Spectra Analysis

DiscovIR- GC™

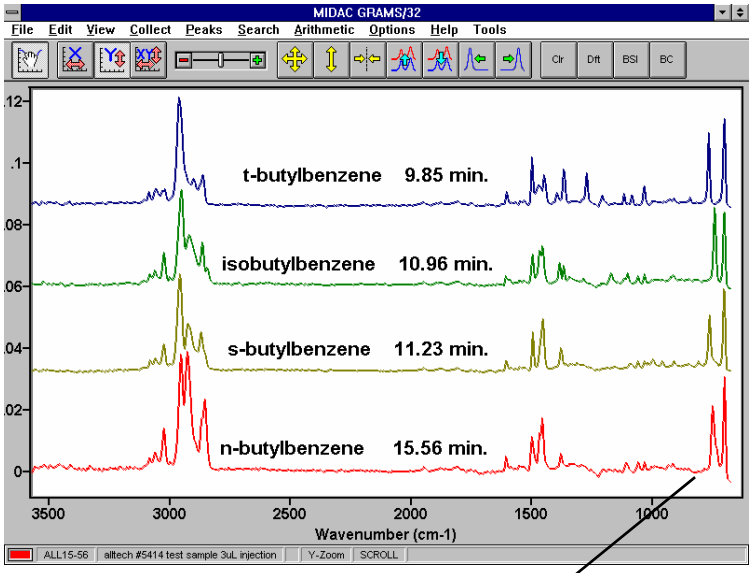
Deposition and Detection System

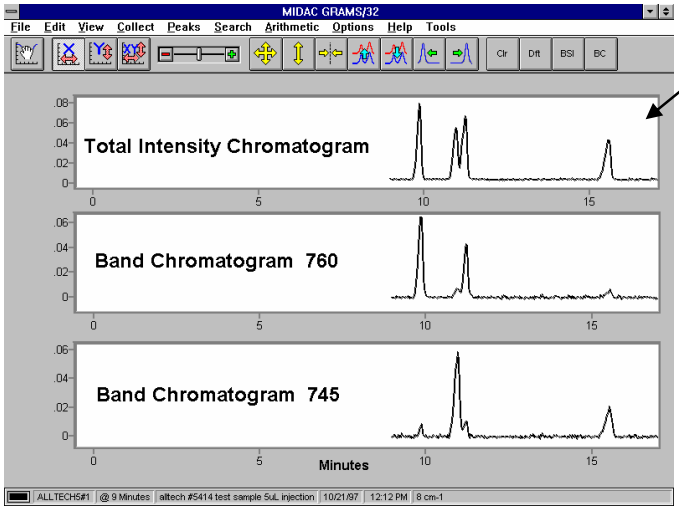
APPLICATION NOTE 001

Analysis of Butylbenzenes by GC-IR

Resolution of overlapping GC Peaks using Spectral Subtraction

Discriminating between Structural Isomers found in a chromatographic separation is often challenging using other detection methods. The DiscovIR-GC™ can define the functional groups preset in each component and help you nail down which isomer is which. And even if the peaks are not well-resolved, you can use the post-run analysis software features such as spectral subtraction to distinguish the isomers.

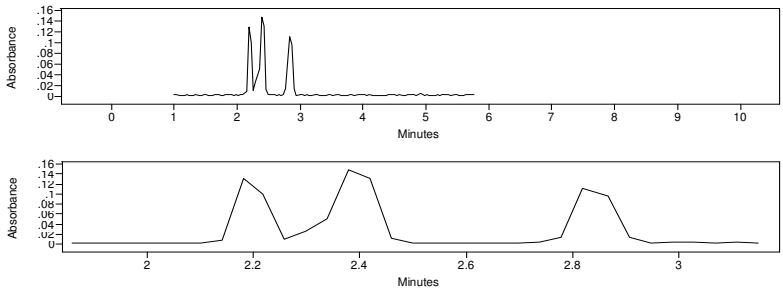




The temperature-programmed separation on the 20-meter column resolved the four isomers, giving clean spectra from the original data.

