



Selected ion flow tube studies of the reactions of H_3O^+ , NO^+ and O_2^+ ions with a series of oxygenated biogenic volatile organic compounds in support of their detection by SIFT-MS

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The Selected Ion Flow Tube – Mass Spectrometry technique (SIFT-MS) has already proven to be a successful technique for the detection and quantification of volatile organic compounds (VOCs) [1]. Although less sensitive than the PTR-MS technique [2], it may be more selective because of the use of multiple source ions (H_3O^+ , NO^+ and O_2^+) which can react with the VOCs in a different way.

In this study, rate constants and product ion distributions of H_3O^+ , NO^+ and O_2^+ ions with geraniol (trans-3,7-dimethyl-2,6-octadien-1-ol, $\text{C}_{10}\text{H}_{18}\text{O}$), nerol (cis-3,7-dimethyl-2,6-octadien-1-ol, $\text{C}_{10}\text{H}_{18}\text{O}$), linalool (3,7-dimethyl-1,6-octadien-3-ol, $\text{C}_{10}\text{H}_{18}\text{O}$), 1,8-cineole ($\text{C}_{10}\text{H}_{18}\text{O}$), cis-3-hexen-1-ol ($\text{C}_6\text{H}_{12}\text{O}$) and 2-methyl-3-buten-2-ol ($\text{C}_5\text{H}_{10}\text{O}$) have been obtained in a SIFT at 150 Pa and 300 K.

Except for 1,8-cineole, which is a saturated monoterpene hydrocarbon containing an ether functional group, all compounds studied here are unsaturated alcohols.

The reactions of H_3O^+ ions with the terpenoid alcohol isomers linalool, geraniol and nerol do not result in the proton transfer product ion, but in ions with masses 137u (H_2O elimination after protonation) and 81u. The reactions of NO^+ ions with nerol and geraniol mainly result in the charge transfer product (154u) and the product ion obtained after elimination of a H_2O molecule (136u). The latter process is even dominant in the reaction between NO^+ and linalool.

The reactions of H_3O^+ ions with 1,8-cineole, 2-methyl-3-buten-2-ol and cis-3-hexen-

1-ol mainly proceed by proton transfer and elimination of a H₂O molecule after protonation, the latter one being the major reaction channel. The reaction of NO⁺ with 1,8-cineole principally results in charge transfer and a small H₂O elimination channel is also observed. The reaction of NO⁺ with cis-3-hexen-1-ol proceeds by several equally important reaction mechanisms (charge transfer, H₂O elimination, hydride transfer, ...). The main reaction channel of NO⁺ with 2-methyl-3-buten-2-ol is elimination of OH, leading to product ions at mass 69 u.

The reactions of O₂⁺ ions with the species studied mostly result in a multitude of product ions and are probably not very useful for detection and quantification by SIFT-MS, except perhaps for the O₂⁺/2-methyl-3-buten-2-ol reaction which mainly proceeds by CH₃ elimination, resulting in an ion at mass 71u.

[1] D. Smith et al., Int. J. Mass Spectrom. 209 (2001) 81.

[2] W. Lindinger et al., Int. J. Mass Spectrom. Ion Proc. 173 (1998) 191.