A detailed analysis of the mechanism of a carbocationic triple shift rearrangement

Cita: Ortega, D., Gutiérrez, S., Tantillo, D., Toro, A. (2015). A detailed analysis of the mechanism of a carbocationic triple shift rearrangement. *Physical Chemistry Chemical Physics, 17*(15), pp. 9771-9779. https://doi.org/10.1039/C4CP03819C

Abstract

The mechanism of a carbocationic triple shift rearrangement is analyzed within the conceptual framework of the reaction force. All the systems were characterized computationally using DFT through B3LYP/6-31+G(d,p) methodology. A complete description of the electronic activity taking place during the reaction emerged through the use of the reaction electronic flux that, together with an NBO Wiberg bond order, produces a detailed picture of the reaction mechanism in terms of chemical events that drive the reaction during the different stages of the process. It is found that a carbocation triple shift occurs asynchronously although in a concerted way.