

Fig. S1. IR spectra of BPY, DHQ and DHQ·BPY (the test temperature was 298K).

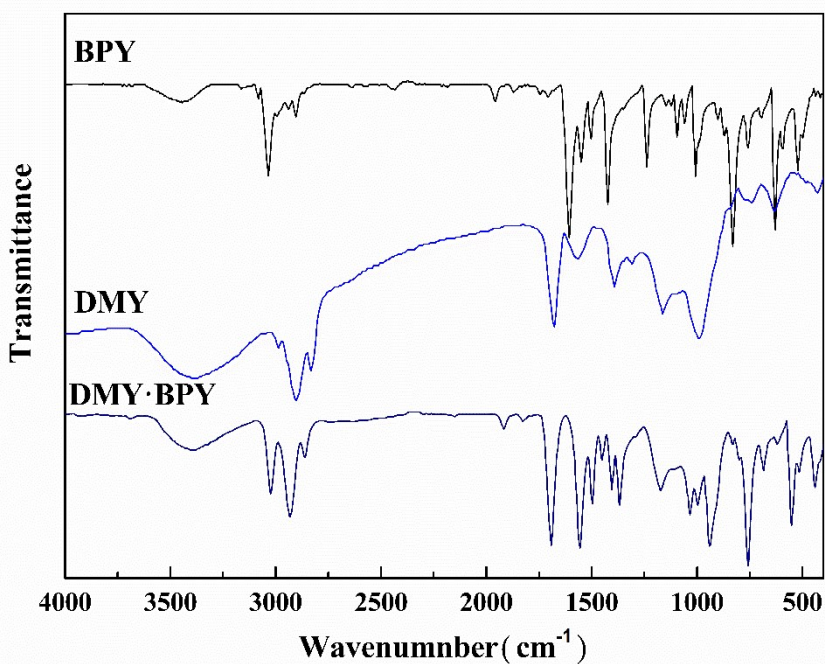


Fig. S2. IR spectra of BPY, DMY and DMY·BPY (the test temperature was 298K).

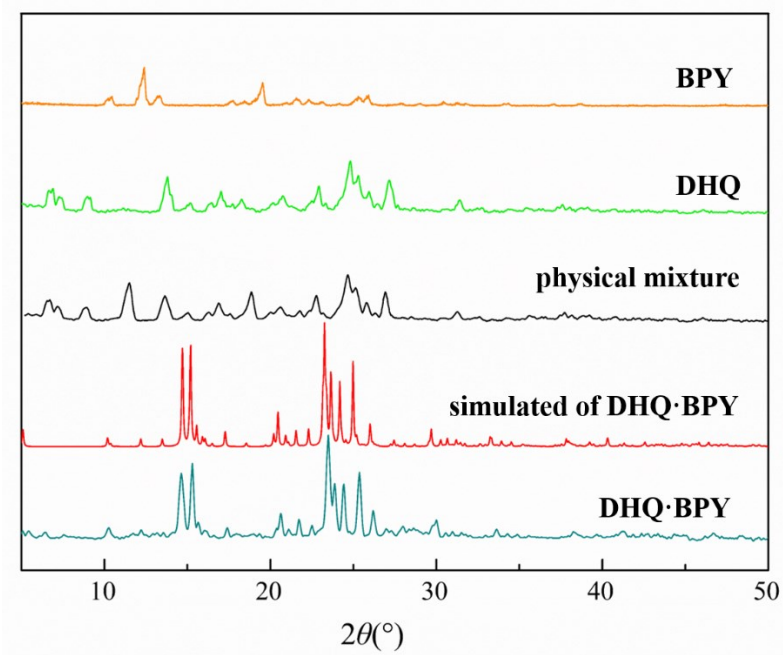


Fig. S3. Comparison of XRD patterns: experimental XRD patterns of BPY, DHQ, DHQ·BPY, physical mixture of BPY and DHQ and the simulated patterns of DHQ·BPY. (the test temperature was 298K).

