

PHOTO-IONIZATION GC×GC-HRTOF/MS FOR AVIATION FUEL CHARACTERIZATION

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Recent application of photo-ionization (PI) coupled with GC×GC-HRTOF/MS for authentic standard mix called century mix along with several groups of petrochemical samples demonstrated PI as an effective soft-ionization technique to characterize volatile mixtures particularly, hydrocarbons [1]. This soft-ionization technology was shown to enhance analyte speciation by providing both molecular ions and structurally significant fragments at low-energy (10.8 eV). The enhanced sensitivity and selectivity stemming from the dramatic reduction in fragmentation at low energies also greatly increases the number of compounds identified, permitting robust statistical comparisons essential for successful chemical fingerprinting of petrochemical base oils.

The need to understand the chemical composition of complex aviation fuels has always been important. This need stems from the shortage of petroleum crude reserves resulted in a transition to alternative crude sources; desire to design and operate high performance jet engines with knowledge of fuel composition; as well as to understand the exposure of fuel components to environment and health. In this study, a reverse phase GC×GC-HRTOF/MS was used to comprehensively characterize highly volatile kerosene based aviation fuel using PI as a soft ionization technique. In addition, different combinations of EI and PI were evaluated to extract useful fragmentation pattern to identify complex isomeric species. Linearity and precision of this application was determined for different groups of paraffins, naphtenes and aromatic compounds. Accuracy of the method was validated by comparing aviation fuel and reference standards with known aromatic contents. As expected, PI revealed the information on the degree of branching particularly for the paraffins in aviation fuel. The technique has provided a much better understanding of complex aviation fuels and has huge potential as an advanced tool for similar products.

[1] Molecular Characterization of Volatiles and Petrochemical Base Oils by Photo-Ionization GC×GC-TOF-MS. A. Giri, M. Courtiade, A. Racaud, K. Okuda, A.J. Dane, R.B. Cody, J-F. Focant. Analytical Chemistry (2017). DOI: 10.1021/acs.analchem.7b00124.