Intramolecular Charge Transfer Enhanced Optical Limiting in Novel Hydrazone Derivatives with D_1-D-A_i-π-A Structure(supporting information)*

Hongjuan Zhu[1], Danyang Zhang[1], Xianghao Sun[1],
Shifeng Qian[1], Eryin Feng[1], Xiaowei Sheng[1*]

1. Anhui Province Key Laboratory for Control and Applications of Optoelectronic Information Materials, Anhui Normal University, Anhui, Wuhu 241000, China

*Correspondence

Xiaowei Sheng, E-mail:xwsheng@mail.ahnu.edu.cn

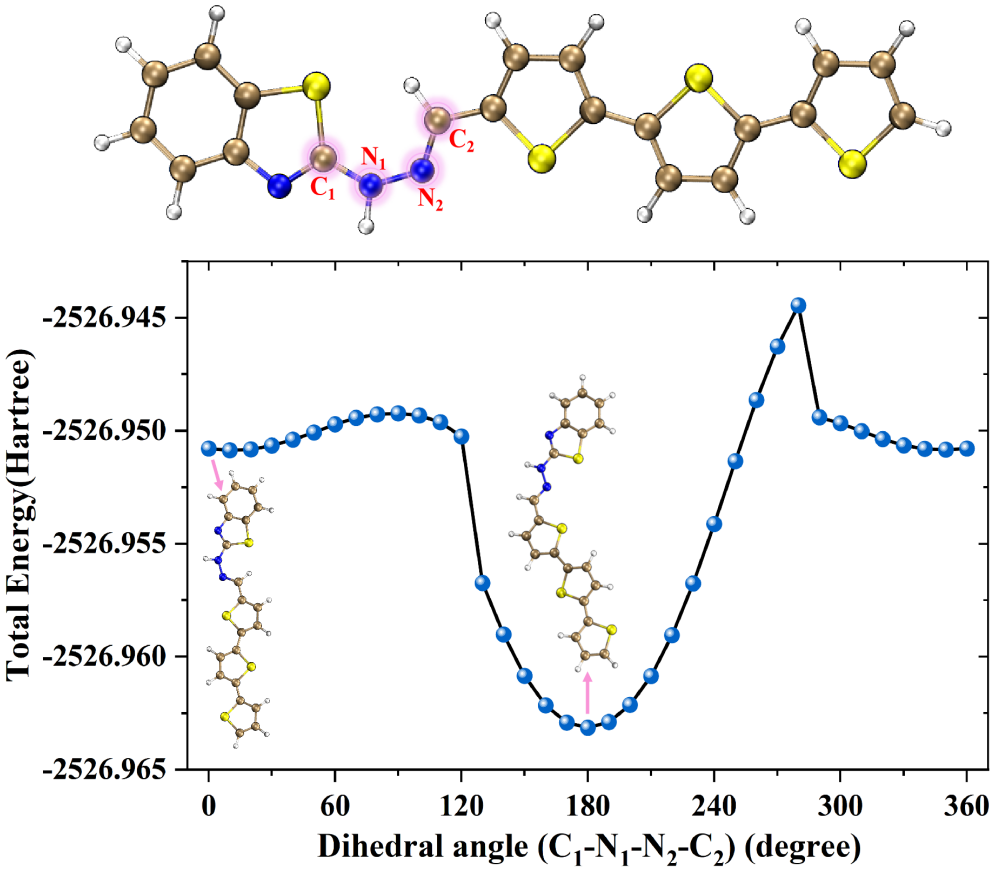

FIG. S1: Potential energy curve of BTH at different dihedral angles.

