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Plastics — Plastics identification using Raman spectrometric methods

Plastiques — Identification des plastiques par spectrométrie Raman

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Foreword

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This document was prepared by Technical Committee ISO/TC 61, *Plastics*, Subcommittee SC 5, *Physical-chemical properties*.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

Plastic is an essential component used in making many types of products. Plastic formulations consist of polymeric or resin material and additives for affecting specific functions, such as plasticizers, foaming agents for low density parts, UV absorbers or colorants.

As a result, plastic and polymer identification and characterization is increasingly becoming more important in several distinct areas including, but not limited to, identification of unknown substances, product development, multi-layer materials, microplastics and environmental impact, including the ability to recycle and to allow informed decisions to be made.

Raman spectroscopy is an inelastic light scattering analysis technique, and is used to provide a structural fingerprint, by which materials can be identified. Monochromatic light, typically from a laser source, interacts with molecular vibrations, resulting in an energy shift. This energy shift is displayed as a spectrum. Raman spectra provide information about the vibrational modes in the sample, allowing materials to be identified. For example, different types of plastics have unique Raman spectral fingerprint. According to this principle, it is possible to identify unknown plastics by comparing them to known materials. The role of Raman spectroscopy is to identify the chemical composition of unknown plastics.

Plastics — Plastics identification using Raman spectrometric methods

1 Scope

This document is applicable to the qualitative analysis of plastic materials in their original form by Raman spectroscopy. It describes procedures to determine the composition of unknown general plastics and multi-layer film plastics.

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 472, *Plastics — Vocabulary*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 472 and the following apply.

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

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

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

3.1
general plastics
wide range of synthetic or semi-synthetic materials that use polymers as a main ingredient, which may also have a colourant added

3.2
multi-layer film plastic
material having two or more thermoplastic polymer layers

3.3
Z stack
set of confocal images taken from the sample so that the image area along the x- and y-axes remains the same but the distance from the objective z-axis is different for each image

3.4
pseudo-colour
colour added during the processing of spectra acquired through mapping to aid interpretation of the spectrum in pictorial form

4 Principle

In order to identify unknown plastics the sample is subjected to monochromatic light, such as laser light, which upon interaction with molecular vibrations or other excitations results in a shift of photons creating a characteristic fingerprint, the Raman spectrum. This fingerprint can be matched to reference spectra

allowing for rapid identification of the unknown plastic. The method is non-destructive and does not require sample preparation for most materials, allowing for use of the plastic directly after identification.

5 Apparatus

5.1 **Raman spectrometer**, of at least one highly stable monochromatic laser source used to excite the sample.

5.1.1 Several **laser wavelength**s are suitable for plastics identification such as 532 nm, 638 nm, 785 nm and 1 064 nm. Infrared excitation is recommended to reduce unwanted background fluorescence signal that can obscure the Raman spectrum.

5.1.2 Optical **power attenuation** of the laser is required to prevent photodamage to the sample, this can be controlled via adjustment of laser current or with neutral density filters.

5.1.3 The excitation light should be focussed on to the sample using high quality optical components such as **objective lenses** and **fibre probes**. The working distance, numerical aperture and magnification of the optics can vary between instrument types, with some systems allowing these components to be exchangeable by the user.

5.1.4 The scattered light shall then be collected by the same optics and filtered using an **edge** or **notch filter** to block the Rayleigh scattered light at the laser wavelength, this allows the weaker Raman scattered light to be detected and analysed.

5.1.5 A high throughput spectrometer with **spectral resolution** of at least 2 cm^{-1} is required to analyse the scattered light to be able to resolve and distinguish fine detail in the Raman spectrum to allow accurate identification. Spectral resolution is defined as the full width half maximum (FWHM) of the line width of a gas emission line measured on the spectrograph with the highest groove density grating. Typically, the pixel resolution should be at least 0,8 cm^{-1}/pixel. The spectral resolution will depend on the focal length of the spectrograph, the entrance slit width, the detector pixel size and the groove density of the diffraction grating. The Raman spectrometer should at least have a spectral range of 500 cm^{-1} to 1 800 cm^{-1} however a wider spectral range of 100 cm^{-1} to 3 500 cm^{-1} is recommended to ensure that the material will be correctly identified.

