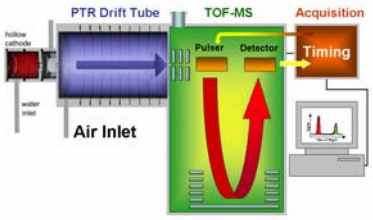
Proton Transfer Reaction Technique for VOC Analysis



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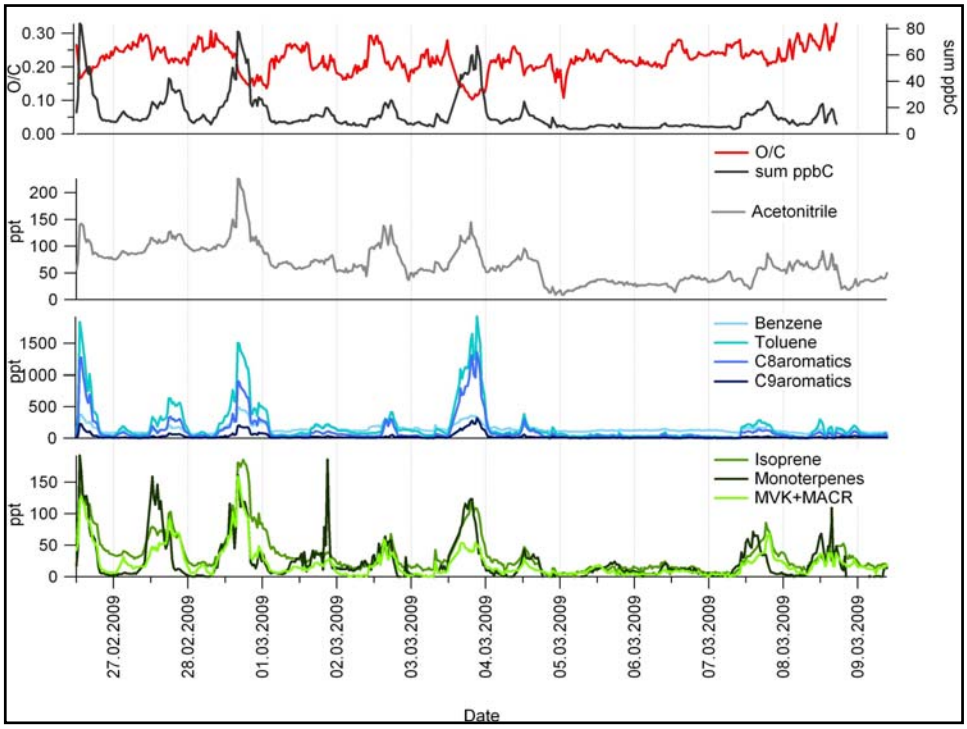
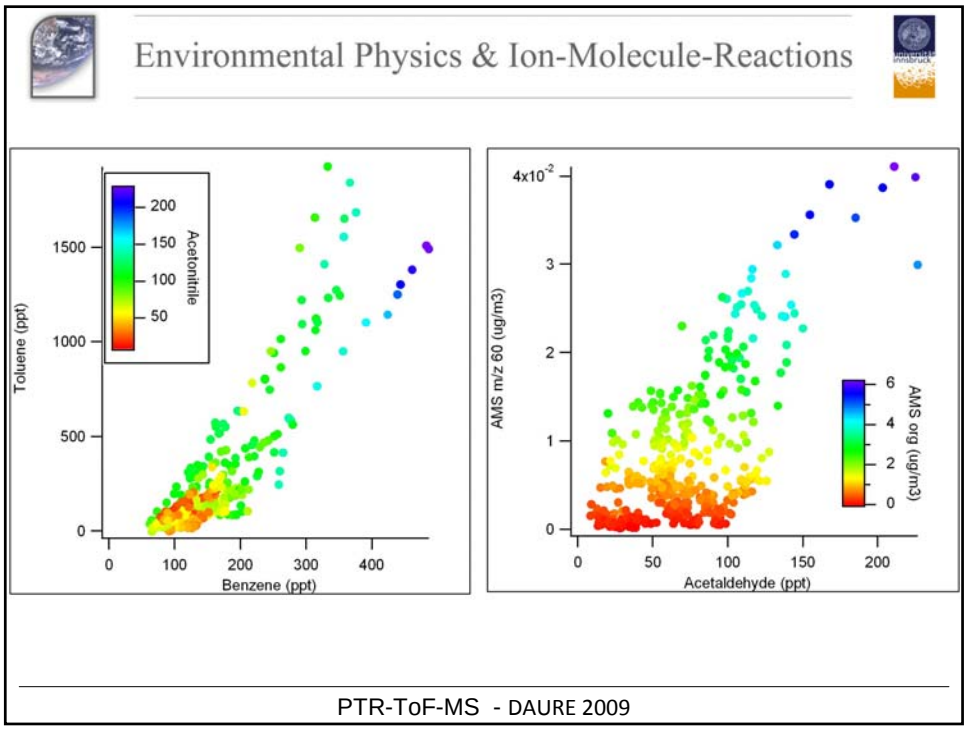
Environmental Physics & Ion-Molecule-Reactions

