

QA/QC CONSIDERATIONS IN GENERATING FTIR REFERENCE SPECTRA

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FTIR reference spectra are used to identify and quantify species found in a sample. Many spectral libraries are available for gas-phase quantitative analysis, especially when used for source or ambient air testing. When a target analyte is not available in a library, it is usually generated in the laboratory. In this paper, quality assurance/control (QA/QC) techniques are illustrated to give the user a high degree of confidence in generating a reference spectrum. Use of spectral simulation techniques and thermodynamic considerations are demonstrated to aid the user in reference spectrum development.