IEC 63085

Edition 1.0 2021-06

INTERNATIONAL STANDARD

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Radiation protection instrumentation – System of spectral identification of liquids in transparent and semitransparent containers (Raman systems)

Instrumentation pour la radioprotection – Système d'identification spectrale des liquides dans des récipients transparents et semi-transparents (systèmes Raman)

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RADIATION PROTECTION INSTRUMENTATION – SYSTEM OF SPECTRAL IDENTIFICATION OF LIQUIDS IN TRANSPARENT AND SEMITRANSPARENT CONTAINERS (RAMAN SYSTEMS)

FOREWORD

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The text of this International Standard is based on the following documents:

FDIS	Report on voting
45B/979/FDIS	45B/984/RVD

Full information on the voting for its approval can be found in the report on voting indicated in the above table.

The language used for the development of this International Standard is English.

This document was drafted in accordance with ISO/IEC Directives, Part 2, and developed in accordance with ISO/IEC Directives, Part 1 and ISO/IEC Directives, IEC Supplement, available at www.iec.ch/members_experts/refdocs. The main document types developed by IEC are described in greater detail at www.iec.ch/standardsdev/publications.

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INTRODUCTION

This document establishes standard test methods and objects for evaluating the capabilities of Raman systems used for the spectral identification of liquids and liquids mixtures. The main focus is made on testing the functionality of the equipment (Raman analyzer); the reliability of identification result for liquids in containers with different light transmittance properties and stability of the equipment performance under various environmental conditions. The design of the optical scheme of the Raman analyzer, geometric and mass characteristics are not discussed and left to the discretion of the manufacturer. This document does not specify the circumstances and purposes of the inspection of liquids, the methods of detection of the container, and also the safety techniques for handling unknown liquids. Hence, the imposed requirements for the functionality of the Raman analyzer are equally suitable for its use in the fields of security, analysis of pharmaceutical solutions and other liquid chemicals. Annex A provides Raman scattering spectra of test samples, referred to in the test methods.

RADIATION PROTECTION INSTRUMENTATION – SYSTEM OF SPECTRAL IDENTIFICATION OF LIQUIDS IN TRANSPARENT AND SEMITRANSPARENT CONTAINERS (RAMAN SYSTEMS)

1 Scope

This document provides technical performance requirements, testing methods, requirements for operational performance and accompanying documents, packaging, transportation and storage conditions for the system of spectral identification of liquids in transparent and semitransparent containers (hereinafter referred to as “system”), based on the method of inelastic (Raman) light scattering by molecules.

This document applies both to stationary and hand-held systems; geometric and mass parameters are not concerned in the tests. This document is applicable to substance identification testing criteria as well as verification, approval and operating criteria of the system. Since this document considers only the functionality of Raman analyzers and their ability to identify single- or multicomponent fluids, it is equally suitable for verifying the Raman analyzers assigned to security screening of threats, inspection of medical solutions, liquid chemicals, etc.

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.

IEC 60038:2009, *Standard voltages*

IEC 60068-2-1:2007, *Environmental testing – Part 2-1: Tests –Test A: Cold*

IEC 60068-2-2:2007, *Environmental testing – Part 2-2: Tests –Test B: Dry heat*

IEC 60068-2-6:2007, *Environmental testing – Part 2-6: Tests – Test Fc: Vibration (sinusoidal)*

IEC 60068-2-78:2012, *Environmental testing – Part 2-78: Tests –Test Cab: Damp heat, steady state*

IEC 60825-4:2006, *Safety of laser products – Part 4: Laser guards*
IEC 60825-4:2006/AMD1:2008
IEC 60825-4:2006/AMD2:2011

IEC 61000-6-1:2016, *Electromagnetic compatibility (EMC) – Part 6-1: Generic standards – Immunity standard for residential, commercial and light-industrial environments*

IEC 61000-6-3:2020, *Electromagnetic compatibility (EMC) – Part 6-3: Generic standards – Emission standard for equipment in residential environments*

ISO 3696:1987, *Water for analytical laboratory use – Specification and test methods*

ISO 9058:2008, *Glass containers – Standard tolerances for bottles*

ASTM D3695 – 95:2013, *Standard Test Method for Volatile Alcohols in Water by Direct Aqueous-Injection Gas Chromatography*

ASTM D5309 – 16, *Standard Specification for Cyclohexane 999*

ASTM E1094 – 04:2015, *Standard Specification for Pharmaceutical Glass Graduates*

ASTM E1840 – 96:2014, *Standard Guide for Raman Shift Standards for Spectrometer Calibration*

