



Simulation of product formation from ozonolysis of monounsaturated omega-9 fatty acid

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Ozonolysis of aerosols of monounsaturated omega-9 fatty acid has been studied for decades in order to observe the effects of reactant loss and product formation on the global climate. Several products were found i.e. 1-nonanal, 9-oxononanoic acid, azelaic acid, nonanoic acid, octanoic acid and Criegee intermediate compounds. Even though a number of studies have been done on the ozonolysis of monounsaturated omega-9 fatty acid, its mechanism and chemical composition are still not completely understood. Aspen Plus V8.8 was used to evaluate all possible reaction mechanisms summarised from previous publications. It was also used to estimate the product composition after ozonolysis. The simulation results show that all molecules of ozone react with monounsaturated omega-9 fatty acid to form 1-nonanal, octanoic acid, and carbon dioxide which are considered to be the major products, whereas trace amounts of azelaic acid, nonanoic acid, and Criegee intermediate compounds are observed. In addition, the chemical composition is similar to the experiment results.

Keywords: Simulation; Product formation; ozonolysis; monounsaturated omega-9 fatty acid