National Institute of Standards & Technology

Certificate of Analysis

Standard Reference Material® 350b

Benzoic Acid (Acidimetric)

C_6H_5COOH

This Standard Reference Material (SRM) consists of highly purified benzoic acid (C_6H_5COOH). SRM 350b is intended for use in acidimetric standardization. A unit of SRM 350b consists of 30 g of benzoic acid.

Certified Values: A NIST certified value is a value for which NIST has the highest confidence in its accuracy in that all known or suspected sources of bias have been investigated or taken into account [1]. The certified values, reported in Table 1 as a mass fraction ($w_{C_6H_5COOH}$) and amount-of-substance content of H^+ ion (ν_{H^+}), are based on coulometric assays of the dried material (see "Drying Instructions") including the effects of air buoyancy. The certified values are based on the results of determinations from 12 randomly selected bottles from the entire lot of SRM 350b. Each determination was obtained by coulometric acidimetric titration [2] to the inflection point (pH ca. 8.15).

Table 1. Certified Values for SRM 350b Benzoic Acid

$w_{C_6H_5COOH}$	99.9978 %	±	0.0044 %
ν_{H^+}	8.188 40 mol kg^{-1}	±	0.000 26 mol kg^{-1}

The uncertainty in the value, calculated according to the method described in the ISO/JCGM Guide [3], is expressed as an expanded uncertainty, U. The expanded uncertainty is calculated as $U = ku_c$, where u_c is the combined uncertainty and k is the coverage factor. The quantity u_c represents, at the level of one standard deviation, the potential combined effects of the uncertainty arising from instrumental sources, chemical interferences, and uncertainties in fundamental constants, and possible material inhomogeneity. The value of k is calculated from the effective degrees of freedom, ν_{eff}. The value $k = 1.96$, corresponding to $\nu_{eff} > 1000$, was used to obtain the cited value for U for $w_{C_6H_5COOH}$. The value $k = 1.97$, corresponding to $\nu_{eff} = 437$, was used to obtain the certified value of U for ν_{H^+}. The coverage factors were each chosen to obtain an approximate 95 % level of confidence. The measurands are the values listed in Table 1 and they are metrologically traceable to the SI units of mass.

Expiration of Certification: The certification of **SRM 350b** is valid, within the measurement uncertainty specified, until **01 April 2024**, provided the SRM is handled and stored in accordance with the instructions given in this certificate (see "Instructions for Use"). The certification is nullified if the SRM is damaged, contaminated, or otherwise modified.

Maintenance of SRM Certification: NIST will monitor this SRM over the period of its certification. If substantive technical changes occur that affect the certification before the expiration of this certificate, NIST will notify the purchaser. Registration (see attached sheet or register online) will facilitate notification.

Overall direction and coordination of the technical activities leading to certification of this SRM was performed by K.W. Pratt of the NIST Chemical Sciences Division.

Statistical consultation was provided by W.F. Guthrie of the NIST Statistical Engineering Division.

Support aspects involved in the issuance of this SRM were coordinated through the NIST Office of Reference Materials.

Carlos A. Gonzalez, Chief
Chemical Sciences Division

Gaithersburg, MD 20899
Certificate Issue Date: 08 June 2015
Certificate Revision History on Last Page

Robert L. Watters, Jr., Director
Office of Reference Materials

Calculation of Certified Value: The certified value was obtained using the present value for the Faraday constant, 96 485.336 C_{90} mol^{-1} [4], currently recommended for coulometric determinations. Corrections for air buoyancy were made using the measured density of 1.3039 g cm^{-3} for SRM 350b. The molar mass of benzoic acid, 122.121 34 g mol^{-1} (calculated from [5]), was used to calculate $w_{C_6H_5COOH}$ from ν_{H^+}. The uncertainty [5] in this molar mass is included in the certified value of $w_{C_6H_5COOH}$. The certified value of $w_{C_6H_5COOH}$ is calculated from ν_{H^+} under the assumption that the replaceable H^+ derives from a substance of net formula $C_7H_6O_2$. No representation is made as to the mass fraction of any impurities present.

INSTRUCTIONS FOR USE

Drying Instructions: Dry at room temperature (22 °C to 23 °C) for 24 h in a desiccator over anhydrous $Mg(ClO_4)_2$. The change in mass on drying is less than 0.005 %, relative. Previous investigations [6] indicate that benzoic acid will not absorb moisture from the atmosphere if the relative humidity does not exceed 90 %.

Stability and Storage: This SRM should be stored in its original bottle at room temperature. It must be tightly re-capped after use and protected from moisture and light.

Homogeneity: Tests indicate that this SRM is homogeneous within the uncertainty limits for sample sizes greater than 300 mg. Samples less than 300 mg are not recommended in order to avoid possible inhomogeneity with smaller sample sizes.

SOURCE AND ANALYSIS[(1)]

The benzoic acid used for this SRM was obtained from a commercial source. The material was examined for compliance with the specification for reagent grade benzoic acid as specified by the American Chemical Society [7]. The material was found to meet or exceed these specifications in all respects.

REFERENCES

[1] May, W.; Parris, R.; Beck, C.; Fassett, J.; Greenberg, R.; Guenther, F.; Kramer, G..; Wise, S.; Gills, T.; Colbert, J.; Gettings, R.; MacDonald, B.; *Definitions of Terms and Modes Used at NIST for Value-Assignment of Reference Materials for Chemical Measurements*; NIST Special Publication 260-136; U.S. Government Printing Office: Washington, DC (2000); http://www.nist.gov/srm/publications.cfm (accessed June 2015).

[2] Pratt, K.W.; *Automated, High-Precision Coulometry* II. *Strong and Weak Acids and Bases*; Anal. Chim. Acta, Vol. 289, pp. 135–142 (1994).

[3] JCGM 100:2008; *Evaluation of Measurement Data - Guide to the Expression of Uncertainty in Measurement*; (GUM 1995 with Minor Corrections), Joint Committee for Guides in Metrology (JCGM) (2008); available at http://www.bipm.org/utils/common/documents/jcgm/JCGM_100_2008_E.pdf (accessed Apr 2015); see also Taylor, B.N.; Kuyatt, C.E.; *Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results*; NIST Technical Note 1297, U.S. Government Printing Office: Washington, DC (1994); available at http://www.nist.gov/pml/pubs/index.cfm (accessed June 2015).

[4] Mohr, P.J.; Taylor, B.N.; *CODATA Recommended Values of the Fundamental Physical Constants*: 2002; Reviews of Modern Physics, Vol. 77(1), pp. 1–107 (2005); available at http://physics.nist.gov/cgi-bin/cuu/Value?f90|search_for=faraday

[5] Commission of Atomic Weights and Isotopic Abundances; *Atomic Weights of the Elements* 2001; Pure & Appl. Chem., Vol. 75(8), pp. 1107–1122 (2003).

[6] SRM 350a; *Benzoic Acid* (*Acidimetric*); National Bureau of Standards, U.S. Department of Commerce: Gaithersburg, MD (1981).

[7] *Reagent Chemicals*, 8th ed.; American Chemical Society: Washington, DC (1993).

Certificate Revision History: 08 June 2015 (Change expiration date; editorial changes); 16 December 2005 (Original certificate issue date).

Users of this SRM should ensure that the Certificate of Analysis in their possession is current. This can be accomplished by contacting the SRM Program: telephone (301) 975-2200; fax (301) 948-3730; e-mail srminfo@nist.gov; or via the Internet at http://www.nist.gov/srm.

[(1)] Certain commercial equipment, instruments or materials are identified in this certificate to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.