Product Note S39 - 10/14

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BRUKER FM ATR Library

As far as we can judge currently no accordant commercial IR libraries are available. Therefore we have set a smart new Bruker MIR-FIR library up consisting of almost 100 different substances. This includes spectra of pure polymers, powdered fillers and composite polymeric materials. The spectral region of all entries ranges from 30 to 4000 cm^{-1}, which allows a complete overview of the molecular and lattice vibrations of all entries. Spectra of the inorganic powder compounds, corrected with the advanced ATR correction algorithm of the OPUS FTIR Software, are also included which allows their identification in the polymeric matrix.[1]

All spectra were measured using the unique Bruker FM wide spectral range MIR-FIR optical components (for details see Bruker FM application note AN118 and AN123) with a spectral resolution of 4 cm^{-1} and zero filling factor 2 which means 2 cm^{-1} digital resolution. For improved spectroscopic library data in the far infrared region a water cooled Hg arc lamp was used for a second set of measurements. The library data contains spectra merged of a mid-infrared spectrum using the internal standard source (4000-50 cm^{-1}) and of a far infrared section of a spectrum using the Hg arc lamp (680-30 cm^{-1}).

The spectra are augmented with the following data (as far as available): Compound name, measurement method, condition, comments, CAS registry number, molecular formula, molecular weight.

The Spectrum Search functionality in OPUS offers a broad toolbox for the identification of the measured substances. For a search example only the pure substances in the library were used as reference. Whereas the polymeric host material can be easily identified with the standard settings the identification of the filler requires more fine tuning of the search options strongly depending on the filler content. However, the identification of a two component system is possible for filler contents above a few percent. Identification of smaller amounts of filler materials requires limiting the region of the search to the FIR limits, the use of an difference spectrum or an existing peak table. In Figure 1 the search function is shown exemplarily for a Styrene Butadiene copolymer (SB) filled with two percent of calcium carbonate. The search function offers the identification of the polymer matrix and the filler material depending on the selected search region.

Spectrum Search

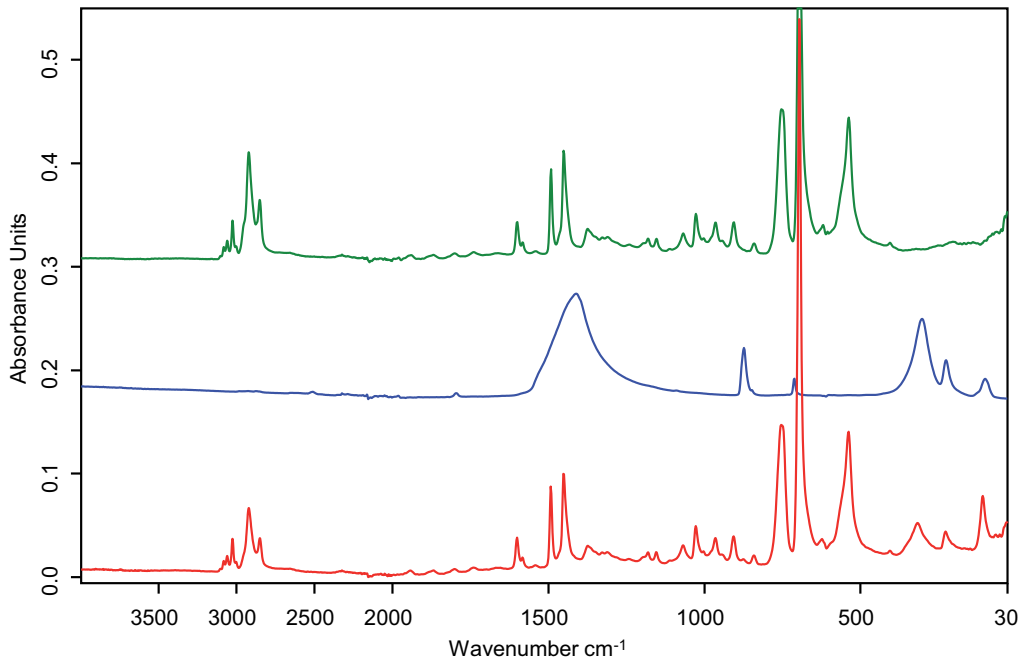

Figure 1: Spectrum search with a sample of Styrene Butadiene copolymer (SB) containing two percent of calcium carbonate. Displayed are the results of a spectrum search with the file limits or the FIR limits.

Search with file limits (4000 -30 cm^{-1}):

Color	Hit Quality	Compound Name	CAS Number	Molecular Formula	Molecular weight
	869	SB	9003-55-8	(C8H8-C4H6)n	

Search with FIR limits (600 -30 cm^{-1}):

Color	Hit Quality	Compound Name	CAS Number	Molecular Formula	Molecular weight
	745	Calcium carbonate	471-34-1	CaCO3	100.9

Color	File
	SB with 2pct calcium carbonate.0

Compound Name	Calcium carbonate
Molecular Formula	CaCO3
Molecular Weight	100.09
CAS Registry Number	471-34-1
Sample Preparation	ATR
Substanzname	Calciumcarbonat
Details	Diamond ATR, corrected
Condition	powder
Entry No.	17
Library name	Bruker FM ATR.S01

Compound classes

- Pure polymer matrices
- Filler materials
- Filled polymer composites

Characteristics

- Full FIR-MIR spectra, spectral range 4000-30 cm^{-1}
- Compound information (see text)
- Single crystal ATR technique

References

[1] Advanced ATR-Transformation, Koichi Nishikida, N & K Spectroscopy, LLC, Honorary Associate/Fellow, Materials Science and Engineering, University of Wisconsin