DART/Orbitrap-HRMS molecular characterization of biogenic secondary organic aerosols generated in the SAPHIR chamber

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Biogenic volatile organic compounds (BVOCs) play an essential role in atmospheric chemistry and form, through a complex set of atmospheric processes, secondary organic aerosols (SOAs) that affect both the air quality and the climate. The organic composition of aerosol is quite complex and its molecular composition is still poorly understood. To gain a better understanding of the molecular composition of atmospheric organic matter (AOM), a total of 12 biogenic secondary organic aerosol samples were generated in the Large Atmospheric Simulation Chamber (SAPHIR) in Jülich from the ozonolysis of individual biogenic SOA precursors including β-pinene, limonene, a mixture of β-pinene/limonene as well as VOCs emitted from Scots pines. Chamber-generated SOAs were subsequently aged with OH radicals primarily formed from the photolysis of HONO and ozone. Each sample was collected on quartz filter and analyzed without further sample preparation in the ambient ionization source DART™ (Direct Analysis in Real Time) coupled to an LTQ-Orbitrap™ high resolution mass spectrometer operated in both positive and negative ionization mode.

Our results show that all chamber-generated monoterpene SOA samples analyzed by DART™ /Orbitrap™-HRMS have a very complex molecular composition with over 1,000 monoisotopic molecular formulas assigned for each sample. Most samples generated 4 series of oligomeric clusters with m/z up to 900 Daltons, whose structural features could be evidenced by collision-induced dissociation (CID) of precursor ions. Data produced from these experiments will be compared using multivariate statistical analysis. Finally, the detailed molecular composition of chamber-generated SOA analyzed by DART™ /Orbitrap™-HRMS will be discussed and compared with that of background aerosols collected from rural and urban areas analyzed using the same method.