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Standard Terminology Relating to Industrial and Specialty Chemicals¹

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1. Scope

1.1 This standard covers terminology relating to industrial and specialty chemicals. It is intended to provide an understanding of terms commonly used in test methods, practices, and specifications throughout the industry.

NOTE 1—The boldface numbers following each definition refer to E15 standards in which the definition appears. Lightface numbers refer to the E15 subcommittee having jurisdiction.

2. Referenced Documents

2.1 ASTM Standards:²

- D891 Test Methods for Specific Gravity, Apparent, of Liquid Industrial Chemicals
- E12 Terminology Relating to Density and Specific Gravity of Solids, Liquids, and Gases (Withdrawn 1996)³
- E70 Test Method for pH of Aqueous Solutions With the Glass Electrode
- E180 Practice for Determining the Precision of ASTM Methods for Analysis and Testing of Industrial and Specialty Chemicals (Withdrawn 2009)³
- E200 Practice for Preparation, Standardization, and Storage of Standard and Reagent Solutions for Chemical Analysis
- E201 Test Method for Calculation of Volume and Weight of Industrial Chemical Liquids (Withdrawn 2001)³
- E222 Test Methods for Hydroxyl Groups Using Acetic Anhydride Acetylation
- E223 Test Methods for Analysis of Sulfuric Acid
- E224 Test Methods for Analysis of Hydrochloric Acid
- E234 Test Method for Total Bromine Number of Unsaturated Aliphatic Chemicals (Withdrawn 2008)³
- E300 Practice for Sampling Industrial Chemicals
- E324 Test Method for Relative Initial and Final Melting

- Points and the Melting Range of Organic Chemicals
- E326 Test Method for Hydroxyl Groups by Phthalic Anhydride Esterification (Withdrawn 2001)³
- E335 Test Method for Hydroxyl Groups by Pyromellitic Dianhydride Esterification (Withdrawn 2002)³
- E347 Test Method for Ash in Polybasic Acids (Withdrawn 2003)³
- E410 Test Method for Moisture and Residue in Liquid Chlorine
- E1899 Test Method for Hydroxyl Groups Using Reaction with *p*-Toluenesulfonyl Isocyanate (TSI) and Potentiometric Titration with Tetrabutylammonium Hydroxide

3. Terminology

3.1 Definitions:

accuracy—the agreement between an experimentally determined value and the accepted reference value. In chemical work, this term is frequently used to express freedom from bias, but in other fields it assumes a broader meaning as a joint index of precision and bias. To avoid confusion, the term *bias* will be used in appraising of the systematic error of test methods for industrial chemicals. See also **bias**. **E180**, E15.04

ash—the residual inorganic matter obtained on ignition of a sample in air at a specified temperature. **E347**, E15.51

Baumé gravity—a unit of density based on specific gravity and defined by the following equation:

$$\text{Baumé gravity} = 145 - [145/\text{sp gr}] \text{ at } 15.5/15.5^\circ\text{C} (60/60^\circ\text{F}) \quad (1)$$

See also **density** and **specific gravity**. **E223**, **E224**, **E324**, E15.51

bias—a constant or systematic error as opposed to a random error. It manifests itself as a persistent positive or negative deviation of the method average from the accepted reference value. See also **accuracy**. **E180**, E15.04

bromine number, total—number of centigrams of bromine equivalent to the total unsaturation present in 1 g of sample. It is a measure of the total ethylenic unsaturation present in the designated aliphatic compound. **E234**, E15.22

coefficient of variation—a measure of relative precision calculated as the standard deviation of a series of values

¹ This terminology is under the jurisdiction of ASTM Committee D16 on Aromatic Hydrocarbons and Related Chemicals and is the direct responsibility of Subcommittee D16.15 on Industrial and Specialty General Standards.

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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.

