Synthesis of Thiophene-Based Twisted Bistricyclic Aromatic Ene with Tricoordinate Boron

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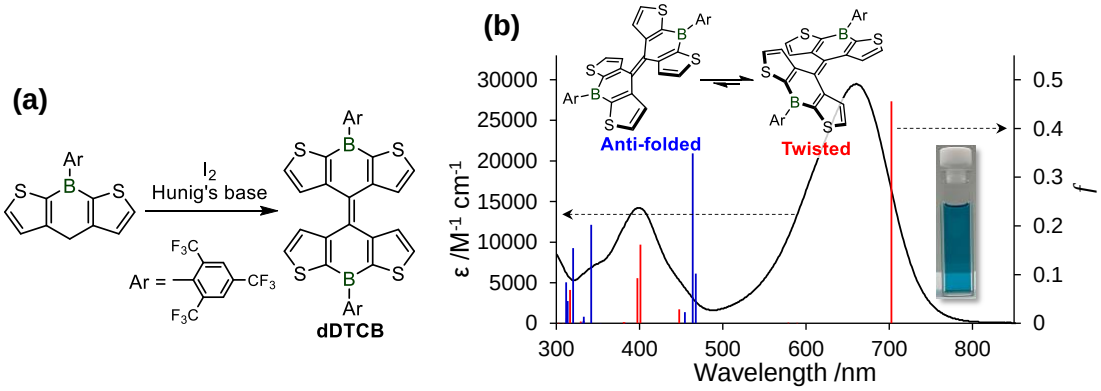
Overcrowded bistricyclic aromatic enes (BAEs) are known as stimulus-responsive materials according to conformational change, e.g., between twisted and anti-folded ones.[1] The twisted conformers of BAEs generally have low-energy absorption relative to the folded one, which is due to the highly twisted central C=C double bond. However, the easy isomerization makes it difficult to apply the twisted conformers to photo absorption/conversion materials. On the other and, the incorporation of tricoordinate boron into conjugated systems is of current interest in the field of materials chemistry as it induces Lewis acidity and specific orbital interactions (p-π* interactions).[2] In this work, we synthesized a tricoordinate boron-embedded and thiophene-based BAE (**dDTCB**) as a new boron-containing conjugated system. The robust sp^2 structure of tricoordinate boron and the relatively low aromaticity of thiophene were expected to impose the twisted conformer.

The predominant population of the twisted conformer of **dDTCB** was confirmed by NMR, absorption, and single-crystal XRD analysis. Electrochemical measurements suggested the electron-deficient character of **dDTCB** (E_{red} = −0.81 V vs $Fc^{0/+}$). Indeed, preliminary studies on the application of **dDTCB** to organic field-effect transistors (OFETs) revealed its moderately high electron mobility of 1.9×10^{-3} cm^2 V^{-1} s^{-1}.[3]



(a) Synthetic scheme of **dDTCB**. (b) Experimental absorption spectrum in toluene (black line) and calculated TD-DFT results of twisted (red) and folded (blue) conformers.

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