meso-1H-TETRAZOLE SUBSTITUTED BODIPYs AS LIGANDS FOR Fe(II) SCO-PL SYSTEMS

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Multifunctional spin crossover (SCO) compounds, with prospective and versatile applications, combine classic SCO properties with additional features e.g. non-linear optics, bulk magnetic ordering, etc.[1]

Since SCO compounds are frequently used as nanomaterials, a promising approach to easily detect the spin state of a system – even in small clusters – is the spin state dependent modulation of photoluminescence (PL). Investigations regarding combined SCO-PL systems are not only interesting when looking at possible future applications, but also due to the fact that the mechanism behind this phenomenon is yet not completely understood.[2]

We developed an easily tunable ligand system consisting of a tetrazole (Tz) and a 1,3,5,7-tetramethyl-BODIPY structure, linked at its *meso* position *via* different spacers (RTzBODIPY; **Figure 1**). The variation of the aforementioned spacers will alter the spatial distance between SCO center and fluorophore. Therefore, a detailed investigation on the mechanism behind future SCO-PL systems, showing synergistic effects, is feasible. To assure such synergy, emission wavelength tuning by means of chemical modifications at the BODIPY core were already realized [3]. In **Figure 2** crystal structures of two RTzBODIPYs are shown.

A detailed photophysical investigation, regarding aggregate formation and its impact on emission properties (aggregation-caused quenching vs. aggregation-induced emission) has already been conducted. These four novel RTzBODIPYs show strong fluorescence even in the solid state and therefore path the way for possible future applications, regarding spin state tracking.

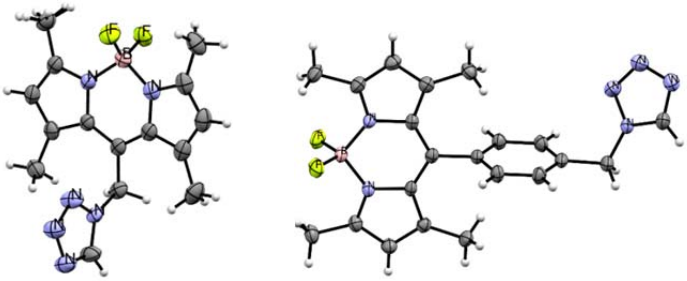

Figure 1: RTzBODIPY; R…-CH_2-, -CH_2CH_2-, -$CH_2CH_2CH_2$-, -CH_2Ph-

Figure 2: single crystal structure of 2TzBODIPY (left) and BnTzBODIPY (right)

[1] Senthil Kumar, K.; Ruben, M. *Coordination Chemistry Reviews* 2017, *346*, 176-205.

[2] Shepherd, H. J.; Quintero, C. M.; Molnár, G.; Salmon, L.; Bousseksou, A. *Spin-Crossover Materials*, 2013, pp. 347-373.

[3] S. Mundigler, M. Huber, M. Schöbinger, B. Stöger, P. Weinberger; Unpublished results