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

divided by their average. It is often multiplied by 100 and expressed as a percentage. **E180**, E15.04

density—the mass of a unit volume of a material at a specified temperature. The units shall be stated, such as grams per millilitre, grams per cubic centimetre, pounds per cubic foot, or other. The form of the expression shall be the following:

$$\text{Density at } x \dots$$

where x = temperature of the material, in <units>, for example, °C. See also **Baumé gravity** and **specific gravity**. **E201**, E15.23

density (of gases)—the mass of a unit volume of a gas at a stated temperature and pressure. The units shall be stated. The form of expression shall be the following:

$$\text{Density at } x, y$$

where:

x = temperature of the gas units, for example, °C, and
 y = pressure of the gas (units, for example, kPa). **E12**, E15.23

density, apparent—the weight in air of a unit volume of a material at a specified temperature. The units shall be stated. The form of expression shall be the following:

$$\text{Apparent density at } x$$

where x = temperature of the material, in <units>, for example, °C. **E201**, E15.23

duplicates—two independent determinations performed by one analyst in a short period of time, for example, one day. **E180**, E15.04

error—*in a statistical sense*, any deviation of an observed value from the true, but generally unknown, value. When expressed as a fraction or percentage of the value measured, it is called a relative error. All statements of precision or bias should indicate clearly whether they are expressed in absolute or relative sense. **E180**, E15.04

error, random—the chance variation encountered in all experimental work despite the closest possible control of variables. It is characterized by the random occurrence of both positive and negative deviations from the mean value for the method, the algebraic average of which will approach zero in a long series of measurements. **E180**, E15.04

hydroxyl number—the milligrams of potassium hydroxide equivalent to the hydroxyl content of 1 g of sample. In the case of a pure compound, the hydroxyl number is inversely proportional to the hydroxyl equivalent weight:

$$\text{equivalent weight (g/equivalent)} = 56100/\text{hydroxyl number} \quad (2)$$

E222, **E326**, **E335**, **E1899**, E15.22

increments (solid sample)—portions of material selected from various parts of a lot, which may be tested individually or composited and tested as a unit. **E300**, E15.05

lot (solid sample)—a discrete quantity of material. It may contain a single batch or several batches or be the product of continuous process broken into units on the basis of time or

shipment. It is very desirable that individual batches in a lot be specifically identified so that they may become individual or stratified units for inspection. **E300**, E15.05

melting point, final—the temperature at which the last crystal disappears into the melt. **E324**, E15.23

melting point, initial—the temperature at which positive evidence of liquefaction is observed. **E324**, E15.23

moisture—the volatile substances evolved during volatilization and purging of the sample-residue flask and absorbed on the desiccant contained in the absorption tubes under the conditions of the test.⁴ **E410**, E15.57

95 % limit (difference between two results)—the maximum absolute difference expected for approximately 95 % of all pairs of results from laboratories similar to those in the interlaboratory study. **E180**, E15.04

pH—defined formally as the negative logarithm to the base 10 of the conventional hydrogen ion activity. The pH of an aqueous solution is derived from E , the electromotive force (emf) of the cell:

$$\text{reference} \parallel \text{solution} \parallel \text{glass electrode}$$

(where the double vertical line represents a liquid junction)

when the electrodes are immersed in the solution, and E_s , the electromotive force obtained when the electrodes are immersed in a standard solution (whose assigned pH is designated pH(S)), by the following equation:

$$\text{pH} = \text{pH(S)} + \frac{(E - E_s)F}{RT \ln 10} \quad (3)$$

where:

F = faraday, 96 487 C·mol⁻¹,
 R = gas constant, 8.314 33 J·K⁻¹·mol⁻¹, and
 T = absolute temperature, (t °C + 273.15). **E70**, E15.23

precision—the degree of agreement of repeated measurements of the same property. Precision statements in ASTM methods for industrial chemicals will be derived from the estimated standard deviation or coefficient of variation of a series of measurements and will be expressed in terms of the repeatability, the within-laboratory, between days variability, and the reproducibility of the method. **E180**, E15.04

range—the absolute value of the algebraic difference between the highest and the lowest values in a set of data. **E180**, E15.04

repeatability—the precision of a method expressed as the agreement attainable between independent determinations performed at essentially the same time (duplicates) by one analyst using the same apparatus and techniques. **E180**, E15.04

replicates—two or more repetitions of a test determination. **E180**, E15.04

⁴ This term or definition is specific to the standard under the test conditions.