European Pharmacopoeia 8.7:2016, 2.2.48, *Raman spectroscopy,* pp.5464-5466

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

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 http://www.iso.org/obp

3.1
container
vessel holding the liquid to be inspected and having a transparent or semitransparent wall or bottom or cap area

3.2
inspection time
time interval between the moment of starting the detection and that of obtaining the identification result

3.3
Raman analyzer
system using the Raman method for spectral identification of organic and inorganic liquids in transparent or semi-transparent containers, producing sample identification data in the form of the chemical name, CAS number or analogous standard substance-identification number, and allowing storage, processing and transfer of identification data for further procedures

3.4
Raman spectroscopy
optical technique of organic and inorganic substance identification based on spectral measurement and analysis of inelastic (Stokes Raman) light scattering by molecules under monochromatic laser illumination

Note 1 to entry: For each type of polyatomic molecule, the light scattering spectrum is composed of a unique set of characteristic peaks shifted in energy from the primary laser line (Raman shift). The method consists of laser light interacting with a substance, collection of the scattered light, spectrum processing and identification by comparison with a reference database of spectra.

3.5
Recognition Reliability Factor
RRF
quantity defining degree of coincidence of Raman spectra of the inspected and reference substances

Note 1 to entry: The recognition reliability factor is represented in a numeric form and is explicitly quantified in 4.3.7.2.

3.6
identification result
data including the common name of the inspected and identified liquid substance, CAS Register number (optional), molecular formula (optional), structural formula (optional) and the recognition reliability factor (optional)

Note 1 to entry: In the event of the identification of several substances, the identification result should include the aforementioned records for every identified substance.

3.7
identification data protocol
data including time and date, Raman analyzer Identification Number (Raman analyzer ID), Operator ID (optional), the identification result, and digital representation of measured and corresponding reference Raman spectra

3.8
test liquid
liquid used for testing system performance

3.9
test sample
combination of a test container subject to 3.1 and a test liquid subject to 3.8

4 Requirements

4.1 Structure and appearance

The connection ports of the Raman analyzer should be designed for easy installation and removal of the test sample, the condition specified in 3.1.

4.2 Functions

4.2.1 Alarm

The Raman analyzer should automatically provide warning in the form of acoustic and/or visual signals when hazardous liquids are identified.

4.2.2 Displayed data

a) The Raman analyzer shall display the identification result in a text or graphical form including optional fields subject to 3.6.

b) The Raman analyzer shall provide an interface for recording an identification data protocol.

4.2.3 Recording and storage of identification data

a) Inspected substance identification data and alarm activation marks should be automatically stored as a time-ordered sequence of data, including identification data protocol subject to 3.7. Users may have the option to disable automatic data logging.

b) Software shall be provided for search and retrieval of identification data.

c) Identification data protocol subject to 3.7 shall be reliably protected in a secure, read-only mode with authorized access to stored data and spectra.

d) The system shall be capable of exporting protocol data (or protocol fragments) and identification results in commonly used non-proprietary text or graphical formats.

e) It should be possible to access and transfer recorded spectral data to external data carriers in digital form.

4.2.4 Error diagnostics and self-verification

The system should have the functionality of error diagnostics and self-verification. Self-verification can be automatic or manual and should cover issues of the device calibration and apparatus functionality. This can be realized via internal calibrated light sources or based on an external etalon sample.

4.2.5 Access control software

The Raman analyzer should have an option to verify the operator's ID. Any unique digital or biometric ID parameters can be used for verification of authorized operators.

4.3 Performance

4.3.1 Testing conditions

4.3.1.1 Environmental conditions

Except where otherwise specified, tests shall be carried out under the standard test conditions shown in the third column of Table 1. For tests performed outside the standard test conditions, the values of temperature, pressure and relative humidity shall be stated and appropriate corrections, if any, made to ensure the expected response under reference conditions (column 2). All the tests mentioned in 4.3 shall be performed with the same system operating parameters. The values of any deviations should be reported. The reference conditions are given in the second column of Table 1.

The values in Table 1 are intended for tests performed in temperate climates. In other climates actual test values shall be stated. Atmospheric pressure lower than 70 kPa is allowed at higher altitudes and shall be similarly recorded.

