Infrared Spectroscopy In Gemstone Testing

As technology marches forward so have techniques in the synthesis and treating of gemstones.

Knowing how to identify, gemstones and treatments is of paramount importance to gemmologists and valuers. This is why we possess the tools of our trade such as microscopes, refractometers, polariscopes, to name just a few.

Knowing which instrument to use, how to use it, and what results to expect is crucial in detecting any anomalies. The experienced gemmologist will further know when their classical instruments are reaching the limits of their capabilities. At this point, they will want to ascertain which of the more advanced equipment may be needed for diagnostics, and when to send it to a laboratory.

The world of visible spectroscopy has taught us much about the absorptions of the various chromophores that are found in most coloured gems. At the atomic level, laboratories use instruments like energy dispersive x-ray fluorescence spectrometers (ED-XRF), or UV-vis-NIR spectrometers. If however a laboratory were to have to choose one single advanced instrument they could have, it would most likely be a Fourier Transform Infrared spectrometer or FTIR, which gathers data in the infrared region and interprets it into a digital spectrum.

**THE EQUIPMENT**

A standard FTIR unit may range from 1250 nanometers, (8000 cm⁻¹) which is about where most digital spectrometers leave off; and from there cover all the way to 380 cm⁻¹, or over 26,000 nanometers! So we can see the detection range of FTIR units covers an area some 25x larger than the visible light range. It offers much potential in diagnostic identification and research.

Some spectrometers render information as displayed in nanometers, others may be in electron volts. With FTIR the units of measurements that are used are wavenumbers expressed in reciprocal centimeters, or cm⁻¹. Readings performed on the FTIR equipment can be obtained by using either a reflectance or a transmission module. Depending on the type of reading desired, these modules are interchangeable attachments that are snapped into place on the machine between the path of the infrared beam which leads to the detector.
When taking readings, there are two regions or ranges of frequencies that are of interest:

**Fingerprint Region.** The wavenumbers that cover from 400 - 1450 cm\(^{-1}\) are referred to as the fingerprint region. This is typically when the reflectance module would be utilized. This type of reading gives us good information on the species of gemstone or mineral type you may have. Fig. 1 shows the reflectance reading of a magnesite imitating turquoise. The bands clearly show the carbonate nature of the magnesite as opposed to the phosphate nature of turquoise.

![Graph showing reflectance reading of magnesite and turquoise](image1)

**Group Frequency Region.** In the wavenumbers between 4000 cm\(^{-1}\) to 1450 cm\(^{-1}\), the peaks are usually due to the stretching vibrations of bonded atoms. This region is sometimes called the 'functional group'. In the functional group reading (Figure 2), the differences in the oxygen-hydrogen (O-H) molecule bonds may be very complex in nature, but as they are stretched by the infrared energy they can become very evident as seen in this synthetic amethyst.

![Graph showing functional group reading of synthetic amethyst](image2)

The **FTIR at Work**

What are some of the other gemmological uses of the FTIR? A variety of diagnostic tests and determinations can be made. As we have seen so far, in the fingerprint region entire mineral species can be identified. Tests can separate some synthetics from natural stones, and in many cases, the heat treatment of corundum can be determined. As treatment techniques involving polymers and synthesizing methods continue to be developed, careful study and tests using infrared continue to be helpful in making the call.

Here are a few more of the many tests that can be run on these infrared spectrometers:

![Graph showing comparison between hydrothermally grown synthetic amethyst and a natural amethyst](image3)

**Fig. 3** While both stones are silicate in nature, as seen in the general outline of this reflectance reading in the fingerprint region, the details of the spectra indicate the differences between a structured quartz and an amorphous glass, yet both are silicas.

![Graph showing ester level differences at 1749 cm\(^{-1}\) and a “Baltic Shoulder” at 1148 cm\(^{-1}\)](image4)

**Fig. 4** Ester level differences at 1749 cm\(^{-1}\) and a “Baltic Shoulder” at 1148 cm\(^{-1}\) give us clear evidence to differentiate this artificially aged copal from a Baltic amber.
Fig. 5  Type Ia irradiated diamond (black line) as compared to a Type IIa diamond.

Fig. 6  The carbon-hydrogen (C-H) stretched molecules seen in the peaks between 2950 and 3300 cm⁻¹ give us undeniable proof that one of these jadeites has been polymer treated.

There are times when we face the limitations of what can and cannot be performed on any one machine. While a very powerful tool, FTIR is not the ‘black box’ that can give out every answer and other equipment may be needed. As any operator of this equipment can tell you, it takes a lot of finesse and practice to learn how to use it. But knowing when to use it, what to expect and why, is an important step in the experience of FTIR usage in gemmology.

Reference
Michigan State University: www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectropy/InfraRed/infrared.htm
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