



# Standard Practice for Qualifying Spectrometers and Spectrophotometers for Use in Multivariate Analyses, Calibrated Using Surrogate Mixtures<sup>1</sup>

This standard is issued under the fixed designation E2056; 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 ( $\epsilon$ ) indicates an editorial change since the last revision or reapproval.

## 1. Scope

1.1 This practice relates to the multivariate calibration of spectrometers and spectrophotometers used in determining the physical and chemical characteristics of materials. A detailed description of general multivariate analysis is given in Practices E1655. This standard refers only to those instances where surrogate mixtures can be used to establish a suitable calibration matrix. This practice specifies calibration and qualification data set requirements for interlaboratory studies (ILSs), that is, round robins, of standard test methods employing surrogate calibration techniques that do not conform exactly to Practices E1655.

NOTE 1—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 in Practices E1655, they do not conform to procedures described therein, specifically with respect to the handling of outliers.

1.2 This practice specifies how the ILS data is treated to establish spectrometer/spectrophotometer performance qualification requirements to be incorporated into standard test methods.

NOTE 2—Spectrometer/spectrophotometer qualification procedures are intended to allow the user to determine if the performance of a specific spectrometer/spectrophotometer is adequate to conduct the analysis so as to obtain results consistent with the published test method precision.

1.2.1 The spectroscopies used in the surrogate test methods would include but not be limited to mid- and near-infrared, ultraviolet/visible, fluorescence and Raman spectroscopies.

1.2.2 The surrogate calibrations covered in this practice are: multilinear regression (MLR), principal components regression (PCR) or partial least squares (PLS) mathematics. These calibration procedures are described in detail in Practices E1655.

1.3 For surrogate test methods, this practice recommends limitations that should be placed on calibration options that are allowed in the test method. Specifically, this practice recommends that the test method developer demonstrate that all calibrations that are allowed in the test method produce statistically indistinguishable results.

1.4 For surrogate test methods that reference spectrometer/spectrophotometer performance practices, such as Practices E275, E925, E932, E958, E1421, E1683, or E1944; Test Methods E387, E388, or E579; or Guide E1866, this practice recommends that instrument performance data be collected as part of the ILS to establish the relationship between spectrometer/spectrophotometer performance and test method precision.

## 2. Referenced Documents

### 2.1 ASTM Standards:<sup>2</sup>

- D6277 Test Method for Determination of Benzene in Spark-Ignition Engine Fuels Using Mid Infrared Spectroscopy
- 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
- E275 Practice for Describing and Measuring Performance of Ultraviolet and Visible Spectrophotometers
- E387 Test Method for Estimating Stray Radiant Power Ratio of Dispersive Spectrophotometers by the Opaque Filter Method
- E388 Test Method for Wavelength Accuracy and Spectral Bandwidth of Fluorescence Spectrometers
- E579 Test Method for Limit of Detection of Fluorescence of Quinine Sulfate in Solution
- E691 Practice for Conducting an Interlaboratory Study to Determine the Precision of a Test Method
- E925 Practice for Monitoring the Calibration of Ultraviolet-Visible Spectrophotometers whose Spectral Bandwidth

<sup>1</sup> This practice is under the jurisdiction of ASTM Committee E13 on Molecular Spectroscopy and Separation Science and is the direct responsibility of Subcommittee E13.11 on Multivariate Analysis.

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<sup>2</sup> For referenced ASTM standards, visit the ASTM website, [www.astm.org](http://www.astm.org), or contact ASTM Customer Service at [service@astm.org](mailto:service@astm.org). For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.