Electronic Supplementary Information (ESI)

The mechanism of ratiometric fluoride sensor and ESIPT process for 2,6-dibenzothiazolylphenol and its derivative

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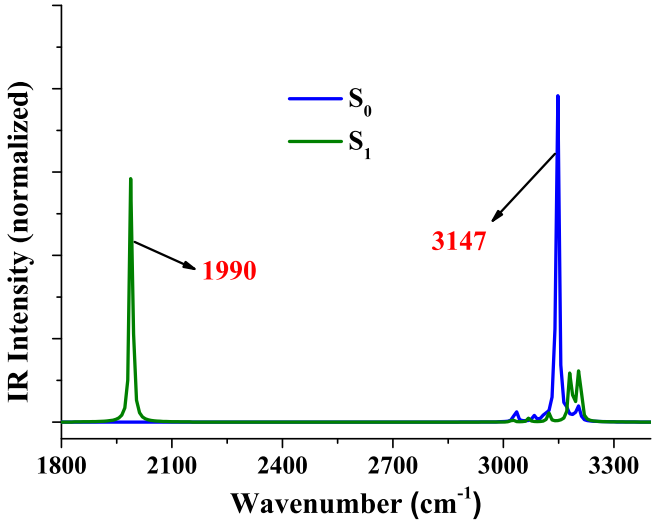

Figure S1: The theoretical IR spectra of 26DB in the spectra region of O1-H2 stretching vibrational mode in both S_0 and S_1 states.

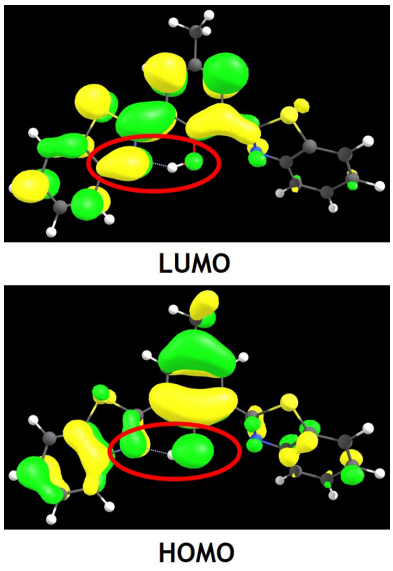

Figure S2: View of the frontier molecule orbitals (HOMO and LUMO) for 26DB molecule. Herein, the red cycle indicates the charge transfer moiety involved in hydrogen bond (O1-H2$\cdots$N3) of 26DB.

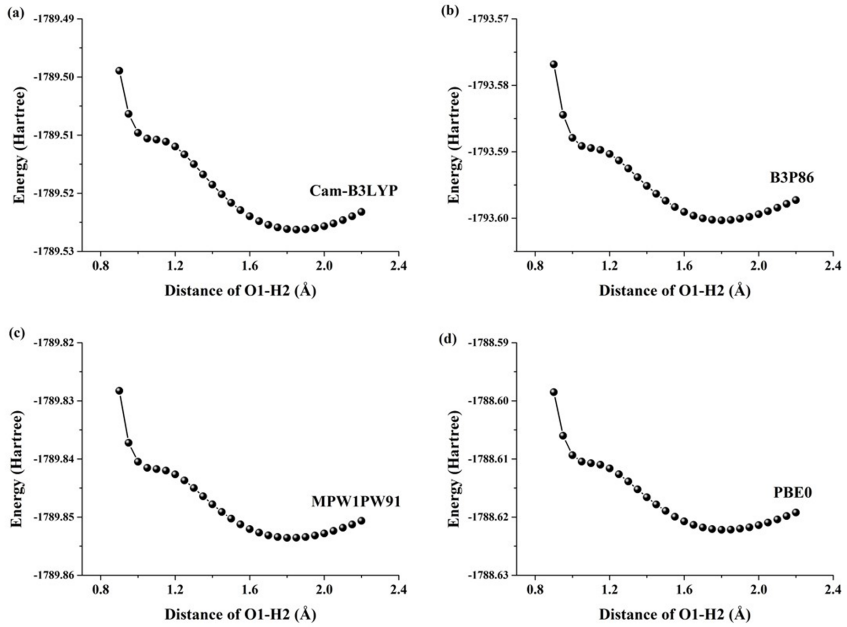

Figure S3: The theoretical S_1-state potential energy curves for 26DB system in step of 0.05 Å based on four kinds of functionals. (a) Cam-B3LYP; (b) B3P86; (c) MPW1MP91; (d) PBE0.

