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Gas phase ozonolysis of sesquiterpenes: kinetics, OH-radical and SOA yields, and reaction mechanism

F. Herrmann, B. Kanawati, A. Sadezky, T. Klüpfel, J. Williams, **R. Winterhalter**, and G. K. Moortgat

Max Planck Institute for Chemistry, Atmospheric Chemistry Division, Mainz, Germany (winterha@mpch-mainz.mpg.de / Phone: +49-6131-305496)

Gas phase ozonolysis of the sesquiterpenes beta-caryophyllene and alpha-humulene was performed in a 570 L static reactor at 730 torr and 296 K in synthetic air. Gas phase products were analysed by FTIR spectroscopy and PTR-MS. Particulate products were studied by LC-MS analysis of collected aerosol particles after extraction with methanol. The aerosol size distribution was monitored by SMPS. The reaction mechanism was investigated by addition of HCHO, HCOOH and water as Criegeeintermediate scavenger. The experiments were also performed in the presence of cyclohexane as OH-radical scavenger and the formation of cyclohexanone monitored by PTR-MS. Due to high time resolution, OH radical yields have been determined for the first double bond of the sesquiterpene as well as for the remaining double bonds of the primary products. Furthermore, the rate constant of the primary products have also been determined by fitting the observed ozone removal. The aerosol yields showed a strong dependence on the added Criegee-Intermediate scavenger. In the absence of scavengers, yields ranging from 5 to 24%, depending on the aerosol mass, were found, whereas by addition of HCOOH and water the yield increased up to a factor of 2. Mechanistic details of the ozonolysis of beta-caryophyllene will be presented.