Does Infrared Spectroscopy Show Mineral Structure?

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We see it reported that Raman spectroscopy reports crystal structure. This is a non-elastic infrared method of study. We see the X-ray diffraction spectroscopy (XRD) reports crystal structure. What about infrared spectroscopy? The study of this is silent because virtually all infrared mineral study involves bashing specimens into powders, mixing them in salt (transparent to infrared), pressing them into pellets and shooting the laser through the wafer. This is transmission infrared.

The idea of transmission infrared is a study of urban mythology, a set of presumptions assumed to be facts. Infrared was first used to study amorphous carbon compounds whose bands are at specific wavenumber positions for various molecular group wobbles and stretches. Then this was applied to mineralogy. The idea is that if you bash a mineral into micron dust and make a salt wafer, this proves that infrared will provide an amorphous response minus any crystallographic effects.

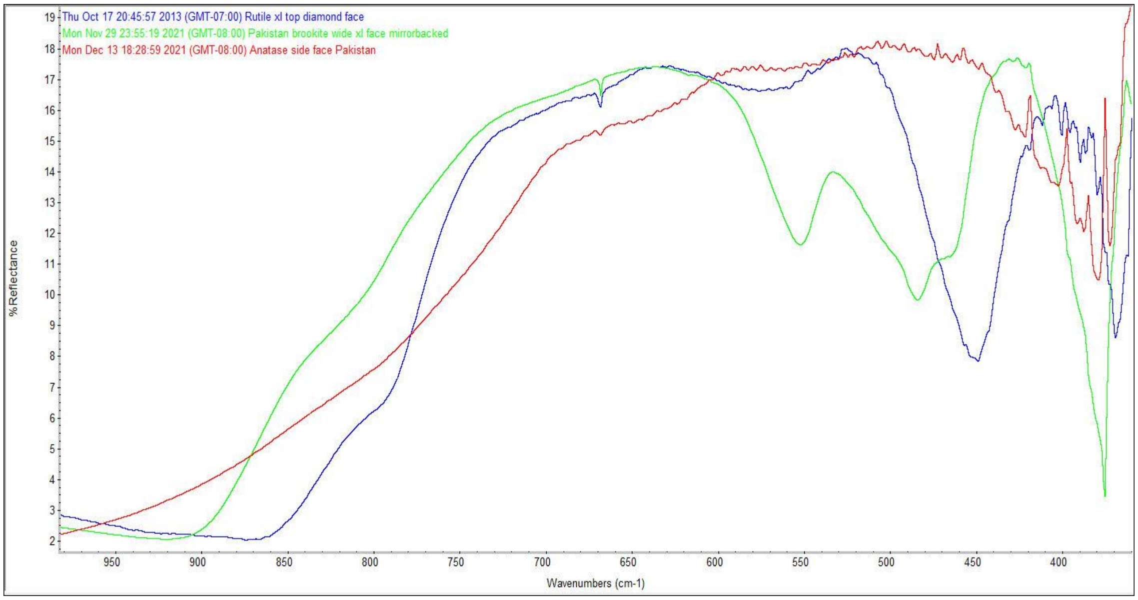
No problem. So now we read off the band positions of various mineral components and we get, oh yeah right, we get total anarchy. The components bands are all over the place. In fact, no master graph of compositional peak wavenumber positions exists for mineralogy and those that tried just made fools of themselves. In place of that, esteemed scientists just pretended it works that way. Then they cannot pretend any more. Then they got mad. Infrared does not work. The bands drift for no reason because they cannot understand what is going on. Infrared is worthless. You can only use it to study mineral water. Today, infrared is only used to study mineral water. This is settled science.

The author has based his 10 years of IR mineralogical infrared study on principles discovered over time that includes:

1. The fundamental region of mineral peak response is based firstly on the mineral refractive index (RI). Higher RI minerals red-shift into far-infrared. An example with the rutile group is shown below.
2. This means the atomic elemental group responses drift because different minerals have different refractive indexes.
3. IR reports a system of crystallography just like every other radiation source used to study matter. An example of rutile, anatase, and brookite is shown below. Every one is TiO_2. Every one has a different spectrum. Every one has the same composition exactly and a different structure, although brookite also has bound OH (hydroxyl) “water”, and the others don’t.
4. When you bash your specimens into dust, you never make a random blend that responds only to atomic composition. If this is true prove it, because no paper proving this exists. Tik, tok, your time is up and you lose. You bash your specimens into powders to make random crystallite face and cleavage plane blends, the blend ratios of each of which shifts your spectra. The solution is to use reflectance infrared on whole mineral specimens, preferably crystal faces. Transmission infrared is an approximation to reflectance infrared.
5. If you think IR is unreliable, take a garnet, take any crystal face, any one or take them all, and generate their spectra. Their spectra never, ever change. Why? Garnets are isometric so have no optical orientation. Those that do in the silicate group will have two dominant spectra. One is along the crystal axis, and the other is perpendicular. Other faces between produce blended graphs. Do this with quartz crystals and try to prove

this wrong. You cannot. There are exactly 5 spectra for all quartz crystals, including up the long axis, and random cuts.

6. IR spectra peaks do not drift because of grain size. They drift because of crystal face blending. Larger grain size reduces the signal throughput and degrades the spectra, but this is not mineral information to put to use, it is noise.
7. In infrared, quartz is hexagonal. All 6 m-faces have identical spectra. It is trigonal only in the minds of early 1830's thinkers and those that repeat their work due to laziness.
8. Different mineral groups have different marker band trend correlations to refractive index and to each other. For example, the silica group and inosilicates have identical trends, offset from each other.
9. The higher the RI for a mineral the more its fundamental region is red-shifted. For silicates, density and RI is strongly correlated, so this means that higher density silicates are red-shifted, some all the way into far-infrared.



Rutile, brookite, and anatase crystal faces. They are all TiO2, the exact same composition. Their spectra are different because their structures are different, and for no other reason. Take the RI value minimum of each. Which one has the lowest wavenumber spectral shift? Correct, rutile has the lowest Christiansen Trough (CT) wavenumber (917 cm-1), the CT being the dominant spectral trough that is on the left here. To the right is the fundamental region. Higher wavenumbers to the CT have no peak response, just water response as troughs in reflectance infrared. Now, which has the highest minimum RI value? Correct, rutile. It is red-shifted relative to the others as we see above.