

Product Note M187 - 12/19

6 Questions about Spectral Resolution in FTIR Spectroscopy



Many manufacturers often specify their devices on the edge of the possible. This is not always sensible and is mostly done to impress customers. **We'd like to create awareness for this.**

We firmly believe that an educated and satisfied customer is our biggest success. Decisions backed by facts, knowledge and understanding will save everyone time and money.

About this document

It is widely believed that the quality of an FTIR spectrometer is defined by only a few parameters such as spectral resolution, signal-to-noise ratio or wavenumber precision and accuracy. The general notion: the "better" the spectral specifications, the better the spectrometer's performance.

But is this really the case?

In this product note we would like to clear up long-standing misconceptions and respond to **your** questions and concerns regarding the specifications of FTIR spectrometers, in particular spectral resolution.

****In the context of this product note we always refer to spectral resolution if the term resolution is used.***

Summary

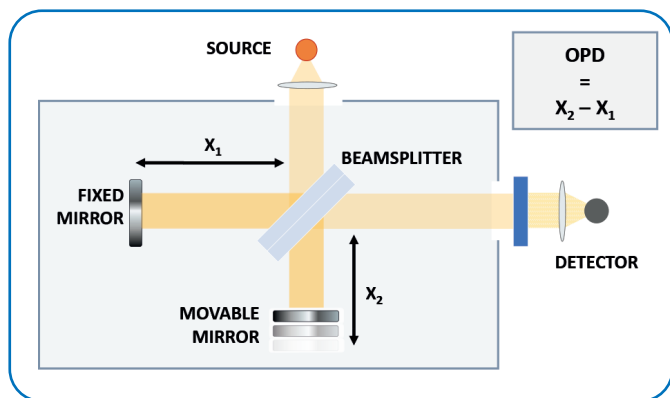
- Spectral resolution describes a spectrometer's ability to separate two spectral lines
- Change of resolution affects signal to noise ratio
- Increasing resolution increases measurement time
- Optimal resolution for solids and liquids: **4 cm⁻¹**
- Standard resolution for most gas applications: **1 cm⁻¹**

1. What is spectral resolution?

The resolution* of an spectrometer can be considered as the ability to separate two spectral lines that are very close in wavelength or frequency. Usually, spectral resolution is given in wavenumbers (cm⁻¹).

The closer the two lines, the higher the resolving power required to separate them.^[1] If the wavenumbers of two lines differ by 2 cm⁻¹, a higher spectral resolution (e.g. 1 cm⁻¹) must be selected to distinguish both spectral features.

The proximity of different lines mainly depends on the chemical and physical properties of the sample. Therefore, it is important to carefully select suitable parameters for the best possible results.



2. How is the spectral resolution determined?

The schematic representation of a Michelson interferometer is shown above. The optical path difference (OPD) between the stationary and moving mirror determines the spectral resolution in an FTIR spectrometer.

3. How can spectral resolution be improved?

A larger OPD will increase the amount of interference at the beam splitter, enabling higher resolving power of the interferometer.

Simply put, the larger the OPD, the higher the resolution.

It must be mentioned that in order to profit from high resolutions an aperture must be set. As a result, IR throughput decreases and S/N ratio suffers. This can be compensated by longer measuring times or even using a liquid N₂ cooled detector.

4. Will increasing resolution affect other parameters?

Yes. With an increased OPD, the moving mirror in the interferometer must travel a longer distance to perform a single scan. Since the noise level in a spectrum is directly proportional to the applied spectral resolution, this will inevitably lead to a lower S/N ratio, as less scans can be recorded within a defined time.

5. Must resolution be set according to sample type?

Yes, definitely. Measuring solids and liquids at a high resolution of 0.5 cm⁻¹ will not get you better results than at e.g. 2 cm⁻¹. Instead, this causes a loss in sensitivity and an increase in measurement time.

As the **natural width** of spectral bands in solids and liquids are **in the order of several wavenumbers**, measurements at high resolutions are ineffective.

The next example will further illustrate this point.

Example #1: FTIR spectroscopy of solids and liquids

Figure 1 shows the spectra of solid polyethylene (PE) and liquid isopropanol. Spectra were collected with a resolution ranging from 8 cm⁻¹ to 0.5 cm⁻¹. The spectral resemblance between the respective resolutions is so close, that virtually no difference can be spotted.

Therefore, it can be safely concluded that a resolution of better than 4 cm⁻¹ is **not** necessary if your only requirement is a reliable identification of raw materials.

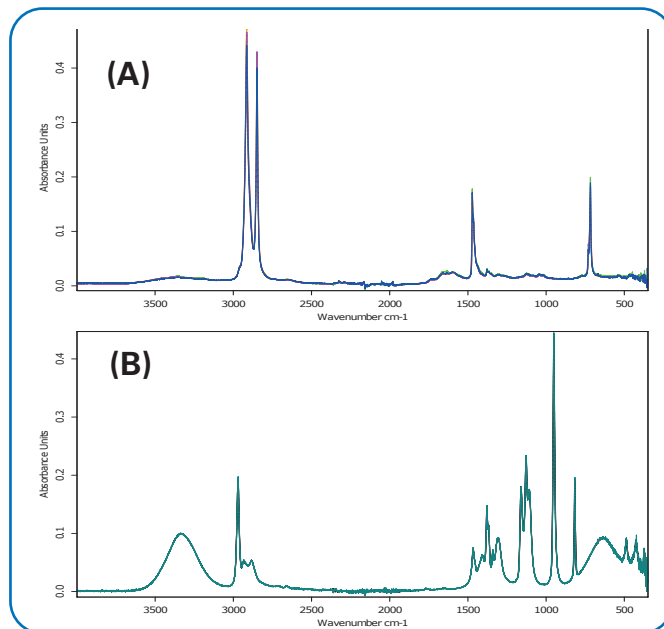


Figure 1: Although looking like a single spectrum, **A** (PE) and **B** (2-propanol) are comprised of 5 spectra recorded at 8 cm⁻¹, 4 cm⁻¹, 2 cm⁻¹, 1 cm⁻¹ and 0.5 cm⁻¹.