Table 1 – Reference condition and standard test conditions

Environment condition	Reference condition	Standard test condition
Temperature	20 °C	15 °C to 35 °C
Relative humidity	65 %	45 % to 75 %
Atmospheric pressure	101,3 kPa	70 kPa to 106,6 kPa
Ambient electromagnetic field	Negligible	Less than the lowest value that causes interference
Ambient magnetic induction	Negligible	Less than twice the value of the induction due to earth's magnetic field

4.3.1.2 Test apparatus

The key apparatus for substance identification tests is shown in Table 2.

Table 2 – Key apparatus for tests and technical requirements

Test sample	Specification and accuracy class
Test sample 1	Glass 100 ml container (subject to ISO 9058:2008) with “Cyclohexane 999” (C_6H_{12}) (subject to ASTM D5309 – 16)
Test sample 2	Glass 10 ml container (subject to ASTM E1094 – 04(2015)) with “Cyclohexane 999” (C_6H_{12}) (subject to ASTM D5309 – 16)
Test sample 3	Glass 100 ml container (subject to ISO 9058:2008) with distilled water (H_2O) (subject to ISO 3696:1987)
Test sample 4	Glass 100 ml container (subject to ISO 9058:2008) with 10 % ethanol (C_2H_5OH) in water (H_2O) (subject to ASTM D3695 – 95:2013)
Test sample 5	Glass 100 ml container (subject to ISO 9058:2008) with a solution of 50 %(volume) methanol (CH_3OH) in 50 %(volume) ethanol (C_2H_5OH) (subject to ASTM D3695 – 95:2013)
Test Sample 6	Glass 100 ml container (subject to ISO 9058) with a solution of 33,3±1%(volume) methanol (CH_3OH), 33,3 ± 1 %(volume) ethanol (C_2H_5OH) and 33,3 ± 1 %(volume) isopropanol (C_3H_7OH) (subject to ASTM D3695 – 95)

4.3.2 Time for single inspection

4.3.2.1 Requirements

Maximum permitted inspection time shall not exceed 10 s.

4.3.2.2 Test method

The system shall successfully identify test sample 1 subject to ASTM E1840 – 96:2014; inspection time is subject to the requirements of 4.3.2.1 (Figure A.1 of Annex A).

4.3.3 Requirements for minimum volume of liquid to be inspected

4.3.3.1 Requirements

The Raman analyzer shall be capable of analyzing a liquid object with minimum volume of 10 ml.

4.3.3.2 Test method

Use test sample 2 for the minimum volume test. The test shall successfully identify cyclohexane by comparison to the reference spectrum given in ASTM E1840 – 96:2014, inspection time is subject to the requirements of 4.3.2.1.

4.3.4 Requirements for container wall thickness

4.3.4.1 Requirements

The Raman analyzer shall be capable of checking a liquid with a container wall thickness up to 10 mm.

4.3.4.2 Test method

The Raman analyzer shall perform a single identification of test sample 1 subject to ASTM E1840 – 96:2014. Insert 5 glass plates (fused silica or similar with (90 ± 5) % transmittance) with thicknesses 2 mm ±0,10 mm, 4 mm ±0,2 mm, 6 mm ±0,3 mm, 8 mm ±0,4 mm, 10 mm ±0,5 mm between test sample 1 and the Raman analyzer sequentially. The glass plate areas shall be sufficient to cover the output and input apertures of the Raman analyzer (see Figure 1). The orientation of glass plates should be reasonably perpendicular (±3 degrees) to the optical axis. The test shall successfully identify cyclohexane by comparison to the reference spectrum given in ASTM E1840 – 96:2014; inspection time is subject to the requirements of 4.3.2.1.

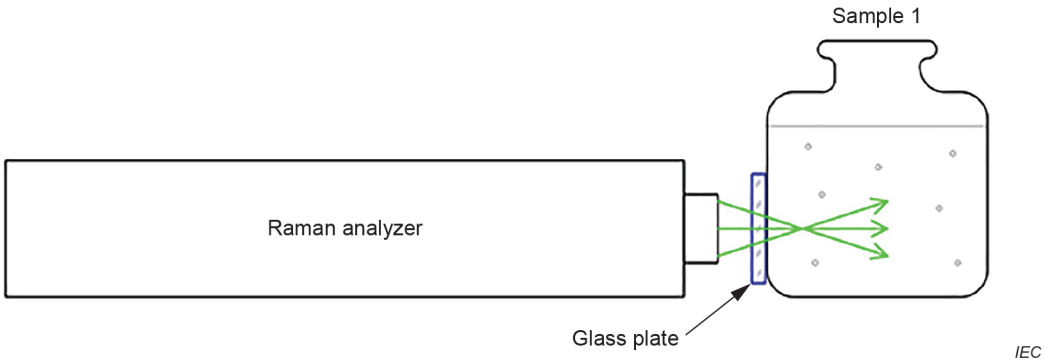

Figure 1 – Test on container wall thickness

4.3.5 Requirements for container wall transparency

4.3.5.1 Requirements

The Raman analyzer shall be capable of checking a liquid in a container with wall transmittance exceeding (25 ± 3) %.

