



Designation: D8470 – 22

Standard Practice for Development and Implementation of Instrument Performance Tests for Use on Multivariate Online, At-Line and Laboratory Spectroscopic Based Analyzer Systems¹

This standard is issued under the fixed designation D8470; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice covers basic procedures that can be used to develop instrument performance tests for spectroscopic based online, at-line, laboratory and field analyzers. The practice is intended to be applicable to Raman spectrometers and to infrared spectrophotometers operating in the near-infrared and mid-infrared regions.

1.2 This practice is not intended as a replacement for specific practices, such as Practices [E275](#), [E925](#), [E932](#), [E958](#), [E1421](#), or [E1683](#) that exist for measuring performance of specific types of laboratory spectroscopic instruments. Instead, this practice is intended to provide guidelines as to how similar practices should be developed when specific practices do not exist for a particular instrument type, or when specific practices are not applicable due to sampling or safety concerns. This practice can be used to develop instrument performance tests for on-line process spectroscopic-based analyzers.

1.2.1 The performance tests described in this practice typically only evaluate the performance of the infrared spectrophotometer or Raman spectrometer part of the analyzer system, referred to herein as the instrument.

1.2.2 Instrument performance tests do not typically evaluate performance of analyzer sampling systems.

1.3 This practice describes univariate level zero and level one tests, and multivariate level A and level B tests which can be implemented to measure instrument performance. These tests are designed to be used as rapid, routine checks of instrument performance. They are designed to uncover malfunctions or other changes in instrument operation, but do not specifically diagnose or quantitatively assess the malfunction or change. The tests are not intended for the comparison of instruments or analyzers of different manufacture.

1.4 The instrument performance tests described in this practice are used during the development of multivariate

calibrations via Practice [D8321](#) to establish the performance level at the time the calibration is developed. The same tests are used during validation of analyzers via Practice [D6122](#) to qualify the working analyzer by demonstrating comparable performance.

1.4.1 Instrument performance tests are used to requalify instruments after analyzer maintenance.

1.4.2 Instrument performance tests are used to qualify instruments in secondary analyzers to which calibrations are being transferred after development on a primary analyzer.

1.5 *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, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.6 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*²

[D4175](#) Terminology Relating to Petroleum Products, Liquid Fuels, and Lubricants

[D6122](#) Practice for Validation of the Performance of Multivariate Online, At-Line, Field and Laboratory Infrared Spectrophotometer, and Raman Spectrometer Based Analyzer Systems

[D7940](#) Practice for Analysis of Liquefied Natural Gas (LNG) by Fiber-Coupled Raman Spectroscopy

[D8321](#) Practice for Development and Validation of Multivariate Analyses for Use in Predicting Properties of Petroleum Products, Liquid Fuels, and Lubricants based on Spectroscopic Measurements

¹ This practice is under the jurisdiction of ASTM Committee [D02](#) on Petroleum Products, Liquid Fuels, and Lubricants and is the direct responsibility of Subcommittee [D02.25](#) on Performance Assessment and Validation of Process Stream Analyzer Systems.

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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.

- D8340** Practice for Performance-Based Qualification of Spectroscopic Analyzer Systems
- E131** Terminology Relating to Molecular Spectroscopy
- E275** Practice for Describing and Measuring Performance of Ultraviolet and Visible Spectrophotometers
- E925** Practice for Monitoring the Calibration of Ultraviolet-Visible Spectrophotometers whose Spectral Bandwidth does not Exceed 2 nm
- E932** Practice for Describing and Measuring Performance of Dispersive Infrared Spectrometers
- E958** Practice for Estimation of the Spectral Bandwidth of Ultraviolet-Visible Spectrophotometers
- E1421** Practice for Describing and Measuring Performance of Fourier Transform Mid-Infrared (FT-MIR) Spectrometers: Level Zero and Level One Tests
- E1683** Practice for Testing the Performance of Scanning Raman Spectrometers
- E1840** Guide for Raman Shift Standards for Spectrometer Calibration
- E1866** Guide for Establishing Spectrophotometer Performance Tests

3. Terminology

3.1 For terminology related to molecular spectroscopic methods, refer to Terminology **E131**. For terminology relating to petroleum products, liquid fuels and lubricants, refer to Terminology **D4175**.