This changes for some specific scenarios. Although PE is easily identified at 4 cm⁻¹, it is also a good example when a slightly increased resolution is needed. In PE, the band at 731 cm⁻¹ is indicative of crystallinity. Since this band is only resolved at 2 cm⁻¹ the resolution must be set accordingly (see Figure 2).

However, resolutions better than 2 cm⁻¹ have no additional value to analysis of solids or liquids and should be avoided to retain optimal S/N ratio and measurement times.

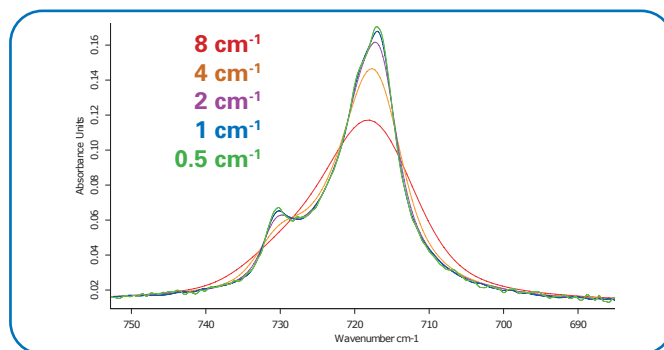


Figure 2: Close up of the band at 731 cm⁻¹. With increasing spectral resolution the band starts to appear at 2 cm⁻¹.

6. Does gas analysis profit from higher resolution?

Molecules in the gas phase do not experience a 'crowded' environment as if they were solids or liquids. This allows the molecules to stretch and rotate more freely without being influenced by intermolecular bonds, interactions or crystal effects.

As these rotations are also excited by infrared light, they can and will be detected by FTIR spectroscopy. Depending on selection rules, stretches and rotations are split in P-, Q- and R-branches. This exclusively applies to gases, as in solids and liquids, these individual rotational states cannot be excited.

As rotational bands are often in close proximity in regards to wavenumber, they can only be distinguished if the measurement is performed at higher resolutions.

Example #2: FTIR measurements of gases

Figure 3 shows the spectra of methane at different resolutions ranging from 8 cm^{-1} and 0.5 cm^{-1} . The absorption at about 3016 cm^{-1} corresponds to the Q-branch of the stretching vibration mode of methane.

Although it is not mandatory to resolve rotational bands, they can be of high interest for research purposes or the analysis of complex gas mixtures.

For identification and quantification purposes, a moderately high spectral resolution of 1 cm^{-1} is recommended, as it combines a well-defined resolution of substance specific bands with a high sensitivity.

Conclusion #1: choosing the appropriate resolution

With this information you are able to select the optimal spectral resolution for your experiment. We give the following recommendation on resolution:

- 4 cm^{-1} for standard solid and liquid samples in material verification, identification and QA / QC
- 2 cm^{-1} to resolve all vibrational bands of a solid or liquid sample. This will increase measurement time if you desire the same S/N ratio
- 1 cm^{-1} for most standard gas applications. Higher spectral resolutions may be required to fully characterize gas mixtures as well as in fundamental research

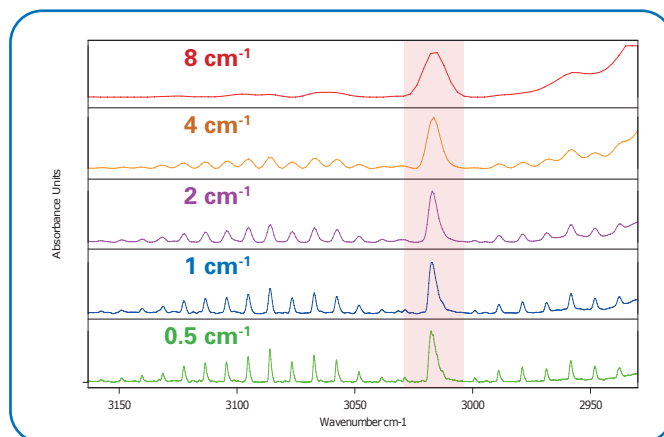


Figure 3: Spectra of methane gas (30s, absorbance). At 1 cm^{-1} the rotational bands are fully resolved.

Conclusion #2: choosing the appropriate instrument

Bruker supplies FTIR spectrometers ranging from basic routine devices to high-resolution research grade instruments. Depending on the customer's requirements each spectrometer has an ideal use case:

- **ALPHA II** offers up to 0.75 cm^{-1} resolution which covers almost all industrial routine applications
- Advanced spectrometers like the **INVENIO** offer high resolutions of up to 0.085 cm^{-1} (**VERTEX** up to 0.06 cm^{-1})
- For the most challenging gas analysis, Bruker offers the world's highest resolving FTIR spectrometer **IFS125HR** with an spectral resolution of 0.0009 cm^{-1}

References

- [1] Chalmers, J. M., Griffiths, P. R., eds. (2002). Handbook of Vibrational Spectroscopy. John Wiley & Sons Ltd.