

Structures of 1-Butene and 1-Heptene Primary Ozonides as Studied by Means of Matrix Isolation FTIR Spectroscopy

S. Strazdaite, J. Ceponkus, V. Aleksa, V. Sablinskas

Department of General Physics and Spectroscopy, Vilnius University
Universiteto str. 3 Vilnius, LT-01513, Lithuania

The investigations of chemical reactions between alkenes and ozone have considerable practical importance in modeling of photochemical smog formation. This reaction starts from breaking down C=C bond of alkene and goes through a few steps forming intermediate unstable species- primary ozonide (POZ), secondary ozonide (SOZ) and *Criegee* intermediates (CI), but spatial structures of these species are still unclear. 1-butene and 1-heptene are the ones of the simplest alkenes, which may have conformational diversity due to rotation around aliphatic radical C-C bond closest to the five membered ring. This conformational diversity should persist in primary ozonides, but the precise nature of the conformational equilibrium has not been determined, yet. Primary ozonide is formed together with secondary ozonide. Due to high instability of primary ozonide it's separation from SOZ is not possible, what makes conformational analysis of this molecule difficult. For such analysis, prior information about conformational diversity of secondary ozonide is needed. Such information allows eliminate spectral bands of secondary ozonide from the mixture of the reaction products. Recently, such information became available from work done in our lab [1-2].

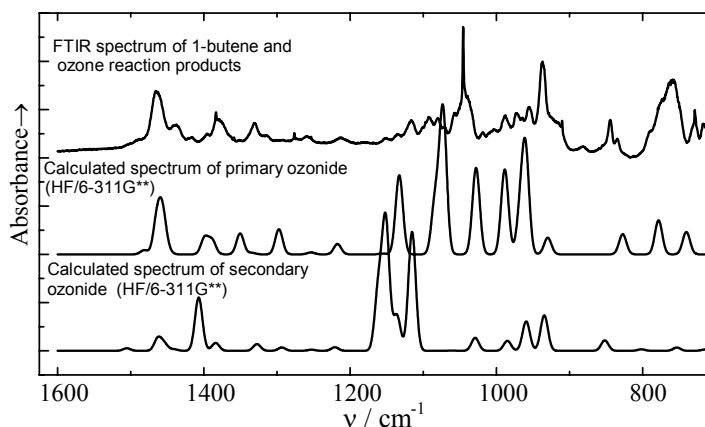


Fig.1: Experimental FTIR spectrum of products of the reaction between 1-butene and ozone in CO₂ matrix and *ab initio* calculated (HF/6-311G**) spectra of *gauche* conformers of primary and secondary ozonides of 1-butene

In this work we obtained FTIR absorption spectra of the ozonization products of 1-butene and 1-heptene, isolated in Xe and CO₂ matrices. Some results for the ozonization products of 1-butene are presented in Fig. 1. From comparison of *ab initio* calculated (HF/6-311G**) and experimental FTIR spectra complete assignment of experimental bands belonging to primary ozonides of 1-butene and 1-heptene was made. It was found that both ozonides preferable exist as *gauche* conformers. Other conformers of the primary ozonides were not found in the mixtures of the reaction product. Contrary, the secondary ozonides of both alkenes exist as mixture of *gauche* and *anti* conformers [1, 2].

[1] R. Bariseviciute, J. Ceponkus, A. Gruodis, V. Sablinskas, Central European Journal of Chemistry 4 (2006) 578-591.

[2] R. Bariseviciute, J. Ceponkus, V. Sablinskas, L. Kimtys, J. Mol. Struct. 844-845 (2007) 186-192.