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Supporting Information

Theoretical Study on Interactions between *N*-butylpyridinium Nitrate and Thiophenic Compounds

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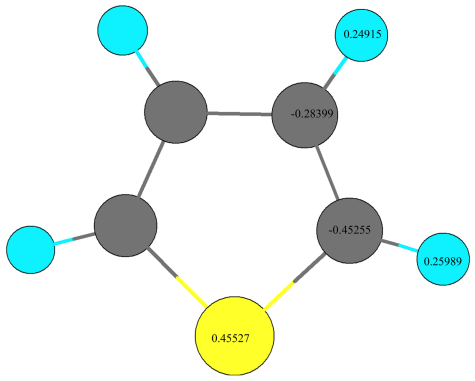
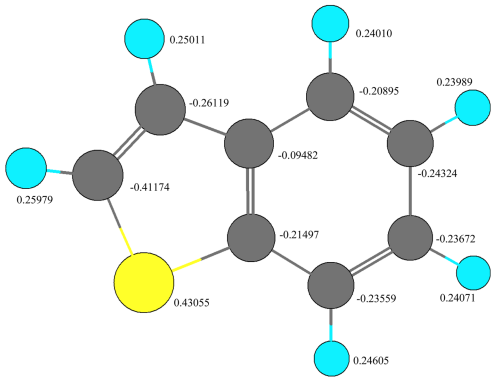
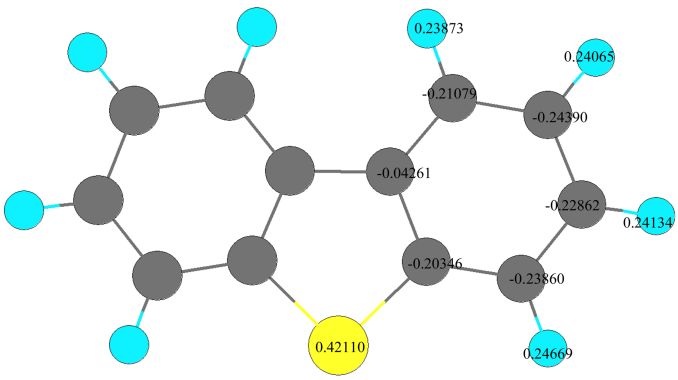


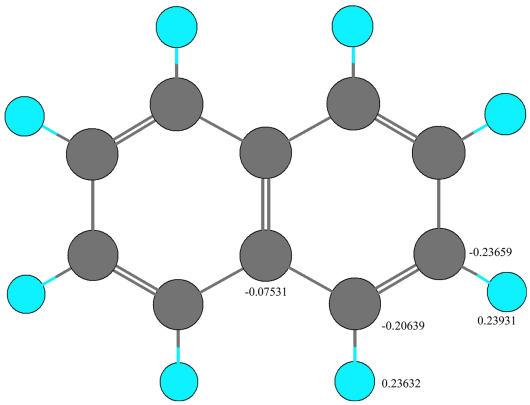
(a)



(b)



(c)



(d)

