These differences are used to distinguish the polymorphic forms of a compound. The presence of solvent or water can be detected using this technique as a result of the "broad–OH" stretch associated with water.

The IRS is applied to studies in a number of ways: by Nujol mull, KBr disc, or the diffuse reflectance (DR) technique. In the KBr disc technique, the compound is mixed with KBr and compressed into a disc by using a press and a die. This compression can be a disadvantage if the compound undergoes a polymorphic transformation under pressure.

Nowadays, most instruments use an FT-infrared (FT-IR) system, a mathematical operation used to translate a complex curve into its component curves. In an FT-IR instrument, the complex curve is an interferogram or the sum of the constructive and destructive interferences generated by overlapping light waves, and the component curves are the IR spectrum. The standard IR spectrum is calculated from the FT interferogram, giving a spectrum in percent transmittance (%*T*) versus light frequency (cm^{-1}).

An interferogram is generated because of the unique optics of an FT-IR instrument. The key components are a moveable mirror and a beam splitter. The moveable mirror is responsible for the quality of the interferogram, and it is very important to move the mirror at a constant speed. For this reason, the moveable mirror is often the most expensive component of an FT-IR spectrometer. The beam splitter is just a piece of semireflective material, usually Mylar film sandwiched between two pieces of an IR-transparent material. The beam splitter splits the IR beam 50/50 to the fixed and moveable mirrors and then recombines the beams after being reflected at each mirror. The FT is named after its inventor, the French geometrician and physicist Baron Jean Baptiste Joseph Fourier, born in 1830.

The FT-IR spectra of amorphous forms are often less well defined and can be used to characterize various polymorphic forms. Heating experiments are also possible by using IRS, where the variable-temperature IRS is conducted to confirm that a solid–solid transition takes place on heating various forms of the compounds.

The disadvantages of the conventional IRS, such as the need to compress the samples, is overcome when the *diffuse reflectance Fourier transform* (*DRIFT*) technique is used, whereby a few milligrams of the compound are dispersed in approximately 250 mg of KBr, and the spectrum is obtained by reflection from the surface.

Many substances in their natural states (e.g., powders and rough surface solids) exhibit DR; that is, the incident light is scattered in all directions, as opposed to specular (mirror-like) reflection, where the angle of incidence equals the angle of reflection. In practice, the DR spectra are complex and are strongly dependent on the conditions under which they are obtained. These spectra can exhibit both absorbance and reflectance features as a result of the contributions from transmission, internal and specular reflectance components, and scattering phenomena in the collected radiation. The DR spectra are further complicated by sample preparation, particle size, sample concentration, and optical geometry effects, to name a few. Specular reflection, whether it occurs from a glossy sample surface or from a crystal surface, produces inverted bands ("Reststrahlen bands") in the DR spectrum, which reduces the usefulness of traditional transmission reference spectra. For highly absorbing samples, these Reststrahlen bands are strong. Grinding and diluting the sample with nonabsorbing powder, such as KBr, KCl, Ge, and Si, can minimize or eliminate these effects. Grinding reduces the contribution of reflection from large particle faces. Diluting ensures deeper penetration of the incident beam, thus increasing the