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Low Band Gap Molecular Dyes

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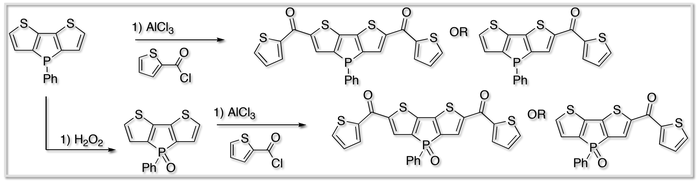
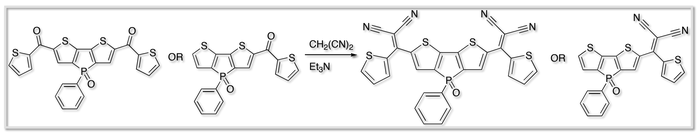
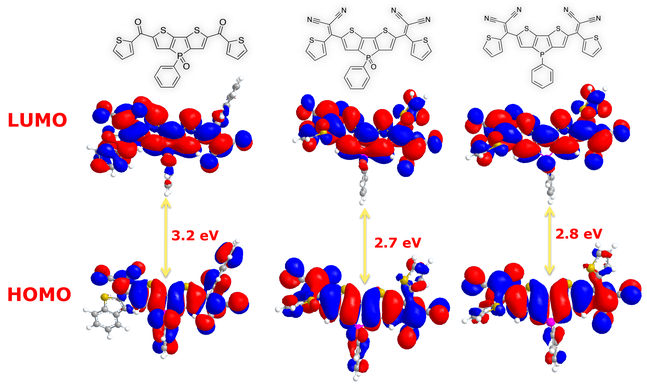
Introduction

Over the last 30 years, organic pi-conjugated materials have been a great interest in development. Organic materials have great potential for application in electronic devices such as polymer-based light emitting diodes (OLEDs/PLEDs), photovoltaic solar cells (OSCs), field effect transistors (OFETs), non linear optical (NLO) devices, or polymeric sensors. Their organic nature allows for the fabrication of lightweight and flexible materials, which can be processed for low power and cost applications. Manipulating the band gap is necessary for applications and using donor-acceptor components is a very good approach. Incorporating the phosphorus centers into π-conjugated materials has recently started to draw an increasing amount of attention. With the versatile reactivity and electronic materials of the phosphorus center, new materials with novel properties can be developed. By using the highly fluorescent dithienophosphole, developed by the group of Dr. Baumgartner, various positions along the backbone can be altered. According to theoretical studies, the phosphole is great for using as a building block to develop an organic pi-conjugated material. The phosphole can be easily modified to make it a n-type semiconductor by allowing for oxidation of the tri-valent phosphorus center to a penta-valent form or complexing the Lewis basic lone pair with a Lewis acid. By substituting at both the thiophene in the 2 and 6 positions and on the phosphole, many new moieties can be developed which will ultimately change the band gap properties of the molecule. A low band gap phosphole material is attempted to be synthesized via the donor-acceptor approach that will serve for valuable applications in electronic devices.

Objective

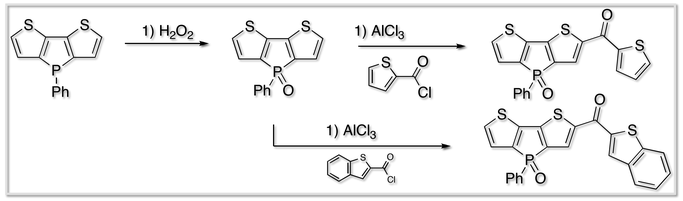


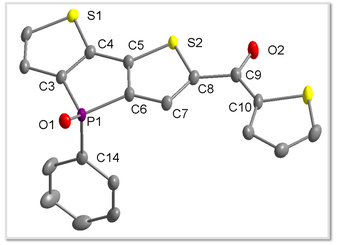




B3LYP/6-31G (d+)