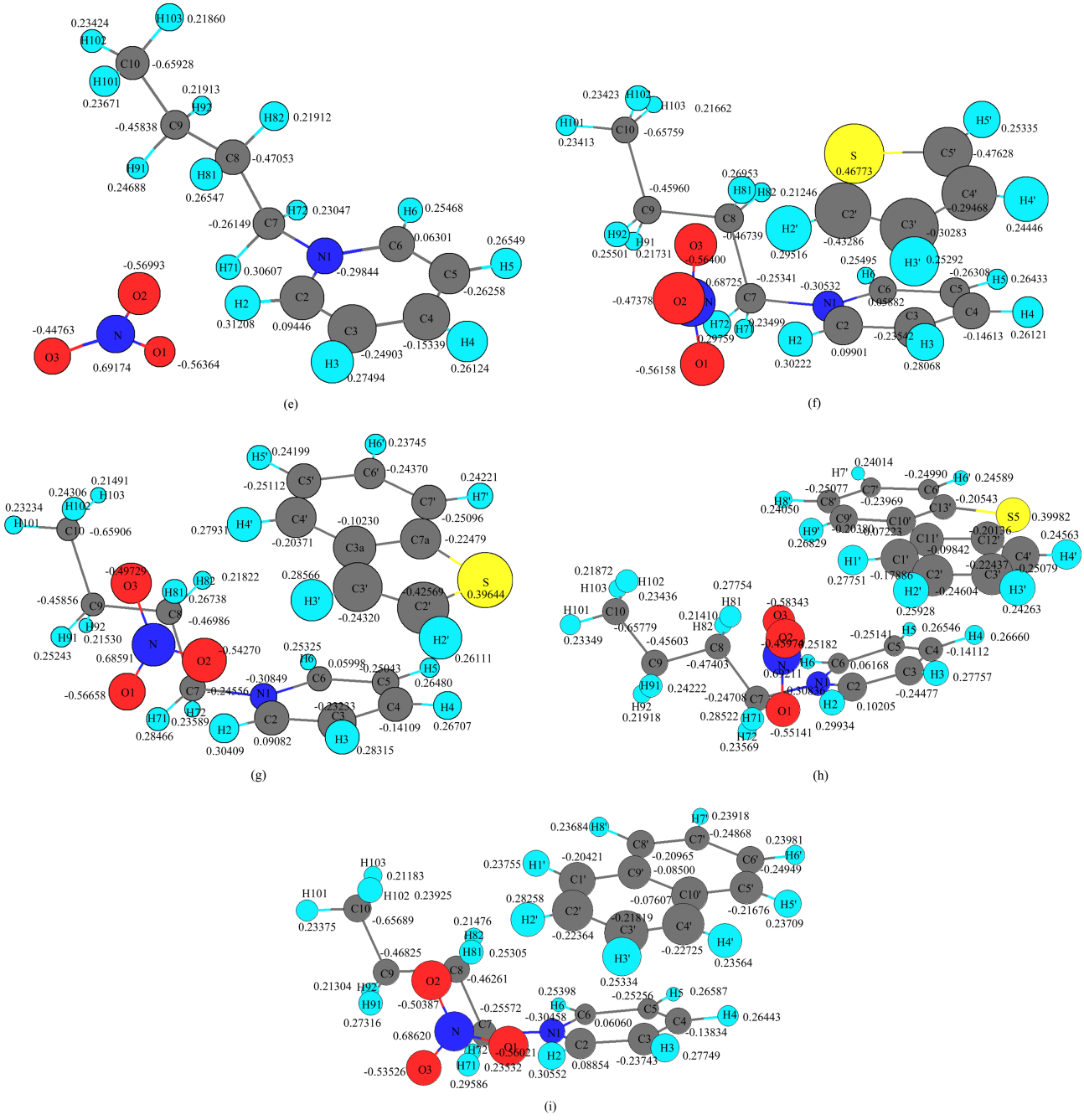


Fig. S1. The NBO charges of (a) TS, (b) BT, (c) DBT, (d) NAP, (e) [BPY]NO_3], (f) [BPY]NO_3]-TS, (g) [BPY][NO_3]-BT, (h) [BPY]NO_3]-DBT, and (i) [BPY][NO_3]-NAP

We have calculated the structures and energies by DFT-D. The results show that the optimized structures are changed with or without DFT-D method. But the optimized structures do not change significantly and we only discussed the optimized structures at GGA/PW91/DNP level. The optimized structures are displayed as following. The interaction energies are shown as following and the energy change trend is similar.

