Standard Guide for Quality Assurance of Laboratories Using Molecular Spectroscopy¹

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 ϵ^1 Note—Section 12 was added editorially in December 1994.

1. Scope

- 1.1 This guideline describes the essential features of quality assurance under the following headings: Validity of Analytical Procedures, Calibration and Standardization, Sample Identification and Storage, Reports of Results, Records Retention, and Internal Audit.
- 1.2 This standard does not purport to address the safety problems 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:
- E 131 Terminology Relating to Molecular Spectroscopy²
- E 168 Practices for General Techniques of Infrared Quantitative Analysis²
- E 275 Practice for Describing and Measuring Performance of Ultraviolet, Visible, and Near-Infrared Spectrophotometers²
- E 386 Practice for Data Presentation Relating to High-Resolution Nuclear Magnetic Resonance (NMR) Spectroscopy²
- E 456 Terminology Relating to Quality and Statistics³
- E 882 Guide for Accountability and Quality Control in the Chemical Analysis Laboratory⁴
- E 925 Practice for the Periodic Calibration of Narrow Band-Pass Spectrophotometers²
- E 932 Practice for Describing and Measuring Performance of Dispersive Infrared Spectrophotometers²

3. Terminology

- 3.1 Definitions:
- 3.2 audit—an examination of the quality assurance system
- ¹ This guideline is under the jurisdiction of ASTM Committee E-13 on Molecular Spectroscopy and is the direct responsibility of Subcommittee E13.02 on Liaison and Communications.
 - Current edition approved Oct. 24, 1984. Published January 1985.
 - ² Annual Book of ASTM Standards, Vol 03.06.
 - ³ Annual Book of ASTM Standards, Vol 14.02.
 - ⁴ Annual Book of ASTM Standards, Vol 03.05.

- to determine adherence to documented procedures.
- 3.3 *calibration*—the relationship of instrumental response to changes in the nature and concentration of reference materials.
- 3.4 *certified test report*—an approved document, containing the results of required tests.
 - 3.5 documented—recorded in proper format.
- 3.6 *standardization*—the procedure used to verify or adjust instrumental response to conform to the analytical curve established during calibration.
- 3.7 *traceability*—the ability to relate an analytical result to a standard reference material.
- 3.8 For definitions of other terms used in this Guideline, refer to Terminology E 131, E 386, and E 456.

4. Summary of Guide

4.1 This guide outlines the requirements for a system of quality assurance for laboratories using molecular spectroscopy equipment. It does not include a detailed description for setting up a quality assurance program. Refer to Guide E 882, Guideline for Data Acquisition and Data Quality Evaluation in Environmental Chemistry⁵, and General and Specific Criteria for Accrediting Testing Laboratories⁶ for other thorough discussions related to this topic.

5. Significance and Use

- 5.1 Quality assurance is a system of activities that provides assurance that the overall quality control program of a molecular spectroscopy laboratory is being carried out effectively. Accepted infra-red quantative procedures are described in Practices E 168. The goals of a quality assurance program are to:
- 5.1.1 Demonstrate adherence to accepted laboratory practices regarding record keeping, instrument maintenance, etc.,
- 5.1.2 Show that individual analyses are performed according to validated methods and meet criteria for precision and accuracy, and
 - 5.1.3 Ensure that data are reported in such a manner that the

⁵ Analytical Chemistry, Vol 52, 1980, p. 2242.

⁶ Federal Register, Vol 46, No. 137, 1981, p. 37034.