

We know that the absorbance value or value of the peaks of interest should be in the vicinity of 0.43A, especially when quantitative results are desired.

If only very small amounts of material are available, then sample size alone will probably limit the analysis to a micro-sampling single reflection device (e.g., the [MVP-Pro](#) accessory or [SplitPea](#) accessory). The exception to this rule of thumb is if the solid sample is actually a paste, foam, or other fairly flexible solid material. In this case, like the [Horizon](#) or [ConcentratIR](#) multiple-reflection ATR accessory would be a possibility.

If there is sufficient solid sample, then either single or multiple reflection ATR are options. The exception to this rule of thumb is if the solid is very hard. In this case, a single reflection ATR accessory is generally required, where the force pushing the sample against the ATR element can be concentrated in the smallest possible area. The ATR element should be harder than the sample. The [Meridian](#), with its single reflection diamond ATR element, would be one accessory which would fulfill these requirements.

If there is sufficient solid sample and the sample is not very hard, then an attempt should first be made to analyze this sample by single reflection ATR. This is probably the simplest method to analyze samples and will probably provide adequate spectral contrast (and S/N) for qualitative studies. If absorbance values of 0.3-0.5A are obtained for peaks to be used for quantitative analysis, then the single reflection technique is, again, chosen.

If absorbance values are too high with single reflection ATR, then, obviously, going to multiple reflection ATR would only exacerbate the problem. In this case, one can choose an ATR material of higher refractive index (e.g., change from ZnSe to Ge with the FastIR accessory), or increase the angle of incidence (e.g., change from 45° to 60° with the variable angle Seagull accessory).

If absorbance values are too low with single reflection ATR, then the spectral contrast can be enhanced by choosing an ATR material of lower refractive index (change from ZnSe to ZnS with the FastIR accessory), or decrease the angle of incidence (e.g., change from 45° to 40° with the variable angle Seagull accessory). These two techniques must be used with care, however, as approaching or exceeding the critical angle, will yield distorted spectra. (The critical angle is that angle, for a given ATR material refractive index and a given sample refractive index, at which total internal reflection no longer occurs. This can be calculated using the [CristalCalc](#) software.)

If absorbance values are still too low, there is sufficient sample, and the sample is not too hard, then, and only then should the analyst try multiple reflection ATR. Based on the preliminary results obtained with single reflection ATR, one should be able to quickly determine the additional number of reflections required to reach the 0.3-0.5A range. The caution here, is that for such a calculation to work, one assumes that the contact with the multiple reflection ATR element is as good as the contact with the single reflection element.