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Theoretical study of Sonogashira reactions on the formation mechanism of several p-carborane compounds

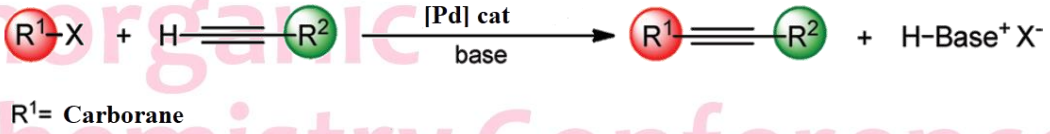
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Cross-coupling is one of the most significant and extensively utilized methods in chemistry for linking two organic substrates using a metal catalyst. In this method, two active groups (such as aryl or alkyl) are connected to each other via an alkyl radical or another reactive group. The palladium-catalyzed Sonogashira reaction [1-3] is one of the most important and widely used methods for preparing arylacetylenes and conjugated enynes, which are precursors for natural products, pharmaceuticals, and materials with specialized optical and electronic properties. The general Sonogashira protocol for coupling terminal alkynes with aryl or alkenyl halides (or triflates) typically involves an organic solvent, a Pd(0)/Cu(I) catalytic system, and at least a stoichiometric amount of a base (Scheme 1). Herein, we have investigated the feasibility of obtaining heteroaryl derivatives of carboranes through Pd-catalyzed B–C cross-coupling reactions involving various organozinc heterocycle. The molecular structures of the compounds studied here, such as reactants, transition states, intermediates and products, have been optimized using the Cam-B3LYP-D3 method in conjunction with the def2-SVP in solution. The Gaussian 09 (revision-D) program package is used for all quantum mechanical calculations. Based on the optimized structures obtained during the solution process,single point energies are determined using the IEF-PCM of the CamB3LYP-D3/def2-TZVP//Cam-B3LYP-D3/def2-SVP theoretical level. As seen in.

Keywords: Cross-coupling reactions, Sonogashira reaction, DFT calculations, Palladium



Scheme 1. General scheme for Sonogashira reactions.

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