Designation: E 1950 – 98 (Reapproved 2003)

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

This standard is issued under the fixed designation E 1950; 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.

2. Referenced Documents

2.1 *ASTM Standards:* [2]

E 29 Practice for Using Significant Digits in Test Data to Determine Conformance with Specifications

E 135 Terminology Relating to Analytical Chemistry for Metals, Ores, and Related Materials

E 1601 Practice for Conducting an Interlaboratory Study to Evaluate the Performance of an Analytical Method

E 1763 Guide for Interpretation and Use of Results from the Interlaboratory Testing of Chemical Analysis Methods

3. Terminology

3.1 *Definitions:*

3.1.1 For definitions of terms, refer to Terminology E 135.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *lower limit, L, n*—the lower limit of the quantitative analyte concentration range.

3.2.2 *low-level reproducibility index,* K_R, *n*—the reproducibility index constant (for low analyte levels) determined in accordance with Guide E 1763.

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 E 29).

4. Significance and Use

4.1 A result should 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. Results that fall below the lower limit, although not quantitative individually, contain compositional information and shall 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.

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 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 in accordance with Section 6 to establish the number of digits and appropriate coding for rounding and reporting the values.

[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 Statistics and Quality Control.

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[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.

TABLE 1 Rounding Guide

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

5.2 Calculated values shall be rounded to the required number of digits in accordance with the rounding-off method of Practice E 29.

5.2.1 The procedure is summarized as follows:

5.2.1.1 When rounding off a number to a specified number of digits, choose that digit that is nearest. If two choices are possible, as when the digits dropped are exactly a five or a five followed only by zeros, choose that ending in an even digit.

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 in accordance with 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 a 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; proceed in accordance with 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*:

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.

6.2.2 Calculate the null limit as follows:

$$NL = L / 4 \tag{2}$$

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 in accordance with 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 a "biased-zero" procedure, treat in accordance with 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:

NOTE 1—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 without enclosing 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 QUANTITATION CRITERIA

A1.1 Quantitation is the ability to determine a result whose value may be compared with specified limiting values. Practice E 29 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 quantitation is found in Practice E 1601 and Guide E 1763. 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. Results at this analyte level are quantitative with approximately one significant digit, and, in accordance with Practice E 29 and common statistical practice, are 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 E 1601) or the equation relating *R* to analyte concentration (for ILS evaluated in accordance with Guide E 1763) 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 E 1763 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 ultimate 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 QUANTITATION CRITERIA

A2.1 The practical basis for quantitation 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 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.

A2.2.3 Class 2 consists of results with values falling within the range *NL* to *L*. Individual results are not quantitative, but averages of values obtained in different laboratories may be quantitative. The number of values needed to obtain a quantitative average ranges from 2 (at analyte levels just less than *L*) to 16 (at analyte levels just greater than *NL*).

A2.3 The classifications in A2.2 meet the requirements in A2.1. The analyst classifies each result by comparing its value with *L* (from the method's scope) and the calculated value of *NL* (*L*/4). Class 1 results are quantitative and are reported uncoded. Class 2 and Class 3 results are not quantitative; this fact is visually indicated by enclosing their values in parentheses. Class 2 results produce quantitative values if a sufficient number of independent results are averaged. Class 3 results are unlikely to produce quantitative average values, a fact visually indicated by enclosing the results in parentheses and adding an asterisk. This type of coding is simple, easy to implement and interpret, and does not affect the readability of tables of data.

APPENDIXES

(Nonmandatory Information)

X1. EXAMPLE DATA SHEET

X1.1 Table X1.1 shows 140 individual "results," values generated to simulate an experiment in which 7 perfectly homogeneous test materials having precisely known analyte contents are analyzed in 20 laboratories. Each laboratory reports one result on each material by a hypothetical method with K_R = 10 ppm. This value defines a lower limit for the method, L = 20 ppm (2 × 10) with a compatible standard deviation s = 3.57 (10/2.8). Each column represents results on one material entered in random order from the 20 laboratories. The simulation was performed by a gaussian random number generator programmed with a target mean given in the second row, and a constant variance, s^2 = 12.75 (3.57^2) at all analyte levels. The last row is the overall mean calculated from the material's set of "results."

X1.2 The variability of the results produced in the "experiment" is illustrated in Fig. X1.1.

