TWO-PHOTON ABSORPTION OF FLUORESCENT DIFLUOROBORATES:

IN SILICO STUDIES

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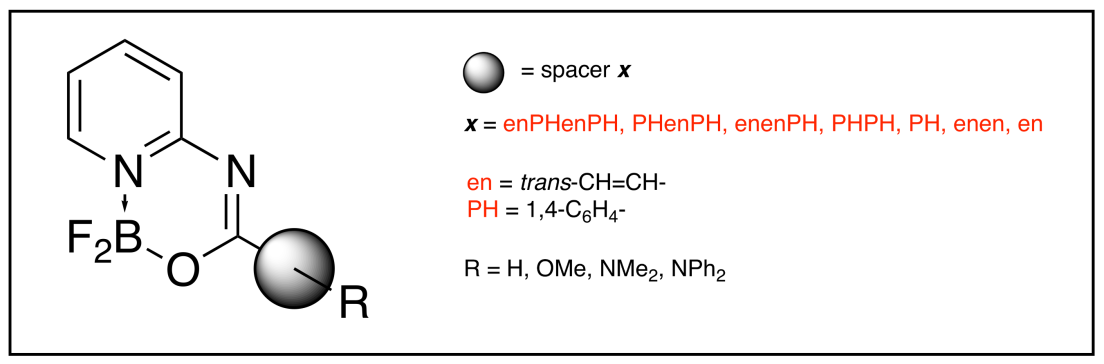
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Two-photon absorption (2PA) process, although predicted on a purely theoretical basis in 30’s of past century, has gained much attention only in last two decades. 2PA is in a limelight mainly due to its potential applications, including three-dimensional data storage or two-photon microscopy. It may also be used to identify symmetry-forbidden transitions or to record high-resolution spectra below the Doppler width. In particular, the applications of 2PA for bio-imaging is rapidly developing area and every year a large numer of 2PA-active dyes are synthesized and studied using both experimental and theoretical methods. The current project aims at contributing to these efforts and focuses on 2PA process for a series of highly fluorescent difluoroborates. To this end, we considered around 30 compounds shown in the figure below.



The geometries of all compounds were optimized at the B3LYP/cc-pVDZ level of theory and used for subsequent electronic structure calculations using Coulomb-attenuated B3LYP functional and the aug-cc-pVDZ basis set. The latter functional was employed to accurately describe long-range intramolecular charge-transfer excitations, which are present in electronic spectra for the studied compounds containing electron-donating/withdrawing substituents. Based on electronic-structure calculations, we formulated structure-property relationships for the studied class of fluorescent difluoroborates and indicated the best candidates for synthesis and experimental measurements (this work is now in progress).

*Authors gratefully acknowledge financial support from the Polish National Science Centre (grant no. 2017/26/M/ST5/00327).*