

# Cross Coupling Selective Diazo Pyrazoles Triggered by Borane

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## Description

Reactive carbene intermediates are produced as a result of the breakdown of donor-acceptor diazo compounds. Products with synthetic utility can be produced through a wide range of carbene transfer reactions on these. To produce N-substituted pyrazoles, we present a borane catalyzed selective cyclization reaction of two distinct diazo compounds. Regioselectively, N-alkylated pyrazoles are produced through the selective decomposition of the more reactive aryl diazoester and subsequent reaction with a vinyl diazoacetate. The pyrazole products were produced in yields ranging from 59 to 70% using catalytic amounts of trisborane. The mechanism of this reaction, which was found to go through two tandem catalytic cycles, both of which were catalyzed has been the subject of extensive DFT. Structure and bonding as well as new approaches to synthetic synthesis were developed as a result of boranes chemistry development.

## Organic Synthesis

Borane compounds are frequently utilized in pharmaceutical synthesis due to their low toxicity. Additionally, they play a significant role in medicinal chemistry and the agrochemical industry. Boranes possess an empty orbital that can be accessed by a lone pair of electrons from a Lewis base leading to a Lewis acid-base adduct. This reactivity has been successfully exploited for the activation of many organic substrates in synthetic transformations. Boranes are also an essential micronutrient for plants and can be found in several natural products. The low toxicity of their hydrolysis products makes their potential use as a catalyst in organic synthesis. It is a heterocycle with a five membered ring made up of three carbon atoms and two adjacent nitrogen atoms that are ortho substituting each other. Celecoxib and the anabolic steroid stanozolol are notable drugs that contain a pyrazole ring. Pyrazole is a weak base; surprisingly our initial experiments showed that catalyzed the selective decomposition of donor-acceptor aryl diazoester compounds in reaction with vinyl diazoacetates. Pyrazole moieties of synthetic value were produced through the formation of one carbene intermediate and subsequent reaction with the vinyl diazoacetates. However, the diazoester based, metal free synthesis of pyrazoles is still under investigation.

## Diazo Compounds

An organic moiety with two connected nitrogen atoms at the terminal position is the diazo group. Diazo compounds are organic compounds that are overall charge neutral and have the diazo group bound to a carbon atom. The electronic structure of diazo compounds is characterized by an orthogonal system with electron density delocalized only over the terminal nitrogen atoms and electron density delocalized over the carbon and two nitrogen atoms. There is a class of diazo compounds called 1,3-dipoles because all octet rule satisfying resonance forms have formal charges. The electron density of diazo diketones and diazo diesters is further delocalized into an electron withdrawing carbonyl group, making them some of the most stable diazo compounds. The majority of diazoalkanes, including diazomethane itself, on the other hand are explosive even when they lack electron withdrawing substituents. Ethyl diazoacetate is a diazo compound with commercial significance. The diazirines are a group of isomeric compounds whose carbon and two nitrogens form a ring and share few properties. In diazo transfer, a weak base like triethylamine causes certain carbon acids to react with tosyl azide. P-toluenesulfonamide, the corresponding tosylamide, is the by product. The synthesis of tert-butyl diazoacetate and diazomalonate are two examples of this reaction, which is also known as the regitz diazo transfer. Methyl phenyldiazoacetate is produced in this manner by treating methyl phenylacetate with p-acetamidobenzenesulfonyl azide in the presence of a base. In physics, chemistry, and materials science, the computational quantum mechanical modeling technique known as Density Functional Theory (DFT) is used to investigate the electronic structure of many body systems, particularly atoms, molecules, and condensed phases. Using functionals, also known as functions of another function, this theory makes it possible to ascertain the properties of a many electron system. These are the spatially dependent electron density functionals in DFT. In condensed matter physics, computational physics, and computational chemistry, DFT is one of the most widely used and adaptable approaches.

Utilizing density functional theory to accurately describe the following is still challenging, despite recent advancements: Intermolecular interactions, particularly van der Waals forces, which are crucial to comprehending chemical reactions; excitations for charge transfer; dopant interactions, transition states, global potential energy surfaces, and some systems with strong correlations; and in semiconductor band gap and

ferromagnetism calculations. The incomplete treatment of dispersion can adversely affect the accuracy of DFT in the treatment of systems that are dominated by dispersion or where dispersion competes significantly with other. Non-uniform classical fluid properties are calculated using a similar formalism in classical density functional theory. The use of the Lewis acidic as a catalyst in  $\text{CH}_2\text{Cl}_2$  at  $35^\circ\text{C}$  produced a complex reaction mixture without the expected product formation. Catalytic amounts of the Brønsted acids trifluoromethane sulfonic acid and p-toluenesulfonic acid had poor regioselectivities and produced the desired product in low yields. Surprisingly, our initial experiments showed that catalyzed the selective decomposition of donor-acceptor aryl diazoester compounds in reaction with vinyl diazoacetates. Pyrazole moieties of synthetic value were produced through the formation of one carbene intermediate and subsequent reaction with the vinyl diazoacetates. The crude

reaction mixture was purified through preparative thin layer chromatography with ethyl acetate as the eluent after all volatiles were removed. The diazoesters discriminatory decomposition of another is rather unusual. According to demonstrated a ligand controlled, gold catalyzed reaction protocol for the selective decomposition of one diazoester over another. However, the topic of metal free pyrazole synthesis made possible by diazoesters is still under investigation. In conclusion, a metal free synthetic protocol has been developed to provide N-alkylated pyrazole products that are synthetically useful in a selective manner of the pyrazole products were produced in yields ranging from 59 to 70% with a catalytic loading at 10%. The possibility of a reaction pathway in which two  $\text{B}(\text{C}_6\text{F}_5)_3$ -catalyzed cycles collaborate to produce regioselective N-alkylated pyrazoles was highlighted by a comprehensive mechanistic using DFT analysis.