

In1-2

THEORY AND PRINCIPLES OF NEAR INFRARED SPECTROSCOPY

Franklin E. Barton

*USDA-Agricultural Research Service, Richard B. Russell Agricultural Research Center,
P.O. Box 5677, Athens, GA 30604-567, USDA-Agricultural Research Service*

The elegant early experiments of Herschel demonstrated that there is light after the visible spectrum in a region we call the near infrared (NIR). This was followed by the work which showed that the spectrum went further into what we call the mid infrared (MIR). The MIR has been used for many years as a qualitative and quantitative region to measure constituent values. The MIR region contains the fundamental vibrations which can be theoretically calculated from symmetry rules and harmonic oscillator equations. The NIR is not as straight forward because the region from 400-2500 nm does not contain any of the fundamental vibrations only combination bands and overtones. Over the past fifty years efforts to understand the NIR have largely been ignored while the quantitative aspects of the region have been utilized. This presentation will focus on the efforts to define terms for NIR, examine the calculation of combination bands and overtones and ways to interpret the spectra. The interpretation of the NIR has been aided greatly in recent years by the use of two dimensional spectroscopy which allows the correlation of bands in one spectral region with that of the NIR.