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Standard Guide for Quality Assurance of Laboratories Using Molecular Spectroscopy¹

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^{ε1} 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

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 quantitative 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

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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.

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

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

reader can evaluate their significance.

6. Calibration and Standardization

6.1 Calibrate the instrument when installed, after major repairs, or as indicated by standardization checks.

6.2 Standardize the instrument as frequently as performance experience indicates.

6.3 Provide written procedures for calibration and standardization.

6.4 Maintain records of standardization runs and adjustments. Include the reference materials used, their certified value, and values obtained by the spectroscopy laboratory. Record the data, shift, and analyst, as well as instrumental parameters.

6.4.1 If standard reference materials are not available for standardization, use secondary reference materials.

7. Validity of Analytical Procedures

7.1 Use fully validated and documented methods for analyses that must be certified. Base validation upon reasonable results for accepted reference materials and define such critical issues as detection limits, precision, and accuracy. *Complete such validation prior to routine quality assurance.*

7.2 Whenever possible, base routine methods of analysis on recognized standard methods (ANSI, ASTM, AOAI, etc.) adapted to specific materials, instrumentation, and analytical requirements. Keep written methods current.

7.3 Qualifications for personnel are usually established by internal management, but may be regulated by external agencies. Maintain a comprehensive training program to instruct all personnel on their responsibilities relative to the quality assurance system.

7.4 Establish routine maintenance procedures for the analytical equipment and include with analytical methods. Include in the maintenance program documented checks for adherence to design specifications, replacement of faulty equipment and stability of instrument outputs (refer to Practices E 275, E 925, and E 932).

7.5 Determination of accuracy and precision are supervisory responsibilities. Procedures to monitor the precision and accuracy of the analytical methods should be established by those who audit the quality assurance system. Document traceability to suitable reference materials in these procedures.

8. Sample Identification and Storage

8.1 *Sample Identification*—Employ a positive identification system to denote the specimen to be analyzed. Maintain sample identification throughout all stages of specimen selection, preparation and analysis, data reporting, and record keeping.

8.1.1 Identify samples in a permanent manner or keep in a permanently identified closeable container, such as an envelope or bag.

8.2 *Sample Storage*—Store samples for a reasonable length of time. Determine storage time for each sample type to satisfy legal and other requirements.

8.2.1 Be able to readily retrieve samples. Protect samples from deterioration and contamination.

9. Reports of Results

9.1 Report results so that they cannot be misinterpreted. For quantitative measurements, report uncertainty or method limitations along with significant figures.

9.2 Statistically treat quantitative results, showing the number of measurements and standard deviations.

10. Records Retention

10.1 Maintain certified test reports as permanent records, for example: original reports; data sheets; computer summaries; microfilm; or other acceptable forms.

10.2 Keep records secure in a convenient location, available for inspection by authorized personnel.

10.3 Retain records for a reasonable period of time. Determine storage time to satisfy legal and other requirements.

11. Internal Audit

11.1 Establish a system of internal audits to monitor quality assurance procedures.

11.2 Maintain a system of verification of analyses. Common techniques involve the analysis of duplicate specimens by other analysts, methods, or laboratories.

11.3 Include in records control sample values, comparisons with assumed true values, reference material values, and corrective action taken.

12. Keywords

12.1 molecular spectroscopy; quality assurance

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