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Characterization of Proton Transfer Reaction Mass Spectrometry for the detection of sesquiterpenes

M. Demarcke (1), C. Amelynck (1), N. Schoon (1), J. Dewulf (2), and H. Van Langenhove (2)

(1) Belgian Institute for Space Aeronomy, Brussels, Belgium (marie.demarcke@aeronomie.be), (2) Research Group Environmental Organic Chemistry and Technology (EnVOC), Faculty of Bioscience Engineering, Ghent University, Ghent, Belgium

It is well-known that terrestrial vegetation is an important source of non-methane volatile organic compounds (NMVOC) of which terpenoid compounds, such as isoprene, monoterpenes and sesquiterpenes, constitute an important fraction. Measurements of sesquiterpenes ($C_{15}H_{24}$) are still sparse and hard to perform because of the low volatility of these compounds and their high reactivity with the main atmospheric oxidants (OH, O_3 , NO_3). Nevertheless, they may well play an important role in atmospheric chemistry because of their high reactivity and their high potential to contribute to secondary organic aerosol (SOA) formation.

Important efforts have been made lately to develop and improve analytical techniques for sesquiterpene detection and recently proton transfer reaction mass spectrometry (PTR-MS) has also been applied for sesquiterpene detection by a limited number of research groups. Further exploitation of the PTR-MS technique for this class of terpenoid compounds may benefit from a better characterization of the ion chemistry inside the PTR-MS reactor at varying instrumental and environmental parameters.

Therefore, product ion distributions of four important sesquiterpenes (beta-caryophyllene, alpha-humulene, longifolene and alpha-cedrene) have been measured in a commercial high sensitivity PTR-MS instrument (Ionicon Analytik GmbH) at different values of the ratio of the electric field strength to the buffer gas number density in the reactor (E/N) and at different water vapour pressures in the inlet line. Although the nascent excited complex, which is formed in the $H_3O^+ \cdot (H_2O)_n$ /sesquiterpene reaction, partially decomposes into a variety of fragment ions, the protonated sesquiterpene remains the major product ion for all four species studied. The product ion distributions show a large dependence on E/N , but, interestingly, are not found to be much influenced by changing relative humidities.

From the results it is expected that sesquiterpene detection sensitivity based on the protonated sesquiterpene ion signal (at m/z 205) can be enhanced by a factor of three when decreasing the E/N value from 140 to 80 Td.

Since some of the sesquiterpene fragment ions have the same m/z value as the common monoterpene PTR-MS fingerprint ions ($C_{10}H_{17}^+$ at m/z 137 and $C_6H_9^+$ at m/z 81), care should be taken when quantifying monoterpenes in the presence of sesquiterpenes.

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