reproducibility—the precision of a method expressed as the agreement attainable between determinations performed in different laboratories. **E180**, E15.04

residue—those substances that remain in the sample flask after sample volatilization under the conditions of the test.⁴ **E410**, E15.57

result—a value, that is, a single determination, an average of duplicates, or other specified grouping of replicates, obtained by carrying out the test method. **E180**, E15.04

sample—a small fraction of a larger bulk having properties sufficiently representative of this bulk.

sample, all-levels (liquid sample)—one obtained by submerging a closed sampler to a point as near as possible to the draw-off level, then opening the sampler and raising it at a rate such that it is about three-fourths full as it emerges from the liquid. An all-levels sample is not necessarily an average sample because the tank volume may not be proportional to the depth and because the operator may not be able to raise the sampler at the variable rate required for proportionate filling. The rate of filling is proportional to the square root of the depth of immersion. **E300**, E15.05

sample, average (liquid sample)—one that consists of proportionate parts from all sections of the container. **E300**, E15.05

sample, bottom (liquid sample)—one obtained from the material on the bottom surface of the tank, container, or line at its lowest point. (Bottom samples are usually taken to check for water, sludge, scale, etc.) **E300**, E15.05

sample, composite, compartment-tank (liquid sample) (ship, barge, etc.)—a blend of individual all-levels samples from each compartment that contains the product being sampled in proportion to the volume of material in each compartment. **E300**, E15.05

sample, composite, single-tank (liquid sample)—a blend of the upper, middle, and lower samples. For a tank of uniform cross section, such as an upright cylindrical tank, the blend consists of equal parts of the three samples. For a horizontal cylindrical tank, the blend consists of the three samples in the proportions shown in **Table 1**. **E300**, E15.05

sample, continuous (liquid sample)—one obtained from a pipeline conveying the product in such a manner as to give

a representative average of the stream throughout the period of transit. **E300**, E15.05

sample, drain (liquid sample)—one obtained from the draw-off or discharge valve. Occasionally, a drain sample may be the same as a bottom sample, as in the case of a tank car. **E300**, E15.05

sample, gross (solid sample)—a composite prepared by mixing the increments. **E300**, E15.05

sample, jar (liquid sample)—one obtained by placing a jar into the path of a free-flowing stream so as to collect a definite volume from the full cross section of the stream. **E300**, E15.05

sample, laboratory (solid sample)—that portion of the subsample that is sent to the laboratory for testing. **E300**, E15.05

sample, middle (liquid sample)—one obtained from the middle of the tank contents. **E300**, E15.05

sample, mixed (liquid sample)—one obtained after mixing or vigorously stirring the contents of the original container, and then pouring out or drawing off the quantity desired. **E300**, E15.05

sample, outlet (liquid sample)—one normally obtained at the level of the tank outlet (either fixed or a swing line outlet). **E300**, E15.05

sample, sub (solid sample)—a smaller sample produced in a specified manner by the reduction in volume or quantity of the gross sample. **E300**, E15.05

sample, top (liquid sample)—one normally obtained 6 in. (152 mm) below the top surface of the tank contents. **E300**, E15.05

sample, tube or thief (liquid sample)—one obtained with a sampling tube or special thief, either as a core sample or spot sample from the specified point in the container. **E300**, E15.05

sample, upper (liquid sample)—one obtained from the middle of the upper third of the tank contents. **E300**, E15.05

sampling (solid sample)—the process of extracting a small fraction of material from a larger bulk, so that it will be

TABLE 1 Sampling Horizontal Cylindrical Tanks

| Liquid Depth, Percent of Diameter | Sampling Level, Percent of Diameter Above Bottom | | | Composite Sample, Proportionate Parts of | | |
|-----------------------------------|--|--------|-------|--|--------|-------|
| | Upper | Middle | Lower | Upper | Middle | Lower |
| 100 | 80 | 50 | 20 | 3 | 4 | 3 |
| 90 | 75 | 50 | 20 | 3 | 4 | 3 |
| 80 | 70 | 50 | 20 | 2 | 5 | 3 |
| 70 | ... | 50 | 20 | 1 | 5 | 4 |
| 60 | ... | 50 | 20 | ... | 5 | 5 |
| 50 | ... | 40 | 20 | ... | 4 | 6 |
| 40 | ... | ... | 20 | ... | ... | 10 |
| 30 | ... | ... | 15 | ... | ... | 10 |
| 20 | ... | ... | 10 | ... | ... | 10 |
| 10 | ... | ... | 5 | ... | ... | 10 |

