MECHANISM OF THE OZONOLYSIS OF 2-METHYL-2-PENTENAL: A COMPUTATIONAL AND EXPERIMENTAL STUDY

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Experimental and theoretical studies were carried out to investigate the ozonolysis of trans-2-methyl-2-pentenal. The experiments were conducted in atmospheric simulation chambers coupled to a FTIR spectrometer and GC/MS/FTIR at room temperature and atmospheric pressure, in the presence of an excess of cyclohexane and in dry conditions (RH ¡ 1theoretically from the results of accurate density-functional (M06-2X) and ab initio (CCSD(T)) computations, employing the AVTZ basis set. The sequence of reaction steps was established and the system of kinetics equations modelled using MESMER. The reaction proceeds mainly via a well-skipping mechanism. In the first step, a primary ozonide is formed, which then decomposes along two pathways. The principal ozonolysis products are propanal, methylglyoxal, ethylformiate and a secondary ozonide. The ozonolysis rate constant and product branching ratio are in excellent agreement with the experimental data that are equally reported in the present work.