4.3.5.2 Test method

The Raman analyzer shall perform a single identification of the test sample 1 subject to ASTM E1840 – 96:2014. Insert sequentially 6 standard absorbing or reflective neutral density filters with transmittance (80 ± 3) %, (63 ± 3) %, (50 ± 3) %, (40 ± 3) %, (32 ± 3) % and (25 ± 3) %; i.e. with an optical density (OD) ranging from 0,1 to 0,6 through 0,1 (transmittance $T = 10^{-OD}$) between test sample 1 and the Raman analyzer. The areas of the neutral density filters shall be sufficient to cover the output and input apertures of the Raman analyzer (see Figure 2). The orientation of glass plates should be reasonably perpendicular (± 3 degrees) to the optical axis. The test shall successfully identify test sample 1 by comparison to the reference spectrum given in ASTM E1840 – 96:2014; inspection time is subject to the requirements of 4.3.2.1.

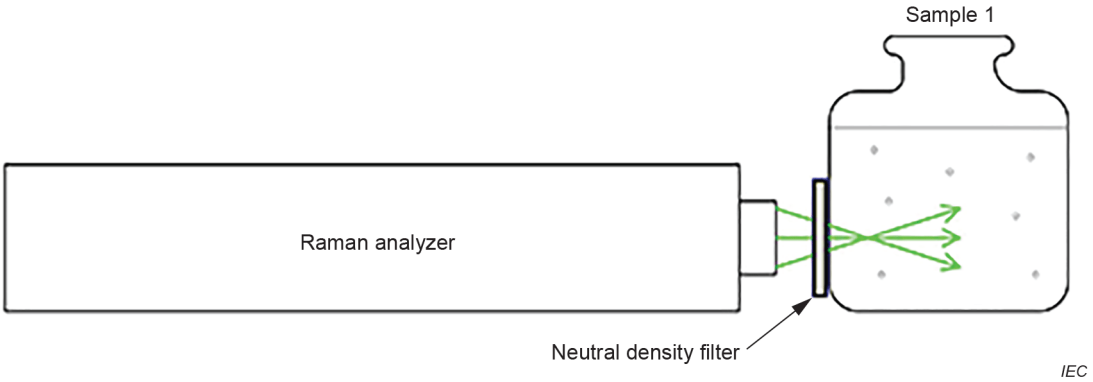

Figure 2 – Test on container wall transparency

4.3.6 Requirements for detectable spectral range

4.3.6.1 Requirements

The Raman analyzer shall be able to record Raman spectra of organic/inorganic liquids in the Raman shift range from 300 cm^{-1} to 3 600 cm^{-1}, the range that contains the characteristic peaks of most known liquids.

4.3.6.2 Test method

The Raman analyzer shall perform single identifications of test samples 1 and 3 and detect the following characteristic Raman features: for test sample 1 subject to ASTM E1840 – 96:2014 – four characteristic peaks at (384 ± 2) cm^{-1}, (801 ± 2) cm^{-1}, (1 444 ± 2) cm^{-1}, and (2 853 ± 2) cm^{-1}; for test sample 3 – the characteristic band ranging from (3 130 ± 30) cm^{-1} to (3 570 ± 30) cm^{-1} (Figure A.1 and Figure A.2 of Annex A). The recorded spectral data shall be either displayed on the embedded monitor or transferred in digital form to an external computer.

4.3.7 Reproducibility of identification result

4.3.7.1 Requirements

The identification result of the same test sample obtained in identical measurement conditions shall coincide with spread of the recognition reliability factor not exceeding 5 %.

4.3.7.2 Test method

Use test sample 1 subject to ASTM E1840 – 96:2014 for the identification reproducibility test (Table 3).

Perform 10 sequential measurement/identification cycles (inspection time is subject to the requirements of 4.3.2.1) and fill in the fields of Table 3, including the result of ID match to test sample 1 (true/false) and the numerical value of the calculated recognition reliability factor. The test is passed if all 10 identification results show the correct substance ID (Cyclohexane) and the coefficient of variation (CoV, defined as the ratio of the standard deviation σ to the mean value) of the recognition reliability factor does not exceed 0,05.