SLOVENSKI STANDARD
oSIST prEN ISO 20595:2022

01-julij-2022

Kakovost vode - Določevanje izbranih lahko hlapnih organskih spojin v vodi - Metoda s plinsko kromatografijo z masno selektivnim detektorjem po statični headspace tehniki (HS-GC-MS) (ISO 20595:2018)

Water quality - Determination of selected highly volatile organic compounds in water - Method using gas chromatography and mass spectrometry by static headspace technique (HS-GC-MS) (ISO 20595:2018)

Wasserbeschaffenheit - Bestimmung ausgewählter leichtflüchtiger organischer Verbindungen in Wasser - Verfahren mittels Gaschromatographie und Massenspektrometrie nach statischer Headspacetechnik (HS-GC-MS) (ISO 20595:2018)

Qualité de l'eau - Dosage de composés organiques hautement volatils sélectionnés dans l'eau - Méthode par chromatographie en phase gazeuse par la technique de l'espace de tête statique et spectrométrie de masse (HS-GC-MS) (ISO 20595:2018)

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Water quality — Determination of selected highly volatile organic compounds in water — Method using gas chromatography and mass spectrometry by static headspace technique (HS-GC-MS)

Qualité de l'eau — Dosage de composés organiques hautement volatils sélectionnés dans l'eau — Méthode par chromatographie en phase gazeuse par la technique de l'espace de tête statique et spectrométrie de masse (HS-GC-MS)

Reference number
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Contents

Page

Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see www.iso.org/patents).

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For an explanation on the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT) see the following URL: www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 147, *Water quality*, Subcommittee SC 2, *Physical, chemical and biochemical methods*.

Introduction

Various methods are available for the determination of highly volatile organic compounds in water. This document specifies a gas chromatographic method with mass spectrometric detection (GC-MS) for the determination of volatile organic compounds using the static headspace technique (HS).

Water quality — Determination of selected highly volatile organic compounds in water — Method using gas chromatography and mass spectrometry by static headspace technique (HS-GC-MS)

WARNING — Persons using this document should be familiar with normal laboratory practice. This document does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user to establish appropriate safety and health practices.

IMPORTANT — It is absolutely essential that tests conducted in accordance with this document be carried out by suitably qualified staff.

1 Scope

This document specifies a method for the determination of selected volatile organic compounds in water (see Table 1). This comprises among others volatile halogenated hydrocarbons as well as gasoline components (BTXE, TAME, MTBE and ETBE).

The method is applicable to the determination of volatile organic compounds (see Table 1) in drinking water, groundwater, surface water and treated waste water in mass concentrations >0,1 µg/l. The lower application range depends on the individual compound, the amount of the blank value and the matrix.

The applicability of the method to further volatile organic compounds not indicated in Table 1 is not excluded, but this is checked in individual cases.

Table 1 — Volatile organic compounds determinable by this method

Name (other name)	Molecular formula	CAS-RN[a]	EC-Number[b]	Molar mass g/mol
allyl chloride[c] (3-chloropropene)	C_3H_5Cl	107-05-1	203-457-6	76,53
benzene	C_6H_6	71-43-2	200-753-7	78,11
biphenyl	$C_{12}H_{10}$	92-52-4	202-163-5	154,21
bromodichloromethane	$CHBrCl_2$	75-27-4	200-856-7	163,83
chlorobenzene	C_6H_5Cl	108-90-7	203-628-5	112,56
2-chloro-1,3-butadiene (chloroprene)	C_4H_5Cl	126-99-8	204-818-0	88,54
2-chlorotoluene	C_7H_7Cl	95-49-8	202-424-3	126,58
3-chlorotoluene	C_7H_7Cl	108-41-8	203-580-5	126,58
4-chlorotoluene	C_7H_7Cl	106-43-4	203-397-0	126,58
dibromochloromethane	$CHBr_2Cl$	124-48-1	204-704-0	208,28
1,2-dibromoethane	$C_2H_4Br_2$	106-93-4	203-444-5	187,86
1,2-dichlorobenzene	$C_6H_4Cl_2$	95-50-1	202-425-9	147,00
1,3-dichlorobenzene	$C_6H_4Cl_2$	541-73-1	208-792-1	147,00

[a] CAS-RN: Chemical Abstracts Service Registry Number.

[b] EC-Number: European Inventory of Existing Commercial Substances (EINECS) or European List of Notified Chemical Substances (ELINCS).