5.1.6 The **detector**, matching the chosen laser source and with an appropriate spectral response to cover the wavelength range required.

Several types of detectors are suitable for these measurements such as:

5.1.6.1 **front or back illuminated charge coupled detectors (CCD)**,

5.1.6.2 **electron multiplied charge coupled detectors (EM-CCD)**, and

5.1.6.3 **InGaAs arrays for infra-red detection**.

All detectors shall have high sensitivity and low noise to be able to detect the Raman signal. Detectors should be cooled to manufacturers recommendations, most require air cooling down to -60 °C, but some detectors require further cooling with water or liquid nitrogen. The system should have comprehensive software to allow hardware control and acquisition of spectra along with file export options compatible with the spectral library.

5.1.7 Use of a **microscope**-based system is recommended due to the versatility it offers when studying plastic materials that come in many formats, shapes and sizes. Portable devices can successfully be used to acquire spectra from bulk materials but have limited use determine composition of micrometre thick layers in the case of multilayer plastics.

5.1.8 A truly **confocal Raman system** with the ability to change pinhole size to allow accurate analysis of multi-layers of plastic material is also applicable and recommended. Additionally, it is recommended that the confocal Raman system has a motorised microscope stage, so that multi-layer plastics can be analysed by regularly taking measurements at set distances, through appropriate software, allowing the layer thickness to be determined. Multiple excitation wavelengths are recommended as plastics can give different background effects with different sources, and these can obscure relevant peaks. It is recommended to start analysis of unknown materials with 785 nm excitation as this usually gives a good balance between Raman signal strength and low background fluorescence.

6 Specimen

This method is suitable for general plastics including bulk plastics, particles, liquids, coloured plastics, single layer and multilayer films. Both transparent and opaque samples can be identified.

Generally, the sample does not need to be pre-processed, it can be directly presented to the Raman apparatus for identification. Depending on the requirements of the apparatus, the sample may need to be placed in a sample holder or on to a microscope stage for testing. The maximum size and thickness of the sample suitable for testing will be specified by the manufacturer of the apparatus, for very large samples a specimen may need to be prepared by cutting the sample to suitable dimensions. For powdered samples, a vessel to contain the sample will be required, such as a microscope slide, vial or dish. If the powder can contain a mixture of materials microscopy investigation is recommended. Other plastics, especially reinforced materials and multilayer film materials can be sliced and then their cross-sections can be tested. Microscopy is more appropriate for identification of specimens containing micrometre thick layers.

7 Testing procedure

7.1 Calibration and parameter settings

The Raman spectrometer should have, at a minimum, two forms of calibration: an underlying wavelength calibration that does not need to be repeated by the user and a Raman wavenumber calibration that shall be run daily when the system is in use, as well as after any apparatus change such as change of laser source or grating.

The wavelength calibration of the spectrometer is performed by the manufacturer using atomic emission lines from a mercury, argon or neon discharge lamp. The wavelength of emission lines are known to a high accuracy and precision. Measuring the position of these emission lines on the detector for each grating and grating angle available on the spectrometer, allows for the detector pixels to be calibrated to the correct wavelength. This is required to acquire accurate spectra that can be compared to other systems as well as cross referenced to spectral databases. The calibration record for the system can be requested from the instrument manufacturer. The Raman wavenumber calibration uses a suitable reference material, such as silicon, which has a known peak at approximately 520,7 cm^{-1} to offset the wavelength calibration of the system. This reference will take into account any environmental changes that can cause small drifts in the calibration of the system. This reference material is generally provided by the manufacturer inside the apparatus, it can also be presented to the apparatus externally by the user. The silicon peak position can vary with stress in the material and, therefore, each manufacturer recommends the exact peak position to use for the wavenumber calibration.

