



Standard Practices for Infrared Multivariate Quantitative Analysis¹

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1. Scope

1.1 These practices cover a guide for the multivariate calibration of infrared spectrometers used in determining the physical or chemical characteristics of materials. These practices are applicable to analyses conducted in the near infrared (NIR) spectral region (roughly 780 to 2500 nm) through the mid infrared (MIR) spectral region (roughly 4000 to 400 cm^{-1}).

NOTE 1—While the practices described herein deal specifically with mid- and near-infrared analysis, much of the mathematical and procedural detail contained herein is also applicable for multivariate quantitative analysis done using other forms of spectroscopy. The user is cautioned that typical and best practices for multivariate quantitative analysis using other forms of spectroscopy may differ from practices described herein for mid- and near-infrared spectroscopies.

1.2 Procedures for collecting and treating data for developing IR calibrations are outlined. Definitions, terms, and calibration techniques are described. Criteria for validating the performance of the calibration model are described.

1.3 The implementation of these practices require that the IR spectrometer has been installed in compliance with the manufacturer's specifications. In addition, it assumes that, at the times of calibration and of validation, the analyzer is operating at the conditions specified by the manufacturer.

1.4 These practices cover techniques that are routinely applied in the near and mid infrared spectral regions for quantitative analysis. The practices outlined cover the general cases for coarse solids, fine ground solids, and liquids. All techniques covered require the use of a computer for data collection and analysis.

1.5 These practices provide a questionnaire against which multivariate calibrations can be examined to determine if they conform to the requirements defined herein.

1.6 For some multivariate spectroscopic analyses, interferences and matrix effects are sufficiently small that it is possible to calibrate using mixtures that contain substantially fewer chemical components than the samples that will ultimately be

analyzed. While these surrogate methods generally make use of the multivariate mathematics described herein, they do not conform to procedures described herein, specifically with respect to the handling of outliers. Surrogate methods may indicate that they make use of the mathematics described herein, but they should not claim to follow the procedures described herein.

1.7 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.8 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 ASTM Standards:²

- D1265 Practice for Sampling Liquefied Petroleum (LP) Gases, Manual Method
- D4057 Practice for Manual Sampling of Petroleum and Petroleum Products
- D4177 Practice for Automatic Sampling of Petroleum and Petroleum Products
- D4855 Practice for Comparing Test Methods (Withdrawn 2008)³
- D6122 Practice for Validation of the Performance of Multivariate Online, At-Line, and Laboratory Infrared Spectrophotometer Based Analyzer Systems
- D6299 Practice for Applying Statistical Quality Assurance and Control Charting Techniques to Evaluate Analytical Measurement System Performance
- D6300 Practice for Determination of Precision and Bias Data for Use in Test Methods for Petroleum Products and Lubricants
- E131 Terminology Relating to Molecular Spectroscopy

¹ These practices are under the jurisdiction of ASTM Committee E13 on Molecular Spectroscopy and Separation Science and are the direct responsibility of Subcommittee E13.11 on Multivariate Analysis.

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² For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

³ The last approved version of this historical standard is referenced on www.astm.org.