

Computational Study of the Ozonolysis Reaction through Criegee Mechanism and Dissociation of Secondary Ozonide

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Abstract

The ozonolysis reactions occur through the so-called Criegee mechanism. These reactions generate various chemical organic and inorganic species. Carbonyl oxides, commonly known as Criegee Intermediates (CI's) are the main intermediates from the gas-phase ozonolysis reaction. A comprehensive computational study for the ozonolysis of sabinene and β -pinene (monoterpenes), methylbutenol, phenanthrene (Polycyclic aromatic hydrocarbons, PAHs), and dissociation of secondary ozonide (SOZ) reaction mechanisms have been computationally studied using the density functional theory (DFT) and *Ab Initio* methods. The Criegee mechanism initially involves a highly exothermic 1,3-dipolar cycloaddition of ozone to the double bond to produce primary ozonide (POZ). The POZ dissociates into a highly reactive carbonyl oxide, non-convertible, distinct zwitterionic Criegee intermediate (*syn* and *anti*) conformers, and an aldehyde or ketone, depending on the structure of the monoterpene and PAHs. The mechanistic pathways and thermodynamics of the unimolecular (Vinyl hydroperoxide- and ester-channels), and bimolecular (Secondary ozonide formation, Insertion of H₂O, 2H₂O) reactions of the CI will be discussed and presented thoroughly.

Keywords: Ozonolysis, Criegee Intermediates, Sabinene, Methylbutenol, Primary Ozonide, Secondary Ozonide

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