

## Supplementary Information

### Theoretical Investigation of Excited-State Intramolecular Double Proton Transfer Process of 2,2'-(benzo[1,2-d:4,5-d']bis(thiazole)-2,6-diyl)diphenol

Yongchao Hao<sup>a,b\*</sup> Xiaoran Li<sup>a</sup> Hongfang Li<sup>a</sup> Shanyan Chang<sup>a</sup> Jiangyu Zhang<sup>a</sup> Lili Dong<sup>a\*</sup>

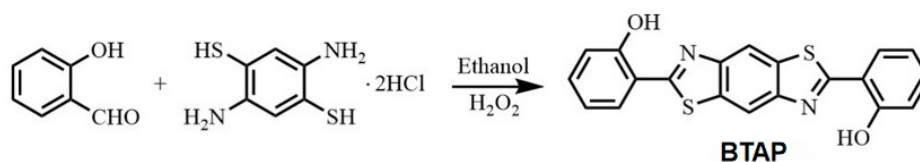
a School of Chemical Engineering and Biotechnology, Xingtai University, Xingtai 054001, China

E-mail: [201610338@xttc.edu.cn](mailto:201610338@xttc.edu.cn) [donglilihanzh@163.com](mailto:donglilihanzh@163.com)

b College of Chemistry and Materials science, Hebei Normal University, Shijiazhuang 050024, China

#### Experimental procedure

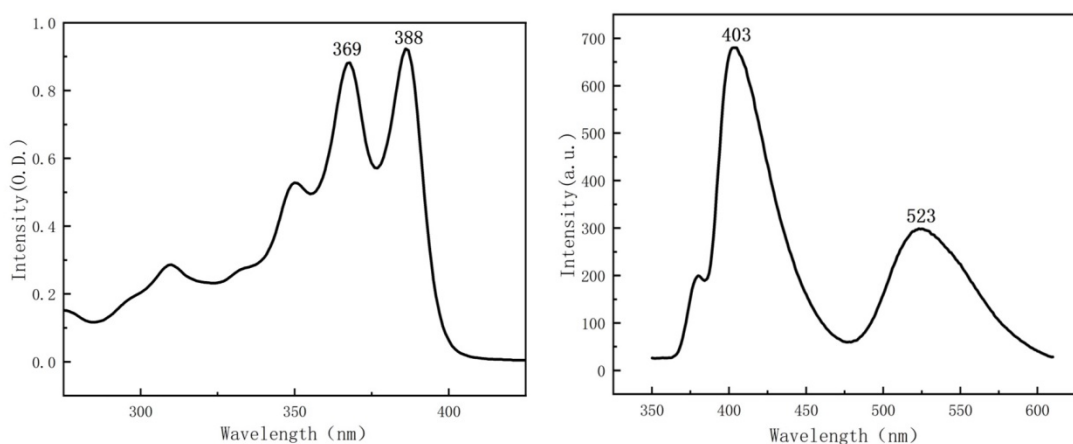
##### Synthesis of BTAP



**Scheme S1.** Synthesis route of BTAP

2,5-diamino-1,4-benzenedithiol dihydrochloride (0.100g, 0.408mmol), salicylaldehyde (0.160g, 1.310mmol) and ethanol (15ml) were mixed into a 100 ml three necked flask, the solution was refluxed for 45 min. After cooling to 50°C, H<sub>2</sub>O<sub>2</sub> (3~5 drops) was added to the above reaction solution, which was reflux for another 10min. Then the mixture was cooled to room temperature, a slightly yellow solid was obtained through centrifugation and it was washed (ethanol, 3\*10ml) and dried to give the product 2,2'-(benzo[1,2-d:4,5-d']bis(thiazole)-2,6-diyl)diphenol (**BTAP**, 0.101g, yield: 66.0%). HRMS C<sub>20</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>, calcd. 376.0340 found: 377.0426 [M+H]

#### Experimental electronic spectrum



**Figure S1.** Absorption spectrum and emission spectrum of **BTAP** in DCM.