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Title: Regioisomeric BODIPY Benzodithiophene Dyads and Triads with Tunable Red Emission as Ratiometric Temperature and Viscosity Sensors†

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Keywords: Aggregate induced emission
Dyes/pigments
Regioisomers
Sensors

Issue Date: 2019

Publisher: Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim

Citation: Chemistry - A European Journal, 25(65), pp. 14870-14880.

Abstract: Regioisomeric acceptor-donor (AD) molecular rotors (p-AD, m-AD and m-ADA) were synthesized and characterized, wherein dyads p-AD and m-AD, and triad m-ADA contained 4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (BODIPY) and benzodithiophene (BDT) as electron-acceptor and electron-donor, respectively. In all the compounds, the donor and acceptor moieties are electronically decoupled by a phenyl spacer, either through a para coupling or through a meta coupling. The dyad counterparts p-AD and m-AD showed distinct photophysical characteristics in which dyad p-AD showed TICT band at ca. 654 nm characterized by a Stokes shift of ca. 150 nm and prominent solvatochromism. However, meta regioisomeric triad m-ADA showed well-defined aggregation in solution. Notably, because of the temperature-tunable and solvent-viscosity-dependent emission, efficient ratiometric temperature sensing with positive and negative temperature coefficients and viscosity sensing was observed for all compounds. Interestingly, the fluorescence of dyad m-AD (in 10/90 v/v THF/water) revealed a near-white light emission with CIE chromaticity coordinates (x, y) of (0.32, 0.29). Furthermore, the fluorescence emission of p-AD in THF at 0 °C also showed a near-white light emission with chromaticity coordinates (x, y) of (0.34, 0.27). Such multifunctional rotors with readily tunable emission in the red region and prominent temperature- and viscosity-sensing abilities are promising for sensing and bioimaging applications.

URI: <https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/chem.201902952>
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