Syntheses and Photophysical Investigations of 2, 1, 3-benzoxadiazole based Luminescent Compounds

Behramand, Fernando Molin, Hugo Gallardo*

Department of Chemistry, Federal University of Santa Catarina, University CampusTrindade,Florianopolis, SC, Brazil

**hugo@qmc.ufsc.br*

Keywords: Benzofurazan, Luminescence, C-C coupling

INTRODUCTION

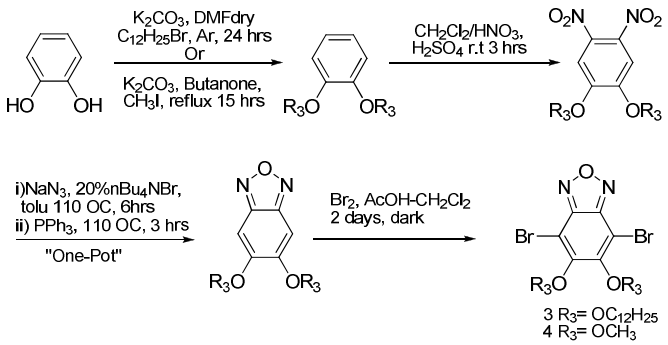
Due to their great advantages over conventional Inorganic luminescent molecules, i.e. facile and economical processing, easy modification of the desired properties etc, Organic luminescent molecules are finding widespread use in modern day's science and technology in search for more efficient and environment friendly functional materials.

The highly fluorescent nature of various conjugated derivatives of 2,1,3-benzoxadiazole, more specifically known as benzofurazan, have been mainly utilized in designing various fluorogenic pre-column labeling reagents for amino acids analysis[1] and heavy metals detection[2]. However contrary to its Sulfur containing analog, i.e. 2,1,3-benzothiadiazole that is exhaustively utilized in solar cells, semiconductors, liquid crystals and conjugated polymers[3], the benzofurazan derivatives are rarely reported for such kind of applications[4].

In this work we present syntheses and photophysical properties of some rationally designed derivatives of benzofurazan with extended conjugation and their potential use in OLEDs

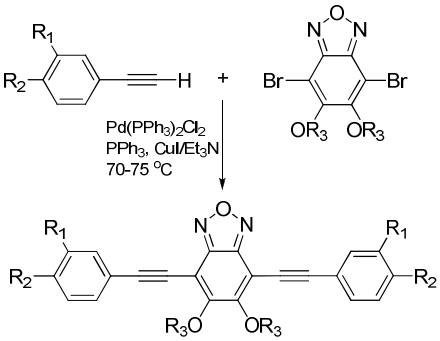
RESULTS AND DISCUSSION

Synthetic plan include syntheses of the terminal alkyne intermediates 1 and 2 according to the methods cited in literature.[5] The activated benzofurazan intermediates 3 and 4 were synthesized as shown in scheme 1.



Scheme1. Syntheses of activated Bromobenzofurazan intermediates 3 and 4

Sonogashira cross coupling of the terminal alkynes with dibromobenzofurazans furnished the target compounds in moderate yields (Scheme 2).



a R_1=H, R_2= $OC_{12}H_{25}$, R_3=CH_3
b R_1=R_2=$OC_{12}H_{25}$, R_3=CH_3
c R_1=H, R_2=$OC_{12}H_{25}$. R_3=$C_{12}H_{25}$
d R_1=R_2=$OC_{12}H_{25}$, R_3=$C_{12}H_{25}$

Scheme 2. Syntheses of target compounds **(a-d)** via Sonogashira C-C coupling.

CONCLUSION

All the intermediates and final compounds were characterized by ^{1}HNMR, ^{13}CNMR and IR spectroscopy. Unlike the brombenzofurazans and terminal acetylenes, the final compounds are intensely fluorescent. The linear acetylenic C-C spacer group helps keeping the aromatic rings in the same plane by eliminating steric repulsion between them and also extends conjugation by connecting the aromatic systems thus rendering highly fluorescent nature to the final compounds.

Quantitative absorption and emission studies of the final compounds and their correlation with molecular structures are in progress.

ACKNOWLEDGEMENTS

CNPq, TWAS, Capes, UFSC, INCT/CAT

REFERENCES

[1] Yanting Song, Takashi Funatsu, Makoto Tsunoda; Journal of Chromatography B, **2011**, 879, 335–340,

[2] Shigehiro Sumiya, Takahiro Sugii, Yasuhiro Shiraishi Takayuki Hirai; Journal of Photochemistry and Photobiology A: Chemistry **2011**, 219,154–158

[3] Guobing Zhang , Yingying Fu , Qing Zhang , Zhiyuan Xie; Polymer **2010**,

51, 2313-2319
[4] Jean Bouffard, Timothy M. Swager; Macromolecules **2008**, 5559-5562.
[5] Gallardo Hugo; Cristiano Rodrigo; Vieira Andre A.; Neves Filho, Ricardo A. W; Srivastava Rajendra M; Synthesis, **2008**, 605-9