Designation: E1950 – 17

Standard Practice for Reporting Results from Methods of Chemical Analysis[1]

This standard is issued under the fixed designation E1950; 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 the approximate number of digits required to express the expected precision of results reported from standard methods of chemical analysis. This practice provides selection criteria and proper form and symbols for coding results when necessary to indicate the relative reliability of results having small values.

1.2 Specifically excluded is consideration of report forms and the associated informational content of reports in which results are tabulated or transmitted. It is assumed that the reporting laboratory has established a report format to ensure proper identification of the materials tested, the nature and conditions of the test, the responsible personnel, and other related information in accordance with existing regulations and good laboratory practices.

1.3 *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]

E29 Practice for Using Significant Digits in Test Data to Determine Conformance with Specifications

E135 Terminology Relating to Analytical Chemistry for Metals, Ores, and Related Materials

E1601 Practice for Conducting an Interlaboratory Study to Evaluate the Performance of an Analytical Method

E1763 Guide for Interpretation and Use of Results from Interlaboratory Testing of Chemical Analysis Methods (Withdrawn 2015)[3]

3. Terminology

3.1 *Definitions:*

3.1.1 For definitions of terms, refer to Terminology E135.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *lower limit, L, n*—the lower limit of the quantitative analyte mass fraction or concentration range (see Annex A1).

3.2.2 *low-level reproducibility index, K_R, n*—the reproducibility index constant (for low analyte levels) determined as directed by Guide E1763.

3.2.3 *null limit, NL, n*—the analyte content below which results are so near zero that averaging is unlikely to yield a value significantly different from zero.

3.2.4 *quantitative, adj—relating to results*, having a numerical value that includes at least one significant digit (see Practice E29).

4. Significance and Use

4.1 A result must be stated to a sufficient number of digits so that a user receives both quantitative information and a measure of the variability of the value reported.

4.2 The range of application of most methods of chemical analysis is based upon the presumption that the quantitative results produced are to be used to compare the analyte content of the test material with specified limiting values. However, analytical results may be used legitimately for other purposes. If the same material is analyzed a number of times or a product is analyzed periodically during an interval of production, each set of results may be averaged to yield an average result having improved reliability, provided nothing has been done between analyses to modify the composition of the analyzed material. Results that fall below the lower limit, although not quantitative individually, contain compositional information and may be reported. The reporting system in this practice permits the analyst to indicate which values are likely to be rendered quantitative by averaging and which are not.

[1] This practice is under the jurisdiction of ASTM Committee E01 on Analytical Chemistry for Metals, Ores, and Related Materials and is the direct responsibility of Subcommittee E01.22 on Laboratory Quality.

Current edition approved Nov. 15, 2017. Published December 2017. Originally approved in 1998. Last previous edition approved in 2010 as E1950 – 10. DOI: 10.1520/E1950-17.

[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.

[3] The last approved version of this historical standard is referenced on www.astm.org.

4.3 The system is simple enough to be used routinely in reporting results from standard methods and assists those untrained in statistics to apply results appropriately.

5. Rounding Calculated Values

5.1 Use information from the precision section of the method to determine the appropriate number of digits to report as follows:

5.1.1 Estimate the reproducibility index, *R*, at the analyte level of the result, *C*, from an equation of *R* as a function of concentration or mass fraction, or from the table of statistical information.

5.1.2 Calculate the percent relative reproducibility index:

$$R_{rel\%} = 100 \times R/C \quad (1)$$

5.1.3 For results within the range of application specified in the method, round the values to the number of digits specified in Table 1 (see A1.1.1 through A1.1.2).

5.1.4 For results less than the lower limit, proceed as directed in Section 6 to establish the number of digits and appropriate coding for rounding and reporting the values.

5.2 Calculated values shall be rounded to the required number of digits in accordance with the rounding method of Practice E29.

6. Procedure

6.1 *Preliminary Precaution*—For a method to be used to analyze materials with analyte content very near zero, the analyst shall determine that it is capable of producing "unbiased" estimates of zero. If the method occasionally yields negative results for low analyte levels, that capability is demonstrated. Proceed as directed in 6.2.

6.1.1 *Test for "Biased-Zero" Methods*—Prepare the method to perform determinations. Include all aspects of instrument preparation and calibration. Apply the method to a "blank" sample or one known to have negligible analyte content but that meets the method's scope requirements in all other respects. If the method yields a negative result, it is not a "biased-zero" method as directed in 6.2. If, during the course of at least ten replicate determinations, several zeros but no negative values are observed, it is a "biased-zero" method. Apply the biased-zero rule of 6.4 in reporting results lower than *NL* (see 6.2.2).

6.2 *Critical Concentrations or Mass Fractions:*

6.2.1 From the method, obtain the value of the lower limit, *L*, to two digits (add a final zero, if necessary). Determine the decimal place of the second digit.

TABLE 1 Rounding Guide

$R_{rel\ \%}$	Number of Digits
5 % – 50 %	2
0.5 % – 5 %	3
0.05 % – 0.5 %	4
< 0.05 %	5

6.2.2 Calculate the null limit as follows:

$$NL = L/4 \quad (2)$$

6.3 *Basic Rules:*

6.3.1 Numerical values shall be reported for every result (including negative values) obtained from a properly conducted method except as provided for certain results from "biased-zero" methods as directed in 6.1.1 and 6.4.

6.3.2 *Results Less Than L*—Round values to the second decimal place of *L*, and enclose in parentheses before reporting. Examples: For *L* equal to 1.5, round to x.x and report (x.x); for *L* equal to 0.22, round to 0.xx and report (0.xx); for *L* equal to 0.00050, round to 0.000xx and report (0.000xx).

