IRD 3 Application Note

Aromatics in Petroleum

Introduction

Due to the complex nature of petroleum and its many by-products, a through characterization of the components present is a formidable task. For gasoline range samples many of the current methods depend on a complete separation of the components on a fused silica capillary column. In this application, a combination of the IRD I and the HP 5970 MSD is utilized to characterize a gasoline range sample for aromatics content. The primary advantages of this system are the two independent types of data obtained from a single injection, and the complete separation of all components on the capillary column is not required.

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 the TRC and TIC of a single injection into the combined system. The chromatographic conditions are listed at the end of this note. The analysis was done using a serial configuration with the IRD followed by the MSD. As seen in these chromatograms, the resolution is very well maintained in passing through the 100ul IRD flow cell to the MSD. One of the primary advantages of the combined IRD/MSD system is the ability to readily extract information from a very complex chromatogram even where the GC peaks are not resolved. Figure 2 illustrates this for a standard mixture containing examples of the four most common classes of compounds found in gasoline range samples. Included are a paraffin, an olefin, and several aromatics. The top chromatogram is the TRC with the bottom chromatogram being a Selected Wavelength Chromatogram (SWC) which was calculated from spectra over the range from 670 to 830 wavenumbers.

As shown, the SWC is easily able to differentiate between the classes of compounds in the mixture. The wavelength range used is specific for the aromatic carbon-hydrogen out-of-plane deformation vibrations, so that only the aromatics are seen in the chromatogram.

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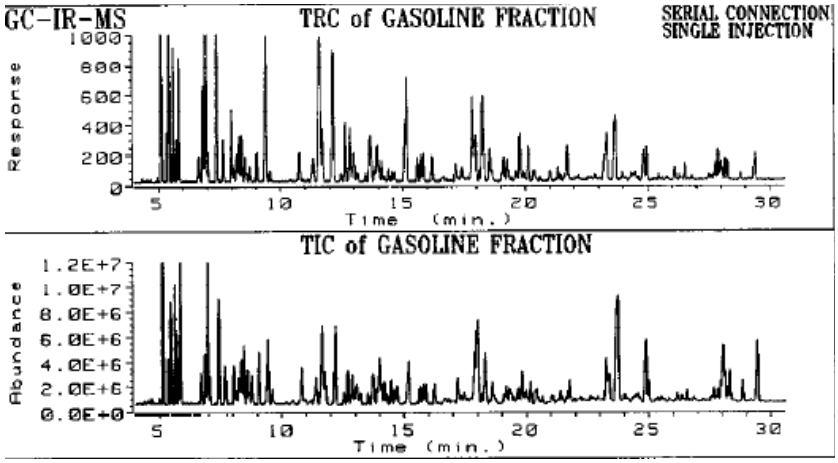
Figure 3 shows the SWC for the gasoline rage sample, as well as some extracted ion profiles from the simultaneously acquired mass spectrometer data. The 91 and 106 amu profiles are indicative of the number of alkyl substituents around the benzene ring. The combination of the two independent types of data is important here as illustrated by the peaks appearing at about 5.9 minutes in the SWC. Since they eluted before benzene, it is clear that they are not aromatic, and this is confirmed by the MS data.

Another example is the small peak at about 27.6 minutes in the 91 amu profile which is too weak to be observed in the SWC, but is readily observable in the MS chromatogram. Since this peak disappears in the 106 amu profile, this is probably the monosubstituted aromatic, propylbenzene.
Both the IRD and MSD have integration capabilities which can be used to quantitate peaks in the SWC and extracted ion profile. Quantitation of the gasoline sample here indicated the presence of about 7.5 weight percent of aromatic compounds.



Conclusion

It has been demonstrated that the IRD/MSD combination is very powerful tool for characterizing complex mixtures such as petroleum samples.