

Abstract

This thesis describes development of the new selected ion flow-drift tube mass spectrometry technique, SIFDT-MS, for online quantification of volatile organic compounds, VOCs, based on gas phase ion-molecule reactions. SIFDT-MS represents a new generation of the successfully used selected ion flow tube, SIFT-MS, analytical method. The essential extension of SIFDT-MS is the uniform electric field E applied across the flow tube reactor, thus converting it to the flow-drift tube where the ion processes can be governed by strength of field E . Newly introduces Hadamard modulation of the gate lens before the flow-drift tube enables direct ion residence, and correspondently ion-molecule reaction, time measurement that is necessary for the precise concentration calculations under variable conditions. The detailed experimental study of these processes results was carried out to form a basis of the analytical method. In order to overcome a well-known issue of SIFT-MS, when mass spectral peaks of isobaric ions overlap, the pseudoinverse matrix multiplication for isobaric mixtures was demonstrated. Finally two data mining approaches were successfully tested on the data of the fragmentation signals of seven monoterpene isomers obtained in SIFT-MS.