



CERTIFIED REFERENCE MATERIAL BCR[®] – 656

CERTIFICATE OF ANALYSIS

ETHANOL			
	Certified value ³⁾	Uncertainty ⁴⁾	Number of accepted sets of data
Site specific deuterium isotope ratio (D/H) _I ¹⁾	102.84 x 10 ⁻⁶	0.20 x 10 ⁻⁶	13
Site specific deuterium isotope ratio (D/H) _{II} ¹⁾	132.07 x 10 ⁻⁶	0.30 x 10 ⁻⁶	13
Relative deuterium isotope ratio R ¹⁾	2.570	0.005	12
δ ¹³ C _{VPDB} measured by IRMS ²⁾	-26.91 ‰	0.07 ‰	12
<p>1) As determined by ²H-NMR</p> <p>2) As determined by IRMS</p> <p>3) Unweighted mean of the means of accepted sets of data, each set being obtained in a different laboratory. The values are traceable to the Vienna Standard Mean Ocean Water (VSMOW) (deuterium ratios) and, via comparison with NBS-22 (using a reference value of -29.73 ‰), to Vienna Pee Dee Belemnite (VPDB), respectively.</p> <p>4) The uncertainty is taken as the half-width of the 95 % confidence interval of the number of accepted datasets.</p>			

This certificate is valid for one year after purchase.

Sales date:

The minimum sample intake is defined in the standard methods (EEC/2676/90; CEN/TC 174 N 108; EEC/2670/90 Annex 8; EEC/2870/00 Annex I).

NOTE

This material has been certified by BCR (Community Bureau of Reference, the former reference materials programme of the European Commission). The certificate has been revised under the responsibility of IRMM.

Brussels, June 2001

Latest revision: November 2014

Signed: _____

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Additional Material Information	
	Mass Fraction
	Value ¹ [%]
Alcoholic grade (t_b)	94
1) These values refer to values that were obtained in the course of the characterisation study.	

DESCRIPTION OF THE SAMPLE

The sample consists of approximately 20 mL neutral ethanol from wine.

ANALYTICAL METHOD USED FOR CERTIFICATION

The method used for the determination of site-specific deuterium ratios of ethanol from wine is given in EEC/2676/90.

The site specific deuterium ratio of a site i is defined as $(D/H)_i = D_i/P_i N_H$ where D_i is the number of molecules with a deuterium atom in site i , N_H is the number of fully protonated molecules, and P_i is the stoichiometric number of hydrogens (deuterons and protons) at site i .

For the ethanol molecule, $(D/H)_I$ represents the site-specific deuterium ratio at site **I** (isotopomer CH_2DCH_2OH) and $(D/H)_{II}$ the site specific deuterium ratio at site **II** (isotopomer CH_3CHDOH). $(D/H)_I$ and $(D/H)_{II}$ are obtained from the corresponding signal intensities in the 2H -NMR spectrum using an internal comparison with a precisely known amount of working standard, N,N,N,N -tetramethylurea (TMU). TMU is a BCR CRM whose values for this parameter are traceable to the internationally-accepted scale VSMOW (Vienna-Standard Mean Ocean Water, supplied by the International Atomic Energy Agency in Vienna).

R is calculated as $2 \times (D/H)_{II}/(D/H)_I$ determined from the ratio of the heights of the peaks in the 2H -NMR spectrum and is therefore dimensionless.

The method used for the determination of carbon-13/carbon-12 ratios of ethanol from wine is given in CEN/TC 174 N 108.

$\delta^{13}C_{VPDB}$ of the sample is determined directly on the carbon dioxide obtained from the total combustion of the ethanol and measured using an isotope ratio mass spectrometer. The results are traceable to the international VPDB scale (Vienna-Pee Dee Belemnite supplied by the International Atomic Energy Agency in Vienna) expressed in parts per thousand.

$$\delta^{13}C_{VPDB} \text{ ‰} = [^{13}C/^{12}C_{\text{sample}}/^{13}C/^{12}C_{VPDB} - 1] \times 1000$$

All measurements were calibrated using NBS-22 with a $\delta^{13}C_{VPDB}$ reference value of -29.73 ‰.

Alcohol grade t_b is the mass fraction of ethanol in this sample, expressed in %. The alcohol grade of the distillates is measured either by the Karl Fischer method as recommended in the official 2H -NMR method (EEC/2670/90 Annex 8) or by electronic densimetry (EEC/2870/00 Annex I).

PARTICIPANTS

Preparation of the material, homogeneity and stability studies

Eurofins Scientific, Nantes (FR)

Certification measurements

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SAFETY INFORMATION

The sample is highly flammable.

INSTRUCTIONS FOR USE

The material is intended for method validation and quality control. For analysis the sample should be taken as it is. Before use it can be stored at room temperature, away from sources of ignition. Once in use, several measurements can be performed from the same flask (reasonably 5 to 7 times), over a period of 7 days maximum, provided that the bottle is kept tightly closed between each use and stored at +4 °C.

Note: The $\delta^{13}\text{C}_{\text{VPDB}}$ value is based on a reference value of -29.73 ‰ for NBS-22. This value has meanwhile been re-assessed and is now stated as -30.03 ‰. When using the new value of NBS-22 for calibration, a different value for the $\delta^{13}\text{C}_{\text{VPDB}}$ of BCR-656 will be obtained. It is not possible to convert the certified value of BCR-656 based on the current reference value of NBS-22.

STORAGE

On receipt, the materials should be stored at room temperature.

However, the European Commission cannot be held responsible for changes that happen during storage of the material at the customer's premises, especially of opened samples.

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NOTE

A technical report on the production of BCR-656 is available on the internet (<http://www.irmm.jrc.be>).

A paper copy can be obtained from IRMM on request.

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