7.2 Measurement of Raman spectrum

7.2.1 Method 1 — General method

The test steps for analysing general use plastics on a Raman spectrometer are as follows.

a) Choose the appropriate excitation wavelength. If available, it is recommended that 785 nm is chosen as the starting wavelength for any sample. If the instrument contains fully integrated lasers and is completely software controlled, go to step c).

b) If the Raman instrument has external lasers or manually exchangeable optical components, follow the set-up procedure given by the manufacturer for the chosen laser wavelength. This alignment and calibration shall be checked before sample analysis begins.

c) Turn on the Raman spectrometer and selected laser. Allow the system to warm up for 30 minutes until the system is stable.

d) Place the sample on a stage or sample holder as recommended by the manufacturer. If not using a microscope go to step f). If using a microscope select a suitable magnification objective, such as x10, x20, or x50.

e) Switch on the microscope lamp to illuminate the sample. Focus on the sample using the microscope camera or eyepieces. Use the fine focus knob to precisely focus on the surface of the material.

f) It is important to adjust the laser power density on the sample, starting at a lower power and then increasing generally starting from 1 mW/µm^2. The approximate area of the excitation spot can be calculated using Formula (1):

$$A = \pi \left(\frac{0{,}61\lambda}{N.A} \right)^2 \quad (1)$$

where

A is the area;

λ is the wavelength;

$N.A$ is the numerical aperture.

The numerical aperture, N.A, of the objective lens or fibre probe should be provided by the manufacturer. The integration time generally should be set to less than 60 s to avoid the sample being heated and damaged by the laser.

g) Set the spectral range from 100 cm^{-1} to 3 500 cm^{-1}. The full extended range is recommended, however if not possible on the apparatus, record the spectral range at least from 500 cm^{-1} to 1 800 cm^{-1}.

h) It is recommended to select at least 3 points on the sample for testing to ensure uniformity across the sample surface. The focal spot size will vary depending on the apparatus used. Line illumination can also be used, which will sample from a larger region of the sample than a gaussian focussed laser spot.

i) Raman peaks should be clearly observed to allow appropriate analysis of the sample to take place. If fluorescence background prevents good quality spectra being acquired, try steps j) to n).

j) If available, close the confocal pinhole to reject the out of focus background signal from contributing to the measurement. This often will require increasing the exposure time to maintain good signal to noise.

k) If the fluorescence background is still too high and reducing the quality of the Raman spectrum, then bleach the fluorescence signal by illuminating the sample with the laser for a set time before taking another measurement. The time required will depend on the sample ranging from 60 s to 60 min. Increasing the power density on the sample can improve the effectiveness of photobleaching.

l) Check that the sample has not been burned by the laser during this time, by checking the microscope image of the sample after each measurement. If burning has been observed, move to a new location on the sample, reduce laser power and repeat sample bleaching step.

m) If previous steps do not achieve a suitable Raman spectrum, changing the laser excitation to a longer wavelength source and repeating the procedure can improve results.

n) If the previous steps do not completely remove background, then post process the data to remove the background signal.

7.2.2 Method 2 — Test method for multi-layer film plastics

7.2.2.1 General

It is advisable to use a microscope-based Raman system with a motorised stage, controllable through software to analyse multi-layer film plastics. For thick multilayer films, manual analysis of a cross section using method 2.2 (see 7.2.2.3) without a microscope is possible when the probe excitation spot is smaller than the layer thickness and can be positioned accurately to measure each layer distinctly. Annex E provides further information on the identification of multilayer plastics. The test steps for analysing these materials are as follows.

7.2.2.2 Method 2.1 — Setup protocol

a) Follow steps a-c of method 1 to set up the instrument.

b) Depending on the thickness and transparency of the sample, additional sample preparation steps may need to be taken before placing the sample on the microscope.

c) If non-destructive sample preparation is required go to method 2.3 (see 7.2.2.4) If destructive sample preparation is required continue to method 2.2 (see 7.2.2.3).

