



Field performance and identification capability of the Innsbruck PTR-TOF

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Over the last one and a half decades Proton Transfer Reaction Mass Spectrometry (PTR-MS) [1, 2] has gained recognition as fast on-line sensor for monitoring volatile organic compounds (VOC) in the atmosphere. Sample collection is very straight forward and the fact that no pre-concentration is needed is of particular advantage for compounds that are notoriously difficult to pre-concentrate and/or analyze by gas chromatographic (GC) methods. Its ionization method is very versatile, i.e. all compounds that perform exothermic proton transfer with hydronium ions – and most VOCs do so – are readily ionized, producing quasi-molecular ions VOC.H⁺. In the quasi-molecular ion the elemental composition of the analyte compound is conserved and allows, in combination with some background knowledge of the sample, conclusions about the identity of that compound. De Gouw and Warneke (2007) [3] summarized the applicability of PTR-MS in atmospheric chemistry but they also pointed out shortcomings in the identification capabilities. Goldstein and Galbally (2007) [4] addressed the multitude of VOCs potentially present in the atmosphere and they emphasized the gasphase-to-aerosol partitioning of organic compounds (volatile and semi-volatile) in dependence of carbon-chain length and oxygen containing functional groups.

In collaboration with Ionicon and assisted by TOFWERK we developed a PTR time-of-flight (PTR-TOF) instrument that allows for the identification of the atomic composition of oxygenated hydrocarbons by exact-mass determination. A detection limit in the low pptv range was achieved at a time resolution of one minute, one-second detection limit is in the sub-ppbv range.

In 2008 the Innsbruck PTR-TOF was field deployed in the icebreaker- and helicopter based Arctic Summer Cloud Ocean Study (ASCOS) to characterize the organic trace gas composition of the High Arctic atmosphere. During the six-week field campaign the PTR-TOF was run without problems even under harsh conditions in the open water and during ice breaking. Continuous time-series of full mass spectra with a one minute time resolution were recorded throughout the campaign between August 2nd and September 7th 2008 running up to a net VOC data set of 745 hours. Over 370 mass peaks have been separated, about 340 show signal intensities above the 30 minute detection limit of ~3pptv. Additionally we analyzed samples from nine helicopter based soundings providing vertical VOC profiles up to 3000 m.a.s.l. The performance of the newly developed instrument will be discussed and ASCOS data will be shown.

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