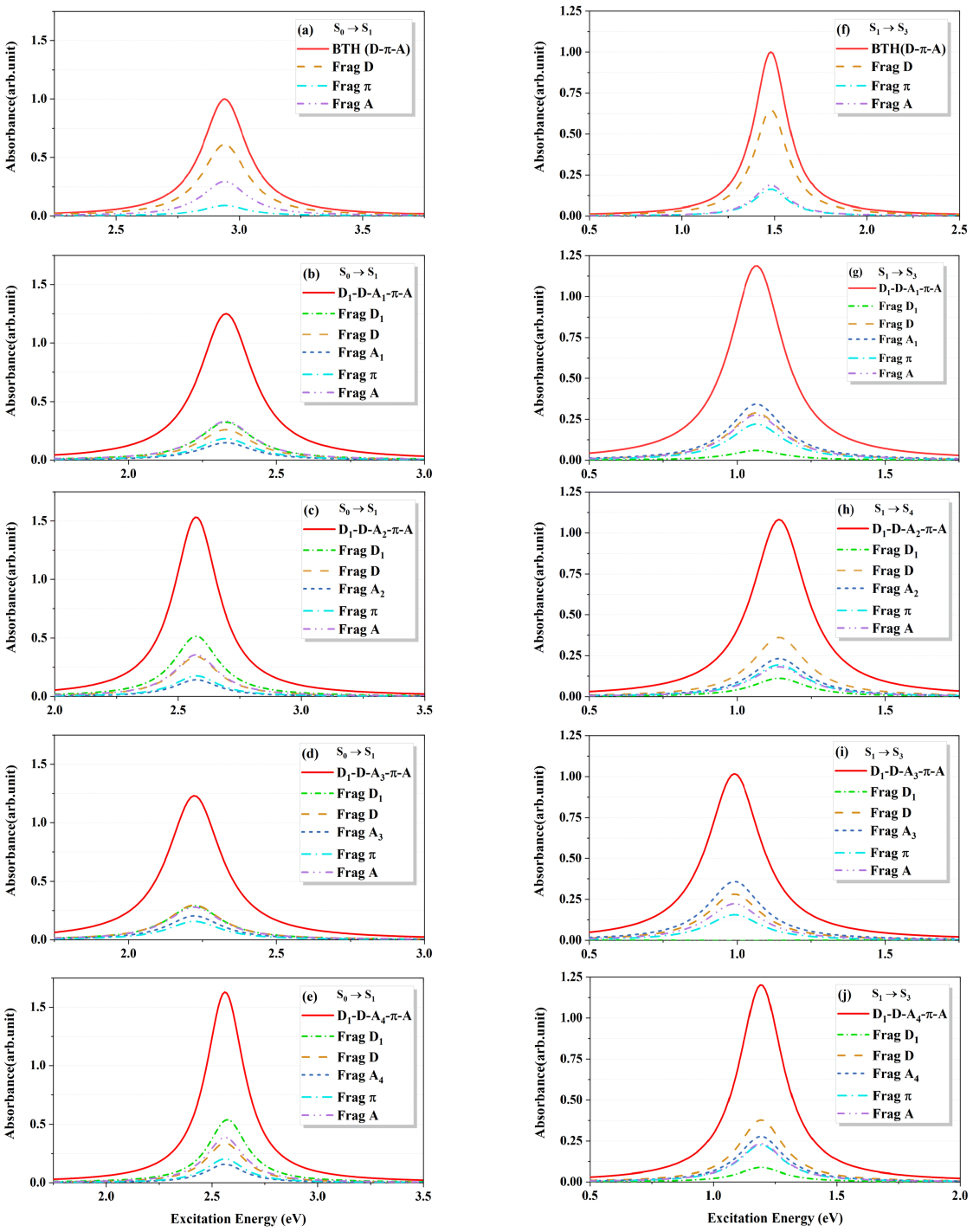

FIG. S2: Contributions of various fragment to the $S_0 \rightarrow S_1$ and $S_1 \rightarrow S_n$ transition spectra in BTH and the present designed four hydrazone derivatives.

