22nd Iranian Inorganic Chemistry Conference, 23-25 August, 2023
University of Kurdistan

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

Elham Soltani and Mehdi Bayat*

Department of Chemistry, Faculty of Chemistry, Bu-Ali Sina University, Hamedan, Iran

**E-mail: mehdi806@gmail.com (mbayat@basu.ac.ir)*

Cross-coupling is one of the most significant and extensively utilized methods in chemistry for linking two organic substrates using a metal catalystIn this method, two active groups (such as aryl or alkyl) are connected to each other via an alkyl radical or another reactive group. Kumada cross-coupling [1-3] is a specific type of cross-coupling that uses magnesium as a catalyst and connects an aryl group with another aryl or alkyl group. Carboranes are boron-rich compounds that have been synthesized through various cross-coupling reactions and hydrogen activation. Due to their unique chemical properties, these compounds are used as new ligands in metal catalysts in various fields of advanced chemistry. For example, in cross-coupling reactions, carboranyl ligands can serve as alternatives to phosphines in palladium and nickel catalysts. Herein, we have investigated the feasibility of obtaining heteroaryl derivatives of carboranes through Pd-catalyzed B–C cross-coupling reactions involving various organozinc heterocycle (See Scheme 1,). 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, Kumada reaction, DFT calculations, Palladium



Scheme 1. General scheme for kumada reactions.

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