[c] Compounds do not have long-term stability.

[d] Compounds can coelute.

[e] Source: Hazardous Substance Data Base University Hamburg (Germany).

Table 1 *(continued)*

Name (other name)	Molecular formula	CAS-RN[a]	EC-Number[b]	Molar mass g/mol
1,4-dichlorobenzene	$C_6H_4Cl_2$	106-46-7	203-400-5	147,00
dichlorodiisopropyl ether	$C_6H_{12}Cl_2O$	108-60-1	203-598-3	171,06
1,1-dichloroethane	$C_2H_4Cl_2$	75-34-3	200-863-5	98,96
1,2-dichloroethane	$C_2H_4Cl_2$	107-06-2	203-458-1	98,96
1,1-dichloroethene	$C_2H_2Cl_2$	75-35-4	200-864-0	96,94
cis-1,2-dichloroethene	$C_2H_2Cl_2$	156-59-2	205-859-7	96,94
trans-1,2-dichloroethene	$C_2H_2Cl_2$	156-60-5	205-860-2	96,94
dichloromethane	CH_2Cl_2	75-09-2	200-838-9	84,93
1,2-dichloropropane	$C_3H_6Cl_2$	78-87-5	201-152-2	112,99
cis-1,3-dichloropropene	$C_3H_4Cl_2$	10061-01-5	233-195-8	110,97
trans-1,3-dichloropropene	$C_3H_4Cl_2$	10061-02-6	602-030-00-5[e]	110,97
2,3-dichloropropene	$C_3H_4Cl_2$	78-88-6	201-153-8	110,97
1,1-dimethylpropyl-methyl ether, *tert*-amyl methyl ether (TAME)	$C_6H_{14}O$	994-05-8	213-611-4	102,17
ethyl benzene	C_8H_{10}	100-41-4	202-849-4	106,17
ethyl *tert*-butyl ether (ETBE)	$C_6H_{14}O$	637-92-3	211-309-7	102,17
hexachlorobutadiene	C_4Cl_6	87-68-3	201-765-5	260,76
hexachloroethane	C_2Cl_6	67-72-1	200-666-4	236,74
isopropylbenzene (cumene)	C_9H_{12}	98-82-8	202-704-5	120,19
methyl *tert*-butyl ether (MTBE)	$C_5H_{12}O$	1634-04-4	216-653-1	88,15
naphthalene	$C_{10}H_8$	91-20-3	202-049-5	128,17
n-propylbenzene	C_9H_{12}	103-65-1	203-132-9	120,19
1,1,1,2-tetrachloroethane	$C_2H_2Cl_4$	630-20-6	211-135-1	167,85
tetrachloroethene	C_2Cl_4	127-18-4	204-825-9	165,84
tetrachloromethane (carbon tetrachloride)	CCl_4	56-23-5	200-262-8	153,82
toluene	C_7H_8	108-88-3	203-625-9	92,14
tribromomethane (bromoform)	$CHBr_3$	75-25-2	200-854-6	252,73
1,2,3-trichlorobenzene	$C_6H_3Cl_3$	87-61-6	201-757-1	181,45
1,2,4-trichlorobenzene	$C_6H_3Cl_3$	120-82-1	204-428-0	181,45
1,3,5-trichlorobenzene	$C_6H_3Cl_3$	108-70-3	203-608-6	181,45
1,1,1-trichloroethane	$C_2H_3Cl_3$	71-55-6	200-756-3	133,40
1,1,2-trichloroethane	$C_2H_3Cl_3$	79-00-5	201-166-9	133,40
trichloroethene	C_2HCl_3	79-01-6	201-167-4	131,39
trichloromethane (chloroform)	$CHCl_3$	67-66-3	200-663-8	119,38
1,1,2-trichlorotrifluoroethane	$C_2Cl_3F_3$	76-13-1	200-936-1	187,38
1,2,4-trimethylbenzene (pseudocumene)	C_9H_{12}	95-63-6	202-436-9	120,19

[a] CAS-RN: Chemical Abstracts Service Registry Number.

[b] EC-Number: European Inventory of Existing Commercial Substances (EINECS) or European List of Notified Chemical Substances (ELINCS).

[c] Compounds do not have long-term stability.

[d] Compounds can coelute.

[e] Source: Hazardous Substance Data Base University Hamburg (Germany).