6.3.3 *Results Less Than NL*—If the method is "biased-zero," treat as directed in 6.4; otherwise, round in accordance with 6.3.2, and enclose in parentheses followed by an asterisk before reporting. Examples: (–0.2)*, (0.04)*, and (–0.00003)*.

6.4 *Special Rule for "Biased-Zero" Methods:*

6.4.1 For results from "biased-zero" methods only, do not report numerical values for results less than *NL*. Replace them with the symbol (– –)*.

6.5 *Reference to the Method:*

6.5.1 Cite the designation of the standard method used to determine each analyte reported.

6.6 *Explanations of Coding Symbols:*

6.6.1 If results less than *L* are reported for any analyte, append the following explanation (results in parentheses are not reliable for individual comparisons):

6.6.2 If results less than *NL* are reported for any analyte, append the following explanation: * These values cannot be distinguished from zero.

6.6.3 If the symbol (– –)* is reported for any analyte, append the following explanation: (– –)* The method cannot report an unbiased estimate at this low analyte level.

7. Use of Uncoded and Coded Values

7.1 *Uncoded Data:*

7.1.1 Numerical values reported not enclosed in parentheses are quantitative results and may be used for comparisons with specified limiting values.

7.2 *Coded Data:*

7.2.1 Values enclosed in parentheses are not quantitative, that is, individual values are not suitable for comparisons. However, data in parentheses not followed by an asterisk may yield values that are quantitative if a sufficient number are averaged (see A2.2.3).

7.2.2 Values coded with an asterisk are from materials that are likely to produce randomly occurring negative values for repeated determinations. They may be averaged, but unless the average includes a large number of individual results (more than 25), even the first digit is not likely to be significant.

8. Keywords

8.1 quantitative results; reporting results

ANNEXES

(Mandatory Information)

A1. STATISTICAL BASIS FOR QUANTIFICATION CRITERIA

A1.1 Quantification is the ability to determine a result whose value may be compared with specified limiting values. Practice E29 adds the concept of significant digits. This term is used in this practice to identify the digits in a value that are not expected to change appreciably if the result is redetermined. The statistical basis for quantification is found in Practice E1601 and Guide E1763. The lower limit (L) of a method's quantitative range is calculated from its reproducibility index, *R*, which is determined in the interlaboratory study (ILS). The analyte content of a material must be greater than that limit if results are to exhibit at least one significant digit.

A1.1.1 *R* represents the largest difference between results obtained in two laboratories on the same material that is not expected to be exceeded in more than 1 in 20 comparisons (95 % confidence level). *L* is arbitrarily defined as the analyte content at which *R* represents a 50 % relative error. At this analyte content, the average difference (50 % confidence level) between results in two laboratories is about 18 % of their mean. A result at this analyte level is quantitative with approximately one significant digit, and, as directed in Practice E29 and common statistical practice, is reported with two digits to preserve the statistical information it contains. Only the first digit is considered significant.

A1.1.2 Users of standard methods (or data obtained from them) can use *R* values reported at the analyte levels of the test materials (Practice E1601) or the equation relating *R* to analyte concentration or mass fractions (for ILS evaluated as directed in Guide E1763) to estimate the reliability of data at any concentration within the quantitative range of the method. If $R_{rel\%}$ is 5 % or less relative to the determined value, report results with three digits (the first two are significant.) If $R_{rel\%}$ is 0.5 % or less, report four digits (the first three are significant.) If $R_{rel\%}$ is 0.05 % or less, report five digits (the first four are significant.)

A1.2 Results from materials with analyte content less than *L* are not quantitative as defined in this practice, but their values contain information concerning the analyte content. These results are reported, but their use for individual comparisons is discouraged.

A1.2.1 Guide E1763 provides calculations for K_R, the constant value *R* achieves at analyte contents near *L* and lower. This value of *R* divided by 2.8 yields the reproducibility standard deviation, s_R, which, added to and subtracted from a result, signifies a confidence interval. While indicating uncertainty, this approach does not lend itself to easy recognition of a value's reliability because the user must apply a rather complex interpretive process to decide how the data may be used.

A1.2.2 The user, if willing to expend time and resources, can reduce variability by averaging a number of results from the same material obtained in different laboratories. For example, if a material having an analyte content of *R* is analyzed once in four laboratories, the relative variability of such an average (four values) is 50 %, the same as the variability of single results from a material with twice the analyte content (that is, at *L*).

A1.2.3 The limit to the enhancement in precision by replication is established only by the resources the user is willing to expend. A reasonable (though arbitrary) limit is the null limit, *NL* = *R/2* (which is equivalent to *L*/4). The null limit is the lowest analyte level at which the average of 16 or more results yields an average value having at least one significant digit. Results below *NL* are, for practical purposes, indistinguishable from zero.

A2. PRACTICAL BASIS FOR QUANTIFICATION CRITERIA

A2.1 The practical basis for quantification must provide guidance to analysts and users of results who have little statistical training. The criteria should be consistent with the ILS statistics and criteria discussed in Annex A1, simple to understand, and convenient to use. The coding applied to each value should give an unmistakable visual indication of its reliability.

A2.2 A system to meet these requirements classifies results into three concentration or mass fraction ranges:

A2.2.1 Class 1 consists of results with values falling between the upper and lower application limits stated in the method. These results are expected to be quantitative as discussed in Annex A1.

A2.2.2 Class 3 consists of results with values less than *NL*. As discussed in A1.2.3, not only are individual results not quantitative, but averages are also unlikely to be quantitative. Individual and average values that are less than *NL* are expected to be estimates of zero.