BODIPY (*meso-phenyl-meso*) dimer as a photovoltaic material

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INTRODUCTION

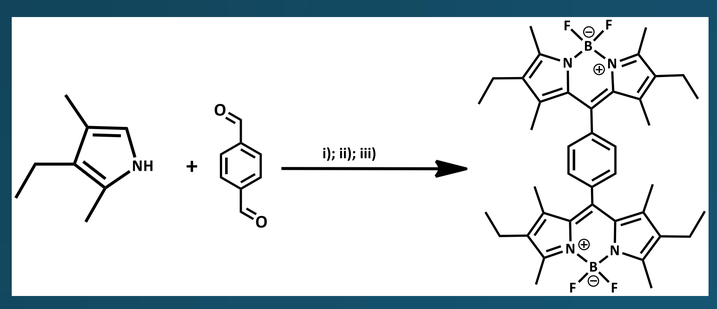
Derivatives of boron-dipyrromethene (BODIPY) constitute an important class of chromophores. The BODIPY dyes can be applied in an extensive variety of applications, such as cellular imaging, photodynamic therapy, drug-delivery or organic photovoltaics [1-4].
The strong absorption in the visible spectra region, the photochemical and chemical stability, good solubility, and general suitable HOMO/LUMO frontier orbital energy levels, made BODIPYs excellent compounds to be applied as electron-donor materials in organic photovoltaic cells.
Following our own work on the use of BODIPYs as photovoltaic materials [5], in this communication we present the synthesis and characterization of a *meso-meso* BODIPY dimer. This BODIPY dimer has all the main properties to work efficiently as electron-donor material since it exhibits strong absorbance in the visible spectrum, good solubility and suitable HOMO and LUMO energy orbitals to work as donor material in the bulky heterojunction BODIPY/PCBM layer, based solar cells.

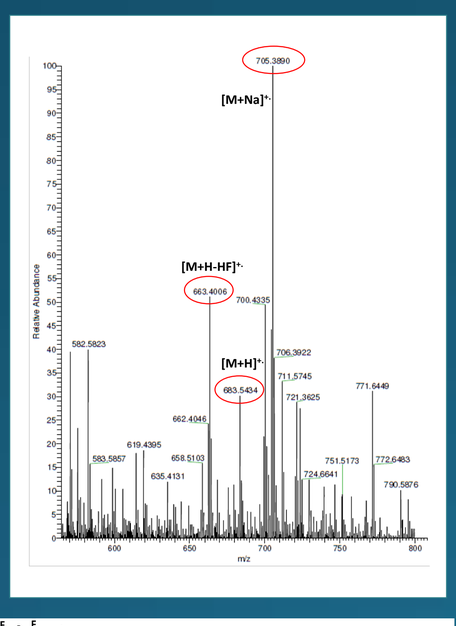
OBJECTIVES

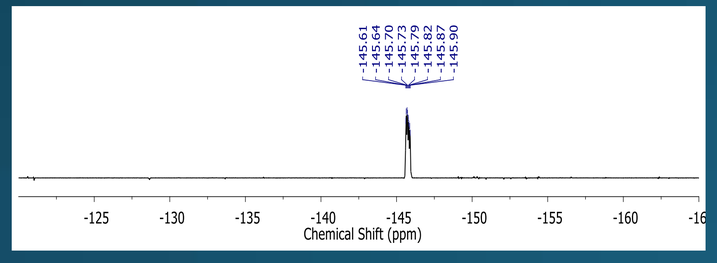
The objective of this work was to synthetize a BODIPY phenyl dimer, evaluate the existence of conformational restrictions on the BODIPY dimer and calculate its HOMO-LUMO gap to evaluate its properties as electron- donor in organic photovoltaic cells.

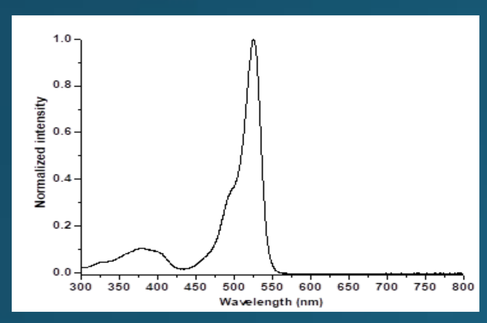
MATERIALS AND METHODS

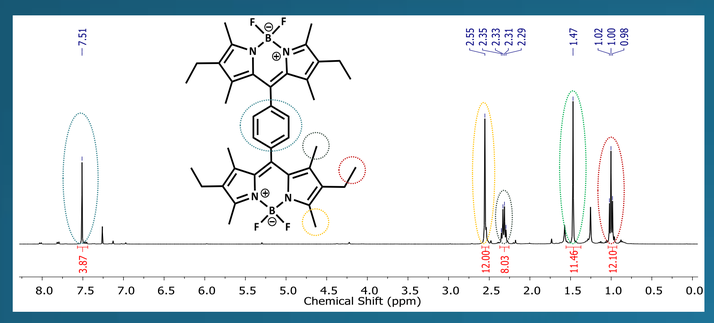
General procedure for the preparation of the BODIPY 10,10'-(1,4-fenilene)bis(2,8-dietil-5,5-difluoro-1,3,7,9-tetrametil-5H-dipirrolo[1,2-c:2',1'-f][1,3, 2] diazaborinin-4-ium-5-uide): i)TFA; ii)DDQ; iii)diisopropylethylamine, $BF_3.O(C_2H_5)_2$.