Table 1 *(continued)*

Name (other name)	Molecular formula	CAS-RN[a]	EC-Number[b]	Molar mass g/mol
1,3,5-trimethylbenzene (mesitylene)	C_9H_{12}	108-67-8	203-604-4	120,19
vinyl benzene (styrene)	C_8H_8	100-42-5	202-851-5	104,15
vinyl chloride (chloroethene)[c]	C_2H_3Cl	75-01-4	200-831-0	62,49
o-xylene	C_8H_{10}	95-47-6	202-422-2	106,17
m-xylene[d]	C_8H_{10}	108-38-3	203-576-3	106,17
p-xylene[d]	C_8H_{10}	106-42-3	203-396-5	106,17

[a] CAS-RN: Chemical Abstracts Service Registry Number.

[b] EC-Number: European Inventory of Existing Commercial Substances (EINECS) or European List of Notified Chemical Substances (ELINCS).

[c] Compounds do not have long-term stability.

[d] Compounds can coelute.

[e] Source: Hazardous Substance Data Base University Hamburg (Germany).

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 3696, *Water for analytical laboratory use — Specification and test methods*

ISO 5667-3, *Water quality — Sampling — Part 3: Preservation and handling of water samples*

ISO 5667-4, *Water quality — Sampling — Part 4: Guidance on sampling from lakes, natural and man-made*

ISO 5667-5, *Water quality — Sampling — Part 5: Guidance on sampling of drinking water from treatment works and piped distribution systems*

ISO 5667-6, *Water quality — Sampling — Part 6: Guidance on sampling of rivers and streams*

ISO 5667-10, *Water quality — Sampling — Part 10: Guidance on sampling of waste waters*

ISO 5667-11, *Water quality — Sampling — Part 11: Guidance on sampling of groundwaters*

3 Terms and definitions

No terms and definitions are listed in this document.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— IEC Electropedia: available at http://www.electropedia.org/

— ISO Online browsing platform: available at https://www.iso.org/obp

4 Principle

An exact volume of an unfiltered water sample is sealed gastight in a headspace vial and heated. After an equilibrium has become established between the volatile organic compounds dissolved in the water and those located in the gas phase above the water level, an exact gas volume is taken from the gas phase and determined by gas chromatography with mass spectrometric detection.

5 Interferences

5.1 General

If a sample consists of several liquid phases, another method shall be applied.

5.2 Interferences in the laboratory

Some of the volatile organic compounds listed in Table 1 are frequently used as solvents in laboratories. Solvent vapours in the laboratory air can lead to overestimates during the analysis. Regular blank value examinations are therefore indispensable (see 9.3.1).

5.3 Interferences by the matrix

Matrix effects that lead to different recoveries and different response factors in samples in comparison to calibration standards can be reduced by adding specific amounts of salt. An increase in the sensitivity can also be attained by adding salt. The use of sodium sulfate or sodium chloride has proven effective. However, interferences can occur depending on the salt used.

5.4 Interferences in the headspace

Some compounds can decompose while the equilibrium forms at e.g. 80 °C. For example, 1,1,2,2-tetrachloroethane decomposes to trichloroethene. If 1,1,2,2-tetrachloroethane is present in the sample, overestimates of trichloroethene can result.

NOTE The decomposition of 1,1,2,2-tetrachoroethane can be eliminated by acidifying the water in the headspace vial with H_2SO_4 to pH <2 and using Na_2SO_4 as salt. But remember that the acid has an immense influence on the life span of the column and the injector.

5.5 Interferences during gas chromatography and mass spectrometry

To rectify interferences that are typically caused by the injection system or by inadequate separation, enlist experts and observe the manufacturer information in the apparatus manuals. The performance and stability of the analysis system shall be checked regularly (e.g. by measuring reference solutions of known composition).

Performance data from an interlaboratory trial held in 2013 are provided in Annex D.

6 Reagents

6.1 General

Unless otherwise indicated, reagents to be used are of purity grade “for analysis” or “for residue analysis”.

6.2 Water, complying with the requirements of ISO 3696, grade 1 or equivalent without any interfering blank values.

6.3 Operating gases for gas chromatograph and mass spectrometer, of high purity and according to the required specification of the manufacturer of the instrumentation, e.g. helium, minimum purity 99,996 %.

6.4 Salts, e.g. sodium sulfate, Na_2SO_4, sodium chloride, NaCl.

6.5 Solvents, for the preparation of stock solutions and as solubilizers in aqueous reference solutions, e.g. methanol, CH_3OH, or dimethylformamide (DMF), C_3H_7NO.

