



## Application Note AN M118

# BRUKER FM: Far and Mid IR Spectral Range Spectroscopy in One Step

### Introduction

The measurement spectral ranges of FTIR spectrometers are defined by their major optical components which are the source, beamsplitter and detector. For modern research FTIR spectrometers software controlled switching of the sources and detectors is available as standard functionality. The bottleneck was the need of an automated beamsplitter changer. Due to the high development costs and technological demand for an automatic beamsplitter changer it was not available for FTIR spectrometers for a long period of time. In 2010 Bruker introduced a 4 position automatic beamsplitter changer BMS-c which works under vacuum condition for its high-end research bench-top FTIR spectrometer VERTEX 80v providing unmatched performance [Ref. 1 and 2].

As a new and unique as well as a cost effective complement to the automatic beamsplitter changer of the VERTEX 80v Bruker has introduced the ultra-wide range mid and far IR beamsplitter (T240/3) for the VERTEX 70v FTIR spectrometers.

By the implementation of this ultra-wide range beamsplitter for the first time it became possible to acquire spectral data in the complete IR spectral range from  $6000\text{cm}^{-1}$  to  $10\text{cm}^{-1}$  with one beamsplitter only [Ref. 3]. There is no longer any

Keywords	Instrumentation and Software
FT-IR, far IR, FIR	INVENIO, VERTEX, OPUS
inorganics	Platinum ATR
filler material	FT-IR beamsplitter and detector
active agent	W240(-T)/x
polymorphism	D201/xD
crystallinity	T240/x



Fig. 1: The next generation intelligent INVENIO R FTIR R&D spectrometer as a VERTEX 70 successor featuring MultiTect™ detector technology, traditional DigiTect™ detector slot and the well-proven RockSolid permanently aligned interferometer, which are fully compatible with the BRUKER FM functionality.

need to open the spectrometers optics bench for manual BMS exchange nor to use a sophisticated automatic beam-splitter changer.

In addition Bruker has then announced the new ultra-wide range room temperature DLaTGS detector which is useable in the spectral range from 12,000 $\text{cm}^{-1}$  to 20 $\text{cm}^{-1}$  [Ref. 4]. These new wide range infrared components together with the internal or external IR source are the basis for the unique BRUKER FM far and mid IR technology. BRUKER FM makes FTIR spectroscopy in the complete IR spectral range extremely easy and efficient because it allows the measurement of a single spectrum from above 6,000 $\text{cm}^{-1}$  to 50 $\text{cm}^{-1}$  in one single measurement.

In 2018 Bruker launched the next generation smart FTIR R&D spectrometer INVENIO R to replace the successful VERTEX 70 entry-level research spectrometer. INVENIO R is fully compatible with the BRUKER FM technology (Fig.1).

### Benefits of BRUKER FM

BRUKER FM option for the INVENIO R purge and VERTEX 70v vacuum R&D spectrometers makes an old dream of FTIR spectroscopists a reality: covering the complete mid and far IR spectral range in one measurement step without any gap and no need to exchange any spectrometer optical components. The additional values of the BRUKER FM technology are obvious and listed in the table below.

The spectra of the powder samples ascorbic acid and calcium

#### Additional values of BRUKER FM functionality

- Full mid and far IR spectrum in one go
- Enormous time saving due to just one single measurement
- Acquisition of the complete molecular vibrational spectral information
- No break of purge or vacuum conditions for optical component exchange
- No danger of touching and breakage of expensive and sensitive optical components
- No need for demanding robot like exchange device
- All optical components are insensitive to humidity

carbonate shown in fig. 2 and 3 have been measured in one go and no gap using the single crystal Platinum diamond ATR unit, the VERTEX 70v vacuum optics bench equipped with the standard internal source and the new and unique ultra-wide range BRUKER FM components.

