**Supplementary Material**

**Computational prediction on photophysical properties of two excited state intramolecular proton transfer (ESIPT) fluorophores bearing the benzothiazole group**

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**Figure S1.** PBE0/TD-PBE0 optimized S0 and S1 structures of deprotonated anion conformers.

**Table S1.** Absorption and emission wavelengths (*λ*, in nm) and the corresponding oscillator strengths (*f*) of molecules **I** and **II** obtained by the TD-PBE0 calculations in combination with a PCM model using hexane and DMF as solvents, respectively, along with previously computational results and experimentally available data.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Conformer | Transitiona | Solvent | *λ*cala | *f*a | *λ*calb | *f*b | *λ*exp |
| **I** |  |  |  |  |  |  |  |
| S0(E) | S0 → S1 | Hexane | 367 | 0.57 | 367 | 0.40 | 369c |
|  | S0 → S2 | Hexane | 322 | 0.28 | - | - | 330c |
| S0(A) | S0 → S1 | DMF | 459 | 0.77 | 516 | 0.67 | 491c |
|  | S0 → S4 | DMF | 323 | 0.16 | - | - | 325c |
| S1(K\*) | S1 → S0 | Hexane | 560 | 0.41 | 624 | 0.28 | 568c |
| S1(A\*) | S1 → S0 | DMF | 491 | 0.79 | 560 | 0.53 | 516c |
| **II** |  |  |  |  |  |  |  |
| S0(E) | S0 → S1 | Hexane | 403 | 0.96 | 389 | 0.71 | 383d |
|  | S0 → S2 | Hexane | 340 | 0.22 | - | - | 312d |
| S0(A) | S0 → S1 | DMF | 547 | 0.98 | 586 | 0.83 | 528d |
|  | S0 → S4 | DMF | 360 | 0.34 | - | - | 372d |
|  | S0 → S10 | DMF | 296 | 0.44 | - | - | 306d |
| S1(E\*) | S1 → S0 | Hexane | 475 | 0.90 | - | - | - |
| S1(K\*) | S1 → S0 | Hexane | 616 | 0.63 | 633 | 0.44 | 626d |
| S1(A\*) | S1 → S0 | DMF | 582 | 0.84 | 648 | 0.63 | 616d |

a TD-PBE0/6-311+G(d,p) calculations from this work.

b TD-B3LYP/6-31+G(d,p) calculations from previous work [1].

c Experimental values from Ref. [2].

d Experimental values from Ref. [1].

**References**

[1] X. Zhang, J.-Y. Liu, W.-W. Ma, and M.-L. Yang, J. Mater. Chem. B **4** 6662 (2016).

[2] X. Zhang and J-Y. Liu, Dyes Pigm. **125** 80 (2016).



**Figure S2.** Frontier molecular orbitals for the investigated molecules in the ground state.