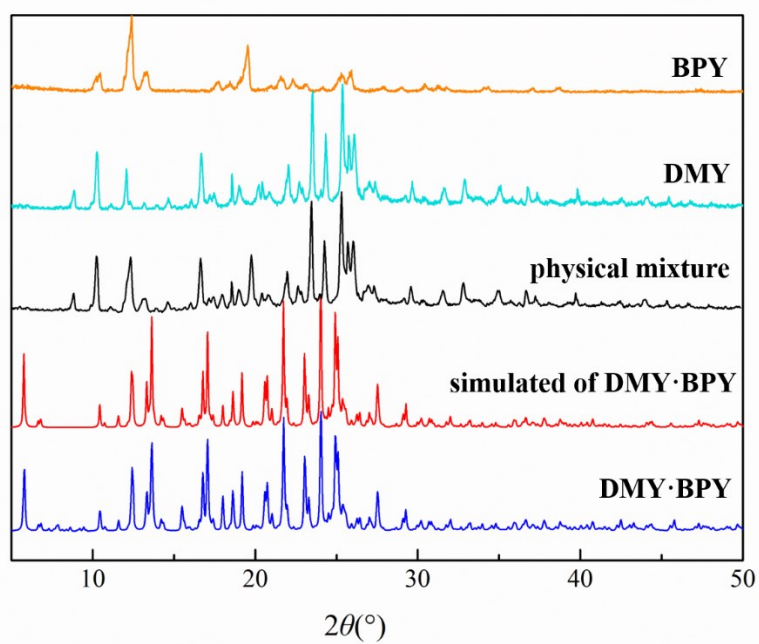


Fig. S4. Comparison of XRD patterns: experimental XPRD patterns of BPY, DMY, DMY·BPY, physical mixture of BPY and DMY and the simulated patterns of DMY·BPY. (the test temperature was 298K).

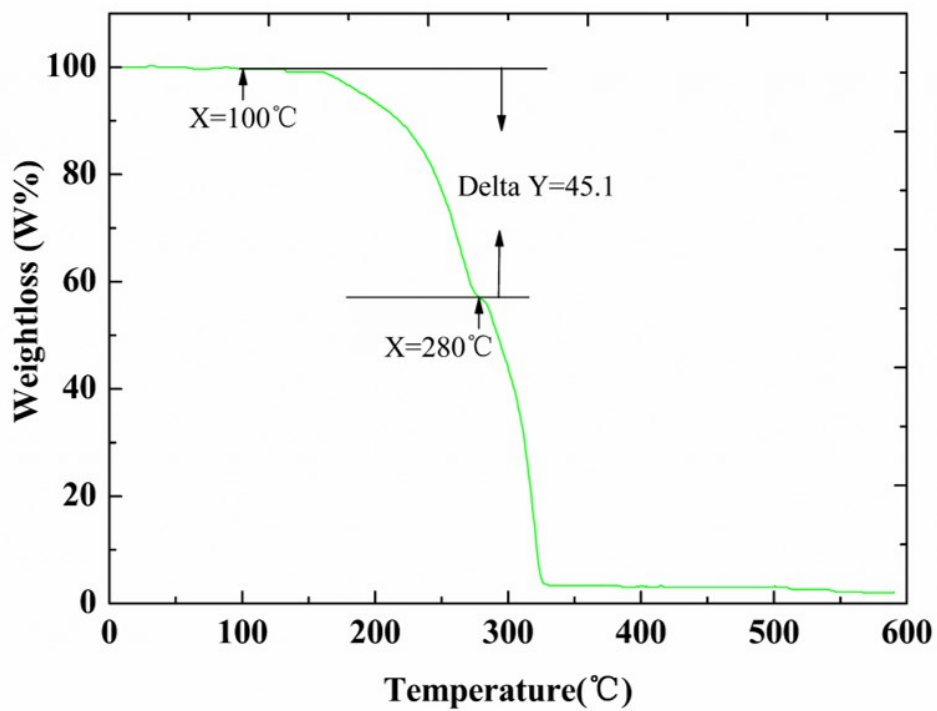


Fig. S5. TGA curve of DHQ-BPY.

