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Investigations on the formation of positive and negative reactant ions in High Kinetic Energy Ion Mobility Spectrometry (HiKE-IMS) by HiKE-IMS-MS

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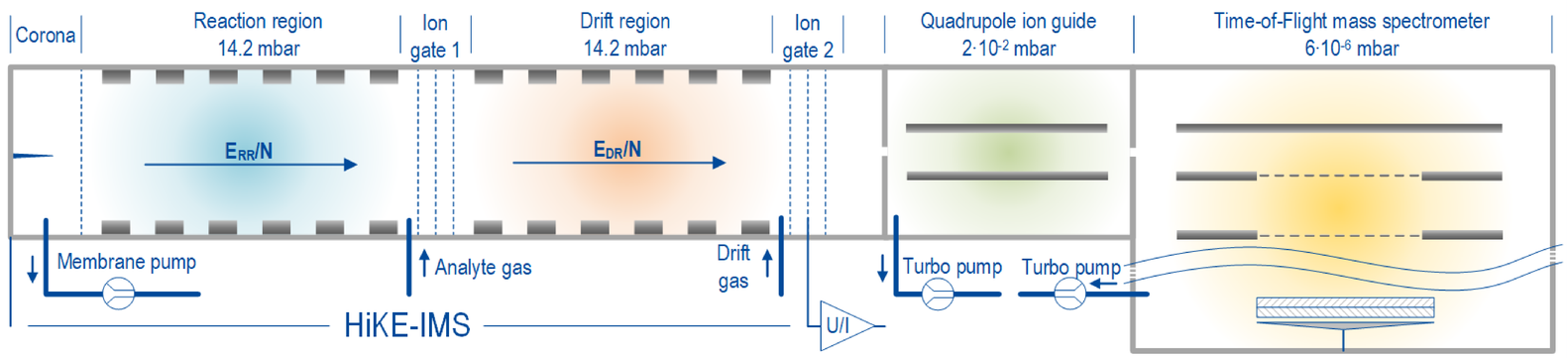
Introduction

Similar to PTR-MS or SIFDT-MS, HiKE-IMS ionize in a reaction region operated at decreased pressures around 20 mbar and high reduced electric field strengths of up to 120 Td. However, instead of a mass spectrometer, an IMS operated at the same pressure as the reaction region is used for ion separation and detection. In this work, the prevailing reactant ion population in HiKE-IMS is analyzed in dependence on the reduced electric field strength in the reaction region E_{RR}/N and the sample gas humidity. To identify individual ion species associated with certain peaks in the ion mobility spectrum, the HiKE-IMS is coupled to a time-of-flight mass spectrometer (TOF-MS) using a simple gated interface allowing to transfer selected peaks of the ion mobility spectrum into the TOF-MS.

For detailed information please see references [1], [2] and [3].

Experimental setup



» Operating pressure: 14.2 mbar; operating temperature: 45 °C.
» Positive ion polarity: E_{DR}/N = const. = 115 Td, E_{RR}/N = variable; Negative ion polarity: E_{DR}/N = const. = 80 Td, E_{RR}/N = variable.
» Unless otherwise stated, drift and sample gas: Purified air containing 70 ppm_v of water (0.35 % rH) and 30 ppm_v of carbon dioxide.

Conclusion

The experimental data suggest the predominant generation of the positive reactant ions NO^+, H_3O^+ and O_2^+ as well as the negative reactant ions O^-, OH^-, O_2^-, and O_3^- in purified air containing 70 ppm_v of water and 30 ppm_v of carbon dioxide. Both the reduced electric reaction field strength and the sample gas humidity significantly affect their relative abundances.

References & Acknowledgment

[1] Allers, Kirk, von Roßbitzky, Erdogdu, Hillen, Wissdorf, Benter, Zimmermann, *"Analyzing Positive Reactant Ions in High Kinetic Energy Ion Mobility Spectrometry (HiKE-IMS) by HiKE-IMS-MS"*, J. Am. Soc. Mass Spectrom., 2020, 31, 812-821.

[2] Allers, Kirk, Eckermann, Schaefer, Erdogdu, Wissdorf, Benter, Zimmermann, *"Positive Reactant Ion Formation in High Kinetic Energy Ion Mobility Spectrometry (HiKE-IMS)"*, J. Am. Soc. Mass Spectrom., 2020, Just accepted.

[3] Allers, Kirk, Timke, Erdogdu, Wissdorf, Benter, Zimmermann, *"Negative Reactant Ion Formation in High Kinetic Energy Ion Mobility Spectrometry (HiKE-IMS)"*, J. Am. Soc. Mass Spectrom., 2020, Under review.

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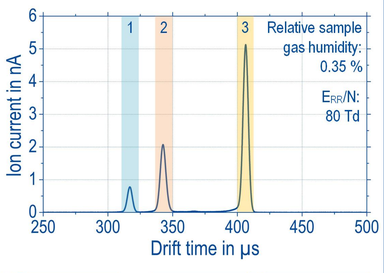
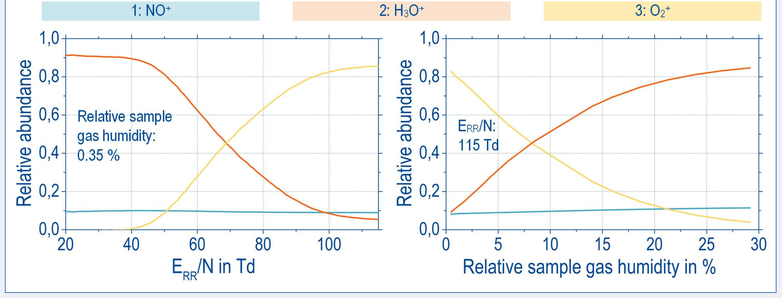
Positive reactant ions

» The positive reactant ion population is determined by the conversion processes of O_2^+ and NO^+ to $H_3O^+(H_2O)_n$.
» Increasing E_{RR}/N inhibits the conversion, increasing the sample gas humidity favors it.





Negative reactant ions

» The negative reactant ion population is determined by the interaction of electrons with neutrals in the reaction region.
» Increasing the sample gas humidity results in the generation of $OH^-(H_2O)_n$ ions.