TUNING THE PHOTOPHYSICAL PROPERTIES OF *MESO*-TETRAZOLE BODIPY LIGANDS FOR LUMINESCENT Fe(II)-SCO COMPLEXES BY CHEMICAL MODIFICATION

Sophia Mundigler, Martin Huber, Matthias Schöbinger, Peter Weinberger

Institute of Applied Synthetic Chemistry, TU Wien, Getreidemarkt 9/163-01-3, 1060 Vienna, Austria
sophia.mundigler@tuwien.ac.at

Luminescent Fe(II)-SCO complexes, which show synergistic effects, are rather rare. Such multifunctional materials are interesting for applications as molecular switches and electronics, spin transition units and information storage.[1,2]

The fluorophore 4,4-Difluoro-4-bora-3a,4a-diaza-s-indacene, better known as BODIPY, is a promising candidate as a luminescent moiety as part of the ligand, due to its strong UV absorbance, sharp peaks of emission and high quantum yields.[3] By decorating this system with functional groups one can direct these properties.[4]

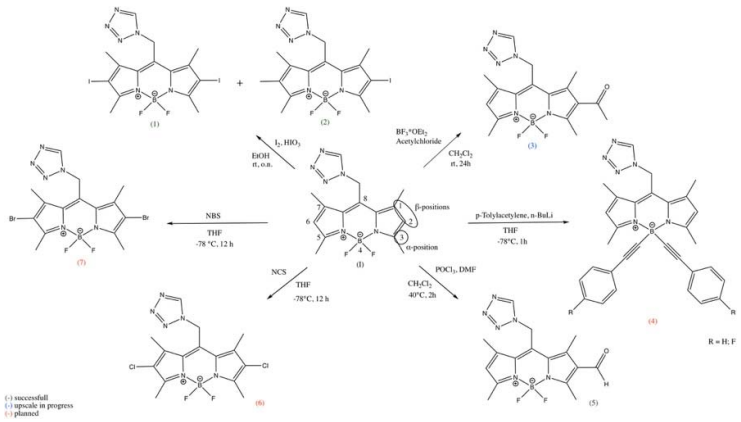

Figure 1: Synthetic pathways of 2TzBODIPY (I) modifications

Such modifications can be applied to the novel ligand 2TzBODIPY (I), which was designed and synthesized by the Weinberger group in order to enable in-depth investigations on novel SCO-PL systems.[5] Especially, the 2,6 position and the boron centre are attractive for functionalization, since steric hindrance is avoided.

In order to create a collection of possible candidates to form luminescent Fe(II)-SCO complexes with synergistic effects, in an accessible wavelength range of 500 – 570 nm combined with high quantum yields ($\Phi > 90$), a literature research was conducted. First experiments (**Figure 1**) exhibit successful functionalization of the initial ligand (I). Moreover, the complexation behaviour of ligand (1) compared to the original ligand (I) was not altered.

---

[1] Zhang W, Zhao F, Liu T, Yuan M, Wang ZM, Gao S. Spin crossover in a series of iron(II) complexes of 2-(2-alkyl-2H-Tetrazol- 5-yl)-1,10-phenanthroline: Effects of alkyl side chain, solvent, and anion. *Inorg Chem*. 2007;46(7):2541-2555. doi:10.1021/ic062062h

[2] Schäfer B, Bauer T, Faus I, et al. A luminescent Pt 2 Fe spin crossover complex. Dalton Transactions. 2017;46(7):2289-2302. doi:10.1039/C6DT04360G

[3] Loudet A, Burgess K. BODIPY dyes and their derivatives: Syntheses and spectroscopic properties. *Chem Rev*. 2007;107(11):4891-4932. doi:10.1021/cr078381n

[4] Ulrich G, Ziessel R, Harriman A. The chemistry of fluorescent bodipy dyes: Versatility unsurpassed. Angewandte Chemie - International Edition. 2008;47(7):1184-1201. doi:10.1002/anie.200702070

[5] M. Huber, M. Schöbinger, B. Stöger, P. Weinberger, unpublished results