A DFT Study of Reaction of Ozone with cyclopropylidenecyclopropane

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In this study, The mechanism of ozone reaction with Alkylidenecyclopropanes to produce carbonyl compounds has been investigated using DFT-B3LYP, CAS(6,6) and UHF quantum chemical method. This calculations for the reaction products, transition states and intermediates were carried out to estimate the activation energies. The potential energy profiles of these processes contain three, five, four and one transition states for A-DFT, A-CAS(6,6), B-CAS(6,6) and C-UHF, respectively. According to the results, calculated energy barriers and product yields, it is concluded that path A is more favorable than path B, and also, path B, in turn, is favored over path C.

Keywords : ozonolysis, alkylidenecyclopropane, DFT, CAS, UHF