Computational Investigation of the Novel Diaminoterephthalate-Based Fluorophores

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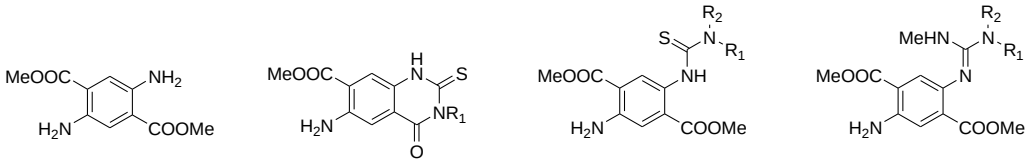
Diaminoterephthalates are typical representatives of the single-benzene-based fluorophores, and they became important building blocks for devising new organic optoelectronic materials [1,2]. The typical fluorescence band of the simple *N*-alkylated 2,5-diaminoterephthalates (**DATA**, Fig. 1) falls above 500 nm, with the observed Stokes shift larger than 100 nm [1]. This was attributed to the specific arrangement of the electron-donating and the electron-accepting groups, leading to the S_1 with highly pronounced charge-transfer character [3]. Besides that, geometry changes triggered by the antiaromaticity in the S_1(FC) region were also recognized as the mechanism that strongly contributes to the large Stokes shift [3,4].

Recently, we found that the PBE0/6-31G(d)//M06-2X/6-31G(d) model presents a simple but quite accurate computational model for predicting absorption and the emission maxima in the selected terephthalate-based fluorophores [5]. Herein, we are presenting calculated basic photophysical properties (λ_{Em} and λ_{Abs}) for the series of thioureas (**1** and **2**, Fig. 1) and guanidines (**3**), as well as the acid/base properties of the guanidine derivatives and their tendency toward intramolecular proton transfer in the S_1 state.



DATA **1** (R_1 = alkyl or aryl) **2** (R_1, R_2 = alkyl or H) **3** (R_1, R_2 = alkyl or H)

Figure 1. Schematic structures of the investigated groups of compounds

References:

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