

## Infrared Detector

### POWER OF THE IRD

Ever since the advent of the gas chromatography the chemist has been trying to figure out, “What is that GC peak?” Sample evaluation from a quantitative sense cannot be done accurately without knowing what compound one is looking at. Hence the need for “smart” GC detectors. The earliest of these were the family of selective detectors, such as electron capture, flame photometric, alkali halide, etc., whose unique properties allowed them to look at certain general chemical phenomena, not molecularly specific characteristics.

With the coupling of the mass spectrometer to the gas chromatograph, the analyst felt that the “ultimate” GC detector has been found. The thousands of MSD’s in the world testify to this notion. The MSD is a “smart” GC detector; it gives important molecular mass related structural information. Through careful spectral interpretation of the fragment ions, the structure of the original molecule can often be pieced together and the molecular weight can be deduced as well.

However, regardless of how great the power of the mass spectrometer is as a GC detector, it has some weaknesses. These specifically relate to the spatial geometry of the molecular, which is destroyed or masked by the ionization/fragmentation/rearrangement processes of the MS. To overcome these inherent difficulties, another “smart” detector was developed. This detector is an infrared detector, the ASAP Analytical IRD 3, which utilizes a flow cell that allows one to analyze the intact molecule. This powerful benefit arises because the molecules are freely rotating and isolated from each other in a low energy environment. The IRD’s vapor phase spectra are not only molecularly unique, but highly reproducible as well. In the IRD the aspects of a molecule’s geometry are kept intact. There are several important areas of structural determination in which the IRD excels. These are highlighted on the following pages.

1. Aromatic Substitution – There is a frequent need to know specifically where on an aromatic ring certain substituents are placed. Mass spectrometry cannot differentiate between the xylene isomers, for instance, while infrared spectroscopy can.
2. Cis-Trans Isomers – The cis-trans spatial geometry about the double bond is destroyed during the impact process in MS while it is preserved in IR.
3. Aliphatic Chain Isomers – In the fragmentation process of conventional electron impact mass spectrometry the character of an aliphatic chain can be confused or even lost. This usually occurs with the chain fragment leaving and the charge remaining on the major residue, often a ring.

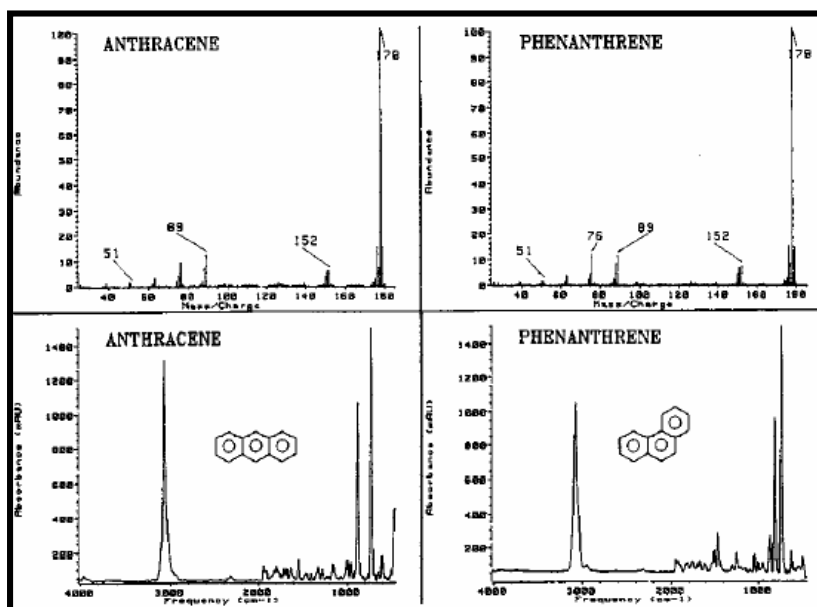


ASAP, LLC  
1511 Neave Street  
Covington, KY 41011  
ph: 877-987-2800 or  
859-581-6990  
fx: 859-581-6821  
info@asapanalytical.com  
www.asapanalytical.com  
date founded: 1999

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- Alcohols – Long chain aliphatic alcohols present a particularly tough problem when analyzed by MS. The spectra of the alcohol and the corresponding dehydration product, an olefin, are identical. To further complicate this, the mass spectrum of the equivalent molecular weight alkyl cyclopropane compound is identical also. The infrared spectra of all of these compounds are different and easily allow the alcohol to be determined.
- Ring Junctions – Polycyclic aromatic hydrocarbons can present a problem when qualitatively analyzed by MS. Most all of the ionization remains in the molecular ion. While this is useful, it gives no clues as to how the rings are joined. For instance, anthracene and phenanthrene give identical mass spectra but unique infrared spectra as can be seen in the figure



- Functional Groups – A very significant property of infrared detection couples the concepts of selected Wavenumber chromatogram and negative information. Total response chromatograms from the IRD can have functional group subset chromatograms extracted from the data. Where GC peaks occur in the SWC it indicates that that compound contains an IR absorption due to a certain wavelength. Where there is no peak, that compound does not contain a functional group of that type.

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Covington, KY 41011  
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