TABLE X1.1 Simulated Results on Seven Materials from 20 Laboratories

Materials	A	B	C	D	E	F	G
True Mean	0.0000	1.0000	3.0000	5.0000	10.0000	20.0000	30.0000
Results:	-1.2055	-1.8667	4.3772	2.5625	9.5295	21.2178	24.5598
	-1.4262	4.4129	0.5831	3.8934	12.2836	13.9872	22.1545
	-0.4879	-2.1661	2.1894	4.1062	8.4187	19.9914	30.2173
	2.7263	0.8737	5.4585	6.3108	8.2525	17.9124	25.2355
	-2.8056	5.5317	-0.5221	6.2797	7.8461	16.6178	40.3682
	-1.4790	6.2286	-1.3163	7.0328	11.4863	22.4489	25.7696
	-5.4582	1.3555	5.1616	6.3471	5.0689	19.5272	27.3613
	-2.3611	1.7518	1.9906	0.2592	6.9597	21.7442	28.9738
	8.0726	-3.8839	-0.9715	5.3175	5.4757	18.1735	27.7038
	3.0421	-1.5017	5.2627	5.2597	12.6711	19.4886	30.9384
	1.3096	5.1467	4.8310	5.5132	5.2709	17.2867	37.3759
	3.8391	2.0727	2.2742	12.2686	5.3672	21.0485	31.2484
	0.5921	3.2007	-0.8770	10.2378	12.7390	17.0270	30.0894
	0.5733	5.9204	-4.7310	6.2747	10.2593	24.9998	31.1189
	3.4663	3.2555	10.8880	7.2903	10.4080	20.5334	35.3467
	-6.3054	0.7760	0.1440	-1.7807	8.2812	16.9223	30.1850
	-2.8220	-2.6817	-0.1913	3.6913	6.3722	21.0028	33.4930
	0.2221	-4.9717	8.0554	10.7651	14.4328	20.4181	20.3663
	-5.3279	3.7239	7.2435	7.8044	9.2613	20.9088	27.6414
	-0.3564	5.8184	9.3255	4.9202	2.0921	16.4079	35.2876
Mean, x	-0.3096	1.6498	2.9588	5.7177	8.6238	19.3832	29.7717

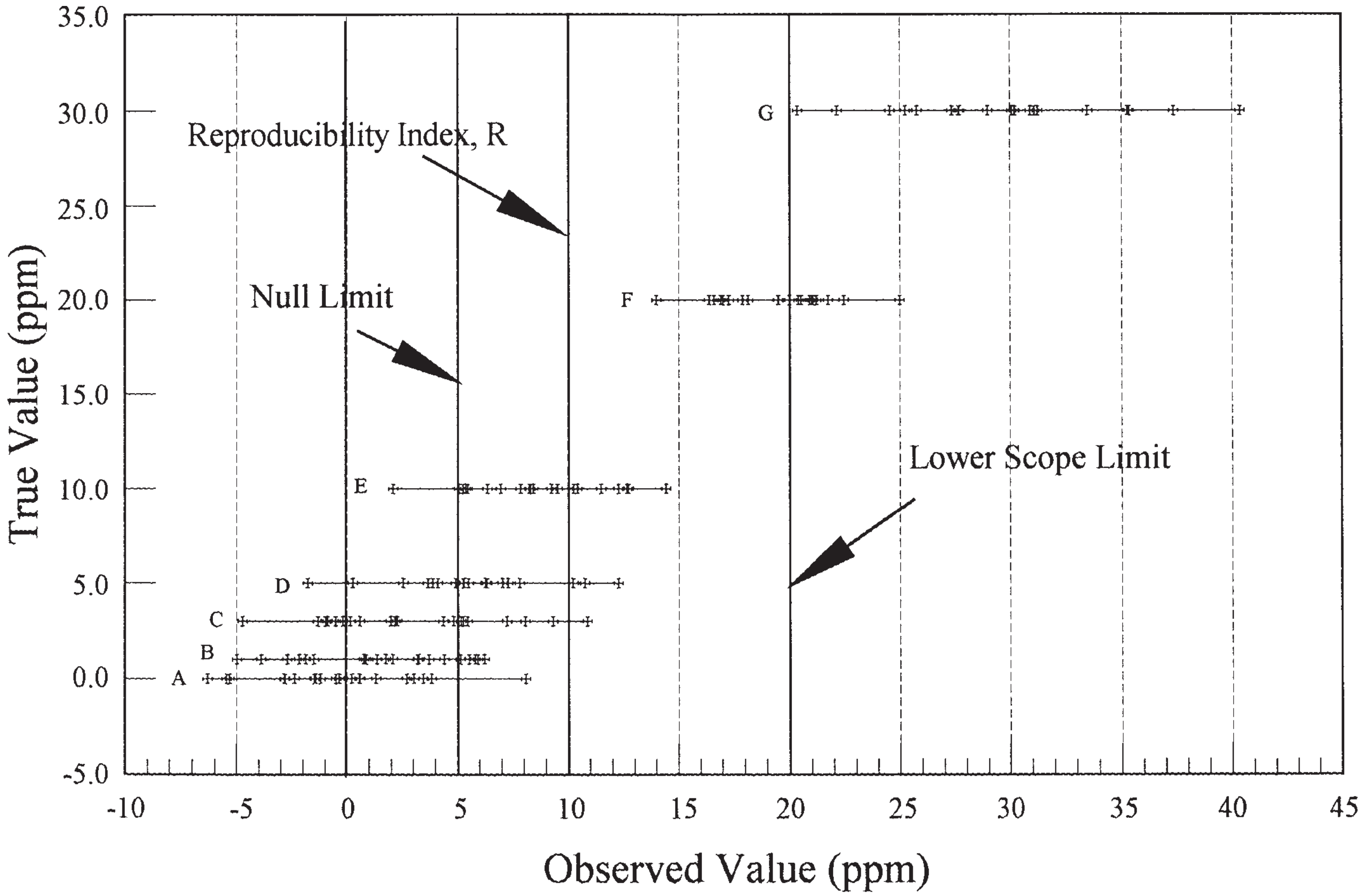

FIG. X1.1 Results From 20 Laboratories

X2. EXAMPLES OF REPORTED RESULTS

X2.1 *Analyst/Laboratory Reports*—Individual results are reported in accordance with procedures outlined in Section 6. In these examples, data values have been selected with the aid of a random number table from the appropriate column of Table X1.1. The method's parameters are: L = 20 and NL = 5.

