IRD 3 Application Note

Functional Group Analysis of Aromatics, Esters and Alcohols

Introduction

Traditional petroleum fluids are very complex. Recent new fuel sources only add to the complexity of fuel and petroleum characterization. Current gas phase analytical methods for petroleum fluids emphasize methods that expect non-polar analytes in the samples.

New fuel source materials introduce a wide range of new analytes into the analysis and characterization of source fuel and mixed petroleum samples. These new fuel related analytes include, new functional groups, as well as more polar chemistry. While this introduces new challenges to the established petroleum analytical techniques, it also allows new opportunities for quick analyze and characterization of these new samples.

New fuel source materials are still developing and they include a wide range of plant based or refuse based materials. These initial source materials are processed to generate a stream that can be further modified and refined for fuel use. Both these source materials and the processing techniques require analytical characterization to assist in optimization. In this application, the ASAP IRD 3, a gas phase infrared detector for GC eluents, is used to provide selectivity and identification in complex samples. The IRD and accompanying software is used with an Agilent 7890 GC with split injection and capillary separations prior to IRD detection.

Product Overview

The IRD 3 is designed from the chromatographer's point-of-view and is the only analytical infrared instrument that seamlessly combines the separating power of the Gas Chromatography with the molecular identification of FTIR.

- Dedicated FTIR for use with GC
- Low maintenance and easy to use
- Small footprint
- Software interfaces with GC control software
- Seamless integration with MS

The IRD 3 is the perfect tool for the chromatographer looking to obtain more information about unknown samples. Using a heater light pipe flow cell, the sample is kept in a vapor state while interacting with IR. This allows the molecules to freely rotate in a low energy environment. Keeping the molecular geometry in tack during analysis provides unique and highly reproducible spectra.

Parameters and Results

Figure 1 is a separation of a complex new source fuel mixture by GC-IRD. First the Total Response Chromatogram (TRC) is shown with response at all wavelengths. This essentially shows the entire chromatogram without selectivity.
We can now look at this same complex sample with functional group selectivity. Figure 2 is a SWC chromatogram at 1750 wavenumbers and now we only see the ester and carboxylic acid analytes (carbonyl groups) in this sample:

This complex sample also contains many alcohols. Here is a SWC chromatogram at 3600 wavenumber (Figure 3) and we see all of the alcohols, phenols and free acids (-OH group) in this sample.

This complex sample also contains many aromatic analytes. Here is a SWC chromatogram at 3070 wavenumbers (Figure 4) and we see the aromatic analytes in this sample:

These three selective SWC chromatograms quickly show examples of a range of functional group distributions for this complex sample. Now we can identify individual peaks or even unresolved peaks with the IR vapor phase libraries.

Conclusion

It has been demonstrated that the GC-IRD system with the ASAP IRD 3 is very powerful tool for the analysis and characterization of new source fuel mixtures.

Figure 1.

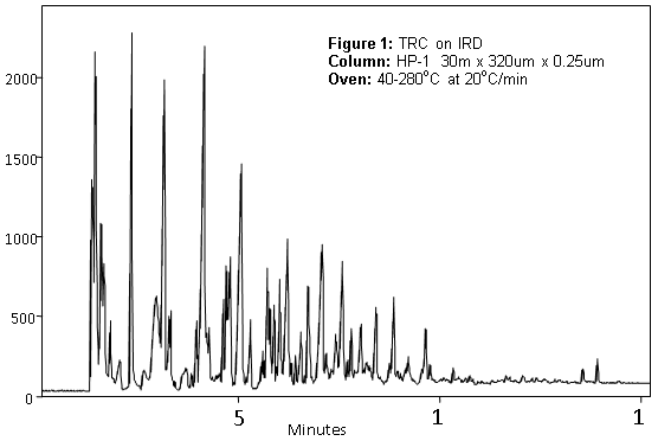


Figure 2

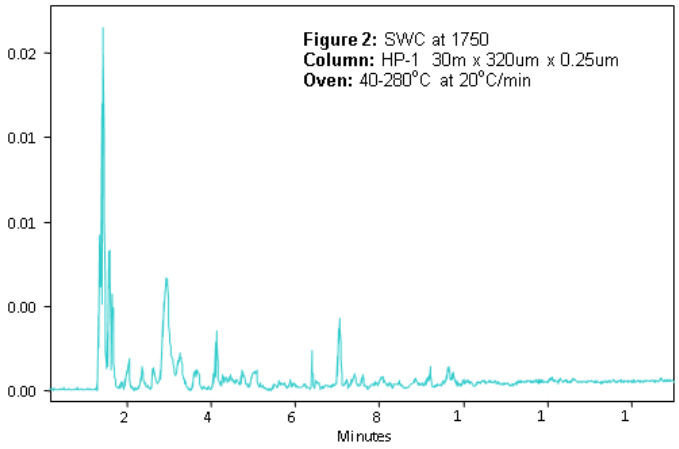


Figure 3.

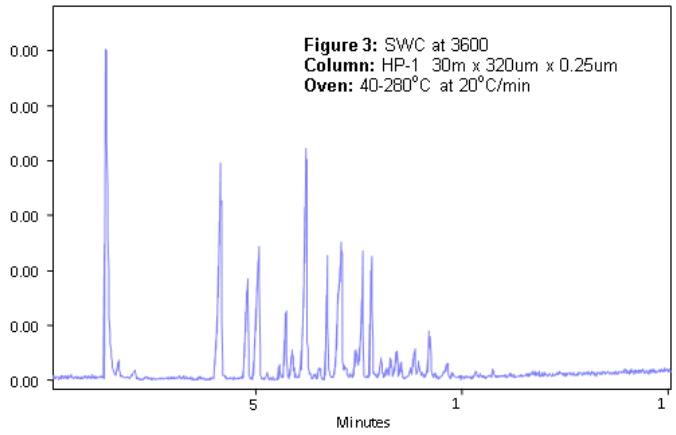
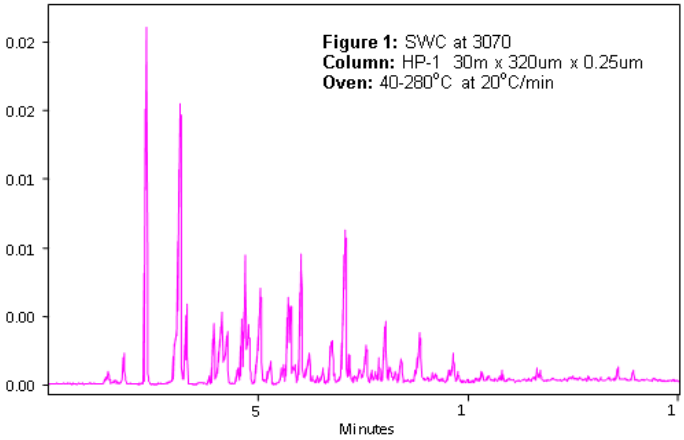


Figure 4.



1511 Neave Street
Covington, KY 41011

p. 859-581-6990
f. 859-581-6821

info@asapanalytical.com
www.asapanalytical.com