



Laboratory studies on sesquiterpene detection by CIMS

F. Dhooghe (1), C. Amelynck (1), N. Schoon (1), E. Debie (2), P. Bultinck (2), F. Vanhaecke (3)

(1) Belgian Institute for Space Aeronomy, Ringlaan 3, B-1880 Brussels, Belgium, (2) Department of Inorganic and Physical Chemistry, Ghent University, Krijgslaan 281, S3, B-9000 Ghent, Belgium (3) Department of Analytical Chemistry, Ghent University, Krijgslaan 281, S12, B-9000 Ghent, Belgium (frederik.dhooghe@aeronomie.be / Fax: +32 2 374 84 23 / Phone: +32 2 790 39 17)

Sesquiterpenes ($C_{15}H_{24}$) are highly reactive biogenic Non-Methane Volatile Organic Compounds (NMVOC) which, until recently, have received much less attention than isoprene and monoterpenes due to their presumed low emission rates. Recent measurements however, have shown that for some plant species sesquiterpene emissions can account for up to 10 % of total NMVOC emissions [1]. Moreover, atmospheric oxidation of sesquiterpenes is expected to contribute significantly to secondary organic aerosol (SOA) formation [2].

Sesquiterpene measurements have mainly been established using time-consuming sampling techniques followed by off-line Gas Chromatographic Mass Spectrometric (GC-MS) analysis. More recently, Proton Transfer Reaction Mass Spectrometry (PTR-MS) has been used for sesquiterpene detection [3]. PTR-MS is a fast and sensitive on-line Chemical Ionization Mass Spectrometry (CIMS) technique which uses the hydronium ion (H_3O^+) as reagent ion species. However, it has the disadvantage that it lacks selectivity for sesquiterpene isomers.

To investigate if other typical CIMS reagent ions, such as NO^+ and O_2^+ , can result in more selective sesquiterpene detection, the reactions of H_3O^+ , NO^+ and O_2^+ ions with a series of seven sesquiterpenes (aromadendrene, β -caryophyllene, α -cedrene, α -humulene, longifolene, isolongifolene and δ -neoclovene) have been studied in a Selected Ion Flow Tube (SIFT) instrument.

H_3O^+ /sesquiterpene reactions are found to result in non-specific fragment ions, so H_3O^+ ions cannot be used to distinguish sesquiterpene isomers. NO^+ /sesquiterpene reactions are found to have some possible selectivity because of the presence of specific fragments with considerable yields for β -caryophyllene and α -humulene. Because of the severe fragmentation encountered for O_2^+ /sesquiterpene reactions, the product ion spectrum of a realistic air sample is expected to be suffering from major interference problems.

Results of this study are presented and the implications for sesquiterpene detection are addressed.

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