7.2.2.3 Method 2.2 — For multilayer films with very thin layers or for thick partially opaque films

a) If layers thinner than 3 µm are expected to be in the sample, then it is recommended to start with cross sectioning the film. This will allow for inspection of individual layer thickness before spectroscopy investigation. If layers are more than 1 mm then a non-microscope-based system could be used if the excitation spot is smaller than the layer thickness.

b) Place the specimen on the stage of the Raman spectrometer. To analyse thin layers select a high numerical aperture objective, such as x50/0,8 N.A. or x100/ 0,9 N.A. this will give suitable spatial resolution to identify layers thinner than 3 µm.

c) If available, switch on the microscope lamp to illuminate the specimen. Focus using camera or eyepieces or by eye until the objective or fibre is in the correct position for analysis. Use the fine focus control to precisely focus on the surface of the specimen. In the case of a portable or probe system position, the probe such that only one layer is investigated at a time.

d) It should be possible to see boundaries between layers in the film. If the specimen can be visualised on a camera, use the digital image and scale bar to measure the thickness of each layer. If no camera is available, then view the specimen with the eyepieces. A graticule eyepiece can be used to estimate the layer thickness.

e) If the layers are thicker than 3 µm then continue analysis with 785 nm laser.

f) If layers thinner than 3 µm are observed it is recommended to use a shorter wavelength excitation source, as this will improve the spatial resolution of the system ensuring very thin layers will not be missed during analysis. If the specimen has high fluorescence, then this may prevent analysis with shorter excitation.

g) After changing the laser source, it is important to adjust the laser power density on the specimen. The approximate area of the excitation spot can be recalculated using Formula (1).

h) If a motorised stage is available, generate a 2D line map across the full width of the cross-section. Set-up the stage coordinates for mapping in the software, use small step sizes of at least 1 µm for automated analysis. Proceed to step j).

i) If only manual sample positioning is available, then translate the sample stage to the first layer. Position the stage such that the known location of the Raman laser is overlayed with the location on the specimen and focus on the layer selected. Go to step j) and then repeat for each layer. This step can also apply for motorised stage control when automated analysis is not suitable.

j) Acquire spectra following steps g) to i) from method 1.

7.2.2.4 Method 2.3 — For thin and thick transparent multilayer films

a) To analyse thin films within the thickness of the intact multilayer film. The film should be secured flat on the microscope stage and held in place with tape.

b) Select a high magnification objective, such as x50/0,8 Numerical aperture or x100/ 0,9 N.A. Note that higher N.A objective lenses will have limited penetration depth into the specimen due to refractive index mis-match and limited working distance. Lower magnification objective lenses would be better suited for analysis of thick transparent films greater than 1 mm in thickness.

c) Switch on the microscope lamp to illuminate the specimen. Focus on the specimen using the microscope camera or eyepieces. Use the fine focus control for precise focussing through layers.

d) Use the microscope image of the specimen or the Raman signal intensity to determine the focus position for the top layer and bottom layer of the film and note the stage co-ordinates for these.

e) Once the Z coordinates have been determined and selected, using software, set a Z stack over the full depth of the film, with steps of at least 1 µm between each layer. In this case, the X and Y co-ordinates of the stage can be kept constant to generate a depth spectral series or a small volume in XY and Z can be sampled.

f) For thick samples >200 µm the laser power density on the specimen shall be increased. The approximate area of the excitation spot can be recalculated using Formula (1).

g) Close the confocal pinhole so that it is set between 25 to 100 µm. The small laser spot from the objective combined with an appropriate confocal pinhole, will allow specimen information to be collected from a small area which can be a small as 1 µm in X/Y and 2 µm in Z, dependent on excitation laser and NA of the optics. Control of the confocal pinhole size can be used to optimise the trade-off between throughput and spatial resolution.

h) Acquire spectra following steps g)-i) from method 1. Set the spectral range from 100 cm^{-1} to 3 500 cm^{-1}. The full extended range is recommended, however if not possible on the apparatus, record the spectral range at least from 500 cm^{-1} to 1 800 cm^{-1}.