- 4m Silco steel inlet (30 C above ambient)
- Teflon filter @ front end of the inlet
- Residence time approx. 1 sec
- Blank measurements every 3hrs
- Calibration every 1-2 days

Environmental Physics & Ion-Molecule-Reactions

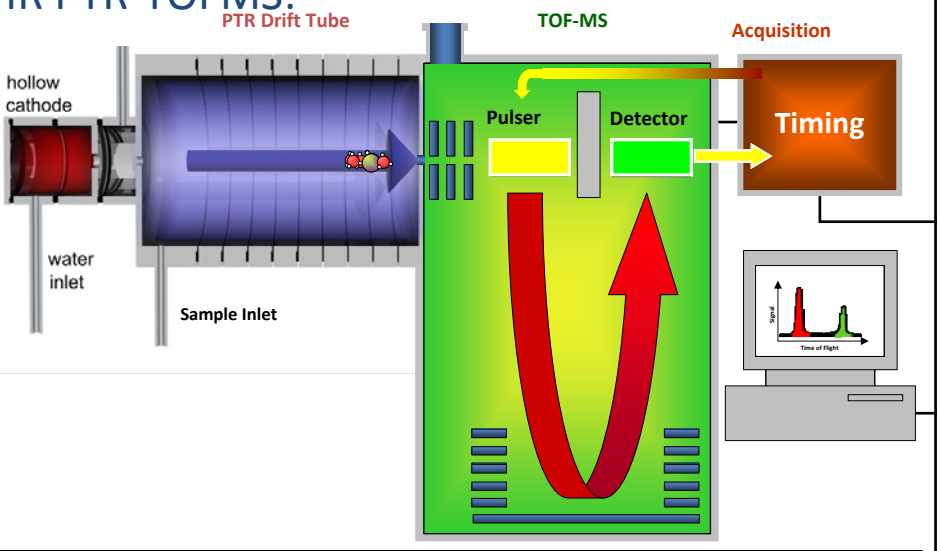
- LOD @ 1min integration time -> 10ppt
- Mass accuracy <15 ppm, Mass Resolution 4000: unambiguous assignment of empirical formulae to a measured exact mass!
- 320 Peaks >> approx.150 compounds.
- 60 compounds >10ppt


O/C
sum ppbC
Acetonitrile
Benzene
Toluene
C8aromatics
C9aromatics
Isoprene
Monoterpenes
MVK+MACR
ppt
Date
27.02.2009
28.02.2009
01.03.2009
02.03.2009
03.03.2009
04.03.2009
05.03.2009
06.03.2009
07.03.2009
08.03.2009
09.03.2009


Environmental Physics & Ion-Molecule-Reactions
Toluene (ppt)
Benzene (ppt)
Acetonitrile
AMS m/z 60 (ug/m3)
Acetaldehyde (ppt)
AMS org (ug/m3)
PTR-ToF-MS - DAURE 2009

THANK YOU

HR PTR-TOFMS:



Proton Transfer Reaction:

- Chemical ionization:
  $H_3O^+ + VOC \rightarrow VOCH^+ + H_2O$
- Reaction controlling parameter: Proton affinity PA
  - $PA_{VOC} > PA_{H2O}$ $\Delta E = PA_{H2O} - PA_{VOC}$
  - PA of main air compounds to low → no PTR ionization
  - Most volatile organic compounds (VOCs) can be detected
- Reaction energy is mostly lower than molecule bonding energies
  → hardly any fragmentation expected
  → soft ionization method

Compound	Proton affinity [kcal/mol]
Argon	88.2
Oxygen	100.6
Nitrogen	118.0
CO	129.2
CO_2	141.7
Water	**165.2**
Formaldehyde	170.4
Benzene	179.3
Methanol	180.3
Ethanol	185.6
Toluene	187.4
Xylene	190.0
DMS	**198.6**

Environmental Physics & Ion-Molecule-Reactions

What do we detect:

- Most hydro carbons and derivates
  - Terpenes
  - Aromatics
- Photo oxidation products and other oxyVOCs
  - Ketones
  - Aldehydes
  - Alcohols
- Aerosol precursors
  - DMS and oxidation products (DMSO)
  - High molecular species (semi volatile)

Performance Summary HR PTR-TOFMS:

- **Detects all ions in one instant**
- **Separation of isobars is possible**
- **Identification of the elemental composition**
- **High sensitivity**
- **Low pptv range LOD**