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DFT study on the Catalytic reaction of selected W(0) and Cr(0) triazolyl Fischer carbene complexes

Fischer carbenes have been explored mainly for their usefulness in the synthesis of organic and natural products in the past. These metal carbene complexes have been further investigated in metathesis catalytic processes and poor activity has been reported [1]. Very few catalytic studies on any other transformations using Fischer carbenes have been reported to date. The focus of our study was to apply the novel Fischer carbene complexes synthesized to metal specific catalytic processes.
Novel Fischer carbene complexes with phenyl ethylene substituents were synthesized and click reactions with azide precursors used to form triazolyl substituted carbene complexes of tungsten and chromium metals [1,2].Classically cycloaddition reactions include the use of different solvents such as THF, at high temperatures which resulted in low yield and two regioisomeric products [3]. In our study, inert, mild and solvent free conditions were explored. The conditions of solvent free reactions resulted in one regioisomeric product which is advantageous to catalytic studies [2,3]. The [3+2] cycloaddition product was obtained using aryl azide as nucleophile which attacked the phenyl ethylene substituent of the Fischer carbene as a dienophile. Further studies will focus on the effect of the electron withdrawing substituent (4-nitrobenzyl) on the catalytic activity of the triazolyl Fischer carbenes compared with ones without electron withdrawing substituents (benzyl, cyclohexyl). The electron withdrawing groups on the aryl azide resulted in low yields of these metal complexes compared to ones without the electron withdrawing group [2]. Density functional theory (DFT) calculations will be done to gain depth understanding of catalytic activity. Aminolysis of the ethoxy triazolyl Fischer carbenes was done using ammonia gas. The catalytic activities of the ethoxy Fischer carbine complexes and aminocarbene complexes will be compared.

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