Synthesis of Azaborines

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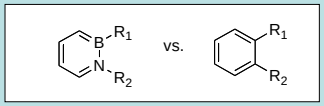
INTRODUCTION

• Azaborines are Benzene rings with adjacent carbons replaced by a nitrogen and a boron atom.



•Azaborines are Isostructural and Isoelectronic to Benzene.

•The synthetic utility of azaborines has been limited due to difficulty of substitution onto the B and N positions.

•Azaborine synthesis into biomimetic molecules is virtually unexplored at this time.

Liu Lab Goals

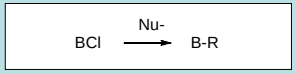
•To expand the functional groups that can be substituted onto B and N positions.

•To explore the classic organic transformation of azaborine.

•To create azaborine bio-molecules.

Substitution onto Azaborine

•Currently Substitution onto Boron is being studied



•-R groups currently being substituted include but are not limited to; Ph, Vinyl, Butyl, tert-Butyl and CN
•Once control of Boron substitution is achieved, substitution onto Nitrogen will be concentrated upon

BNCT- Boron Nuclear Capture Therapy

•Uses ^{10}B containing compounds within human tissue and a high energy neutron beam. Fig 1.
•Results in nuclear fission of ^{10}B and death of cell in target area, but is harmless to non ^{10}B containing tissue.
•Of the currently approved for trial medications, only one attempts to mimic a biologically occurring molecule.

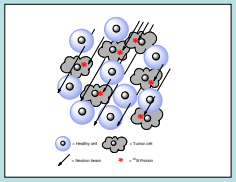
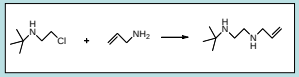


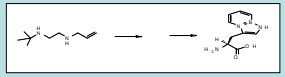
Figure 1

Sampling of Reactions Performed

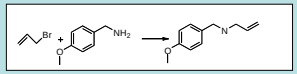
Reaction A



This product may be used to prepare B,N Tryptophan in the future

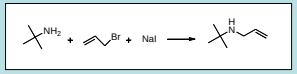


Reaction B



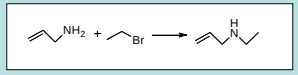
This product will be used in the de-protection of Nitrogen

Reaction C



This product will be used in the de-protection of Nitrogen

Reaction D



This product will be used for the substitution of Nitrogen

Common Procedures Used

•**Distillation**-Uses the difference of boiling points in a solution for separation. Figure 2.

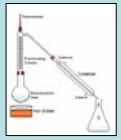


Figure 2

•**Thin Layer Chromatography (TLC)**-Uses silica on a glass plate. Capillary action of solvent up silica separates small amounts of compounds with varying solubility's. Figure 3.

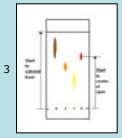


Figure 3

•**Column Chromatography**-Uses silica gel in glass column. Gravity pulls solvent down column separating compounds with varying solubility's.

•**Rotavap-** Used to separate compounds with lower boiling points from compounds with higher boiling points. Lowers air pressure in apparatus lowering temperature at which compounds can vaporize. Uses condensing column to collect vaporized compounds. Figure 4.

Figure 4

^{1}H NMR- Nuclear Magnetic Resonance

•Uses a magnetic field to measure the magnetic moments of hydrogen atoms. Figure 6.

•Groups chemically equivalent hydrogen atoms together on spectrum.

•Placement of peak on spectrum is determined by the shielding of ^{1}H neutron by electrons. Less electrons results in peak being farther to left (Downfield).

•Integration shows relative number of atoms.

•Splitting shows number of hydrogen atoms within 3 σ bonds.

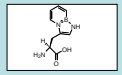
Figure 6

FUTURE DIRECTIONS

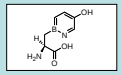
•Continuing study of substitution onto the Boron

•Substitution onto the Nitrogen

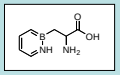
•Synthesis of biomimetic compounds for use in BNCT



B,N Tryptophan



B,N Tyrosine



B,N Phenylamine

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