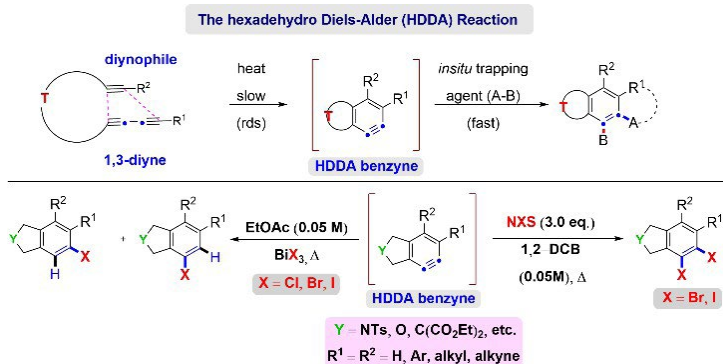


The mono and di-halogenation reactions of the HDDA benzynes

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The HDDA reaction forms polycyclic benzyne intermediates via [4+2] cycloaddition between tethered alkyne and 1,3-diyne, yielding complex benzenoid products after trapping reactions. We devised and developed a versatile method for crafting mono and dihaloarenes by trapping HDDA benzynes using Bismuth halides and N-halosuccinimides respectively. Here, we show how BiX₃ reagents stimulate the hydrohalogenation reactions of HDDA benzynes to produce complicated aryl halides. Each of the three bismuth(III) halides, Cl-, Br-, or I-, can serve as the source for the corresponding halide. The type of substituent at the diyne terminal determines the regiochemical preference for hydrohalogenation. Natures of the linker and the BiX₃ reagent have no effect on the regiochemical outcome of these reactions. This process exhibits broad substrate scope in terms of tethering units and diyne substituents, with good yields and moderate regioselectivity. Extending this, HDDA reactions with N-halosuccinimide gives vicinal di-halogenation of arenes as well as radical di-halogenation of HDDA benzynes. This presentation unveils our effort towards HDDA arynes using halogen based reagents.



Biography

Siddique Khan is a research scholar pursuing his doctoral studies (PhD) under the supervision of Prof. Beeraiah Baire. He joined the Department of Chemistry, at IIT Madras in Jan 2019. His research focuses mainly on strategies for halogenation of the hexadehydro Diels-Alder reaction based Benzynes.

Received: September 13, 2024; **Accepted:** September 16, 2024; **Published:** December 14, 2024