X2.1.1 *Example 1*—A laboratory is requested to perform a single determination on samples B, D, E, and F. It reports the following results:

SAMPLE	Analyte, ppm	REMARKS
B	(4)*	Note: Results in parentheses are not reliable
D	(6)	for individual comparisons.
E	(7)	* These values cannot be distinguished from
F	(17)	zero.

X2.1.2 *Example 2*—An investigator wishes to find the analyte content of materials B, D, E, and G. He sends a test portion to four laboratories requesting a single determination from each. The results from the individual lab reports, each of which should be similar to Example 1, are shown in Table X2.1.

NOTE X2.1—The investigator and analysts in real life have no way of knowing "true" values. However, in this simulation, "true" values are the "true mean" values in Table X1.1. They may be compared with the calculated "average" in Table X2.1 to find the actual "error." For averages of 4, NL = 2.5, R = 5, and L = 10 (the method statistics divided by 2).

TABLE X2.1 Results for Four Materials[A]

Laboratory	Material B	Material D	Material E	Material G
1	(3)[B]	(7)	(14)	31
2	(1)[B]	(10)	(10)	28
3	(6)	(11)	(13)	28
4	(3)[B]	(7)	(10)	20
Average	(3)	(9)	12	27
Rel. error, %	+200 %	+80 %	+20 %	-10 %

[A] Values in parentheses are not reliable for individual comparisons.
[B] These values cannot be distinguished from zero.

X2.2 *Use of Standard Methods at Extremely Low Levels*—To illustrate the improvement averaging achieves, consider the first 16 results for materials A, C, E, and G as data obtained by a research group from various laboratories. The group wishes to know the level of analyte in each material. The group knows that the method has a lower limit of 20 ppm, null limit of 5 ppm, and that s_R is 3.57. These statistics are for single results. Averaging 16 results divides these values by 4, the square root of 16. For averages of 16 results, the standard deviation is 0.89, NL is 1.25, R is 2.5, and L is 5.0. This level of improvement assumes results from 16 independent laboratories, not 4 replicate results from only 4 laboratories, for example. Table X1.1 represents individual results from independent laboratories, so its data should demonstrate the expected improvement. Table X2.2 shows the data received by the group and the averages and standard deviations calculated from them.

TABLE X2.2 Data from 16 Laboratories[A]

NOTE—The root-mean-square average of the "experimental" standard deviations for A, C, E, and G is 3.73. Divided by 4, it gives an "average" standard error of the mean of 0.93 (means of 16). This compares well with the predicted value of 0.89. The group (correctly) identifies the experimental mean for A as an estimate of zero because it is less than 1.25, the *NL* for means of 16. The experimental mean for C is not an estimate of zero because it is greater than *NL*, but it is inappropriate for comparison with limiting values because it is less than 5.0, *L* for means of 16. The means for E and G are greater than 5.0 and may be compared with limiting values. Both are quantitative with a significant first digit and a second digit to convey variability information. This information is compactly displayed in the report format exhibited after the equals sign in the "Mean Value" column. If this were real experimental data, the group would have no way of knowing how close the means calculated from the experimental data are to the "true" values. It would depend upon the laws of probability to support an expectation that 19 of 20 comparisons made in this manner would achieve correct conclusions.

Material	Results	Mean Value	Calc. SD
A	(-1)[B] (-1)[B] (0)[B] (3)[B] (-3)[B] (-1)[B] (-5)[B] (-2)[B]	0.31 =	3.5
	(8) (3)[B] (1)[B] (4)[B] (1)[B] (1)[B] (3)[B] (-6)[B]	(0.3)[B]	
C	(4)[B] (1)[B] (2)[B] (5) (-1)[B] (-1)[B] (5) (2)[B]	2.06 =	3.8
	(-1)[B] (5) (5)[B] (2)[B] (-1)[B] (-5)[B] (11) (0)[B]	(2.1)	
E	(10) (12) (8) (8) (8) (11) (5) (7)	8.62 =	2.8
	(5) (13) (5) (5) (13) (10) (10) (8)	8.6	
G	(25) (22) (30) (25) (40) (26) (27) (29)	29.8 =	4.6
	(28) (31) (37) (31) (30) (31) (35) (30)	30	

[A] Values in parenthesis are not reliable for individual comparisons.
[B] These values cannot be distinguished from zero.