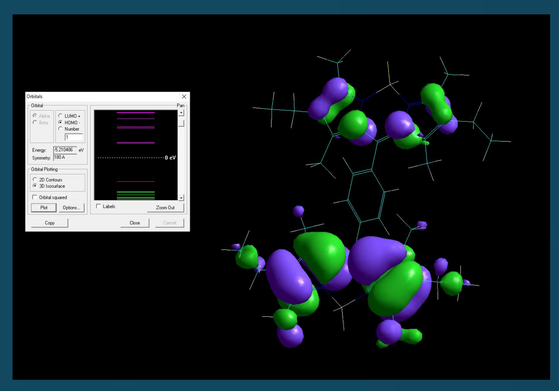


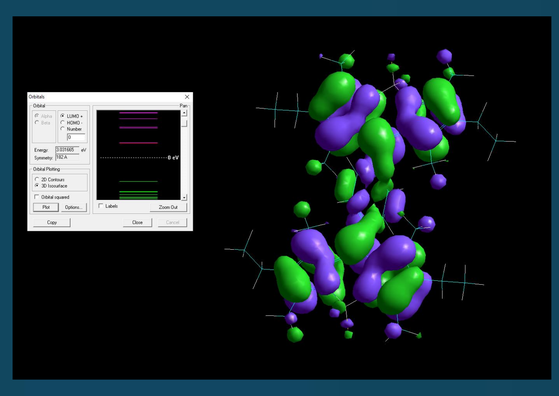


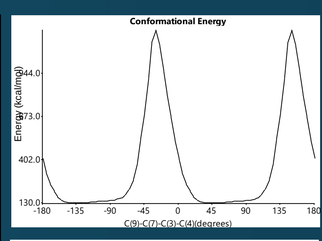


The ^1H NMR, ^{19}F NMR and mass spectra confirm the structure; The absorption spectra shows strong absorbance in visible region ($\varepsilon = 1 \times 10^5$).

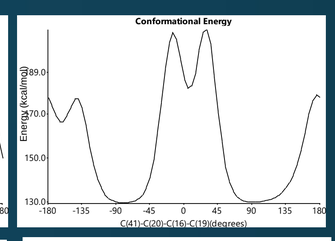
RESULTS AND DISCUSSION



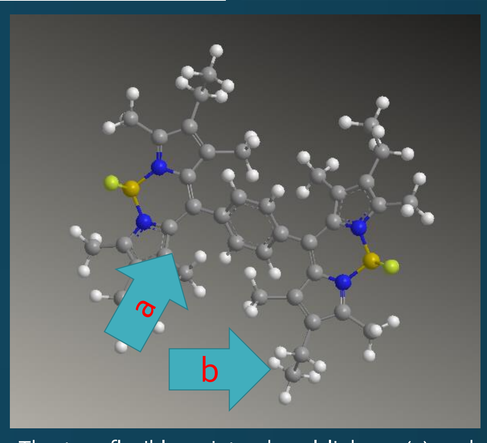




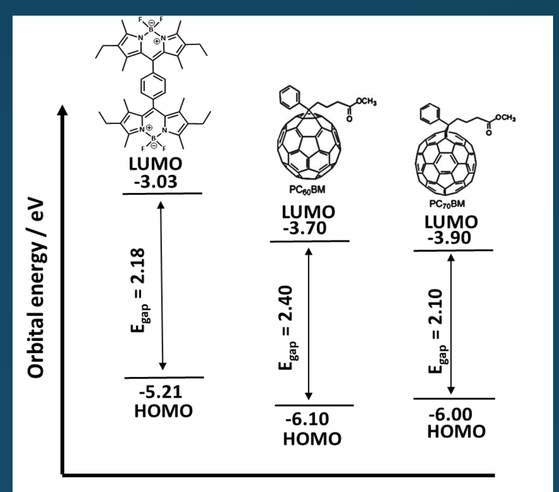
Dihedral Map for the phenyl-BODIPY rotation, maximum at E(150°) = 1293.34 kcal/mole and minimum at E(-135°) = 207.67 kcal/mole.



Dihedral Map for the ethyl-BODIPY rotation (maximum E(-150°) = 207.88 kcal/mole and minimum at E(-90°) = 129.92 kcal/mole.



The two flexible points phenyl linkage (a) and the ethyl groups (b). (via Chem3D, Cambrideg Soft.)



HOMO (left) (-5.21 eV) and LUMO (right) (-3.03 eV) After *ab initio* in Hyperchem with Minimal Basis Set (STO-3G) with (HyperGauss with 298 basis functions and 894 primitive gaussians). Geometry minimization with a Polak-Ribiere algoritm with a RMS of 0.5 kcal/(A mol).

Very suitable HOMO and LUMO energy levels to work as donor material in a BODIPY:Fullerene blend.

CONCLUSIONS

Form this study we can conclude that this BODIPY dimer has an accessible synthesis, simple purification steps, high absorbance in the visible region, and presents a rigid structure which is important for layer homogeneity. Also presents suitable HOMO/LUMO orbitals to be used as electron-donor in organic photovoltaic cells, blended with fullerene ($PC_{60}BM$ or $PC_{70}BM$) acceptors. Therefore is a excellent candidate for bulk heterojunction organic solar cells.

References

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[5] "Synthesis, characterization and application of meso-substituted fluorinated boron dipyrromethenes (BODIPYs) with different styryl groups in organic photovoltaic cells", António Aguiar, Joana Farinhas, Wanderson da Silva, Mariana Emilia Ghica, Christopher M.A. Brett, Jorge Morgado, Abílio J.F.N. Sobral, Dyes and Pigments Vol. 168 (2019) 103-110.

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