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ANALYTICAL CHEMISTRY DIVISION
COMMISSION ON ANALYTICAL NOMENCLATURE

RECOMMENDATIONS FOR THE PRESENTATION OF THE RESULTS OF CHEMICAL ANALYSIS

A Report prepared by

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Introduction. This report was prepared by R. W. Fennell (U.K.) and T. S. West (U.K.) on behalf of the commission. It was circulated to all members of the Division and, following moderation, was presented for further comment in the IUPAC Information Bulletin No. 26. This final version is presented in the light of all comments received.

The value of much published research work on chemical analysis is diminished by the lack of a generally accepted system of reporting numerical results. It is seldom that a research worker is able to plan collaborative work for detailed statistical study or, indeed, to carry out more than a short series of replicate determinations in his own laboratory. In the development of a new analytical method, synthetic samples or standard materials of known (assumed) composition are normally used to test the proposed method and it is further assumed that the materials are homogeneous and that sampling errors are negligible. The results of chemical analyses done under the conditions outlined above are, however, amenable to simple statistical treatment.

The following list is designed to provide the necessary means for reporting results in a standardized form with the intention that, by using these terms and symbols, an author may report his data unambiguously without further explanation of terminology or method of computation. Only if other terms were used would it be necessary for the author to define his meaning.

The proposed list includes both statistical terms, *e.g.* 'standard deviation', and other non-statistical terms, *e.g.* 'per cent absolute', which are required by the analytical chemist, but which frequently cause confusion even though they are in common use, because differing meanings are attributed to them. The statistical terms are defined according to the practical requirements of the analytical chemist who is normally only concerned with short series. Only the minimum of requirements has been incorporated in the list, but the same terms may be used in more advanced statistical treatment.

Readers who are unfamiliar with the elementary theory of statistics may find it useful to consult an introductory text before using these terms.

1. General terms

1.1. MEASURED VALUE. The observed value of the weight, volume, meter-reading or other quantity found by the chemist in his analysis of a material.

1.2. RESULT. The final value reported for a measured quantity after performing a measuring procedure including all sub-procedures *and* evaluations.

1.3. VARIATE. The numerical value taken for statistical handling; it may, for example, be a measured value or result. Symbol: x†.

1.4. SERIES. A number of variates (x_1, x_2, $x_3 \ldots x_n$) equivalent to each other with respect to statistical considerations, *e.g.* the results of repeated analyses using only one analytical method on a substance which is presumed to be homogeneous.

2. Reliability of results

2.1. ACCURACY. Accuracy relates to the difference between a result (or mean) and the true value.

2.2. PRECISION. Precision relates to the variations between variates, *i.e.* the 'scatter' between variates.

3. Expression of results

A. In relation to precision

The reported data should include items 3.01, 3.03 or 3.04 and 3.07.

3.01. MEAN (AVERAGE). The sum of a series of variates divided by the number of variates in the series. Symbol: $\bar{x}$.

3.02. DEVIATION. The difference between a variate and the mean of the series to which it belongs. Symbol: d‡.

3.03. RANGE§. The difference between the highest and lowest results of measured values in a series.

3.04. STANDARD DEVIATION‖. The square root of the sum of the squares of the deviations between the variates and the mean of the series, divided by one less than the total number¶ in the series. Symbol: s**.

3.05. VARIANCE††. The square of the standard deviation. Symbol: V.

3·06. RELATIVE STANDARD DEVIATION‡‡. The standard deviation divided by the mean of the series. Symbol: S_r§§.

3.07. NUMBER OF VARIATES. The total number of variates in the series. Symbol: n‖‖.

† In circumstances where 'x' may cause confusion another symbol, *e.g.* 'z', may be used.

‡ The symbol 'e' (French: écart) is recommended in place of the commonly used symbols 'd' or 'δ' (Greek, delta) where their use may cause confusion.

§ This term should only be used where there are insufficient data available for calculation of standard deviation. The estimation of standard deviation from range-tables under these circumstances is not recommended.

‖ The term 'Standard error' in place of 'Standard deviation' is not recommended.

