

ABSTRACT

The addition reaction of diazoalkanes to alkyne(pentacarbonyl) chromium leads to the formation of 3H-pyrazole complexes. There are two pathways that can explain this reaction. One path is the addition of diazoalkane to the free alkyne forming the 3H-pyrazole which will react with the solvated $\text{Cr}(\text{CO})_5$, the other path is the addition of diazoalkane to the coordinated alkyne with chromium carbonyl followed by rearrangement step to give the 3H-pyrazole complex.

The aim of present work is to assign which of the two pathways is more thermodynamically favorable. Computational calculations are done for all compounds in both paths, based on the hybrid density function theory (B3LYP), supplemented by high accuracy basis set (6-311++g (3df,pd)).

The obtained results show that the reaction prefers to proceed by the addition of the diazoalkane to the coordinated alkyne followed by rearrangement, since a lower energy barrier exist for the formation of the 3H-pyrazole. The bonding interaction type of each compound is also explained by these computational calculations.

As a result, chromium carbonyls act as a catalyst, that reduces the activation energy for the reaction to proceed faster.