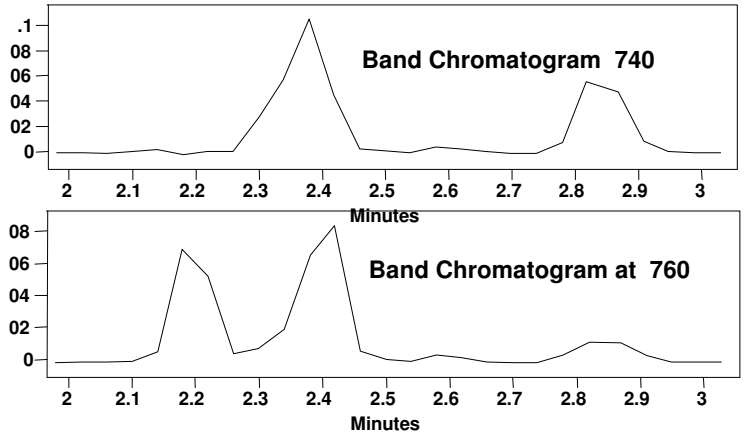
Sample Conditions:

Sample	Alltech 5414 Aromatic Hydrocarbon Mixture (equal portions of the 4 isomeric butyl benzenes)
Concentration	1 mg each component per mL hexane solvent
Injection:	1 - 3 *u*L using split/splitless injector, split 50:1
Column:	DB5, 20-meter x 0.32-mm ID, 0.25-*u*m film for normal separation 10-meter length used for demonstration of overlapping GC peaks
Conditions:	Helium carrier, 1 mL/min Temp program: 70^0 for 3 min, 6^0/min up to 200^0 for normal separation 110^0 Isothermal used for demonstration of overlapping GC peaks Injector, transfer line, restrictor tip all at 250^0 Sample window -100^0



Using the short column in an isothermal run, the isobutyl and the sec-butyl isomers merged into a severely overlapping GC peak, centered at 2.4 minutes.

Looking at the spectra near 750 cm^{-1} across the chromatogram between 2.25 and 2.5 minutes, we see a clean spectrum of the ***iso*** isomer at 2.34 minutes. All of the ***s***-butyl spectra in this time range are contaminated with the ***iso***-butyl isomer. We can obtain the clean spectrum of ***s***-butylbenzene shown on the next page by subtracting the spectrum at 2.34 minutes from that at 2.42.



