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Cluster analysis on mass spectra of biogenic secondary organic aerosol

C. Spindler (1), A. Kiendler-Scharr (1), E. Kleist (2), A. Mensah (1), T. Mentel (1), R. Tillmann (1), and J. Wildt (2)

(1) Forschungszentrum Jülich, ICG-2, Germany (c.spindler@fz-juelich.de), (2) Forschungszentrum Jülich, ICG-3, Germany

Biogenic secondary organic aerosols (BSOA) are of high importance in the atmosphere. The formation of SOA from the volatile organic compound (VOC) emissions of selected trees was investigated in the JPAC (Jülich Plant Aerosol Chamber) facility. The VOC (mainly monoterpenes) were transferred into a reaction chamber where vapors were photo-chemically oxidized and formed BSOA. The aerosol was characterized by aerosol mass spectrometry (Aerodyne Quadrupol-AMS). Inside the AMS, flash-vaporization of the aerosol particles and electron impact ionization of the evaporated molecules cause a high fragmentation of the organic compounds. Here, we present a classification of the aerosol mass spectra via cluster analysis. Average mass spectra are produced by combination of related single mass spectra to so-called clusters. The mass spectra were similar due to the similarity of the precursor substances. However, we can show that there are differences in the BSOA mass spectra of different tree species. Furthermore we can distinguish the influence of the precursor chemistry and chemical aging. BSOA formed from plants exposed to stress can be distinguished from BSOA formed under non stressed conditions. Significance and limitations of the clustering method for very similar mass spectra will be demonstrated and discussed.