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Chemical Identification: Infrared Spectroscopy (FTIR)

Infrared (IR) spectroscopy is an experimental technique that is used to obtain information about the structure of molecules. Molecules absorb infrared light at frequencies that match the energy of molecular vibrations. Infrared spectroscopy is therefore often called vibrational spectroscopy. This absorption of light can be very useful because similar functional groups, such as O-H bonds, C=O bonds and N-H bonds will often absorb infrared light in a small range of frequencies regardless of other structural features. That means all compounds containing carbonyl groups will show absorptions in a small range of frequencies in an infrared spectrum.

Fourier transform infrared (FTIR) spectroscopy is a powerful analytical tool for characterising and identifying organic molecules. Using the IR spectrum, chemical bonds and the molecular structure of organic compounds can be identified.

Within Resolve, we offer a wide range of FT-IR techniques including:

- microscopy
- attenuated total reflectance (ATR)
- imaging technology
- time resolved measurement for kinetic studies (spectra frequency > 60/s).

Specimens that are unusable for transmission measurements (for example black materials) can usually be analyzed by the ATR technique.

What can we do for you?

For elastomers, FTIR spectroscopy is a fast, non-destructive technique that can be used to chemically characterise an organic sample, such as parts, foils, coatings (down to 3-5 µm), contaminations, deposits, powders etc. We use a large database containing 250,000 FTIR spectra to precisely identify the FTIR functional groups.

Typical applications for elastomers are:

- quantitative determination of the monomer content
- quantitative analysis of the amount of Maleic acid anhydride
- analysis of blooming
- identification of surface conternimations (discolerations).

FTIR also provides very useful information for analyzing samples from competitors, including:

- polymer type (type of rubber: SBR, isoprene rubber, ethylene propylene diene rubber (EPDM and NBR)
- filler type (chalk, clay, talcum).

Analysis of chemical distribution and reaction monitoring can be performed as well. FTIR spectroscopy can be applied to a variety of chemical businesses.

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Sample size

The typical amount of sample required is 10 to 100 mg. For the quantitative analysis (FTIR transmission measurement) of the monomer composition of EPDM, 1-2 grams of sample is needed. With FTIR, measurements can also be performed on very small particles and inclusions using an IR microscope. The spot size can be down to 5 µm. This analysis can performed on a compound or profile.

Quantitative analysis of the monomer composition of EPDM

A method has been developed to quantitatively analyse EPDM on it's monomer composition. From the sample, a thin film is pressed and this film is analysed in transmission mode. An example of the determination of the monomer (C2/C3 and diene) in Keltan 5508 grade is shown in the table below.

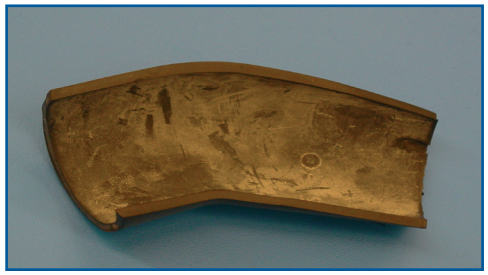
No	Description	% C2	% C3	% C9 ENB
1	EPDM K5508	69.8	26.3	4.51

Table 1: Monomer composition of EPDM K5508 (typical values).

Identification of blooming on a compound

Figure 1 shows visible blooming on the surface of a profile. The FTIR-ATR crystal was placed on the surface and an FTIR spectrum was recorded at a penetration depth of 1-3 µm to obtain chemical information about the blooming.

Figure 1: blooming on the surface of a profile.



The FTIR spectrum measured at the surface was identified as talcum. See Figure 2.

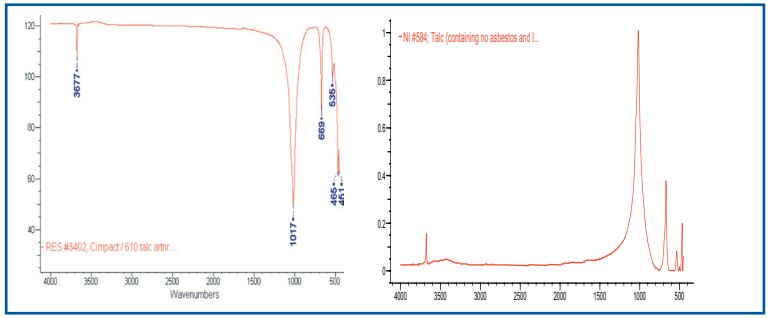
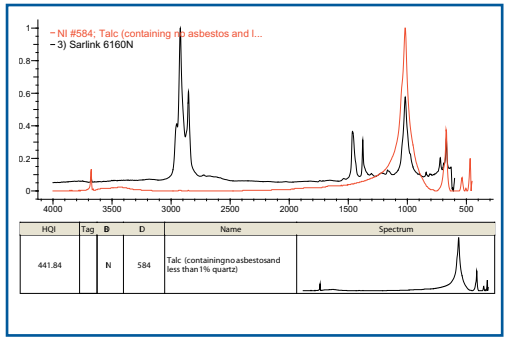


Figure 2: FTIR spectrum (left) of the blooming on the surface of a profile compared with a spectrum of talcum from the FTIR library (right).

Identification of the filler in a Thermo Plastic Vulcanisate (TPV)

An FTIR spectrum in a TPV was recorded and looked up in the FTIR library. The filler in the compound was identified as talcum. See Figure 3.

Figure 3: FTIR spectrum of a TPV (black spectrum). In addition to the EPDM, Polypropylene (PP) and talcum (red spectrum) were also identified after a search using our database.



Stretch your thinking in polymers

We think about polymers differently because we understand the complete spectrum of polymers - from research and development to production and end of life disposal. Credit our decades of experience in materials analysis and processing, chemical engineering and safety testing, as well as product enhancement and polymer recycling issues. We can help you think beyond the way you're currently producing polymers.

DSM RESOLVE R&D SOLUTIONS

In cooperation with Lanxess Elastomers LANXESS Energizing Chemistry