

# INFRARED SPECTROSCOPY IN GEMSTONE TESTING

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

*Bear Williams*

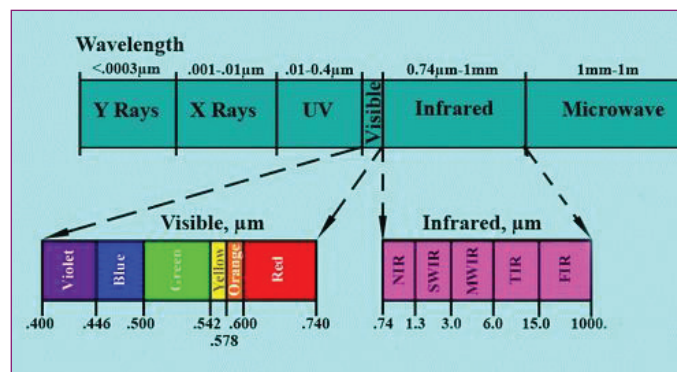
Knowing how to identify, gemstones and treatments is of paramount importance to gemmologists and valuers. This is why we possess the tools of our trade such as microscopes, refractometers, polariscopes, to name just a few.

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.

## INFRARED

Across the entire electromagnetic spectrum, there is a seemingly infinite range of frequencies to utilize in testing and obtaining data. In the infrared region alone, there is a vast amount of bandwidth to explore. With a UV-vis-NIR spectrometer one looks at absorptions or emissions as a function of the atoms in gemstones and how they interact with visible light. With the FTIR spectrometer, we observe molecules and how they are affected by the incoming infrared light. The peaks and valleys seen in the graphs of FTIR are indicative of a molecule's signature vibration as it releases the energy. The process starts as the infrared light source hits the test sample and is absorbed. The molecules will then stretch or bend and release at a characteristic 'wavenumber'. It's important to note that a customer need not be concerned of damage to their stone as the FTIR performs non-destructive tests.



Two adjoining areas shown are part of a much larger electromagnetic spectrum. While not to scale, we can see that the visible light area covers the area from 400nm to 740nm. The infrared region like the ultraviolet, is basically invisible to humans. Here we see the infrared resuming the readings in the 'near infrared' (NIR) at 740nm and going all the way through the end of the 'far infrared' to one million nanometers.

## THE EQUIPMENT

A standard FTIR unit may range from 1250 nanometers, (8000  $\text{cm}^{-1}$ ) which is about where most digital spectrometers leave off; and from there cover all the way to 380  $\text{cm}^{-1}$ , 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  $\text{cm}^{-1}$ . 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  $\text{cm}^{-1}$  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.

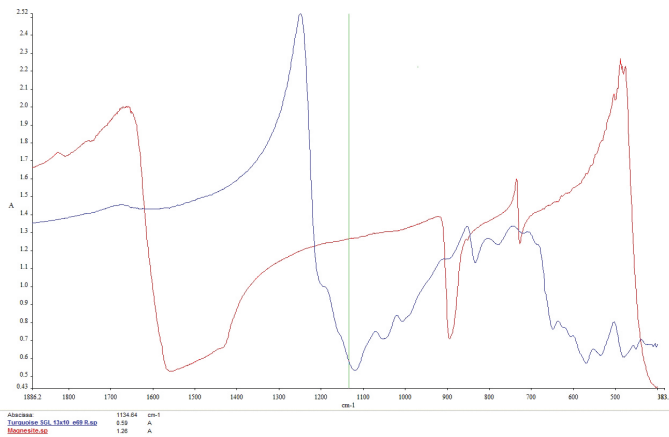


Fig. 1 Magnesite (red trace) is a carbonate. Turquoise (blue line) is a phosphate mineral. The reason for the name “fingerprint region” becomes clear.

**Group Frequency Region.** In the wavenumbers between 4000  $\text{cm}^{-1}$  to 1450  $\text{cm}^{-1}$ , 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.

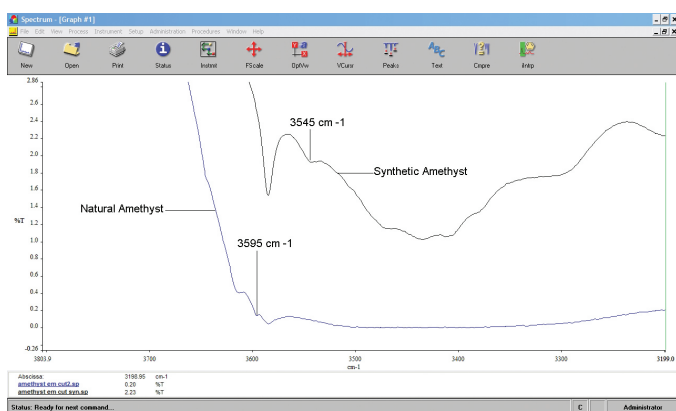


Fig. 2 The differences between a hydrothermally grown synthetic amethyst and an amethyst of natural origin.