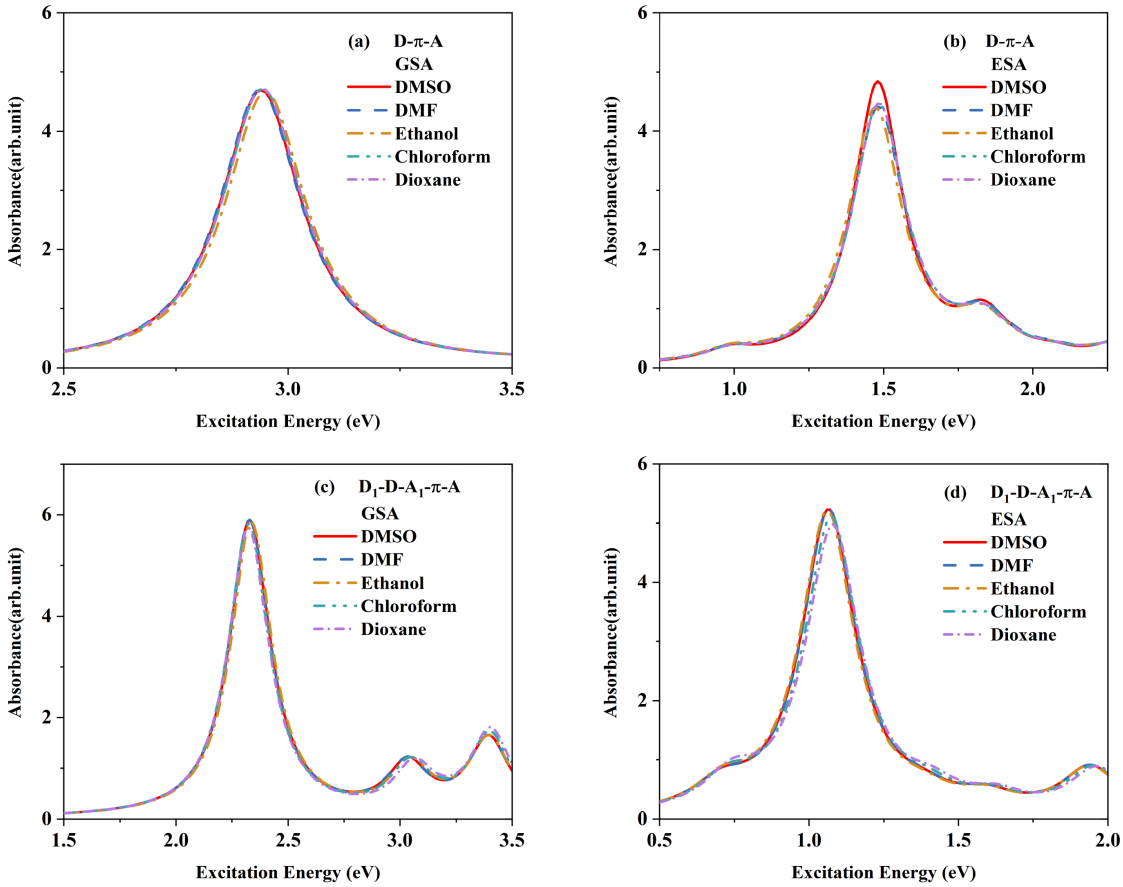

FIG. S3: GSA and ESA spectra of BTH and D_1-D-A_1-π-A in various solvents.

TABLE S1: Distance between centroid of hole and electron (D), hole delocalization index(HDI) and electron delocalization index (EDI) for the $S_0 \rightarrow S_1$ transition of the BTH and D_1-D-A_i-π-A molecules.

	D($\AA$)	HDI	EDI
D-π-A(BTH)	0.14	6.01	5.77
D_1-D-A_1-π-A	2.13	5.01	5.36
D_1-D-A_2-π-A	1.72	4.91	4.58
D_1-D-A_3-π-A	2.63	4.78	4.90
D_1-D-A_4-π-A	1.50	4.83	4.72