sufficiently representative of the bulk for the intended purpose. **E300**, E15.05

significance level—the decimal probability that a result will exceed the critical value. **E180**, E15.04

simple liquid—a single-phase liquid having a vapor pressure of less than 16 psi Reid vapor pressure at 100°F (830 mm Hg at 37.8°C) and a Saybolt viscosity of less than 10 000 s (2160 cSt) at 25°C. **E300**, E15.05

slurry—a suspension of solid particles in a liquid that can be separated by filtration or sedimentation (does not include emulsions). **E300**, E15.05

solid—a state of matter in which the relative motion of molecules is restricted and in which molecules tend to retain a definite fixed position relative to each other. A solid may be said to have a definite shape and volume. **E300**, E15.05

specific gravity—the ratio of the mass of a unit volume of a material at a stated temperature to the mass of the same volume of gas-free distilled water at a stated temperature. The form of expression shall be the following:

$$\text{Specific gravity } x/y \text{ } ^\circ\text{C} \dots$$

where:

x = temperature of the material <units>, and

y = temperature of the water <units>.

See also **Baumé gravity** and **density**. **E201**, E15.23

specific gravity (of solids and liquids)—the ratio of the mass of a unit volume of a material at a stated temperature to the mass of the same volume of gas-free distilled water at a stated temperature. If the material is a solid, the volume shall be that of the impermeable portion. The form of expression shall be the following:

$$\text{Specific gravity } x/y \text{ } ^\circ\text{C}$$

where:

x = temperature of the material (<units>), and

y = temperature of the water (<units>). **E12**, E15.23

specific gravity, apparent (of solids and liquids)—the ratio of the weight in air of a unit volume of a material at a stated temperature to the weight in air of equal density of an equal volume of gas-free distilled water at a stated temperature. If the material is a solid, the volume shall be that of the impermeable portion. The form of expression shall be the following:

$$\text{Apparent specific gravity } x/y \text{ } ^\circ\text{C}$$

where:

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x = temperature of the material (<units>), and
 y = temperature of the water (<units>). **D891**, **E201**, **E12**, E15.23

standard deviation—a measure of the dispersion of a series of results around their average, expressed as the square root of the quantity obtained by summing the squares of the deviations from the average of the results and dividing by the number of observations minus one. It is also the square root of the variance and can be calculated as follows:

$$s = \sqrt{\frac{\sum (X_i - \bar{X})^2}{n - 1}} \quad (4)$$

where:

s = estimated standard deviation of the series of results (<same units as X >),

X_i = each individual value (<units>),

\bar{X} = average (arithmetic mean) of all values (<units>), and

n = number of values. **E180**, E15.04

standard volumetric solution—a solution of accurately determined concentration used in the quantitative analysis of chemicals and other products. The concentration of such solutions is usually expressed in terms of normality or molarity. **E200**, E15.03

variance—a measure of the dispersion of a series of results around their average. It is the sum of the squares of the individual deviations from the average of the results, divided by the number of results minus one. **E180**, E15.04

within-laboratory, between days variability—the precision of a method expressed as the agreement attainable between independent determinations (each the average of duplicates) performed by one analyst using the same apparatus and techniques on each of two days. **E180**, E15.04

DISCUSSION—This definition is almost synonymous with repeatability. Other sources than **E180** define *within-laboratory variability* as the precision of a test method that a laboratory is likely to achieve on average. The practical meaning of it is that this form of precision is relevant for the customers of the laboratory. It can be used to assess the uncertainty of each result that the laboratory provides to the plants and to the certification or logistics departments. In this context it is not restricted to one analyst or to a two-day period, but can extend to more analysts and a longer period of time, for example, one year. It can be derived from, for example, control charts. In this definition it would be synonymous with “laboratory precision” or “intermediate precision.”

4. Keywords

4.1 accuracy; Baumé gravity; bromine number; density; hydroxyl number; industrial chemicals; melting point; moisture; pH; precision; residue; sampling; specific gravity