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Contraction Designation

Designation: D 596 – 91 (Reapproved 1995)

AMERICAN SOCIETY FOR TESTING AND MATERIALS 100 Barr Harbor Dr., West Conshohocken, PA 19428 Reprinted from the Annual Book of ASTM Standards. Copyright ASTM

Standard Practice for Reporting Results of Analysis of Water¹

This standard is issued under the fixed designation D 596; 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.

This standard has been approved for use by agencies of the Department of Defense. Consult the DoD Index of Specifications and Standards for the specific year of issue which has been adopted by the Department of Defense.

1. Scope

1.1 This practice provides guidelines for the reporting of results of water analyses, including drinking water, wastewater, process water, ground water, and surface water, to laboratory clients in a complete and systematic fashion. Adequate documentation must be provided on the sample analyzed, the methods of analysis used, the results obtained, the precision and bias of the measurements, and related quality assurance information.

1.2 Results of chemical analysis of water shall be reported as a weight/volume ratio, such as milligrams per litre (mg/L), milliequivalents per litre (meq/L), etc., when concentration is being determined.

1.3 Results of other tests, such as pH, radioactivity, or turbidity, shall be reported as specified in the individual test methods.

1.4 The values stated in SI units are to be regarded as the standard.

1.5 This standard does not purport to address all of the safety concerns, if any, 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:

- D 933 Practice for Reporting Results of Examination and Analysis of Water-Formed Deposits ²
- D 1129 Terminology Relating to Water³
- D 2777 Practice for Determination of Precision and Bias of Applicable Methods of Committee D-19 on Water ³
- D 3856 Guide for Good Laboratory Practices in Laboratories Engaged in Sampling and Analysis of Water ³
- D 4210 Practice for Intralaboratory Quality Control Procedures and a Discussion on Reporting Low-Level Data ³
- D 4460 Practice for Calculating Precision Limits Where

² Annual Book of ASTM Standards, Vol 11.02.
³ Annual Book of ASTM Standards, Vol 11.01.

Values are Calculated from Other Test Methods ⁴ E 29 Practice for Using Significant Digits in Test Data to Determine Conformance With Specifications ⁵ ES 16 Practice for Generation of Environmental Data Related to Waste Management Activities ⁶

3. Terminology

3.1 Definitions—For definition of terms used in this practice, refer to Terminology D 1129 and Practice ES 16.

3.2 Definitions of Terms Specific to This Standard:

3.2.1 *milliequivalent per litre* (meq/L)—a weight-volume measurement obtained by multiplying the concentration expressed in moles per litre by the ionic charge or by the change in oxidation number of the substance in a defined reaction.

3.2.2 milligrams per litre (mg/L)—a weight-volume measurement that expresses the concentration of a solute in milligrams (10^{-3} g) in a litre of solution.

3.2.3 micrograms per litre ($\mu g/L$)—a weight-volume measurement that expresses the concentration of a solute in micrograms (10⁻⁶ g) in a litre of solution.

3.2.4 *surrogates*—compounds that are similar to analytes of interest in chemical composition and behavior, separation, and measurement, but that are not normally found in environmental samples. These compounds are added to blanks, standards, samples, or spiked samples prior to analysis to confirm the proper operation of the analytical system.

4. Significance and Use

4.1 The proper use of analytical data requires adequate documentation of the source and history of the sample, laboratory performing the analysis, method of analysis, date of analysis, precision and bias of the measurements, and related quality assurance information.

4.2 Tables are included for interconversion of data between units in common use.

4.3 Other information on reporting results may be included in individual test methods for the analysis of water.

4.4 For corresponding information regarding the reporting of results for water-formed deposits, see Practice D 933.

¹ This practice is under the jurisdiction of ASTM Committee D-19 on water and is the direct responsibility of Subcommittee D19.02 on General Specifications, Technical Resources, and Statistical Methods.

Current edition approved Sept. 15, 1991. Published February 1992. Originally published as D 596 – 40. Last previous edition D 596 – 83.

⁴ Annual Book of ASTM Standards, Vol 04.03.

⁵ Annual Book of ASTM Standards, Vol 14.02.

⁶ See 1991 Annual Book of ASTM Standards, Vol 11.04.