3.2 Definitions:

3.2.1 *absorbance* (A), n —the logarithm to the base 10 of the reciprocal of the transmittance, (T).

$$A = \log_{10}(1 / T) = -\log_{10} T$$

E131

3.2.1.1 *Discussion*—Absorbance is a measure of the capacity of a substance to absorb light of a specific wavelength.

3.2.2 *action limit*, n —for multivariate spectroscopic analyzers used in the analysis of liquid petroleum products and fuels, the limiting value from an instrument performance test, beyond which the multivariate spectroscopic analyzer is expected to produce potentially invalid results. **D6122**

3.2.3 *calibration*, n —in multivariate spectroscopic measurement, a process for creating a multivariate model relating component concentrations or sample properties to spectra for a set of known samples, referred to as calibration samples. **D8321**

3.2.4 *control limits*, n —limits on a control chart that are used as criteria for signaling the need for action or for judging whether a set of data does or does not indicate a state of statistical control.

3.2.5 *extractive sampling*, n —for spectroscopic process analyzers used in the analysis of liquid petroleum products and fuels, the process of transporting a sample from the process, performing any necessary sample conditioning and finally presenting the sample to the analyzer so as to produce a spectrum of the process sample.

3.2.6 *in situ sampling*, n —for spectroscopic process analyzers used in the analysis of liquid petroleum products and fuels, the process of transporting light from the analyzer to a sample

probe located in the process wherein the light interacts with a process sample, and collecting the transmitted or scattered light, returning it to the analyzer where it is analyzed by the instrument to produce a spectrum of the process sample.

3.2.6.1 *Discussion*—For some NIR and nearly all Raman analyzers, the light will typically be transported to and from the analyzer using fiber optics.

3.2.7 *instrument*, n —for spectroscopic analyzers used in petrochemical service, the spectrometer or spectrophotometer, associated electronics and computer, spectrometer or spectrophotometer cell, and if utilized, transfer optics. **D6122**

3.2.8 *instrument performance verification sample*, n —for multivariate spectroscopic analyzers used in the analysis of liquid petroleum products and fuels which employ extractive sampling, a material representative of the product being analyzed which is adequately stored in sufficient quantity to be used as a check on instrument performance; instrument performance verification samples are used in instrument performance tests and as checks on calibration transfer, but the samples and their spectra are generally not reproducible long term **D6122**

3.2.8.1 *Discussion*—In **E1866** and previous versions of **D6122** and this practice, an instrument performance verification sample was referred to as a test sample.

3.2.9 *instrument qualification sample*, n —for multivariate spectroscopic analyzers used in the analysis of liquid petroleum products and fuels, a single pure compound, or a known, reproducible mixture of compounds whose spectrum is constant over time such that it can be used in an instrument performance test. **D6122**

3.2.9.1 *Discussion*—In **E1866** and previous versions of **D6122** and this practice, an instrument qualification sample was referred to as a check sample.

3.2.10 *level A test*, n —for spectroscopic analyzers used in the analysis of liquid petroleum products and fuels, a pass/fail instrument performance test in which the spectrum of a check or instrument performance verification sample is compared against historical spectra of the same sample via a multivariate analysis.

3.2.11 *level B test*, n —for spectroscopic analyzers used in the analysis of liquid petroleum products and fuels, a pass/fail instrument performance test in which the spectrum of a check or instrument performance verification sample is analyzed using a multivariate model, and the results of the analysis are compared to historical results for prior analyses of the same sample.

3.2.12 *level one (1) test*, n —for spectroscopic analyzers used in the analysis of liquid petroleum products and fuels, a simple series of measurements designed to provide quantitative data on various aspects of spectrophotometer performance and information on which to base the diagnosis of problems.

3.2.13 *level zero (0) test*, n —for spectroscopic analyzers used in the analysis of liquid petroleum products and fuels, a routine check of instrument performance, which can be done in a few minutes, designed to visually detect significant changes in instrument performance and provide a database to determine instrument performance over time.