8 Analysis of Raman spectrum

8.1 General

To identify unknown plastic samples using Raman spectrometer, the characteristic peaks in the collected Raman spectrum are compared with spectra of a known plastics using a Raman spectral database. This can either be a commercially available database or can be created by the laboratory. Commercial databases should also be supplemented with spectra taken of reference materials in the laboratory. Commercial databases come with a spectral matching and search tool, which automates the identification process and improves accuracy of results. The spectral database search should match both relative peak intensities and peak positions to find the correct match. Functional group analysis can also provide additional information to the user to make an informed decision on the composition of the unknown plastic. The Raman spectra can also be processed by baseline correction, differentiation, integration and normalization to improve the accuracy of identification.

For multi-layer film plastics, the spectrum for each layer can be given a pseudo-colour. By doing this, and giving each layer a different colour, a 3D representation of the specimen can be visualised. As the stage co-ordinates have also been logged, the analysis of these materials can give information on layer thickness as well as the chemical composition of the materials used present in the specimen.

8.2 Plastic identification

a) Post process spectra to remove cosmic rays and unwanted background signal using data processing tools in the Raman system control software.

b) Compare the spectrum with a suitable library. Manually inspect the top 10 entries to determine the best match. Annex A provides examples of Raman shifts of characteristic peaks of some plastics as well as functional groups.

c) The best match will be determined by comparing the peak position and relative intensities of the characteristic peaks of the measured sample matches the library spectrum closely over the full spectral range. Annex B provides additional examples of use of spectral libraries to identify unknown plastics.

d) If additional peaks are present and not matched to the top result then a 2nd component may be present which should also be identified. Annex D provides an example of identifying a multi component material.

e) Once verified, record the compound with the best match to the unknown spectrum, you may export a report showing the spectral overlay of the match a table of the peaks of the measured spectrum compared to the reference spectrum can be included in the report. For commercial database the score of the match result can also be recorded.

9 Test report

The test report of Raman spectrum shall include at least the following contents:

a) a full description of the sample and sample preparation if any, a reference to the document used including its year of publication;

b) the test instrument:

   1) the instrument model;

   2) test conditions including spectral range, laser wavelength, laser power and its attenuation value, exposure time, slit, pinhole and objective lens;

c) Raman spectrum correction process as background correction and smoothing;

d) the identification results to show the best match to the library reference spectrum;

e) any deviations from the procedure, noting any additional peaks or peaks that are shifted from the reference spectrum;

f) any unusual features observed;

g) the date of the test.

Example test reports are shown in Annex C and D.

Annex A
(informative)

Raman shift characteristic peaks of some plastics and functional groups

Table A.1 summarises some characteristic Raman peaks for common plastics. This information alone is not sufficient for plastic identification, the full spectrum should be analysed, and the relative peak intensities compared to the reference before an identification can be made. The peak positions of the key functional groups are given in Table A.2 and can also be used to identify the plastic.

Table A.1 — Raman shift characteristic peak of some plastics

No.	Plastics	Raman shift 1 cm^{-1}	Raman shift 2 cm^{-1}	Raman shift 3 cm^{-1}	Raman shift 4 cm^{-1}
1	PMMA	602	813	1 184	1 729
2	PC	637	887	1 176	1 230
3	PE	1 062	1 125	1 418	1 440
4	PP	841	1 157	1 322	1 451
5	PET	857	1 283	1 602	1 716
6	PS	621	1 001	1 032	1 602
7	PVAc	632	1 351	1 441	1 733
8	ABS	622	1 003	1 668	2 237
9	POM	921	1 093	1 492	2 925
10	PA6	933	1 128	1 309	1 638
11	PA66	953	1 130	1 443	1 653
12	PVC	636	694	1 427	2 939

Table A.2 — Raman shift range of key functional groups

Functional group	Mode	Raman shift range (cm^{-1})
C-C	Aliphatic chain vibrations	600 – 1 300
C-O	Symmetric stretching	820 – 1 050
C-O	Antisymmetric stretching	1 070 – 1 130
CH_2	Deformation - twisting	1 230 – 1 280
CN	Stretching	1 250 – 1 290
CH_2	Deformation-wagging	1 330 – 1 370
CH_2	Bending	1 440 – 1 480
C=O	Amide I ,Stretching	1 640 – 1 690
C=O	Stretching	1 715 – 1 735
CH	Stretching	2 880 – 2 890
CH_2	Symmetric stretching	2 850 – 2 900
CH_2	Antisymmetric stretching	2 910 – 2 960

Annex B
(informative)

Spectral database identification

For accurate identification of plastics, it is important to take into account the relative peak intensities as well as peak positions. This can be done by using a spectral database which matches the complete spectral profile to identify unknown samples. Built in spectral database search tools automate this process and show overlays of the measured unknown spectrum with the best match in the database.