5. Sample Documentation

5.1 Information regarding the source and history of the sample to be included in the analytical report should define the sample and include the following, as appropriate:

5.1.1 Laboratory performing analysis,

5.1.2 Name and address of organization or person requesting analysis,

5.1.3 Specific location of sampling and complete identification of sample,

5.1.4 Date and time of sampling,

5.1.5 Sample identification number, and

5.1.6 Sampling method, treatment, and preservation.

5.2 In addition to the information in 5.1, the following information should be included as appropriate:

5.2.1 Identification of sampling organization and individual sampler,

5.2.2 Pressure and temperature of system sampled,

5.2.3 Flow rate of water in a stream,

5.2.4 Copies of sampling logs with signatures,

5.2.5 Chain of custody forms with signatures,

5.2.6 Results of field measurements, and

5.2.7 Description information (color, odor, etc.) clearly presented.

6. Analysis Documentation

6.1 As described in Guide D 3856, the test method of analysis should be specified in the analytical report for each determination performed on a sample. A reference of sufficient definition or a copy of the test method should be provided to the requestor of the analytical services.

6.2 The precision, bias, and detection limit of each analytical test method should be disclosed as part of either the test method or the analytical report. Consult Guide D 3856 for the quality control system from which estimates of precision and bias could be made, or review the procedure for determining single-operator precision of a test method as provided in Practice D 2777 for guidance. The procedure used to derive the detection limit should be identified along with any specific definitions associated with the derivation. Practice D 4210 is one of many sources for computing detection limits.

6.3 The date on which each determination is performed should be reported, as should other time-critical processes such as extractions. In some cases, such as in microbiology tests, it is critical to record the time that the test was started.

6.4 The analytical reports should clearly specify the form in which multi-atomic analytes, such as nitrate and orthophosphate, are reported.

6.5 If a sample is diluted prior to analysis, the sample dilution ratio(s) for the sample or involved constituents, and the reason for the dilution(s) should be documented on the analytical report.

7. Significant Figures

7.1 When recording direct measurements, test results should be reported by recording all digits that are known plus one that may be subject to change on repeated analysis. When calculating results from test data, rounding should be performed only on the final result, not upon the intermediate values employed in the calculation. For a discussion of the principles and practices for determining significant figures, refer to Practice E 29.

7.2 When a value is computed from two or more other test results, refer to Practice D 4460 for techniques of determining precision limits of the calculated value.

8. Documentation of Quality

8.1 Each sample analysis may have different quality needs based on the use of the data. This information should be determined before sampling and analysis. Based on this information, an analytical report may include the following information, as appropriate:

8.1.1 Recovery of any surrogate compounds with laboratory control limits,

8.1.2 Results of corresponding check samples or blank spikes with laboratory control limits,

8.1.3 Results of analysis of duplicate samples or duplicate matrix spiked samples and the percent difference with laboratory control limits,

8.1.4 Recoveries of any matrix spikes (and matrix spike duplicates) with laboratory control limits,

8.1.5 Results of all blanks,

8.1.6 Results of any reference samples run during sample analysis with laboratory control limits,

8.1.7 Calibration and tuning data, and

8.1.8 Chromatograms.

9. Review of Analytical Results

9.1 The deviation from a perfect balance between cations and anions determined in water samples may be appraised by totalling separately the determined concentrations in milliequivalents per litre (meq/L) of anions and cations. This can only be done if all major ions have been determined. The cation-anion difference, either positive or negative, may be calculated from the following empirical formula in which cations and anions are expressed in meq/L: ⁷

percent cation-anion difference =
$$\frac{\Sigma \ cations - \Sigma \ anions}{\Sigma \ cations + \Sigma anions} \times 100$$

Note 1—With careful work, the difference will not generally exceed 2 % of the total cations or anions in waters of moderate concentrations (250 for 1000 mg/L). A somewhat larger percentage can be tolerated if the sum of cations and anions is less than about 5.00 mg/L. ⁸

9.2 A comparison of results from the dissolved solids determination with dissolved solids calculated from individual major ion determinations is a helpful review procedure.

9.3 The procedure used to report analytical values when constituents of interest are found in a blank analysis should be described by the laboratory.

