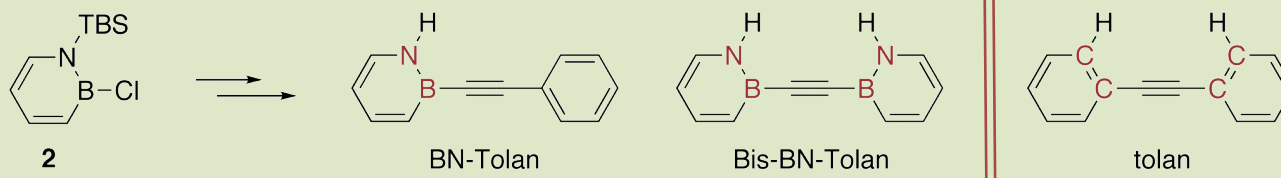


# Exploring the B-N/C=C Isosterism in Carbon-Rich Compounds

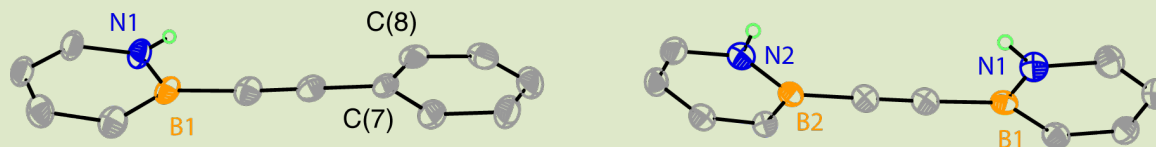
Shih-Yuan Liu, Department of Chemistry, University of Oregon, Eugene OR 97403

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-Tolan and Bis-BN-Tolan have been characterized crystallographically. Unique N–H $\cdots\pi$ (CC) hydrogen bonding that is intermediate between a typical N–H and an arene C–H $\cdots\pi$ (CC) hydrogen bonding has been observed in the solid-state for Bis-BN-Tolan.



- Both BN-Tolan and Bis-BN-Tolan exhibit an absorption band at 299 nm, which is broadened significantly relative to the corresponding absorption in tolan. The emission of BN-Tolan is bathochromically shifted relative to tolan, while the emission of Bis-BN-Tolan is shifted to an even longer wavelength.
- Our next goal is to synthesize more complex conjugated scaffolds based on the 1,2-azaborine core and to understand their observed photophysical properties using high-level computational calculations.

