Near-Infrared Spectrophotometers

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Spectrophotometers used within the laboratory for near-infrared (NIR) measurements may function using a variety of optical and mechanical design configurations. Spectrophotometers are defined in technical terms as devices designed to furnish the ratio (ratiometric function) of the radiant power of two beams as a function of spectral position (i.e., wavelength or frequency). The two beams may be separated in time, space, or both. This definition, paraphrased from the American Society for Testing and Materials (ASTM) International E131 definition for spectrophotometer reveals enough information to determine the basic characteristics of measurements taken using this ratiocination method. The measurement spectrum for any NIR spectrophotometer is given by the ratio of the photometric (i.e., transmittance or reflectance) measurement of the sample at a wavelength or set of wavelengths divided by the measurement of a reference material at the same wavelength or wavelengths. If the measurements are taken with transmittance geometry, this ratio is equal to the transmittance, \( T \), with a value of from 0 to 1.0. If the measurements are taken with reflectance geometry, then this ratio is equal to the reflectance, \( R \), with a value from 0 to 1.0. For transmittance reference measurements a blank or ambient air is generally used. For reflectance reference measurements a highly reflective, diffuse reflection sample is used. This reflective reference is generally a ceramic, or Spectralon (Labsphere, North Hutton, NH), each having a surface that is 95 to 99% reflective for the NIR wavelength region measured.

A common assumption in spectrophotometric measurements is that Beer’s Law relationship applies for a change in instrument response due to a change in concentration of the analyte material present within a sample specimen. Beer’s Law assumes that the transmittance of a sample within an incident beam is equivalent to 10 exponent the negative product of the absorptivity in liters per mole per centimeter, times the concentration of the analyte in solution in moles per liter, times the pathlength in centimeters of the sample in solution. The units can obviously be converted to other units for convenience when necessary. However changes in sample and instrument temperature, atmospheric pressure within the instrument, and interferences caused by overlapping absorption bands will create deviations from the ideal case. For most analytical situations Beer’s Law relationship holds well enough for useful quantitative measurements.