CDS solutions

APPLICATIONS INFORMATION USING ADVANCED SAMPLE HANDLING TECHNOLOGY

Identifying Additives in a Pyrogram using Deconvolution Software

Pyrolysis-GC/MS is a simple technique which may be used to study the composition of complex polymeric materials. Automobile tire rubber, for example is made with polymers, and also additives such as carbon black, antioxidants and other processing agents. The pyrogram of rubber shown in Figure 1 reveals that the polymeric material was formulated using styrene, butadiene and isoprene. Additional information about the additives used is generally also present, requiring the investigation of peaks not related to the rubber pyrolysis products.

Deconvolution software can facilitate this investigation by comparing specific ions in the mass spectra of the various peaks with a library of known compounds. Searching the total ion chromatogram produces a reconstructed TIC made up of the likely matches for compounds in the method library. The peaks are identified by compound name and retention time, making it simple to confirm the identification in the original chromatogram.

Figure 2 shows a deconvolution search of the rubber in Figure 1 performed using the IFD software from Ion Signature and a method library prepared at CDS. At 19.42 minutes, a large peak is indicated for N-(-1-methylethyl)-N'-phenyl-1,4-benzenediamine (called Antioxidant IP among other names). The IFD software indicates the masses used for matching as well as the actual and expected abundances of these masses.

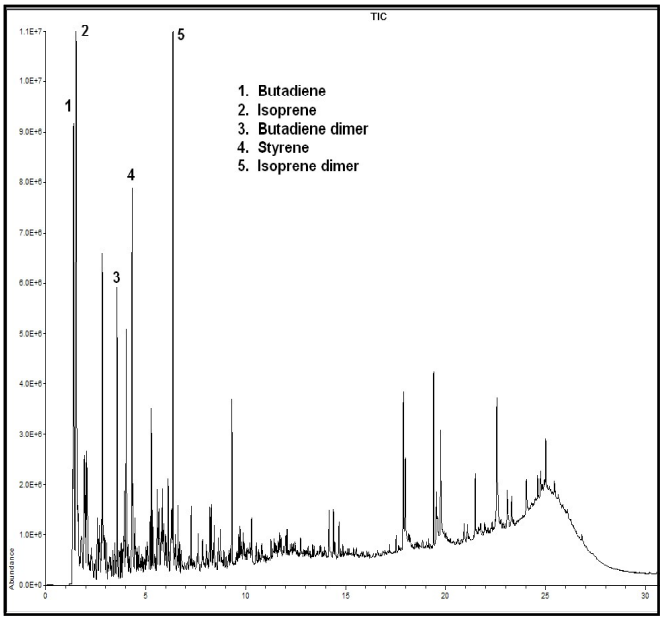

Figure 1. TIC of rubber pyrolyzed at 750°C.

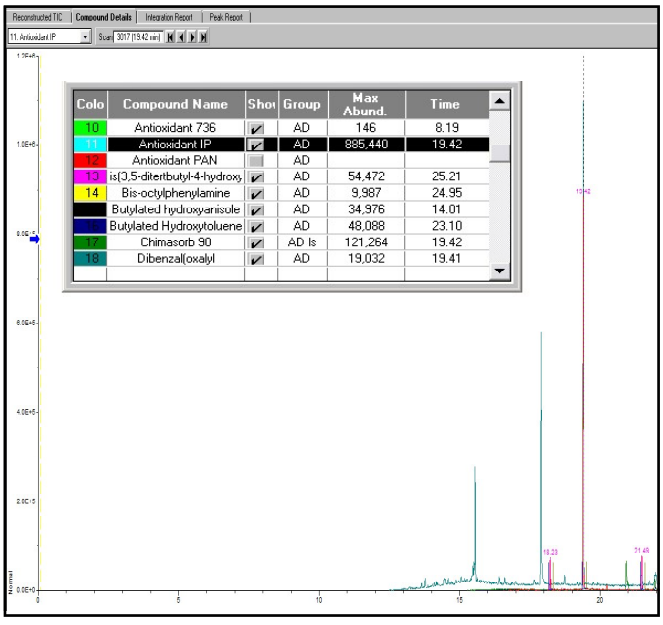

Figure 2. Search results for rubber, indicating Antioxidant IP at 19.42 minutes.

Equipment

These samples were analyzed using a CDS Model 5200 Pyroprobe, interfaced to an Agilent gas chromatograph/mass spectrometer.

Model 5200 Conditions

Valve Oven:	300°C
Transfer Line:	325°C
Temperature:	750°
Time:	10 seconds
Interface:	300°C
Interface time:	4 min

GC Conditions

Carrier:	Helium
Injector:	300°C
Split:	75:1
Column:	5% phenyl (30m X 0.25mm)
Detector:	Agilent MSD
Range:	35 - 550

GC Program:

Initial:	40°C for 2 minutes
Ramp:	10°C/min.
Final:	300°C

Deconvolution Software

Ion Signature
100-01 Quantitative Deconvolution Software

FOR MORE INFORMATION CONCERNING THIS APPLICATION, WE RECOMMEND THE FOLLOWING READING:

Determination of Polymer Additives using Analytical Pyrolysis, K. D. Jansson et al., J. Anal. Appl. Pyrolysis 79, (2007) 353-361.

Additional literature on this and related applications may be obtained by contacting your local CDS Analytical representative, or directly from CDS at the address below.

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