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Atmospheric Pressure Gas Chromatography Mass Spectrometry (APGC/MS) for Novel Applications in Petroleum and Chemical Research

(Ionization Combined with Gas Phase Chemical Reactions for Compound ID and Compound Type Determination)

Douglas Stevens1, Chang S. Hsu2, Steven Lai3, Adam Ladak3

1. *Waters Corp., 34 Maple Street, Milford MA 01757*
2. *Future Fuels Institute, 1800 East Paul Dirac Drive, Tallahassee, FL 32310*
3. *Waters Corp., 100 Cummings Center Suite 407N, Beverly MA 01915*

Atmospheric pressure chemical ionization for gas chromatography using a QTof mass spectrometer has demonstrated utility across applications such as petrochemical/fuel analysis and the analysis of extractables from polymers. Soft ionization produced by the APGC source provides spectra with intense molecular ions. This results in GC/MS data that can be processed using the same workflow as has been successfully applied to electrospray QTof data using liquid chromatography (LC) since the mid 1990's in applications where unknown identification is required. APGC is more flexible than traditional CI GC/MS due to the range of reagents that can be used. Vacuum CI sources are limited to reagents that are gases at room temperature such as methane and ammonia. Due to the fact that it is not a vacuum pumped region and, therefore, easily accommodates reagents that are liquid at room temperature, APGC can provide access to a wider range of ionization types which results in improved selectivity. Added to improve sensitivity, it has subsequently been found to provide the advantage of also allowing real time gas phase chemical reactions to be used to add selectivity to GC/MS of complex samples. This possibility of combining a variety of ionization types with chemical reactions that reveal details such as the presence or absence of an aromatic ring in an unknown structure increases the utility of the technique even beyond the QTof's ability to provide routine accurate mass measurements for elemental composition determination. The ability to cover a wide range of analytes in different matrices is of value to fuel researchers investigating fossil fuels from new sources as well as those with interest in sustainable, renewable, and alternative fuels from biological sources. The identification of individual unknown compounds is often required in petroleum and chemicals research. The Classification of structurally related compounds, such as compound type analysis is also important. API techniques matched with gas chromatographic separations provides unique and complementary information needed for a more accurate and comprehensive description of samples. The advantages of real time gas phase HDX will be discussed.