In figure 4 measurement results acquired with the INVE-

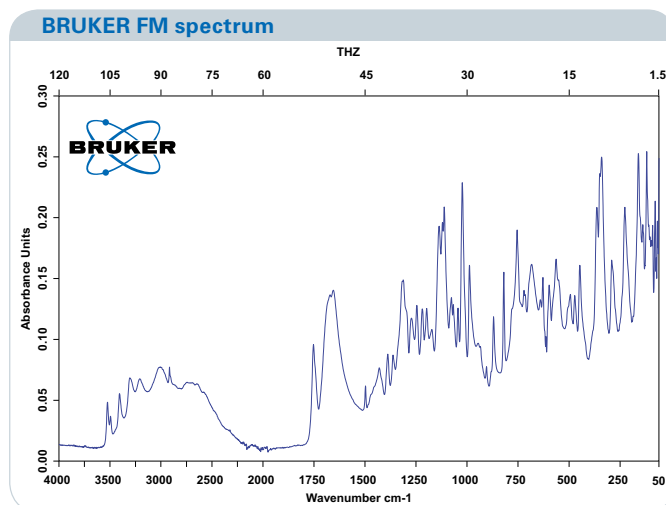


Fig. 2: Active agent ascorbic acid measured with VERTEX 70v vacuum FTIR, Platinum Diamond ATR, standard internal IR source and the new ultra-wide range BRUKER FM optical components from 4000  $\text{cm}^{-1}$  to 50  $\text{cm}^{-1}$  in a one-step measurement without any gap.

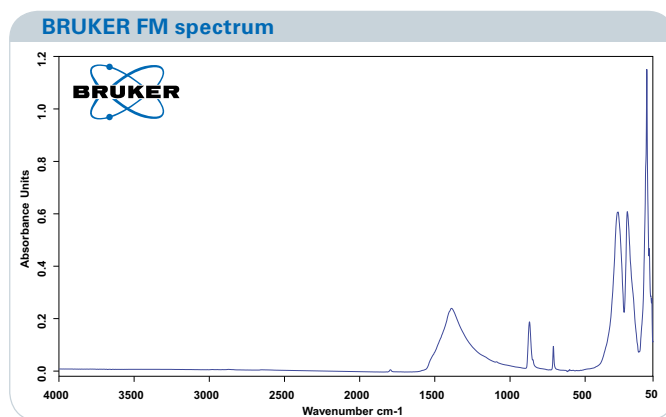


Fig. 3: Polymer filler material Calcite (calcium carbonate,  $\text{CaCO}_3$ ) powder measured with VERTEX 70v vacuum FT-IR spectrometer, Platinum Diamond ATR and BRUKER FM technology in one go.

NIO R and BRUKER FM far and mid IR functionality re shown. The spectra demonstrate clearly the additional value of the far IR spectral range beyond 400 $\text{cm}^{-1}$ . In the mid IR region the two measured ABS polymer samples could not be distinguished. Only in the far IR region around 250 $\text{cm}^{-1}$  the characteristic bands of the filler material  $\text{CaCO}_3$  in one of the samples could be identified.

It should be noted that for high quality spectra in the far IR spectral range below 400 $\text{cm}^{-1}$  purge of the optics bench with dry air (dew point lower than  $-50^\circ\text{C}$ ) or dry nitrogen is mandatory. Technical nitrogen is definitely not useful

because its H<sub>2</sub>O vapor content is too high. The purge flow needs to be adjusted according to the numbers listed in the instruments document "Installation Requirements". For sure it is obvious and should not be necessary to mention that the best far IR spectra quality will be achieved by using a VERTEX vacuum optics bench. Details regarding the vacuum advantages will be found in Ref. 5.

