Real-time monitoring of dynamic isomer populations with CI-SLIM IMS-MS

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Ion mobility spectrometry (IMS) using Structures for Lossless Ion Manipulations (SLIM) is an emerging powerful tool for rapid isomer separations. This technology offers high mobility resolution due to prolonged ion mobility path lengths that are achieved on a small form factor separation device. In this work, we interface SLIM IMS separation with a chemical ionization source, which allows one to sample from the gas- and particle-phases directly. As such, one can monitor dynamic isomer populations in ambient air in real-time without prior sample preparation. This technology opens the door to new possibilities in atmospheric chemistry where isomer distribution is expected to play a key role in gas phase processes and in the formation of organic aerosols.

The CI-IMS-TOF instrument built by TOFWERK produces ions via a two-step chemical ionization process, which involves 1) producing reagent ions and 2) ionizing neutral analyte molecules via the reagent ions through either charge transfer or adduct formation. Once generated, these secondary ions travel into the SLIM IMS region, where a series of DC- and AC-electrodes on printed circuit boards create a traveling wave driving force. As the ions travel through the helium buffer gas, they separate based on their rotationally averaged collision cross-sections.

In the present work, various experiments were performed using an aerosol flow tube reactor and an atmospheric simulation chamber to recreate atmospheric conditions. Gas-phase oxidation of isoprene was used to explore the capabilities of the CI-SLIM IMS-MS under atmospheric relevant conditions. Firstly, the most important oxidation products produced from the OH-oxidation of isoprene were used including methacrolein, methyl vinyl ketone, isoprene epoxy diols (IEPOX), isoprene hydroxy hydroperoxide (1,2 and 4,3-ISOPOOH), and other $C_5H_{10}O_3$ reactive uptake products as a single component or as a mixture to first evaluate the capabilities of the CI-SLIM IMS-MS at resolving the different isomers. Secondly, the reactive uptake of IEPOX onto acidic particles and OH-initiated oxidation (low and high NO regimes) of isoprene were studied to characterize the dynamic of the isomers generated within the simulation chamber under various environmental conditions. Results will be presented to demonstrate the capabilities of the newly developed CI-SLIM IMS-MS at resolving isomers in real time.

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