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Atmospheric sampling Townsend discharge ionization tandem mass spectrometry

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On-line techniques are particular convenient for the study of reaction products from oxidation of biogenic volatile organic compounds (VOCs). The development of these techniques has advanced significantly over the past years, and they do not suffer from the same inherent disadvantages as off-line techniques do.

Here we report the application of atmospheric sampling Townsend discharge ionization (ASTDI) triple quadrupole mass spectrometry for on-line sampling. A signal to noise ratio of S/N = 7 was determined by online ASTDI sampling of 7 ppb toluene (m/z 92). The on-line ASTDI mass spectra of 57 different VOCs within 11 mono- and difunctional groups were tested and evaluated. The sample air was introduced directly into the Townsend discharge ionization source, which produced mainly O_2^+, NO^+ and NO_2^+. Ion-molecule reactions of hydride abstraction, charge exchange and NO^+ addition resulted in ASTDI spectra, which resembled those of nitrous oxide chemical ionization (NO CI) and related techniques. The mass spectra contained detailed fragmentation suitable for structure elucidation, in addition to ions related to the molecular mass. Mass spectra resembling conventional methane chemical ionization were recorded by mixing methane with the air sample prior to the Townsend source (ASTDI(Me)). The combination of ASTDI and ASTDI(Me) allowed for a determination of the molecular mass in most cases. Identification of the functional group was also possible in most cases, since most classes of functional groups exhibited a unique combination of quasi molecular- and NO^+-adduct ions in ASTDI and ASTDI(Me). Analysis of complex mixtures can be achieved by use of the MS/MS option on molecular- or quasi-molecular ions.