# COMPUTATIONAL "DIVE" INTO A NICKEL(0)-CATALYZED ARENE C-F ACTIVATION WITH ALKYNES

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The development of new reactions to functionalize C-F bonds has become more and more relevant with the years due to the increasing implementation of fluorinated compounds in areas like medicine, material sciences and catalysis [1]. In addition, the implementation of alkynes to create new C-C bonds that ends up in cyclized products, has emerged as a practical tool in synthesis [2]. We developed a Nickel(0)–Catalyzed C-F activation that reacts with alkynes to yields an aromatic homologation (double insertion) product and/or a monoalkyne annulation product (depending on the electronic properties of the alkyne). Further, we isolated and characterized a reaction intermediate that inspire us to study some mechanistic aspects of the reactions using theoretical calculations. Here, we report some of the result obtained from those computational investigations with DFT and the way we rationalize them to gain a better insight of the mechanism and the behavior of the reaction.
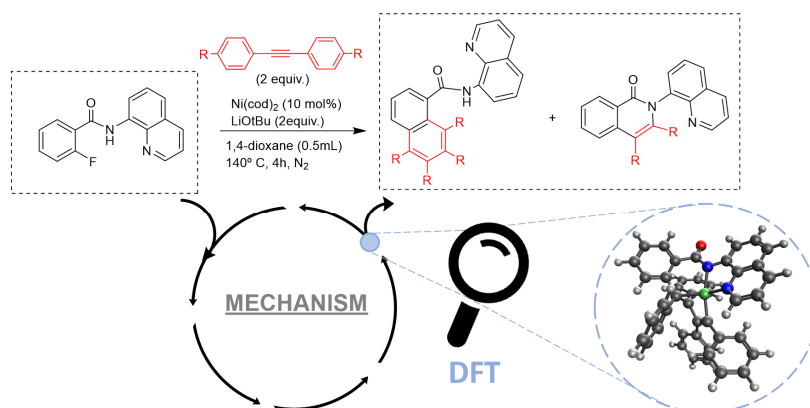
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