,y,z.