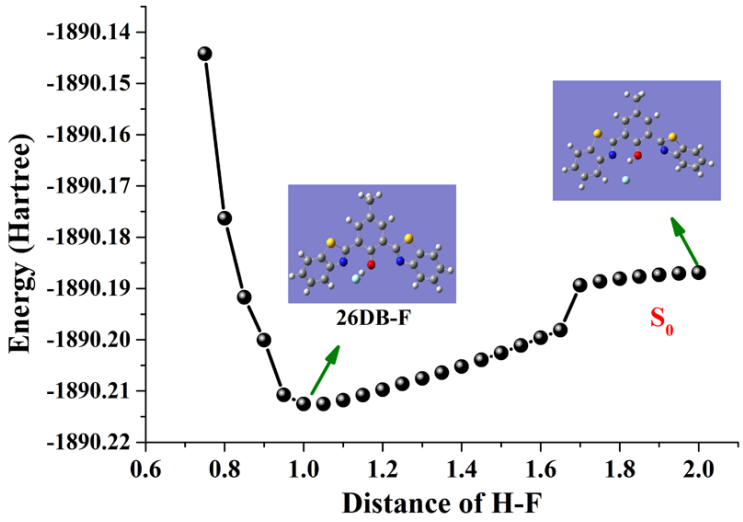

Figure S4: Potential energy curve of S_0 state for 26DB with the addition of fluoride anion, which is the function of H-F distance.

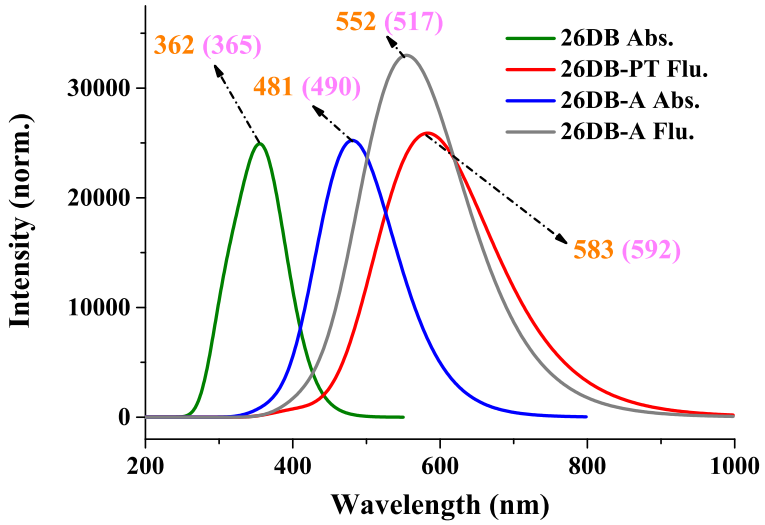

Figure S5: The theoretical electronic spectra of 26DB, 26DB-PT and 26DB-A structures in THF solvent. Herein, the previous experimental results are listed in the brackets.

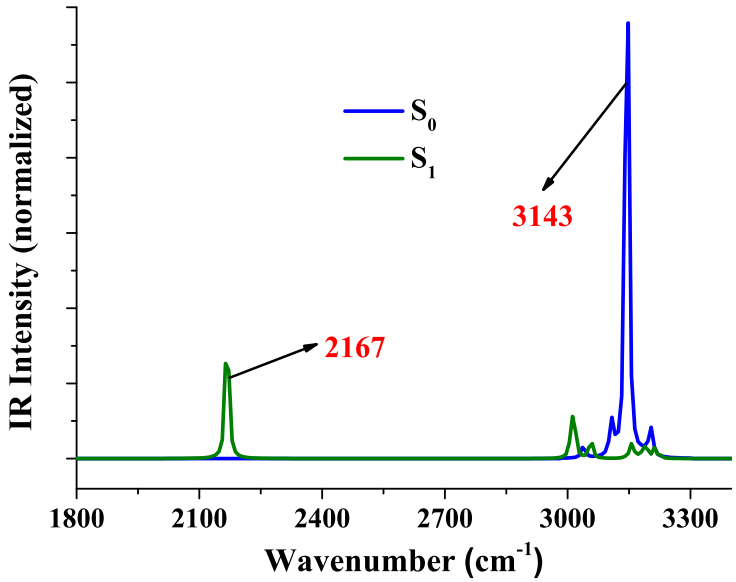

Figure S6: The theoretical IR spectra of Bis-26DB in the spectra region of synergetic O1-H2 and O4-H5 stretching vibrational mode in both S_0 and S_1 states.