¶ The number of variates necessary to obtain a meaningful standard deviation may be assessed by reference to *Table 1*, Appendix I.

** The symbol 'σ' (Greek, sigma) should not be used.

†† This term is not normally reported by the analytical chemist, but is used in the process of statistical calculation.

‡‡ It is recommended that Relative standard deviation should be reported as a decimal fraction *not* as a percentage, in order to avoid confusion where results themselves are reported as percentages.

§§ The term 'Coefficient of variation' in place of 'Relative standard deviation' is not recommended.

‖‖ This number should *always* be reported.

B. In relation to accuracy

3.08. ERROR. The value of a result† minus the true value.

3.09. PERCENTAGE ERROR‡. The error expressed as a percentage of the true value.

3.10. BIAS. The mean of the differences, having regard to sign, of the results from the true value. This equals the difference between the mean of a series of results and the true value.

3.11 PERCENTAGE RECOVERY. A result expressed as a percentage of the true value.

4. Symbols

Variate	x
Series	$x_1, x_2, x_3. \dots x_n$
Number in series	n
Series sum	$\sum x$
Mean (Average)	$\bar{x}$
Deviation	d
Variance	V
Standard deviation	s

5. Methods of computation

A. From a series of variates at one level of the quantity being determined

Mean $\bar{x} = \frac{1}{n}\sum x$

Deviation $d = | x - \bar{x} |$

Standard deviation $s = \left(\frac{1}{n-1}\sum d^2\right)^{\frac{1}{2}} = \left(\frac{1}{n(n-1)}[n\sum x^2 - (\sum x)^2]\right)^{\frac{1}{2}}$

$$= \left(\frac{1}{(n-1)}\left[\sum x^2 - \frac{(\sum x)^2}{n}\right]\right)^{\frac{1}{2}}$$

Variance $V = s^2$

Relative standard deviation $s_r = \frac{S}{\bar{x}}$

B. Computation of pooled standard deviation (symbol: s_g) from more than one series of variates over a range of levels of the quantity being determined

(i) For each series, having $n_1, n_2, \dots . n_g$ variates respectively, compute the mean and sum the squares of the deviations. $\sum d_1{}^2 + \sum d_2{}^2 + \dots \sum d_g{}^2$

(ii) Divide the above sum of squares by the total number of variates

† Where a result is reported as a percentage this term will, of course, appear as a percentage. In these circumstances, in order to differentiate between this term and 'Percentage error'—see 3.09—it is permissible to refer to the error as 'Percent absolute'.

‡ The term 'Percentage error' must be quoted in full rather than 'Error' to avoid confusion with the term 'Error' as defined above. The term 'Relative error' should not be used.

$(n_1 + n_2 + n_3 + \ldots . n_g)$ minus the number of series being considered (g).
(iii) Derive the square root of the above quotient.

$$s_g = \left[\frac{\sum d_1^2 + \sum d_2^2 + \ldots . \sum d_g^2}{(n_1 + n_2 + \ldots . n_g) - g}\right]^{\frac{1}{2}}$$

APPENDIX I

In reporting results in relation to the precision of working, it should be noted that the number of variates '*n*' should always be quoted because this allows readers of a paper to form an opinion of the reported data. This is particularly important where only a standard deviation (s) is recorded. The distribution of variates about the mean closely follows a normalGaussian law in chemical analysis. The probability of a single value falling within $\pm\, t{\cdot}s$ of the mean, $\bar{x}$ of a finite series depends on the number, n, in the series. *Table 1*, based on Gaussian distribution, shows the appropriate value of '*t*' for different probability levels and values of '*n*'.

Table 1

Probability level, n	*t* 95%	99%	99·7%
2	12·71	63·66	235
3	4·30	9·92	19·2
4	3·18	5·84	9·22
5	2·78	4·60	6·62
6	2·57	4·03	5·51
7	2·45	3·71	4·90
8	2·37	3·50	4·53
9	2·31	3·36	4·27
10	2·26	3·25	4·09
25	2·06	2·80	3·34
∞	1·96	2·58	3·00