IRD 3 Application Note

Cis/Trans Isomers

Introduction

While the mass spectrometer produces powerful structural information based on molecular fragmentation, often including molecular weight data, MS can be weak in the area of isomer differentiation. Conversely, the Infrared spectrometer is strong in this area. This note highlights the power of the IRD to aid in the distinguishing of isomers, specifically eugenol and cis-trans isoeugenol. While this example is chosen from the area of flavors and fragrances, isomer differentiation has broad applicability in all areas where structural identification is important.

Eugenol occurs in allspice, cinnamon leaf, bay, myrrh, patchouli in cloves where it constitutes 85% of the oil. Clove leaf oil is the raw material for the production of eugenol, which is further used to make isoeugenol and eugenol esters. Small amounts are used as a dental antiseptic. An important alternate source of eugenol is from the California bay leaf. Eurgenol is a carminative compound in that it has the ability to release hydrogen sulfide, methane and hydrogen in the digestive tract. Isoeugenol differs from eurgenol only in the location of the double bond in the hydrocarbon side chain. This shifts the odor from clove-like to nutmeg-like. The spice nutmeg is derived from the ground seeds of the nutmeg tree while mace comes from the seed coatings.

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

It can be seen from Figure 1 that the mass spectra of eugenol and cis-trans isoeugenol are very similar. The only difference of note is a slightly larger fragment at m/z 137 in the spectrum of eugenol due to a loss of part of the hydrocarbon side chain. On the other hand, the infrared spectra, Figure 2, have many subtle differences, which allow a higher confidence structural determination.

These differences are highlighted in Figure 3 where a comparison of the fingerprint region is shown. Visual differences are easily spotted and the IRD library search routine confirms the identities, finging the correct match in all three cases. Some

peaks shift a little but in a totally reproducible manner due to the nature of vapor phase spectra and the highly precise manner in which the IRD collects spectra. The most important spectral difference is the out-of-plane deformation of the vinyl hydrogens of eugenol at 916 wavenumbers compared to the out-of-plane deformation of the trans-disubstituted hydrogens of trans isoeugenol at 959 wavenumbers.

Conclusion

The use of the GC/IRD has been shown to be useful in the differentiation of similar isomeric compounds where spectral information has provided only molecular weight and general structural information.

Figure 1.

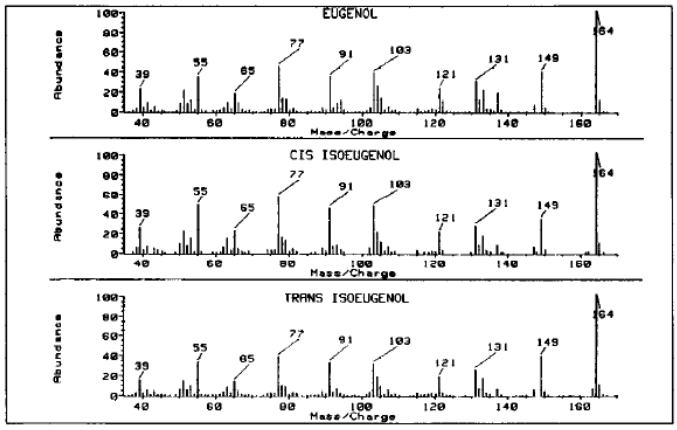


Figure 2.

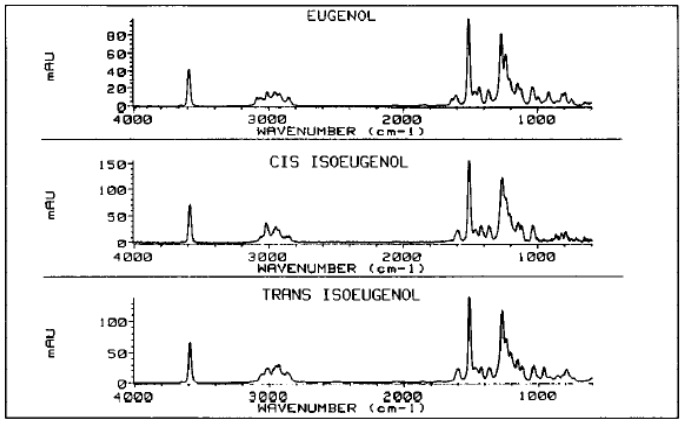
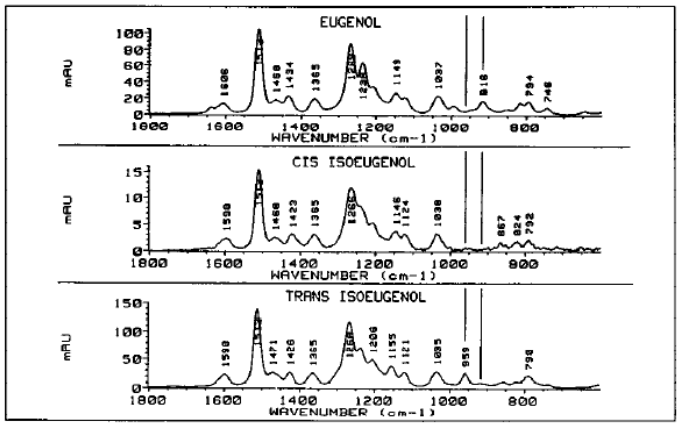


Figure 3.



1511 Neave Street
Covington, KY 41011

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

info@asapanalytical.com
www.asapanalytical.com