### Product configuration

BRUKER FM is available as the packages W240(-T)/IRD(S) for the INVENIO R down to 80 cm<sup>-1</sup> and as W240/BDV for the vacuum VERTEX 70v achieving to 50 cm<sup>-1</sup>. In order to

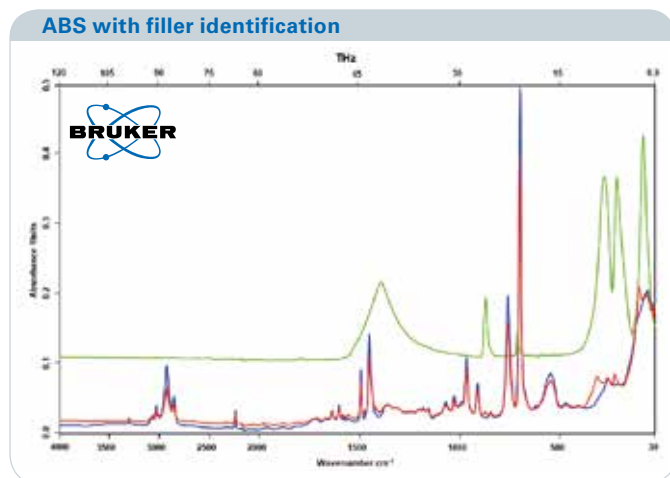


Fig. 4: BRUKER FM spectra of two ABS polymer samples measured with an INVENIO R spectrometer equipped with Platinum Diamond ATR and internal standard source. The spectral resolution was set to 4 cm<sup>-1</sup> and the measurement time around 50 sec.

Blue curve: ABS polymer sample without Calcite filler material (CaCO<sub>3</sub>); Red curve: ABS polymer sample with Calcite; Green curve: Pure CaCO<sub>3</sub> powder spectrum (off-set and compressed) for comparison.

### References

- [1] Bruker Product Note M128-02/11: Automatic beamsplitter exchange unit for VERTEX 80v FT-IR
- [2] A. Simon, G. Zachmann / Vibrational Spectroscopy 60 (2012) 98–101
- [3] Product Note M143-03/13 : T240/3 Ultra-Wide Range Beamsplitter
- [4] Product Note D201/BD: Wide range MIR-FIR DTGS Detector
- [5] Product Note PN\_T18\_Vacuum Advantage

improve the signal to noise ratio in the spectral range below 100 cm<sup>-1</sup> the externally adapted water cooled mercury arc lamp is available.

The wide range room temperature (RT) DLaTGS detector D201/BD is available for all the INVENIO and VERTEX series spectrometers means VERTEX 80-80v as well. In principle it is usable in the spectral range from ca. 12,000 cm<sup>-1</sup> in the near IR down to 20 cm<sup>-1</sup> (500 μm wavelength) in the far IR/THz spectral range. It has to be noted that the covered spectral range is defined by the interplay with the combined optical components namely the sources and beamsplitters [Ref. 4].

### Importance of BRUKER FM for vibrational spectroscopy

- Inorganic and organometallic chemistry
- Semiconductor development and research
- Studies on polymer filler material and color pigments
- Geological and rock analysis
- Pharmaceutical fillers and active agent measurements as well as polymorphs differentiation
- Crystallinity investigations
- Product and material comparison
- Low temperature matrix isolation spectroscopy

### Conclusion

The innovative and unique BRUKER FM technology extends the VERTEX 70v and INVENIO R FTIR spectrometers to the far IR and THz spectral range in an easy and efficient way. No exchange of optical components is required and the complete mid and far IR spectral range is accessible in one go without any gap. No manual or automated components exchange is necessary. That BRUKER FM technology offers new opportunities for molecular vibrational spectroscopy in the areas of pharmaceutical, inorganics and polymorphs analysis. In the table above example areas of application are listed.

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#### ● Bruker Optik GmbH

Ettlingen · Deutschland  
Phone +49 (7243) 504-2000  
Fax +49 (7243) 504-2050  
info.bopt.de@bruker.com

#### Bruker Optics Inc.

Billerica, MA · USA  
Phone +1 (978) 439-9899  
Fax +1 (978) 663-9177  
info.bopt.us@bruker.com

#### Bruker Shanghai Ltd.

Shanghai · China  
Phone +86 21 51720-890  
Fax +86 21 51720-899  
info.bopt.cn@bruker.com

[www.bruker.com/optics](http://www.bruker.com/optics)

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