W-59-13

Designation: E 137 – 82 (Reapproved 1987)

Standard Practice for Evaluation of Mass Spectrometers for Quantitative Analysis From a Batch Inlet[1]

This standard is issued under the fixed designation E 137; 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 provides general criteria and tests that are generally helpful for evaluating a mass spectrometer for use in ASTM mass spectrometric methods of chemical analysis. The number of types of mass spectrometers available, and the variety of materials that may be analyzed, preclude a discussion in this practice of the capabilities of each type of mass spectrometer for each specific method of analysis. Neither is it intended to include all the technical considerations involved in procuring a new mass spectrometer. Such considerations as mass range, sample introduction facilities, programming and data handling systems, scan rate, maintenance requirements, and price must all be evaluated relative to the needs and facilities available in a specific laboratory.

1.2 *This standard may involve hazardous materials, operations, and equipment. This standard does not purport to address all of 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. Reference to This Practice in Standards

2.1 The inclusion of the following paragraph, or suitable equivalent, in any ASTM mass spectrometric method (preferably after the section on Scope) shall constitute due notification that mass spectrometers to be used with that method are to be evaluated in accordance with the recommendations set forth in this practice.

Evaluation of Mass Spectrometers—The suitability of mass spectrometers for use with this method of analysis shall be evaluated by means of performance tests described in this method and in ASTM Practice E 137, for Evaluation of Mass Spectrometers for Quantitative Analysis from a Batch Inlet.

3. Terminology

3.1 *Mass Spectrometer or Mass Spectrometric*—The term mass spectrometer or the adjectival form, mass spectrometric, shall apply to all apparatus in which an analysis of matter is effected by means of ionization of the matter followed by separation of the ions according to mass-to-charge ratio and recording of a measure of the numbers of the various ions.

3.2 *Background*—The term background refers to the response (mass spectrum) obtained from a mass spectrometer with operating conditions the same as those used for sample analysis except that the sample is absent.

3.3 *Sensitivity*—The sensitivity of a mass spectrometer for a particular compound is a measure of the response of the instrument, per unit of sample, at a specified mass peak under specified operating conditions.

3.4 *Resolution*—The resolution of a mass spectrometer refers to the ability of the instrument to distinguish between two adjacent mass peaks under given experimental conditions: Two adjacent peaks of equal height are said to be resolved when the minimum height above base line in the valley between them is less than 10 percent of the common peak height. The resolution exhibited by two adjacent peaks of equal height is defined numerically as the ratio of their average mass to the mass difference between them when a valley condition of 10 percent prevails. A statement of mass-to-charge ratios for the peaks used is pertinent to a comparison of resolution data, because different instrument types show differences in the variation of resolution with mass-to-charge ratio.

NOTE 1—Alternatively, the resolution R achieved at any isolated peak in a mass spectrum may be calculated from the equation $R = m/\Delta m$, where m is the mass corresponding to the peak and Δm is the width (in mass units) at 5 percent of the peak height.

The equation is better adapted to typical experimental data than the 10 percent valley definition, but is technically equivalent to it, provided the peak is symmetrical and the mass spectrometer system linear in the range between the 5 and 10 percent levels of the peak. The equation and definition are in practice equivalent within the range of typical deviations from symmetry and linearity.

3.5 *Interference*—The term interference refers to an instrumental condition which prevents attaining the usual accuracy in determining the concentration of a component in a sample mixture.

3.6 *Test Mixture*—The term test mixture refers to a mixture of known composition that is similar to the composition of a sample to be analyzed. A test mixture is usually obtained by mixing measured quantities of pure materials.

4. General Criteria

4.1 The suitability of a particular mass spectrometer for use in a given analysis may be judged on the basis of the answer to these questions:

4.1.1 Has the design of the apparatus previously been proven acceptable for this or a similar analysis?

[1] This practice is under the jurisdiction of ASTM Committee E-14 on Mass Spectrometry and is the direct responsibility of Subcommittee E 14.14 on General Practices.

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In 1968, the practice was revised editorially, its scope was clarified, Section 3 was revised to recommend a definition of resolution, and the discussion of reproducibility in Section 4 was referenced to ASTM Recommended Practice E 177.