Infrared Detector

Analysis of Polynuclear Aromatic Hydrocarbons by GC-IRD

Introduction

While the mass spectrometer produces powerful structural information based on molecular fragmentation, often including molecular weight data, MS can be weak differentiating polynuclear aromatic hydrocarbons (PNA) ring bonding. Conversely, the infrared spectrometer is strong in these areas.

This note highlights the power of the IRD 3 to aid in the distinguishing of the some polynuclear aromatic hydrocarbons. While this example is chosen from the area of industrial chemistry, knowledge of PNA ring bonding has broad applicability in all area where structural identification is important.

The PNAs are naturally present in fossil and synthetic fuels, and can be formed during incomplete combustion of these fuels. PNAs have been found in diesel exhaust, wood smoke, coal, coal liquifaction and gasification products, creosote, and oil shale. From a health and environmental standpoint the mutagenic and carcinogenic properties of the some PNAs are of concern. The PNAs were one the earliest compound classes to be shown as carcinogenic from the studies of chimney sweeps and coke-oven workers. The carcinogenic and mutagenic activity apparently stems from the oxidation products of the PNAs. Thus controlling emissions and site characterization and remediation are of great importance.

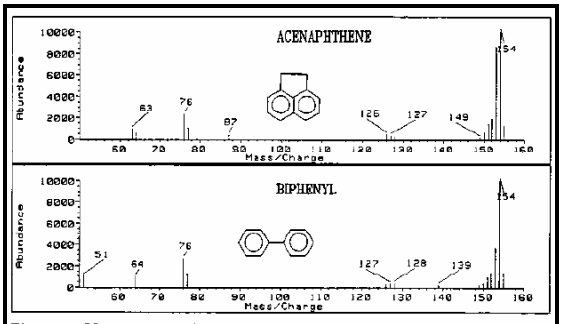

Figure 1. Mass spectra of acenaphthene and biphenyl

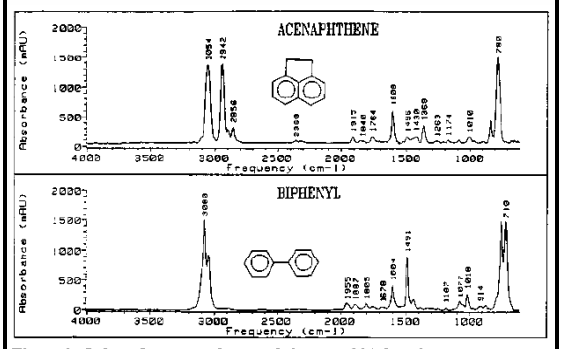

Figure 2. Infrared spectra of acenaphthene and biphenyl

Polynuclear aromatic condensed ring compounds absorb in the same general regions as benzene derivatives, with the carbon-hydrogen stretching vibrations at 3030 to 3100cm-1 and the with out-of-plane deformations occurring from 675 to 900cm-1. Specifically these deformations are as follows: one isolated aromatic hydrogen atom, 830 to 900cm-1; two adjacent aromatic hydrogen atoms, 810 to 850cm-1; three adjacent aromatic hydrogen atoms, 730 to 760cm-1 and 785 to 815cm-1; and four adjacent aromatic hydrogen atoms, 740 to 770cm-1. Out of plan ring vibrations occur at wavenumbers less then 500.

As can be seen in the figures, mass spectra of PNAs give strong molecular ions and little definitive fragmentation information. This leads to considerable uncertainty in making identifications based on mass spectral information alone. However, the infrared spectra of PNAs of the same molecular weight are different and identifications can easily be made based on infrared data.

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

ASAP
Analytical Solutions
And Providers

Infrared Detector

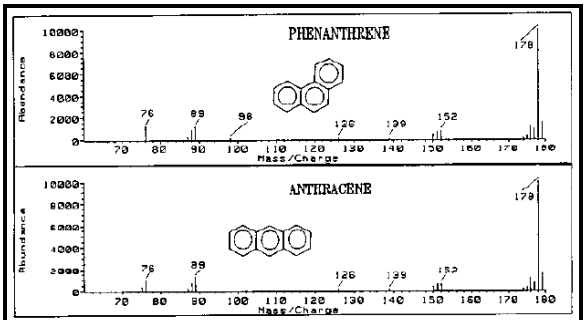

Figure 3. Mass spectra of phenanthrene and anthracene

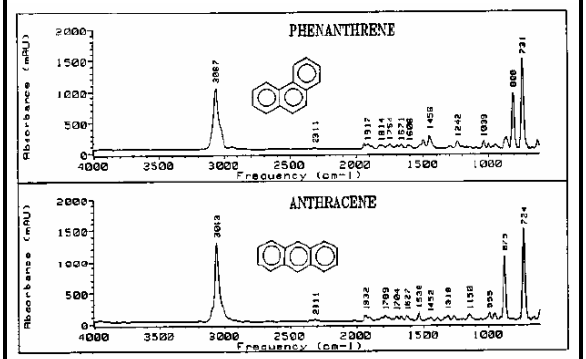

Figure 4. Infrared spectra of phenanthrene and anthracene

PBM library searches of the NBS or the Wiley mass spectral libraries cannot differentiate between anthracene and phenanthrene. This is understandable when one examines their mass spectra, see Figure 3. Their infrared spectra, see Figure 4, are entirely different and a search of the EPA Vapor Phase Library easily tells them apart. In order to achieve a very high confidence determination, a combined IR and MS library search was performed.

Conditions:

IRD: scan from 4000 to 550 wavenumbers
Optical Resolution: 8 cm^{-1} wavenumber
Transfer Line Temperature: 280°C

Summary

The GC-IRD has been shown to be useful in the differentiation of similar polynuclear aromatic hydrocarbons, specifically in this example of phenanthrene and anthracene. The combined IRD and MSD provide higher confidence results than either technique alone.

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

ASAP
Analytical Solutions
And Providers