9.4 A quality assurance narrative should be used to explain any discrepancies in the data or unusual conditions that resulted in data of questionable quality (that is, matrix

⁷ Friedman, L. C., and Erdmann, D. E., "Quality Assurance Practices for the Chemical and Biological Analyses of Water and Fluvial Sediments," *Techniques of Water-Resources Investigations of the U.S. Geological Survey*, Book 5, Chapter , U.S. Government Printing Office, 1982.

⁸ Hem, J. D., "Study and Interpretation of the Chemical Characteristics of Natural Water," U.S. Geological Survey Water-Supply Paper 2254, 1985.

TABLE 1 Conversion Factors Between Units in the Specific Test Method and Other Units in Common Use

TABLE 2	Factors for Interconversion Between Milli	grams Per
	Litre and Milliequivalents Per Litre A B	-

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To Convert	Into	Multiply By
mL (or cm ³) of dissolved oxygen/L	. mg/L	1.429
grains/US gal	mg/L	17.12
grains/Imperial gal	mg/L	14.25
grams/L	mg/L	1000
normality	meq/L	1000
mg/L as CaCO ₃	meq/L	0.0200
grains/US gal as CaCO ₃	meq/L	0.342
grains/Imperial gal as CaCO ₃	meq/L	0.285
mg of dissolved oxygen per L	mL (or cm ³) of dissolved	0.700
	oxygen per L	
mg/L	grains/US gal	0.0584
mg/L	grains/Imperial gal	0.0702
mg/L	grams/L	0.001
meq/L	normality	0.001
meq/L	percent of normal	0.1
meq/L	mg/L as CaCO ₃	50.0
meq/L	grains/US gal as CaCO ₃	2.92
meq/L	grains/Imperial gal as CaCO ₃	3.51

interferences, elevated detection limits).

9.5 The report should include the signature of the laboratory manager or a designee attesting to the review of the results reported and that the results meet the specified quality of data.

10. Conversion Factors

10.1 Table 1 lists factors for interconversion between units in common use.

10.2 Table 2 lists factors for interconversion of milligrams per litre and milliequivalents per litre of common ions.

11. Keywords

11.1 analysis; blank; cation-anion balance; results; surrogate; water

lon	Mu	Multiplier	
ION	mg/L to meq/L	meq/L to mg/L	
Al ⁺³	0.1112	8.994	
Ba ⁺²	0.01456	68.67	
Br [–]	0.01252	79.90	
Ca ⁺²	0.04990	20.04	
CI -	0.02821	35.45	
CN -	0.03844	26.02	
CO ₃ -2	0.03333	30.00	
Cr +3	0.05770	17.33	
Cr +6	0.1154	8.666	
CrO ₄ ⁻²	0.01724	58.00	
Cu ⁺²	0.03147	31.77	
F ⁻	0.05264	19.00	
Fe ⁺²	0.03581	27.92	
Fe ⁺³	0.05372	18.62	
H +	0.9921	1.008	
HCO ₃ ⁻	0.01639	61.02	
HPO ₄ ⁻²	0.02084	47.99	
H₂PO₄ [−]	0.01031	96.99	
HS -	0.03024	33.07	
HSO ₃ [–]	0.01233	81.07	
HSO ⁴ -	0.01030	97.07	
I	0.007880	126.9	
K *	0.02558	39.10	
Mg ⁺²	0.08229	12.15	
Mn +2	0.03640	27.47	
Mn ⁺⁴	0.07281	13.73	
Na ⁺	0.04350	22.99	
NH_4 +	0.05544	18.04	
Ni ⁺²	0.03407	29.35	
NO ₂ -	0.02174	46.01	
NO ₃ -	0.01613	62.00	
OH -	0.05880	17.01	
Pb +2	0.009653	103.6	
PO ₄ ⁻³	0.03159	31.66	
S ⁻²	0.06238	16.03	
SiO ₃ ⁻²	0.02629	38.04	
SO ₃ ⁻²	0.02498	40.03	
SO ₄ ⁻²	0.02082	48.03	
Sr +2	0.02283	43.81	
Zn ⁺²	0.03059	32.69	

^ABased on ${}^{12}C = 12$ amu (atomic mass units).

^BIt is assumed that reactions proceed to the zero oxidation state.

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