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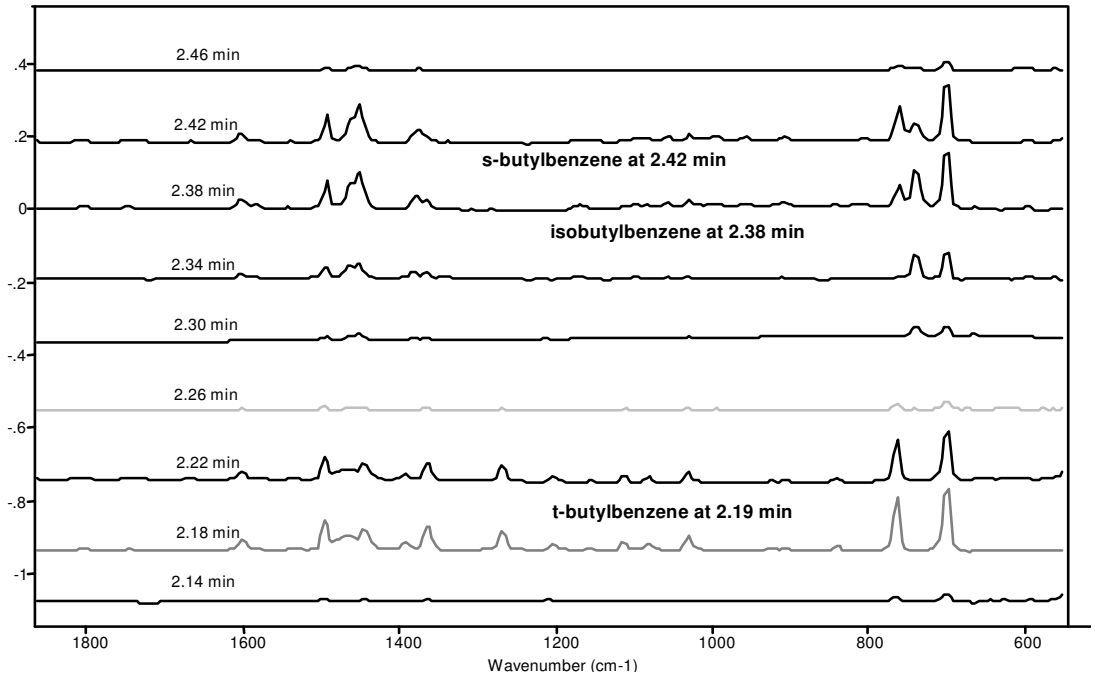
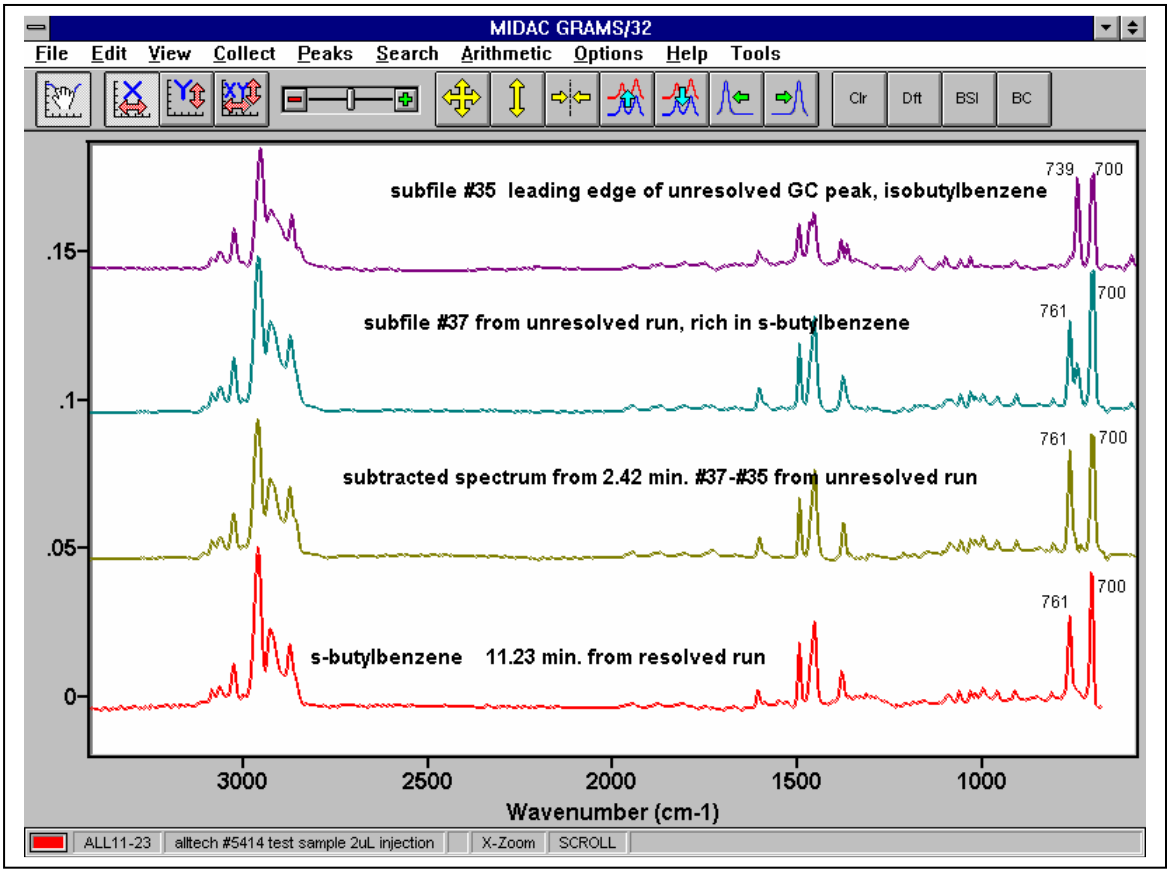


Traces of Iso-butylbenzene can be seen from from 2.26 through 2.5 minutes on this run, making both isomers difficult to identify.



By subtracting The top spectrum (#35) from the next one (#37), we can create a spectra that clearly matches that of s-butyl benzene from a fully-resolved run.

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