Proton-Transfer-Reaction Mass Spectrometry (PTR-MS)

PTR-MS is a state-of-the-art chemical ionization mass spectrometry technique that allows for fast (seconds) and highly sensitive (detection limits in the tens of pptv range) of volatile organic compounds (VOCs). A detailed description of the measurement principle and the instrument can be found at:

http://en.wikipedia.org/wiki/Proton-transfer-reaction_mass_spectrometry

The technique was developed in the mid-1990ies at the University of Innsbruck in Austria and has since then become a routine and integral part of most tropospheric chemistry field campaigns including INDOEX 1999, SOS 1999, TEXAQS 2000, AOE 2001, BEWA 2002, ECHO 2003, ARCTAS-2008, DISCOVER-AQ 2011 – just to name a few of the campaigns in which the University of Innsbruck measurement team has been involved. An interactive presentation of the airborne PTR-MS instrument can be found at:

http://discover-aq.larc.nasa.gov/instruments.php (click on interactive viewer and on PTR-MS)

During SEAC⁴RS, the PTR-MS instrument will measure organic trace gases from all major emission sources in Southeast Asia: biogenic (isoprene, monoterpenes, oxygenated VOCs), biomass burning (acetonitrile, oxygenated VOCs, aromatics) and anthropogenic (aromatics, oxygenated VOCs). The list of analytes (see Table 1) includes compounds of different photochemical lifetimes (including very short-lived species such as isoprene) and different solubility (including water-scavengable species such as acetic acid). These data will provide important information on the amount of boundary layer air that reaches the upper troposphere, convective transport times, as well as wet removal and photochemical transformation processes in the convective outflow.



Figure 1: The Innsbruck PTR-MS instrument onboard the NASA DC-8

	m/z	detection limit ¹	accuracy	interferences
methanol	33	100 ppt	± 20 %	none
acetonitrile	42	10 ppt	± 10 %	none
acetaldehyde	45	100 ppt	± 15%	none ²
acetone	59	35 ppt	± 10 %	propanal ³ , glyoxal
acetic acid ⁴	61	N/A	N/A	glycolaldehyde
isoprene	69	20 ppt	± 10 %	methylbutenol ⁵ , furan ⁵
MVK + MACR	71	20 ppt	± 10 %	crotonaldehyde ⁶
benzene	79	20 ppt	± 10 %	none
toluene	93	20 ppt	± 10 %	none
monoterpenes	137	50 ppt	± 10 %	none

The list of species to be routinely measured onboard the DC-8 during SEAC⁴RS is given in Table 1 together with conservative values for the expected analytical performance:

 $\frac{1}{3} \frac{2\sigma}{3}$ typically < 10% of acetone $\frac{2}{3}$ measured only in the lower troposphere, artifacts in UT/LS $\frac{4}{3}$ acetic acid measurements are exploratory $\frac{6}{3}$ only in urban environments

List of species to be measured with the Innsbruck PTR-MS during SEAC⁴RS Table 1: together with typical analytical performance characteristics

In the current flight version of the Innsbruck PTR-MS instrument, m/z-signals are sequentially measured in a quadrupole mass analyzer using a 0.5-1 second signal integration time per m/z. The complete set of signals will be collected at 10-15 seconds time resolution.