Friedel-Crafts Acylation of Dithieno[3,2-*b*:2',3'-*d*]phosphole



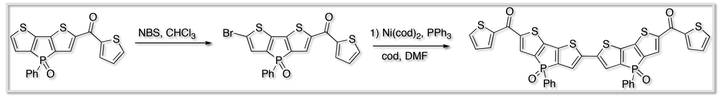


Molecular Structure in the Solid State

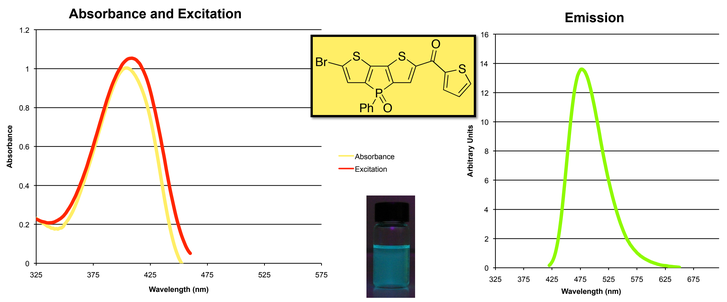
Selected Parameters [pm]

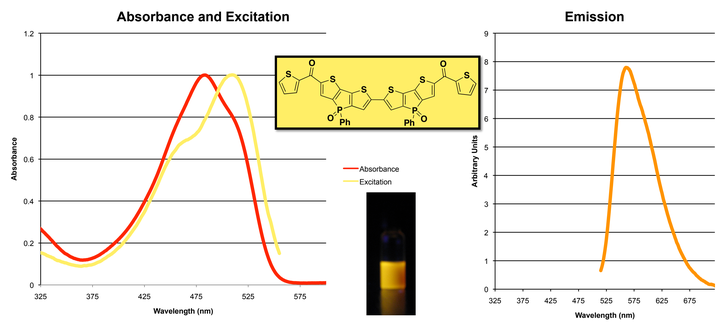
C9-O2:	122.8(3)
C9-C8:	146.7(3)
C9-C10:	147.2(3)
P1-O1:	148.37(17)
P1-C3:	181.0(2)
P1-C6:	180.0(2)
P1-C14:	180.2(2)
C4-C5:	145.6(3)
C3-P1-C6:	91.66(11)
C3-P1-C14:	106.13(11)
C6-P1-C14:	106.17(11)

Yamamoto Cross Coupling



Optoelectronic Properties





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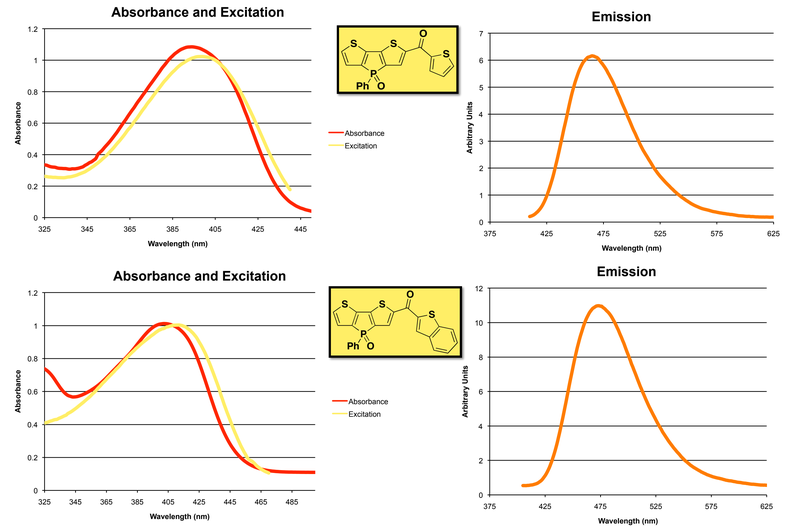

Conclusions

Although the originally planned strategy from achieving a low band gap molecular dye through the Knoevenagel Condensation turned out to be an impossible approach, a new method was achieved that successfully got the compound into the desired region needed for solar cells or bio markers. This project allowed for asymmetrically substituted dithienophosphole that are otherwise very difficult to obtain. Results that have been obtained in this project are promising in that if the conjugated can be extended even further, the molecule will emit further into the red region.

Friedel Crafts Acylation can be carried out on the phosphole system. However, only the mono substituted product could be synthesized. Due to the system being so electron deficient after the first Friedel Crafts Acylation that the di-substituted product could not be obtained.

When preparing for the Yamamoto Coupling, the bromination was quantitative for one side of the mono substituted "Friedel Crafts oxide". This product can be then be carried out through the Yamamoto Coupling to increase the conjugation, therefore inducing a red shift within the molecule.

References

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