

CDSolutions

APPLICATIONS INFORMATION USING ADVANCED SAMPLE HANDLING TECHNOLOGY

Identifying Additives in Pyrograms using CDS Additive Library and AMDIS

Thermal analysis can be used to help analysts identify additives in manufactured polymers. Many times, additives desorb at sub pyrolysis temperatures, so the sample can first be heated to a lower temperature, like 300°C to release additives in a simple looking chromatogram containing just a few compounds. If a single-step pyrolysis is preferred, deconvolution software like AMDIS, equipped the CDS Additive library can be used. The CDS Additive Library is a database which contains, among others, flame retardants, plasticizers, antioxidants, and solvents.

Operation of AMDIS is relatively simple. After the additive library is loaded into the correct folder, it is selected in the software. A loaded pyrogram is analyzed against the library using the "Simple" analysis type. The program yields two types of results: component and target. Component results contain single components identified in the pyrogram. Target results are those components identified by the loaded library.

The target results display has a the total ion chromatogram, a profile of key ions in the discovered additive, an information list which contains all the identified additives, a comparison of the raw mass spectrum and the deconvoluted spectrum, and finally, a comparison of the deconvoluted spectrum and library match (Figure 2).

A flame retardant polycarbonate pyrolyzed at 700°C for 15 seconds, resulted in a very complex pyrogram (Figure 1). A good hit for Tribromophenol arises when searched against an additive library specific for flame retardants (Figure 2). This compound was completely buried in the valley of two peaks. AMDIS was able to deconvolute the spectrum, when a simple background subtraction would not (Figure 3). The CDS additives library contains over 400 additives. Coupled with AMDIS, the CDS Additives library can be a valuable screening tool for additives.

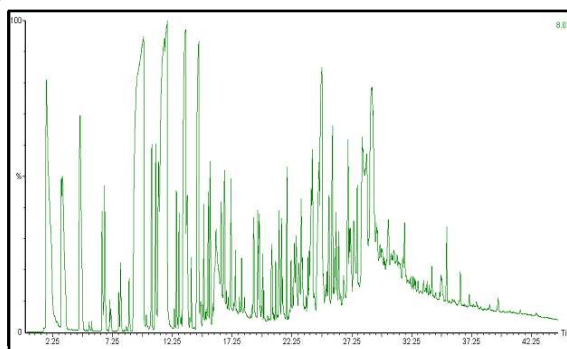


Figure 1: Pyrogram of Flame Resistant Polycarbonate.

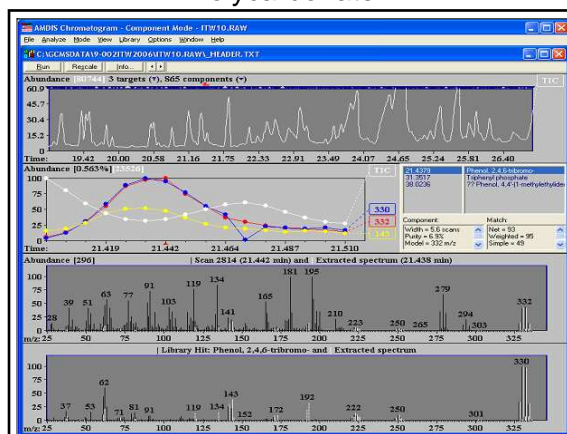


Figure 2: AMDIS Results Display.

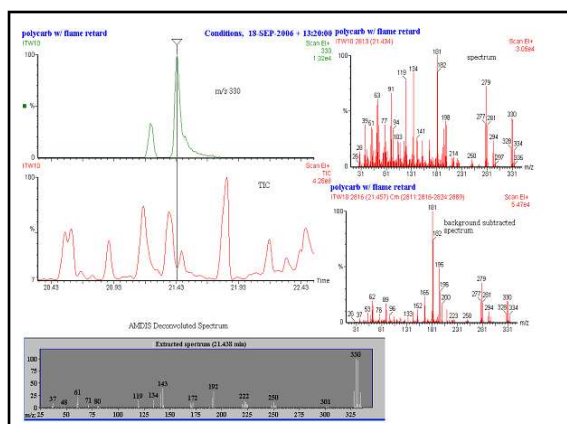


Figure 3: Deconvoluted spectrum found the flame retardant hidden in a valley.

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

To download AMDIS- go to the following link:

<http://www.amdis.net/index.html>

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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