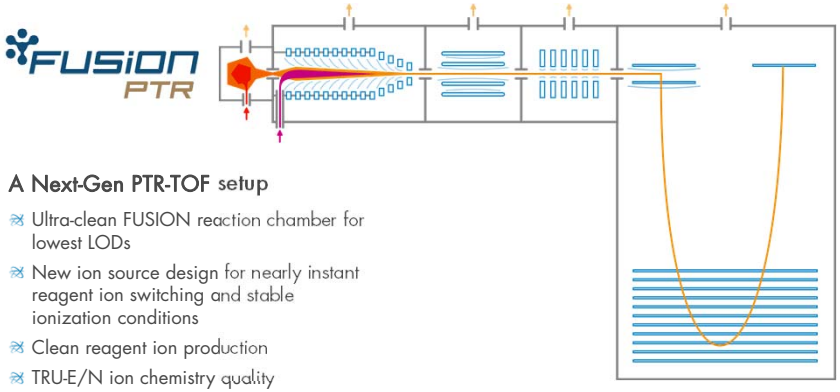
FUSION PTR-TOF 10k - Next Generation PTR-TOFMS

IONICON Analytik GmbH., Eduard-Bodem-Gasse 3, 6020 Innsbruck, AUSTRIA
https://www.ionicon.com/technologies/details/fusion-ptr

Introduction

We present a novel proton-transfer-reaction mass spectrometry (PTR-MS) [1] instrument. FUSION PTR-TOF 10k (IONICON, Austria) features several enhancements compared to state-of-the-art PTR-MS technology.
The novel ion source improves the decoupling from the reaction chamber providing lowest interferences with neutrals and parasitic reagent ions. Within a single second, this source switches from quantitative proton-transfer-reaction with H_3O^+ reagent ions to almost fragmentation-free adduct ionization with NH_4^+. Ion-molecule reactions with organics occur in a fully-controlled environment of a novel ion-focusing RF reaction chamber (FUSION) operated at reduced pressures of 2-4 mbar. This guarantees the needed clean ion chemistry with ion-molecule reactions at predictable reaction energies (E/N) and reaction rates that are crucial for quantitative operation of PTR-MS. With these enhancements, FUSION PTR-TOF 10k achieves lowest limits of detection (< 1 pptV in 1 s) and extremely high sensitivities up to 80000 cps/ppbV at a TOF-MS mass resolution > 10000 m/dm.

Overview



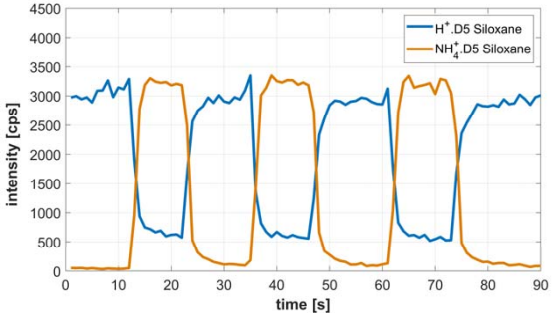
A Next-Gen PTR-TOF setup

- Ultra-clean FUSION reaction chamber for lowest LODs
- New ion source design for nearly instant reagent ion switching and stable ionization conditions
- Clean reagent ion production
- TRU-E/N ion chemistry quality
- ioniTOF MS 10k with a mass resolution of typically 10000 – 15000 m/Δm (FWHM)

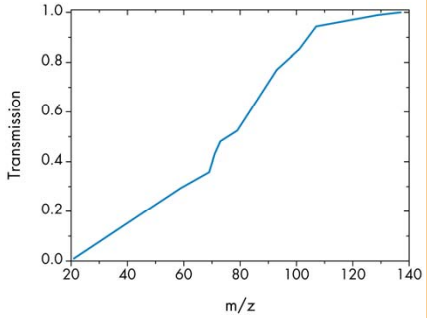
FUSION Ion Source

Fast switching between proton transfer (H_3O^+) and adduct ionisation (NH_4^+) [2]

- Possible reagent ions include [3]: H_3O^+, NH_4^+, NO^+, O_2^+
- Switching time ~ 1s
- Switching between high and low reaction energy (E/N)

