

How do I choose an ATR accessory for my application?

Attenuated Total Reflectance (ATR) spectroscopy can be used for samples that are difficult to analyze by a transmission technique. Internal reflectance measurements are made by using an ATR crystal in contact with the sample. Choice of an appropriate ATR accessory is wholly dependent upon the amount and physical state of the sample that you wish to analyze.

The range of ATR accessories currently available from Specac are a vertical 25 reflection system, horizontal 6 reflection system (Gateway ATR) and two horizontal single reflection systems (Quest and Golden Gate ATR systems). The multiple reflection ATR accessories (25 and 6 reflections) require a larger amount of sample to cover an ATR crystal, whereas smaller amounts of sample are required to just cover the ATR crystals used in the single reflection ATR accessories. For the crystal size on both the Quest and Golden Gate ATR systems, the sample can be as small as 2mm by 2mm.

The physical state of the sample is an important factor in determining an appropriate ATR system. The sample must be in very good contact with the ATR crystal to obtain a good ATR spectrum. Hence liquids usually exhibit better ATR spectra than solid samples. A clamping system is used with solid samples to force the sample into good contact with the ATR crystal. It helps if the solid sample has a high degree of homogeneity to obtain consistent spectra between like samples. Issues such as reproducibility and sensitivity can become important, due to the way a sample makes contact with a specific ATR crystal.

The frequency range that can be studied by the ATR technique in the Mid IR region is determined by the choice of ATR crystal. Typically, ZnSe (zinc selenide) is popularly used as an ATR crystal, because of its relative cost, allowing for study of a Mid- IR spectrum over a spectral range from 4000 cm^{-1} to 550 cm^{-1} .

However, it must always be considered that although the crystal may offer the spectral range, it may not be chemically compatible with a particular sample and could be damaged on contact. To this extent diamond as an ATR crystal material is now a common, universally applicable crystal material to choose because of its chemical resistance, durability and wider spectral transmission range in the Mid-IR for ATR measurement of 4000 cm^{-1} to 400 cm^{-1} . Other crystal materials used for ATR study include germanium, silicon and KRS-5 (a mixed salt of thallium bromide and thallium iodide).

In summary, along with the sample amount and type, it is often a compromise between chemical performance and spectral range of a crystal material that determines the choice of an ATR accessory for a particular experimental application.

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