



Identification of new oxidation products in the aerosol particles of β -caryophyllene ozonolysis using LC/MS-MS-TOF

B. Kanawati, F. Herrmann, A. Sadezky, R. Winterhalter, G. K. Moortgat

Max-Planck Institute for Chemistry, Atmospheric Chemistry Division, Mainz, Germany.
(kanawati@mpch-mainz.mpg.de)

Sesquiterpenes, a very reactive class of biogenic VOC, play an important role in new particle formation in the atmosphere. The ozonolysis of β -caryophyllene was studied in a glass reactor under atmospheric conditions. Secondary organic aerosol (SOA) formed was collected on a PTFE filter and extracted in methanol, then analyzed by using HPLC coupled to a hybrid Triple Quadrupole TOF mass spectrometer, for high-resolution mass detection. Both APCI+ and ESI- operational modes of the ion sources were used and provided useful insights on the identification of a large number of multifunctional oxidation products. Detailed structural information have been deduced using collision induced fragmentation experiments of molecular ions. For example, an oxocarboxylic acid believed to be formed from the ester channel of a Criegee Intermediate generated in the first steps of the mechanism has been identified unequivocally. Moreover, the identification of several isomers with e.g. molecular weight 252 was accomplished with this method and confirmed by theoretical investigations of the fragmentation pathways. An electrospray method was developed to ionize not only organic acids but also aldehydes in the negative mode, extending widely the range of oxidation products that can be detected in one analysis step. Examples of the identification of some oxidation products will be presented.