CONFORMATIONAL ANALYSIS OF 1-ALKENE SECONDARY OZONIDES BY MEANS OF MATRIX ISOLATION FTIR SPECTROSCOPY

VALDAS SABLINSKAS, SIMONA STRAZDAITE, JUSTINAS CEPONKUS, *Dept. of General Physics and Spectroscopy, Faculty of Physics, Vilnius University, Sauletekio av. 9 bl. 3, LT-01222, Vilnius, Lithuania*.

An ability of ozone to break double C=C bond in olefins is known for more than five decades. Understanding of those reactions is very important in atmospheric chemistry. During different steps of the reaction the primary ozonide (POZ), carbonyl oxide (COX) and the secondary ozonide (SOZ) are formed. Fate of the reaction depends on many parameters such as type of radical, conformation of alkene, temperature of the reaction and environmental effects. Despite of numerous studies of the reaction by different spectroscopic techniques the precise mechanism of the reaction is still unknown. It is experimentally observed that the SOZ is more stable than POZ. Stability of the SOZ depends on the size and configuration of the radical. Unfortunately, it is not much known about the spatial structures of the SOZes. The aim of this study is to define the geometrical structures and stability of the different conformers of the 1-butene and 1-heptene secondary ozonides by combined analysis of the matrix isolation FTIR spectral data with the results of Density Functional Theory (DFT) calculations.