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Computational Investigation of Carbonyl Positioning Mechanism in Mn (CO) $_5CH_2F$ Complex by Functional Density Theory

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Abstract

In this study, quantum computation was performed by density functional theory (DFT) on carbon monoxide placement in the Mn (CO) 5CH2F complex. First, all geometric optimization structures and then CO depositional mechanisms were evaluated in different states. it placed. The pathway for the placement reaction was through the migration of the alkyl group. The initial complex will have four different paths to reach the product. The computational results indicate that a route is preferable to other paths, which is attributed to spatial and electron effects.

Keywords: Density Function Theory, Mn (CO) 5CH2F, Reaction Reaction.