## 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:

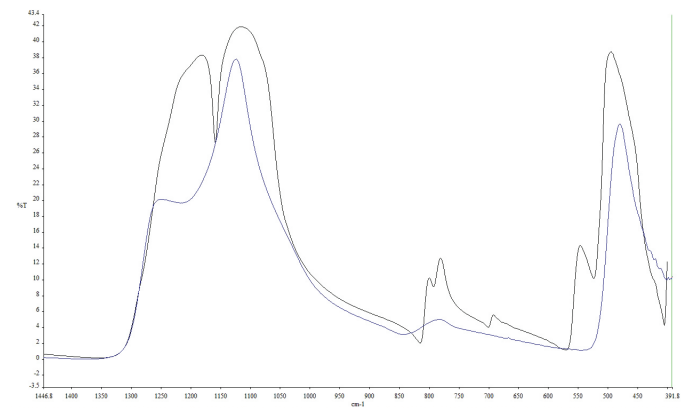


Fig. 3 While both stones are silicate in nature, as seen in the general outline of this reflectance reading in the fingerprint region, the details of the spectra indicate the differences between a structured quartz and an amorphous glass, yet both are silicas.

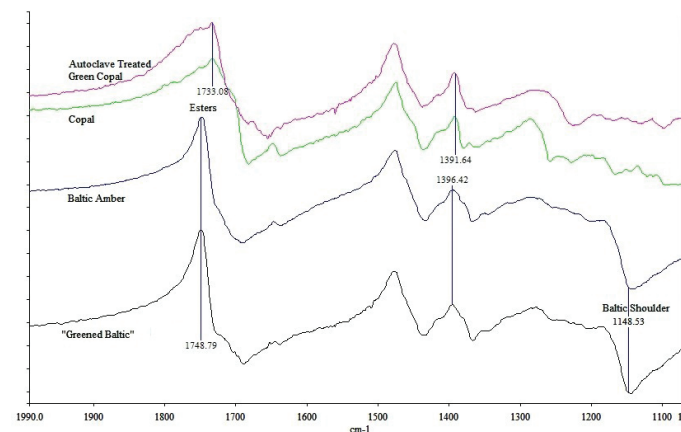


Fig. 4 Ester level differences at 1749  $\text{cm}^{-1}$  and a “Baltic Shoulder” at 1148  $\text{cm}^{-1}$  give us clear evidence to differentiate this artificially aged copal from a Baltic amber.

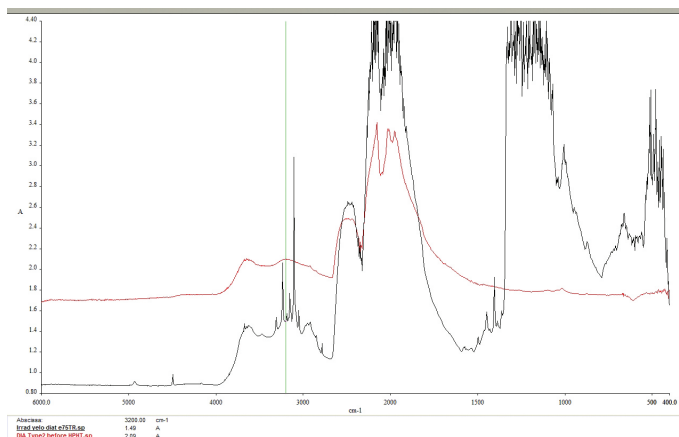
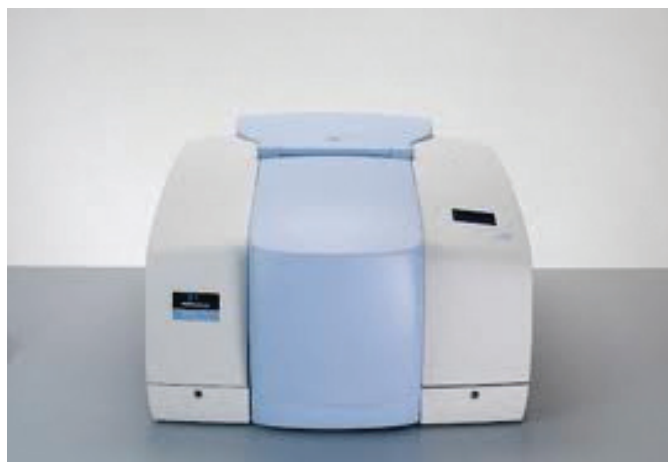


Fig. 5 Type Ia irradiated diamond (black line) as compared to a Type IIa diamond.



Perkin Elmer FTIR Unit as used by Stone Group Laboratories (USA) and Spectra (Australia)

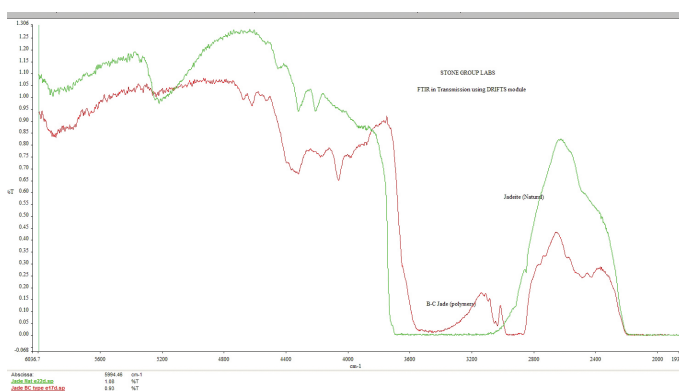


Fig. 6 The carbon-hydrogen (C-H) stretched molecules seen in the peaks between 2950 and 3300  $\text{cm}^{-1}$  give us undeniable proof that one of these jadeites has been polymer treated.

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/Spectrpy/InfraRed/infrared.htm](http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/InfraRed/infrared.htm)

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Author Contact: [bear@stonegrouplabs.com](mailto:bear@stonegrouplabs.com)

