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A Comparative Study of the Carbonyl Positioning Mechanism in the Mn (CO) 5 CH2F and Mn (CO) 5CHF2 Complex through Quantum Chemistry

Zahra Pakdel*

Ph.D. in Chemistry, Islamic Azad University, Science and Research Branch, Tehran, Iran.
*Corresponding Author e-mail Address: dr.zpakdel@yahoo.com
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Abstract

In this study, quantum computation was performed by density functional theory (DFT) on carbon monoxide CO placement in Mn (CO) 5CH2F and Mn (CO) 5CHF2 complexes, and all structures were geometric optimization and the CO deposition mechanism in different states on They were evaluated. The pathway for locating the reaction in both complexes was through the migration mechanism of the alkyl group. The initial complex will have four different paths to reach the product.

The computational result shows that a path is preferable to other paths, which is attributed to spatial and electron effects

Keywords: Mn (CO) 5CH2F, Reaction Reaction, DFT, Mn (CO) 5CHF2.

1. Introduction