SHIMADZU
Excellence in Science

Effect of Resolution on FTIR Spectra – A Teaching Laboratory Exercise

Synopsis:

This teaching experiment aims to explore how varying the resolution of Fourier Transform Infrared (FTIR) spectroscopy affects the quality and interpretability of spectral data. Students will engage in a hands-on investigation, using FTIR instruments to collect spectra of a known sample at different resolutions.

Objectives:

1. To understand the principles of FTIR spectroscopy and the role of resolution in spectral analysis.
2. To examine how changes in resolution impact the clarity, peak identification, and overall quality of FTIR spectra.
3. To develop skills in data collection, analysis, and interpretation in the context of vibrational spectroscopy.

Instrument and measurement conditions:

In this experiment, the IRSpirit with the QATR-S accessory (shown in Fig. 1) is recommended for analysis. The measurement conditions are listed in Table 1.

Fig. 1 IRSpirit with QATR-S

Table 1 Measurement Conditions

Instrument	: IRSpirit QATR-S (Diamond Puck)
Resolution	: 4cm^{-1}
No. of Scans	: 45
Apodization Function	: Happ-Genzel
Wavenumber Range	: 4000-400cm^{-1}

Sample preparation:

Sample Selection: A suitable sample (e.g., a common organic compound like ethanol or paracetamol) will be chosen for its distinct absorption features.

Operating procedure:

1. Open *Spectrum* from *LabSolutions™ IR.*
2. Connect the IRSpirit to *Spectrum* using the [Instrument] Drop Down menu, clicking [Connect].
3. Set method parameters as per *Table 1.*
4. Insert your file name and sample name in the sample labelling section.

5. Select BKG Scan ensuring nothing is on the crystal.
6. Once completed, add a small amount of sample to cover the crystal and clamp the sample in place.
7. Select [Sample Scan] to produce a spectrum.
8. Remove the sample and clean the ATR crystal with IPA
9. Repeat steps 3-7 but vary the resolution of the subsequent scans
10. Once all resolutions have been tested, print the spectra.

Questions and discussions:

1) What change was observed in the spectrum as the resolutions was lowered (16 cm^{-1} -> 0.9 cm^{-1})?
2) When and how would a higher resolution (e.g. 0.9 cm^{-1}) be beneficial for analysis?

Expected outcomes:

By the end of this experiment, students will have a deeper understanding of how resolutions affect the final spectrum in FTIR spectroscopy and when it can be applied to different sample types. They will develop critical thinking and analytical skills and gain an appreciation of the complexities and considerations involved in FTIR spectroscopy. This experiment aims to highlight the relevance of FTIR in various fields form the pharmaceutical industry, gas generation and materials science.