A typical entry for a common plastic in the database is shown in Figure B.1. All peak positions are clearly labelled and the relative peak intensities can be tabulated allowing for manual verification of results.

Peak Table

Pos (cm^{-1})	Height
621.87	0.24
747.22	0.0986
1002.75	1
1032.64	0.29
1080.85	0.11
1157.02	0.15
1183.06	0.19
1200.42	0.21
1276.59	0.29
1304.56	0.37
1438.59	0.38
1584.19	0.18
1603.47	0.35
1641.08	0.23
1668.08	0.61
2237.95	0.14
2845.43	0.42
2908.10	0.71
3001.63	0.34
3054.67	0.39

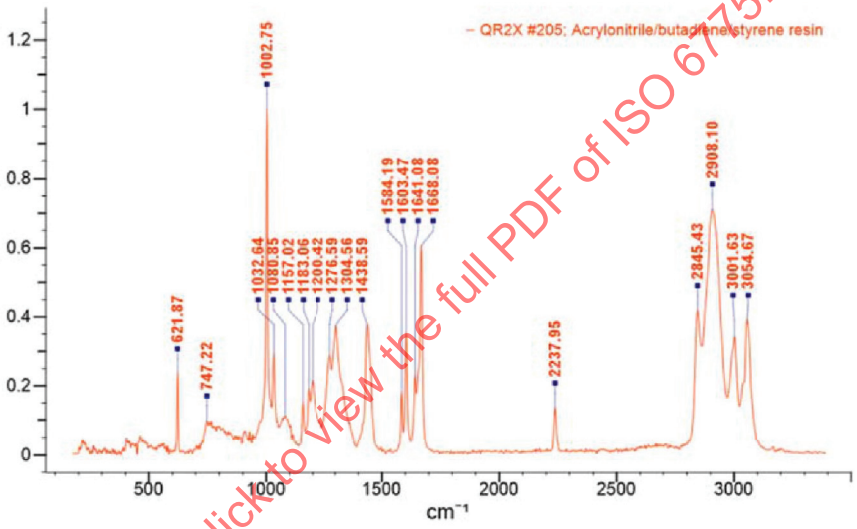


Figure B.1 — A typical entry for a common plastic in a spectral database

The database software also allows the spectra to be analysed by inspection of the functional groups providing additional information that can be used to select and interpret the correct match. An example of functional group analysis is shown in Figure B.2.

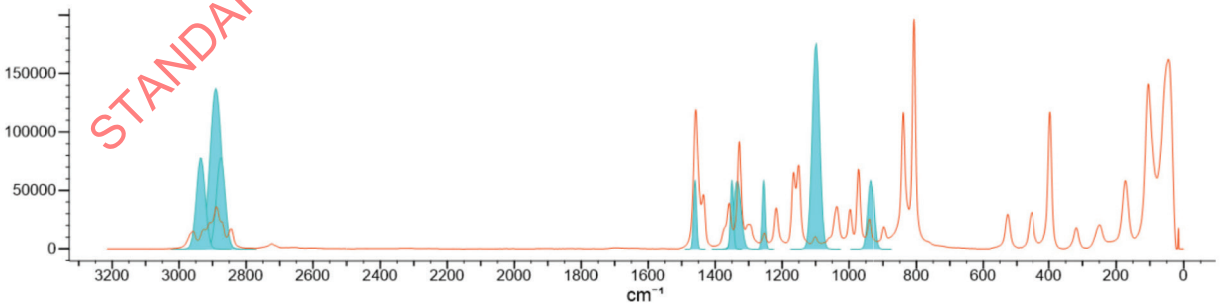


Figure B.2 — Functional group analysis

TableB.1 provides the functional group analysis of a heat resistant polypropylene carried out using KnowItAll®[1)] spectral library, shown with the functional group peak position overlayed on the spectrum.