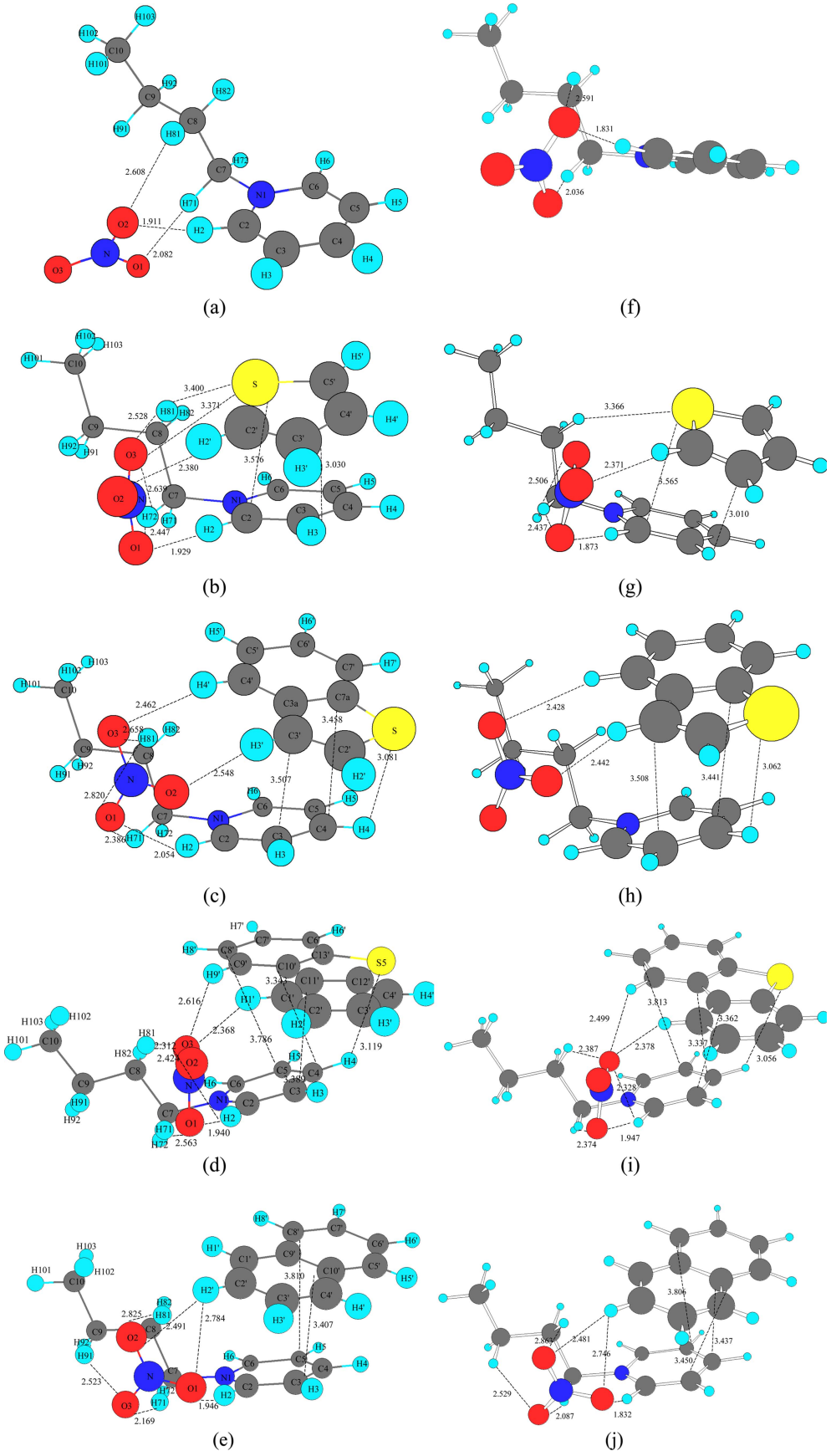


Fig. S2. The optimized structures and some interacting distances of (a) $[BPY]^+[NO_3]^-$, (b) $[BPY]^+[NO_3]^-$-TS, (c) $[BPY]^+[NO_3]^-$-BT, (d) $[BPY]^+[NO_3]^-$-DBT, (e) $[BPY]^+[NO_3]^-$-NAP at GGA/PW91/DNP level. (f) $[BPY]^+[NO_3]^-$, (g) $[BPY]^+[NO_3]^-$-TS, (h) $[BPY]^+[NO_3]^-$-BT, (i) $[BPY]^+[NO_3]^-$-DBT and (j) $[BPY]^+[NO_3]^-$-NAP at DFT-D level.

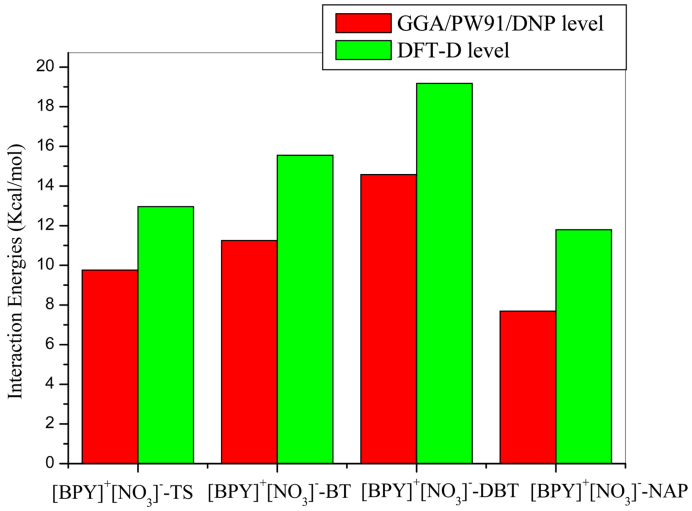


Fig. S3. The interaction energies calculated at GGA/PW91/DNP level and DFT-D level.