Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.13876

Gas-phase kinetic and mechanistic study of degradation of a several of first-generation oxidation products of monoterpene by Ozone.

MARIAM FAKIH

GSMA (group of molecular and atmospheric spectrometry)

Presenting Author: fakih_mariam@outlook.com

Biogenic Volatile Organic Compound (BVOC) emissions are the largest land source of Organic Compounds in the atmosphere. Among BVOCs compounds [1], monoterpenes (C10H16), presents an important fraction of BVOCs [2].Their low-volatility contribute to the formation of secondary organic aerosols (SOA) as well as the formation of tropospheric ozone. Thus, an evaluation of their impact on climate and air quality requires many studies of their reactivity and atmospheric degradation pathways. However, atmospheric oxidation of these products still less well understood in terms of kinetic and mechanism especially considering their first-generation oxidation products.

In this work we report, for the first time, the kinetics and mechanistic measurements of the gasphase reactions of three first-generation oxidation products of monoterpenes including myrtenal, limononaldehyde, and ketolimonene with O3.Experiments have been performed in a 63 L Pyrex atmospheric simulation chamber over the temperature range 298-353 K in air and at near atmospheric pressure of 760 Torr.The reaction is followed using PTR-ToF-MS and GCMS-SPME to monitor the concentration of the reactants and formed products.Kinetic experiments were carried out using an absolute kinetic method, in which O3 was quantified by a UV absorption.

Our results show that the rate constants, k, of the reactions of myrtenal, limononaldehyde and ketolimonene with O3 were found to exhibit a positive temperature dependence under our experimental conditions. Products formation and mechanistic investigations from the reaction

of studied species with O3 reveal the formation of several multifunction carbonyls such as glycolaldehyde, glyoxal and methylglyoxal.According the mechanistic results, the gas-phase degradation mechanism will be presented and discussed in detail. Atmospheric lifetimes and reactivity trends are presented considering the compounds rate coefficients obtained.The impact of studied compounds on air quality will be discussed considering its atmospheric life times.

[1] Guenther, and al.The Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN2. 1): an extended and updated framework for modeling biogenic emissions. Geoscientific Model Development, 2012, vol. 5, no 6, p. 1471-1492.

[2] Messina,and al.Global biogenic volatile organic compound emissions in the ORCHIDEE and MEGAN models and sensitivity to key parameters. Atmospheric Chemistry and Physics, 2016, vol. 16, no 22, p. 14169-14202.