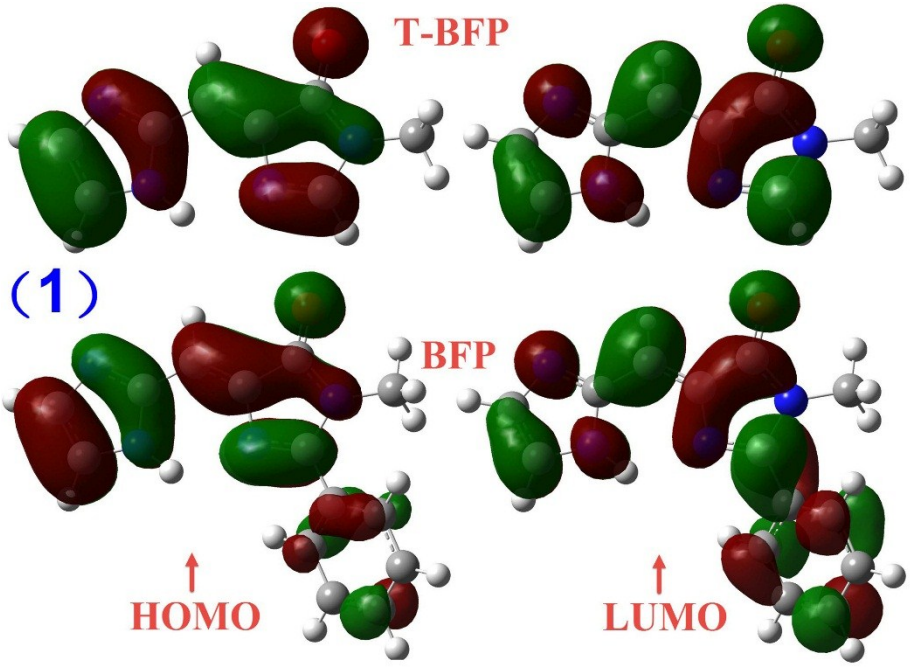
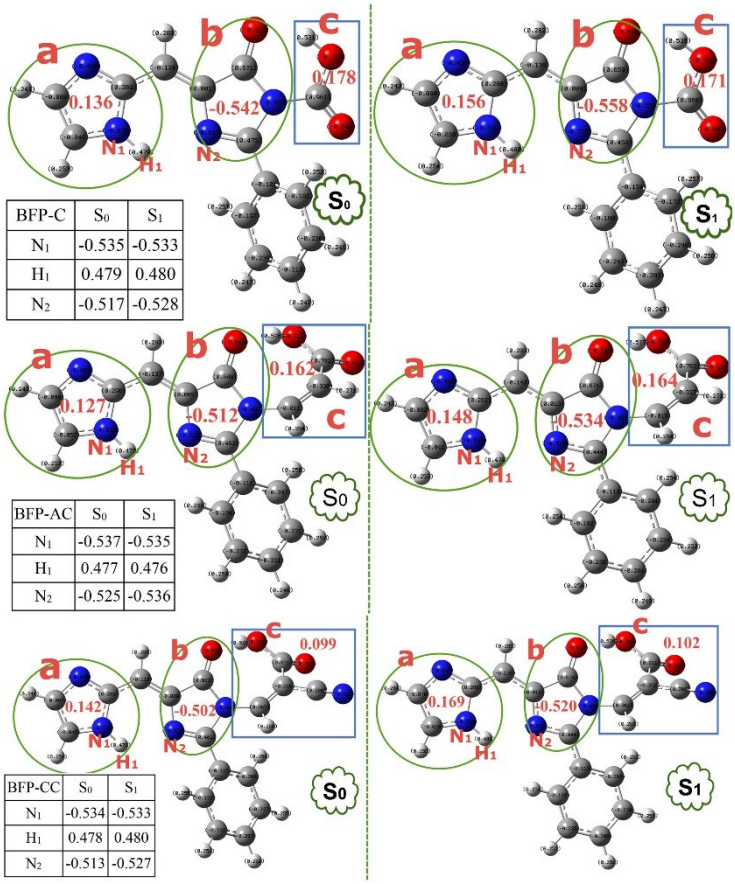


Fig. S1 The HOMO/LUMO orbitals of T-BFP and BFP molecules.



BFP-C	S_0	S_1
N_1	-0.535	-0.533
H_1	0.479	0.480
N_2	-0.517	-0.528

BFP-AC	S_0	S_1
N_1	-0.537	-0.535
H_1	0.477	0.476
N_2	-0.525	-0.536

BFP-CC	S_0	S_1
N_1	-0.534	-0.533
H_1	0.478	0.480
N_2	-0.513	-0.527

Fig.S2 The NBO charges of BFP-AC, BFP-C and BFP-CC in both S_0 and S_1 states.

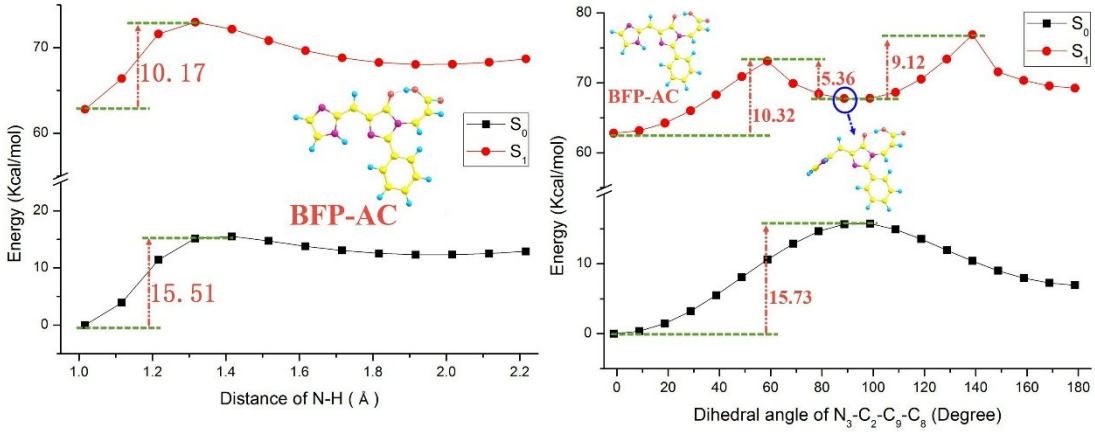


Fig. S3 The potential energy lines of BFP-AC molecule with a serious of bonds and angles.

Table S1 The potential energy barriers.

		BFP	BFP-C	BFP-AC	BFP-CC	BFP-MC	BFP-MN
Bond	**S_0**	**14.62**	**15.38**	**15.51**	**16.09**	**17.02**	**17.28**
	S_1	**9.08**	**10.69**	**10.17**	**10.38**	**9.69**	**1.17**
Angle	**S_0**	**14.26**	**15.81**	**15.73**	**16.11**	**14.79**	**14.98**
	S_1	**12.94**	**7.77**	**10.32**	**8.01**	**23.11**	**23.98**