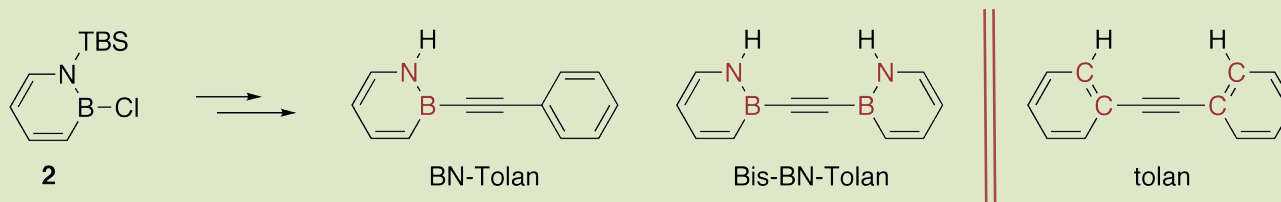


Exploring the B-N/C=C Isosterism in Carbon-Rich Compounds

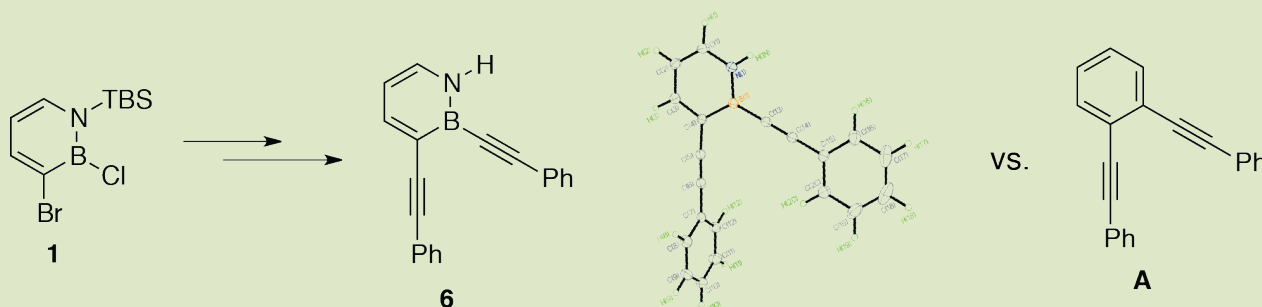
Shih-Yuan Liu, Department of Chemistry, University of Oregon, Eugene OR 97403

Objective: investigate the effects of B-N vs. C=C isosterism in conjugated carbon-rich compounds using BN-substituted benzene derivatives (i.e., 1,2-azaborines) as model.

- BN-Tolan and Bis-BN-Tolan have been synthesized from precursor **2**.



- BN-bis(phenylethynyl)benzene has been prepared from the versatile precursor **1**.



• The absorption spectrum of **6** shows a broad absorption maximum at 328 nm ($\epsilon = 23316 \text{ M}^{-1}\text{cm}^{-1}$). By comparison, the absorption spectrum of 1,2-bis(phenylethynyl)benzene **A** shows an absorption at 315 nm ($\epsilon = 10723 \text{ M}^{-1}\text{cm}^{-1}$). The fluorescence spectrum of heterocycle **6** displays a peak at 378 nm ($\Phi_{\text{PL}} = 0.08$). In contrast, 1,2-bis(phenylethynyl)benzene **A** shows an emission at 356 nm ($\Phi_{\text{PL}} = 0.24$). The bathochromic shift observed for compound **6** relative to its carbon analog is consistent with our previous study of BN-doped analogs of diphenylacetylene.

- Our next goal is to synthesize more complex donor-acceptor-substituted conjugated scaffolds based on the 1,2-azaborine core and to understand their observed photophysical properties using high-level computational calculations.