Atmospheric Chemistry and Physics
An Interactive Open Access Journal of the European Geosciences Union

Atmos. Chem. Phys., 6, 4973-4984, 2006
www.atmos-chem-phys.net/6/4973/2006/

Investigating the composition of organic aerosol resulting from cyclohexene ozonolysis: low molecular weight and heterogeneous reaction products

J. F. Hamilton[1], A. C. Lewis[1], J. C. Reynolds[1], L. J. Carpenter[1], and A. Lubben[2]
[1]Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK
[2]Bruker Daltonics, Banner Lane, Coventry , CV4 9GH, UK

Abstract. The composition of organic aerosol formed from the gas phase ozonolysis of cyclohexene has been investigated in a smog chamber experiment. Comprehensive gas chromatography with time of flight mass spectrometric detection was used to determine that dicarboxylic acids and corresponding cyclic anhydrides dominated the small gas phase reaction products found in aerosol sampled during the first hour after initial aerosol formation. Structural analysis of larger more polar molecules was performed using liquid chromatography with ion trap tandem mass spectrometry. This indicated that the majority of identified organic mass was in dimer form, built up from combinations of the most abundant small acid molecules, with frequent indication of the inclusion of adipic acid. Trimers and tetramers potentially formed via similar acid combinations were also observed in lower abundances. Tandem mass spectral data indicated dimers with either acid anhydride or ester functionalities as the linkage between monomers. High-resolution mass spectrometry identified the molecular formulae of the most abundant dimer species to be $C_{10}H_{16}O_6$, $C_{11}H_{18}O_6$, $C_{10}H_{14}O_8$ and $C_{11}H_{16}O_8$ and could be used in some cases to reduce uncertainty in exact chemical structure determination by tandem MS.

Final Revised Paper (PDF, 832 KB) Discussion Paper (ACPD)

Citation: Hamilton, J. F., Lewis, A. C., Reynolds, J. C., Carpenter, L. J., and Lubben, A.: Investigating the composition of organic aerosol resulting from cyclohexene ozonolysis: low molecular weight and heterogeneous reaction products, Atmos. Chem. Phys., 6, 4973-4984, 2006. Bibtex EndNote Reference Manager