

## Difluoro-triazaborinines containing benzo-fused imidazo-, oxazolo-, and thiazolo-pyrimido fragment as new luminescent frameworks

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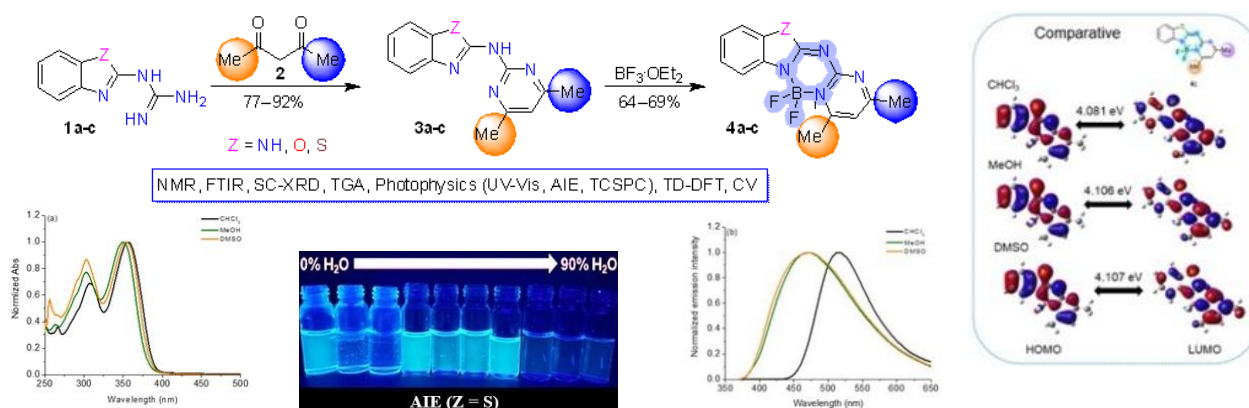
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### ABSTRACT

In the present work the results of an efficient method for synthesizing three novel tetra-coordinated BF<sub>2</sub> complexes, specifically namely, 6,6-difluoro-2,4-dimethyl-6*H*-5λ<sup>4</sup>,6λ<sup>4</sup>-benzo[4,5]imidazo(oxazolo/thiazolo)[3,2-*c*]pyrimido[2,1-*f*][1,3,5,2]triazaborinines (**4**) is reported by us. The compounds **4** were synthesized via the reaction of selected *N*-(4,6-dimethylpyrimidin-2-yl)-benzo[*d*]imidazo(oxazolo/thiazolo)-2-amines (**3**) with BF<sub>3</sub>·OEt<sub>2</sub>, employing Et<sub>3</sub>N as a base[1,2]. Compounds **3** were previously obtained from the reaction of aminoguanidines (**1**) with pentane-2,4-dione (**2**). Optimized yields up 64% were achieved when the reactions were conducted in anhydrous CHCl<sub>3</sub> at room temperature for 24 hours. The structural characterization of BF<sub>2</sub> complexes **4** was elucidated through a combination of multinuclear NMR, FTIR, SC-XRD, and HRMS techniques. Compounds **4** demonstrated thermal stability up to 150 °C. The spectroscopic properties (in both solution and solid states) and the electrochemical properties of the synthesized derivatives were thoroughly investigated using UV-Vis spectroscopy, steady-state, time-resolved fluorescence emission, TD-DFT calculations, and redox potential measurements. The results of this study highlighted a dependence of the compounds' properties on the heteroatom (N, O, S) present within the heterocyclic scaffolds (Scheme 1).



Scheme 1. A summary of this study: Synthesis and photophysical properties of 6,6-difluoro-2,4-dimethyl-6*H*-5λ<sup>4</sup>,6λ<sup>4</sup>-benzo[4,5]imidazo(oxazolo/thiazolo)[3,2-*c*]pyrimido[2,1-*f*][1,3,5,2]triazaborinines **4**.

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