Syntheses and Properties of BAr_2-Bridged Azafulvene Compounds Base on Five-Membered Chelate Rings

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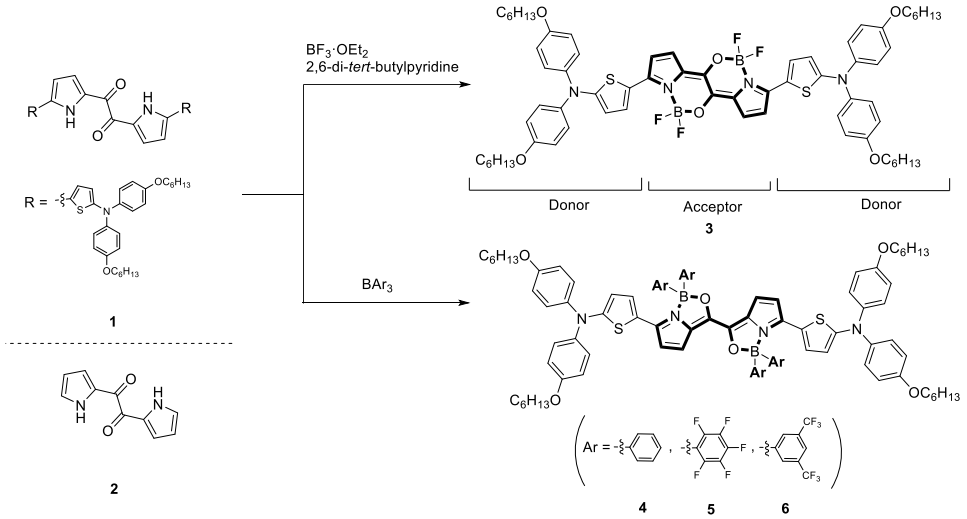
In a previous study, we developed a strong electron acceptor based on BF_2-bridged azafulvene dimer with six-membered chelate rings. Featuring this acceptor, the donor-acceptor-donor molecule **3** functions as a near-infrared (NIR) absorbing dye with high photostability.[1]

In the present study, the fluorines on boron atom are substituted with aryl groups in order to further tune the energy gap. BAr_2-bridged azafulvene with six-membered chelate rings was readily synthesized by refluxing **2** with BAr_3 in toluene. Interestingly, the reaction of **1** with BAr_3 gave products **4**–**6**, all featuring BAr_2 five-membered chelate rings. The structures of **5** and **6** were confirmed by single crystal X-ray analysis.

The substituent effect was investigated using cyclic voltammetry. The first reduction potential of **4** in CH_2Cl_2 shows at $E_{1/2}$ = –1.01 V (vs. Fc/Fc^+), whereas that of compound **5** and **6** were observed at more positive potentials of $E_{1/2}$ = –0.87 V and –0.82 V, respectively. The introduction of electron withdrawing groups on the boron atoms led onto the enhancement of electron-accepting ability. In this presentation, we will discuss the synthesis of these compounds, as well as their electronic and optical properties.



1) H. Shimogawa, Y. Murata, A. Wakamiya, *Org. Lett.* **2018**, *20*, 5135.