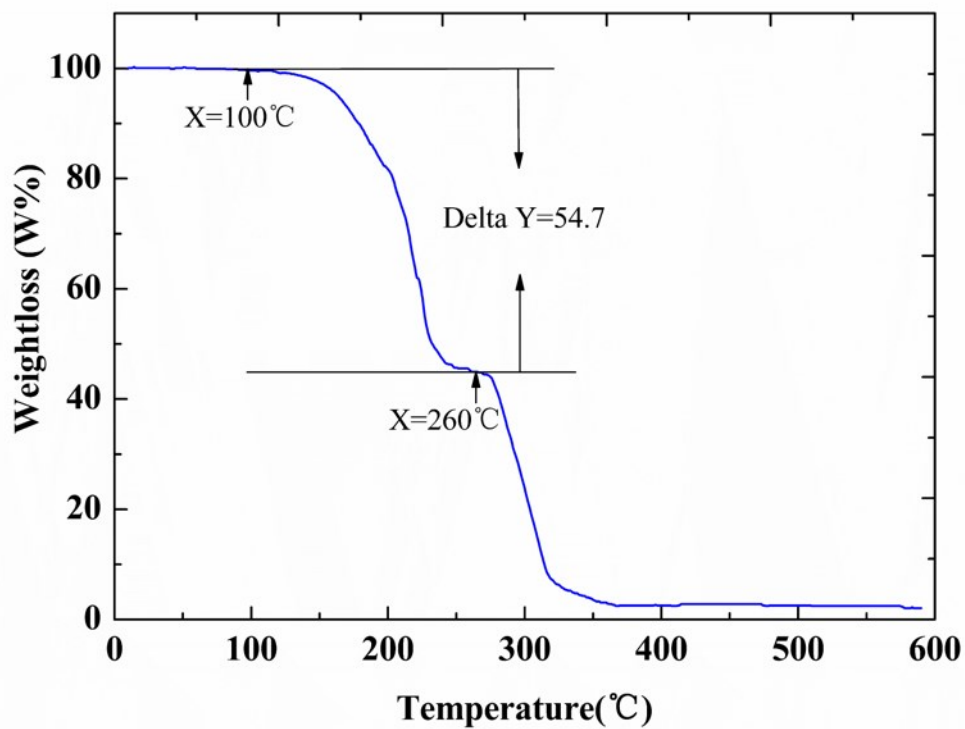


Fig. S6. TGA curve of DMY-BPY.

Table S1 Hydrogen bond lengths/Å and angles/° for DHQ·BPY.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O1-H1···O2	0.82	2.32	2.748(4)	113
O1-H1···N2 ^{#1}	0.82	2.00	2.735(5)	150
O2-H2···O3 ^{#2}	0.82	2.16	2.979(4)	172
O3-H3···N6 ^{#2}	0.82	1.94	2.718(4)	159
O5-H5···O4	0.82	1.86	2.588(4)	147
O6-H6···N4 ^{#3}	0.82	1.86	2.659(4)	164
O8-H8···O10	0.82	1.87	2.593(4)	147
O9-H9···N5	0.82	1.88	2.669(4)	163
O11-H11···N3 ^{#4}	0.82	1.91	2.721(4)	170
O13-H13···O11 ^{#5}	0.82	2.20	3.014(5)	174
O14-H14···O13	0.82	2.30	2.725(5)	113
O14-H14···N1	0.82	2.01	2.727(5)	146
C16-H16···O14 ^{#6}	0.93	2.55	3.443(5)	161

#1 =x,-1+y,1+z; #2=-1-x,-1/2+y,-z; #3=-1+x,-1+y,z; #4=-1-x,-1/2+y,-1-z; #5=-2-x,1/2+y,-1-z;
#6=-1-x,1/2+y,-1-z

Table S2 Hydrogen bond lengths/Å and angles/° for DMY·BPY.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O1-H1···N3	0.82	1.91	2.711(4)	165
O2-H2···O3	0.82	2.24	2.669(4)	113
O2-H2···N2 ^{#1}	0.82	2.14	2.917(5)	159
O3-H3···N1	0.82	1.89	2.670(5)	159
O5A-H5A···O6	0.82	2.39	2.722(17)	105
O5A-H5A···N4 ^{#2}	0.82	1.95	2.697(17)	150
O7-H7···N5 ^{#3}	0.82	1.87	2.662(5)	161
O8-H8···O6	0.82	1.84	2.571(4)	148
C7A-H7A···O7 ^{#3}	0.98	2.54	3.470(8)	158
C27-H27···O5A ^{#4}	0.93	2.38	3.303(16)	170
C27-H27···O5B ^{#4}	0.93	2.55	3.48(4)	177
C29-H29···O5B ^{#5}	0.93	2.47	3.40(5)	174
C32-H32···O2 ^{#6}	0.93	2.43	3.079(5)	127
C35-H35···O6 ^{#2}	0.93	2.43	3.137(6)	133

#1=2-x,1-y,1-z; #2=1-x,3-y,2-z; #3=-x,2-y,1-z; #4=-1+x,y,z; #5=-x,2-y,2-z; #6=x,1+y,z.