

Comparison of FTIR Spectra Collected by Transmission and ATR Sampling

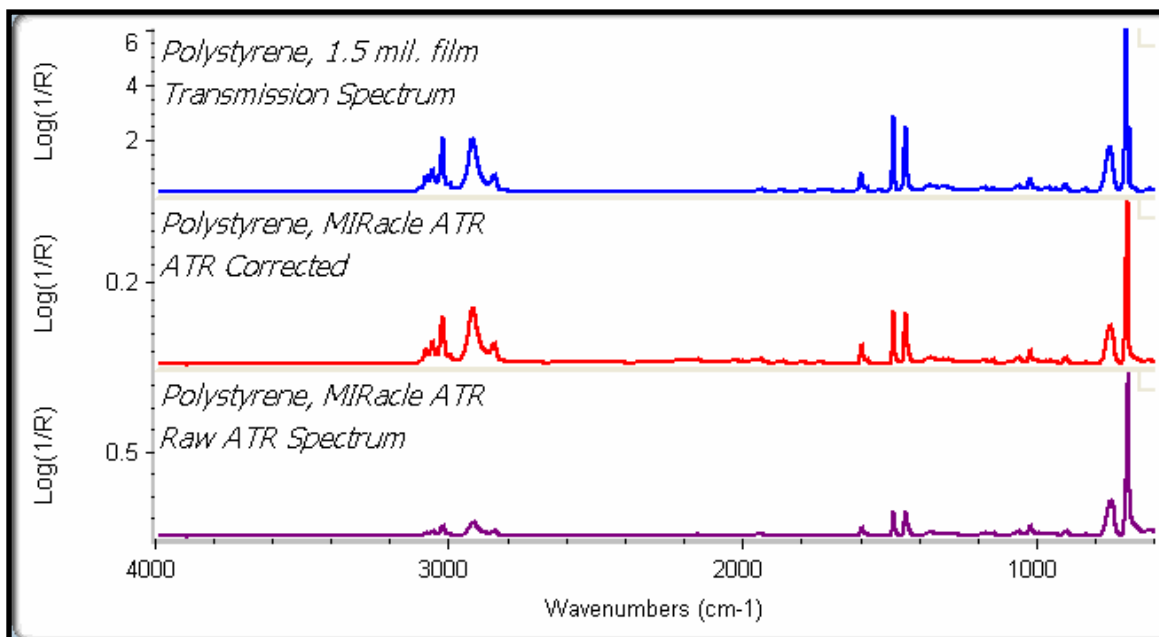
Attenuated total reflectance (ATR) spectra measured by FTIR are similar to those collected by transmission measurements. However, subtle differences exist for the following physical phenomenon;

ATR sampling depth or **depth of penetration** (d_p) is relative to the wavelength of light. Technically, this is defined as the distance required for the electric field amplitude to fall to e^{-1} of its value at the surface

where λ is the wavelength of light, θ is the angle of incidence of the IR beam relative to a perpendicular from the surface of the crystal, n_1 is the refractive index of the ATR crystal and n_2 is the refractive index of the sample. The result of this is that IR absorbance bands at long wavelength will be of higher absorbance than those of shorter wavelength.

This is shown in Figure 1 for polystyrene.

The ATR correction feature of the FTIR software package will make a correction for the relative band intensity and its result will more closely resemble the transmission spectrum. Performing the ATR correction may also improve library search results and is a recommended procedure for qualitative analysis.



and is further defined by:

$$d_p = \frac{\lambda}{2\pi(n_1^2 \sin^2 \theta_1 - n_2^2)^{1/2}}$$

Figure 1. Polystyrene collected by transmission (upper spectrum) and by ATR (lower spectrum). The middle red spectrum is after ATR correction.