

Abstract: Chemical ionization mass spectrometry (CI-MS) is a powerful analytical technique, capable to detect trace levels of organic molecules diluted in air samples in real-time. Processes leading to ionization of organic molecules, necessary for their detection and identification, are however often strongly affected by the presence of water vapours in form of sample humidity. In the present work, I studied the influence of water vapours on ion chemistry and, subsequently, the respective influence on sensitivity and selectivity of CI-MS techniques.

Studies were carried out using several soft chemical ionization mass spectrometry instruments, including Selected Ion Flow Tube Mass Spectrometry (SIFT-MS), Proton Transfer Reaction Mass Spectrometry (PTR-MS) and Selected Ion Flow-Drift Tube Mass Spectrometry (SIFDT-MS). Experimental studies were also supplemented by theoretical simulation of proposed ion chemistry using the Kinetic of Ion-Molecular Interaction simulator (KIMI), developed by the author.

In this thesis, I present a study of formaldehyde, glyoxal and phthalates ion chemistry with H_3O^+ , NO^+ and O_2^+ reagent ions, focusing on secondary reactions with water vapours. Additionally, I also studied secondary reactions of protonated hydrated acetic acid with acetone. Finally, I have carried out experiments with fast gas chromatography (CG) coupled with the SIFT-MS instrument, to reduce humidity influence and improve the selectivity of monoterpenes.