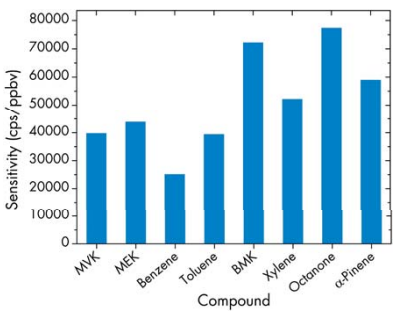


Fusion Reaction Chamber



Well defined ion chemistry

- Predictable sensitivities, based on reaction rate constants
- No mass cut-off towards lower and higher m/z

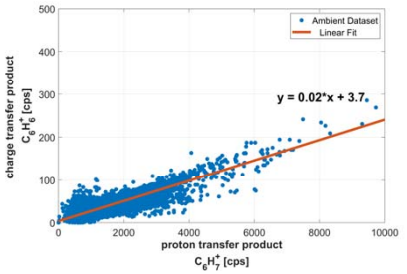


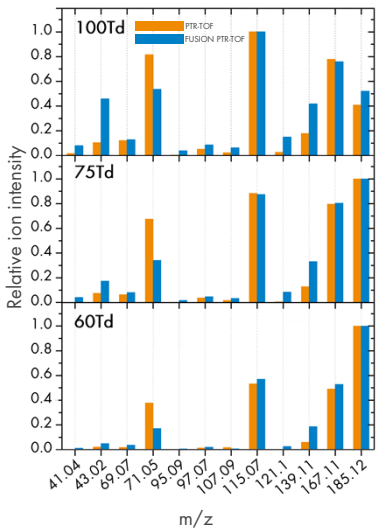
Sensitivities for different compounds

- High sensitivities ~ 80000 cps/ppbv
- Limit of Detections < 1pptv in 1 s

Reagent ion purity

- Measurement of benzene in H_3O^+ mode
- Data taken from ambient dataset (2 weeks)
- Varying humidity level
- Ratio of charge transfer product (O_2^+) vs. proton transfer product (H_3O^+)
- Ultra clean reagent ion production with:
  $C_6H_6^+/C_6H_7^+$ ~ 2%
  independent of moisture level





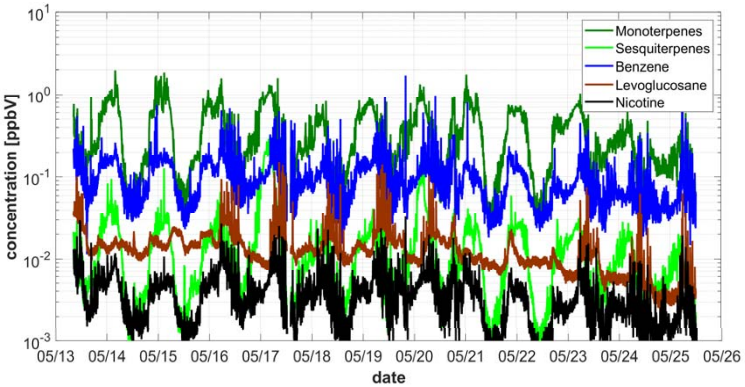
Reaction kinetic evaluation

- Branching ratios are very sensitive to the applied reaction energy (E/N)
- TRU-E/N method (US10074531, EP3309817) allows to reproduce intensity ratios for all relevant pinonic acid product ions corresponding to E/N values down to 60 Td

Results

Two weeks continuous measurement of ambient air in Innsbruck, Austria

- FUSION PTR-TOF 10k enables robust and stable long term measurements
- Selected compounds over the course of two weeks
  - Anthropogenic compounds like benzene
  - Biogenic compounds include monoterpenes and sesquiterpenes
  - Local emissions from smoking (levoglucosan and nicotine)
- Real time measurements in the sub-pptv range
- Fast response time
- Simultaneous detection of large range of volatility classes (e.g. levoglucosan and nicotine)



References
[1] W. Lindinger and A. Jordan, Proton-transfer-reaction mass spectrometry (PTR–MS): on-line monitoring of volatile organic compounds at pptv levels, Chem. Soc. Rev., 27, (1998) 347-375, DOI: 10.1039/A827347Z
[2] M. Müller et al., A novel method for producing NH_4^+ reagent ions in the hollow cathode glow discharge ion source of PTR-MS instruments. Int. J. Mass Spectrom. 447 (2020) 116254. DOI: 10.1016/j.ijms.2019.116254
[3] A. Jordan et al., An online ultra-high sensitivity Proton-transfer-reaction mass-spectrometer combined with switchable reagent ion capability (PTR + SRI – MS). Int. J. Mass Spectrom. 286 (2009) 32-38. DOI: 10.1016/j.ijms.2009.06.006