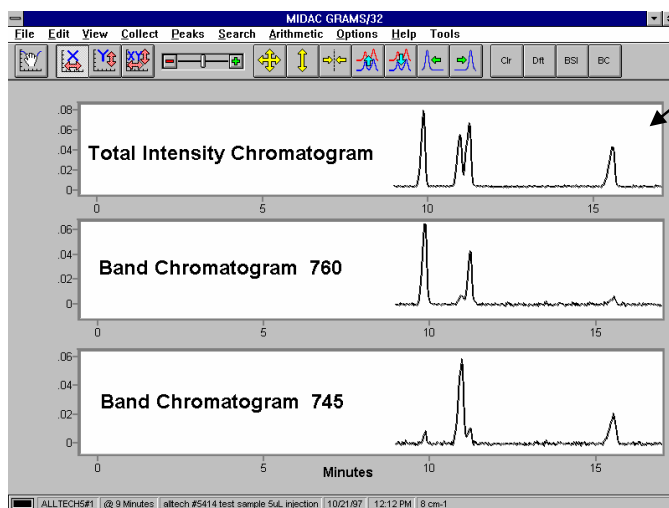
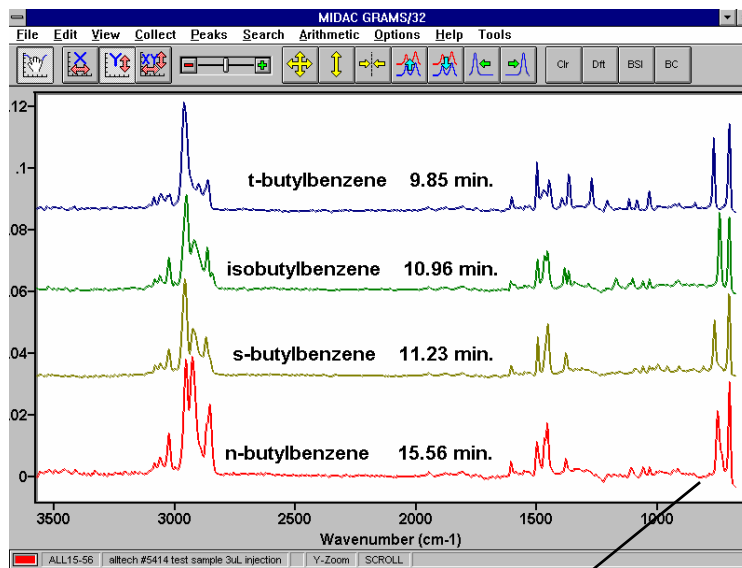


Analysis of Butylbenzenes by GC-IR Resolution of overlapping GC Peaks using Spectral Subtraction

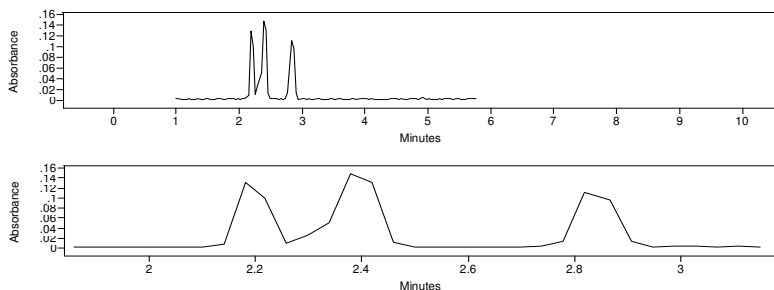
Discriminating between Structural Isomers found in a chromatographic separation is often challenging using other detection methods. The DiscovIR-GC™ can define the functional groups preset in each component and help you nail down which isomer is which. And even if the peaks are not well-resolved, you 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.

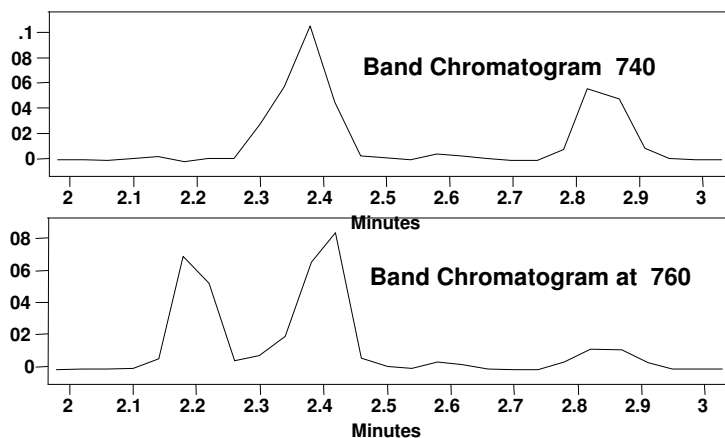
Sample Conditions:

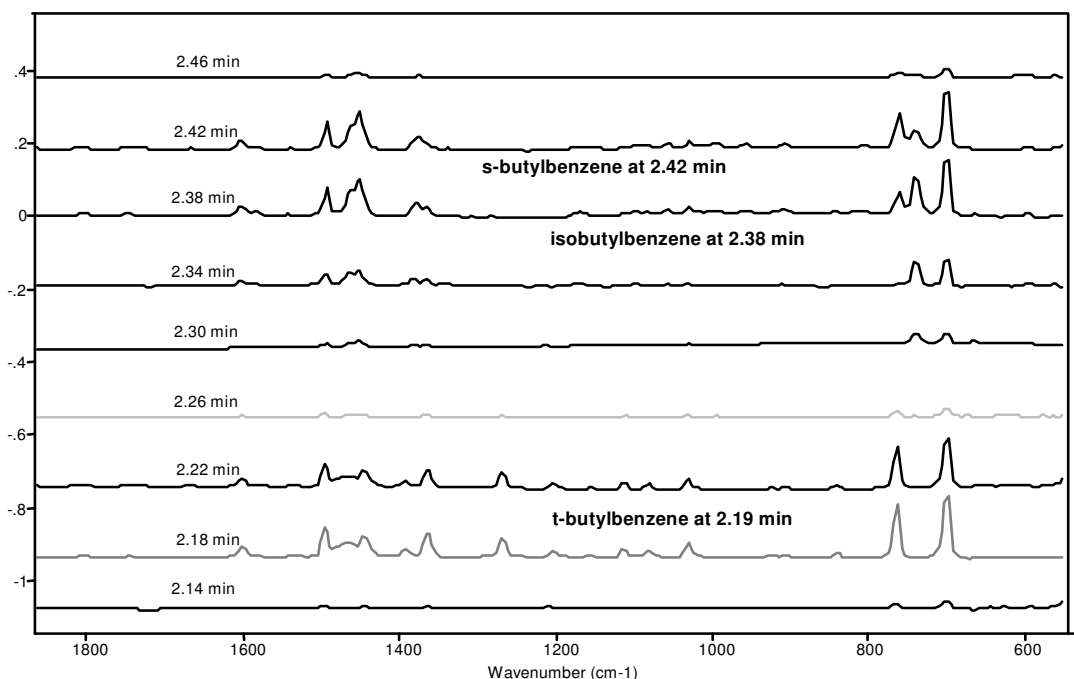
Sample Alltech 5414 Aromatic Hydrocarbon Mixture
 (equal portions of the 4 isomeric butyl benzenes)
Concentration 1 mg each component per mL hexane solvent
Injection: 1 - 3 μ L using split/splitless injector, split 50:1
Column: DB5, 20-meter x 0.32-mm ID, 0.25- μ m film for normal separation
 10-meter length used for demonstration of overlapping GC peaks
Conditions: Helium carrier, 1 mL/min
 Temp program: 70⁰ for 3 min, 6⁰/min up to 200⁰ for normal separation
 110⁰ Isothermal used for demonstration of overlapping GC peaks
 Injector, transfer line, restrictor tip all at 250⁰
 Sample window -100⁰



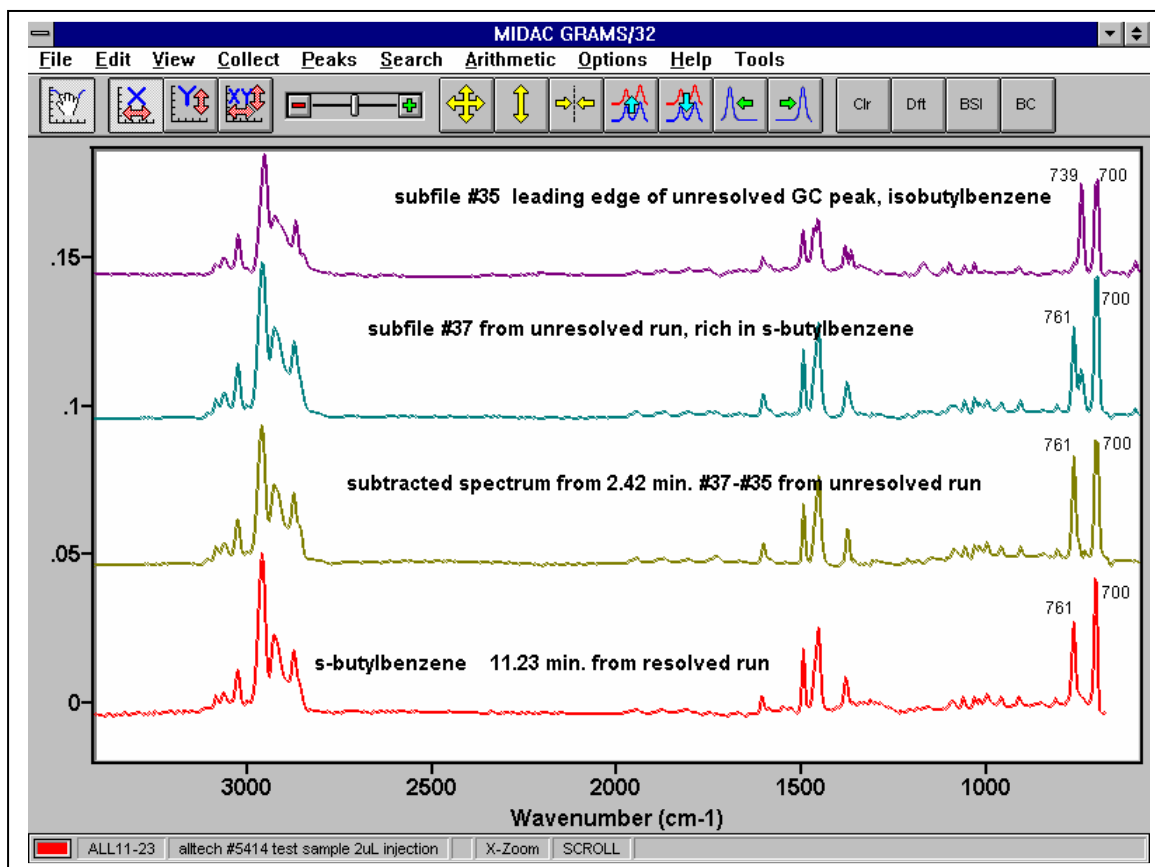
Using the short column in an isothermal run, the isobutyl and the sec-butyl isomers merged into a severely overlapping GC peak, centered at 2.4 minutes.

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.





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.