Ion-Molecule-Reactions & Environmental Physics

Performance Assessment of a High Resolution PTR-TOFMS Instrument

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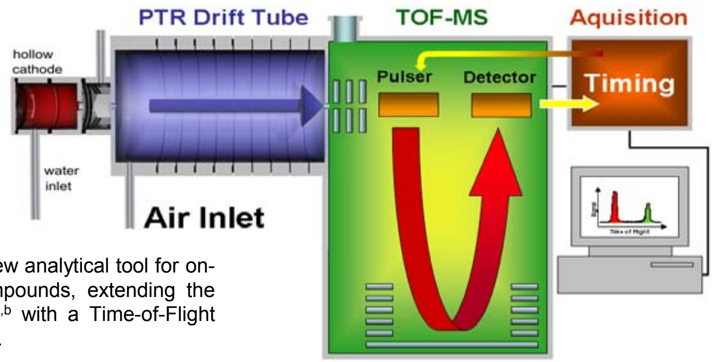
Introduction

A High Resolution Proton Transfer Reaction Time-of-Flight Mass Spectrometer (HR PTR-TOFMS) was recently developed at the University of Innsbruck.



The HR PTR-TOFMS is a powerful new analytical tool for on-line analysis of volatile organic compounds, extending the approved PTR technique (PTR-MS)[a,b] with a Time-of-Flight Mass Spectrometer (PTR-TOF-MS)[c,d].

Performance Assessment

The biggest advantage of the HR PTR-TOFMS is it's high **mass resolving power** $R=m/\Delta m$. Figure (1) demonstrates the characteristics of the mass resolving power. A mass resolving power of R=5500 (FWHM) that slightly decreases to lower masses can be achieved. All data of Figure (1) are gained by one 60 seconds integrated spectrum.

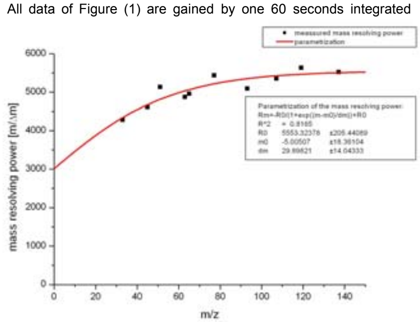


Figure (1): Characteristics of the mass resolving power of the HR-PTR-TOFMS

Analysis of the detector noise around m/z=107.5 (no chemical background expected) yields in a LOD lower than **20pptv** applying a 60s integration period (2σ LOD).

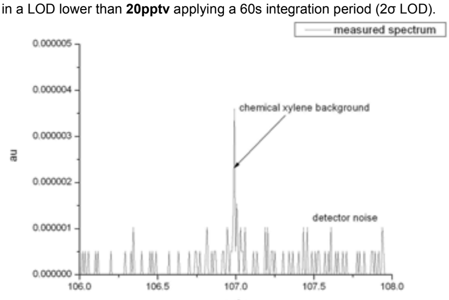


Figure (2): Chemical and detector noise at m/z=107: The chemical noise can be separated from the statistical distributed detector noise.

Data Examples

In the following, the performance of the HR PTR-TOFMS is demonstrated by separation of isobars. With an example protonated ions of **glyoxal** ($C_2H_2O_2.H^+$) and **acetone** ($C_3H_6O.H^+$), figure (3) demonstrates, that two compounds can be distinguished.

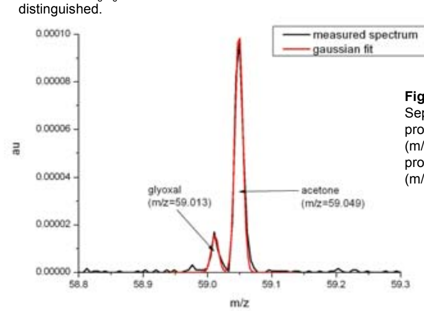


Figure (3): Separation of protonated glyoxal (m/z=59.013) and protonated acetone (m/z=59.049)

Figure (4) shows three peaks at m/z=47 (protonated **formic acid**, $\mathbf{N_2H_3O^+}$ and protonated **ethanol**), which can be separated. Identification of the mass peaks (**empirical formula**) is done by their respective exact mass and verified by their **isotopic patterns**.

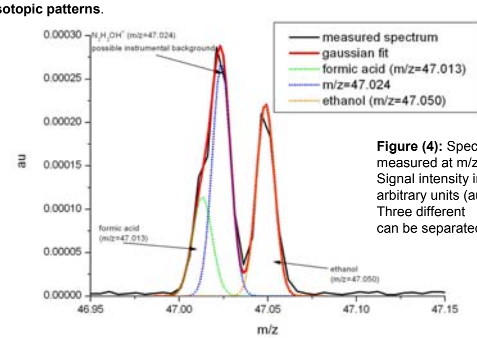


Figure (4): Spectrum measured at m/z=47. Signal intensity in arbitrary units (au). Three different peaks can be separated.

Conclusion

This new PTR instrument is a very powerful and quantitative tool for trace gas analysis. It's high mass resolving power and high time resolution as well as it's size are opening many challenging applications, positioned in environmental and atmospheric physics as well as medical science and food chemistry.

Acknowledgement
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References

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