Synthesis of carbazole-linked isoindole-pyrromethene- boron complexes showing red-emission in solid state

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Organic dyes with far-red and near-infrared emission in a solid state have great promise for application in optoelectronics including OLED and organic solid-state lasers. However, such emissive dyes are rare because the emission is significantly suppressed or quenched in high-concentrated, solid state or aggregation state, due to non-radiative excimer or exciplex by the strong π-π stacking of the π-backbone in the aggregates. Recently, π-conjugated systems with distorted conformation have emerged as an important subject because engineering distortion in the molecules would lead to AIE-active luminophores, organic fluorescent rotor molecules with TICT character, and TADF materials based on well-tailored donor and acceptor designs. In this study, carbazole-linked isoindole-pyrromethene-boron complexes (**CarB1** and **CarB2**) have been designed and synthesized (Fig. 1). The isoindole-pyrromethene unit is a substructure of asymmetrical benzo[*a*]-fused BODIPYs.[1]

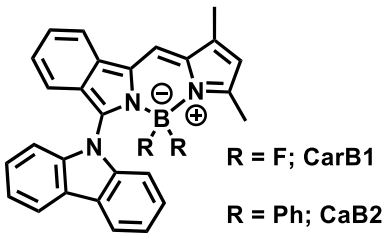

Fig. 1. Structure of target molecules

Target **CarB1** was synthesized via multi-step from phthalimide, which absorbed visible light at 563.5 nm ($\varepsilon = 9.1 \times 10^4$ cm^{-1} M^{-1}) and had an emission at 588 nm ($\Phi_F = 0.88$) in THF when excited at 530 nm (Fig. 2). As one of the features is to find far-red and near-infrared emission at around 697 nm in the solid state. In order to get insight into the underlying the origin, single-crystal X-ray diffraction analysis was conducted, where the intermolecular packing structure were obtained with a significant π-π interaction between isoindole unit and pyrrole ring of adjacent molecule. In the presentation, details of the characterization as well as synthesis of **CarB2** are discussed.

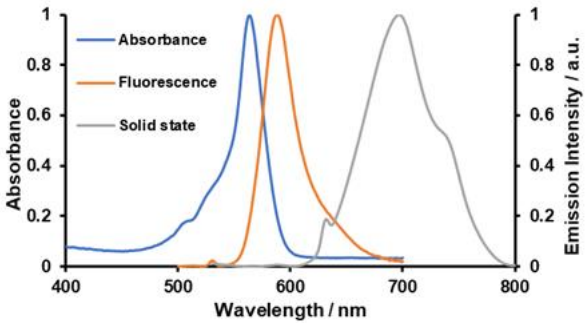

Fig. 2. Absorption and PL spectra of **CarB1** in THF and solid state. c = 1.0 μM. λ_{ex} = 530 nm (THF), 420 nm (solid state).

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