Table B.1 — Functional group analysis

Bond	Range	Intensity	Mode
CH	2 900 - 2 880	weak	stretching
CH	1 350 - 1 320	weak	deformation
CH2	2 960 - 2 910	medium	antisymmetric stretching
CH2	2 900 - 2 850	medium	symmetric stretching
CH2	1 480 - 1 440	medium	deformation/bending
CH2	1 370 - 1 330	medium	deformation/wagging
CH2	1 280 - 1 230	medium	deformation/twisting
C-O	1 130 - 1 070	strong	antisymmetric stretching
C-O	1 050 - 820	medium-weak	symmetric stretching

1) KnowItAll® is a registered trademark of Wiley & Sons, Inc. This information is given for the convenience of users of this document and does not constitute an endorsement by ISO of the product named. Equivalent products may be used if they can be shown to lead to the same results.

Annex C
(informative)

Example test measurement 1

Figure C.1 presents the measurement conditions and results for the identification of a general use plastics. This is a single point measurement on the surface of a sample. KnowItAll® Raman Database was used to identify the sample.

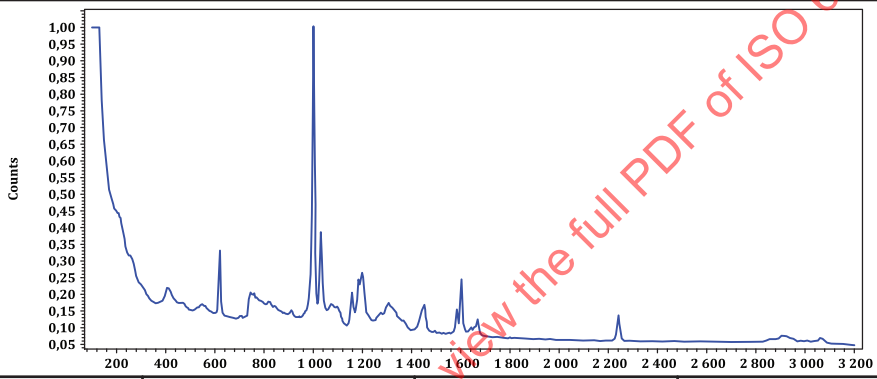
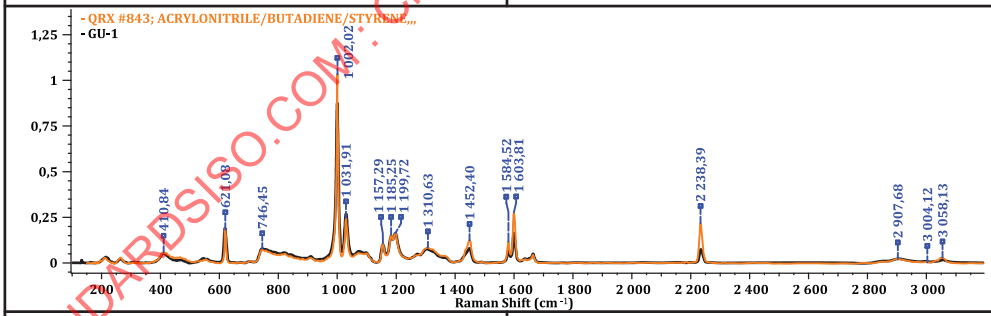
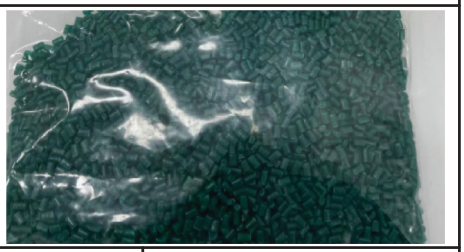
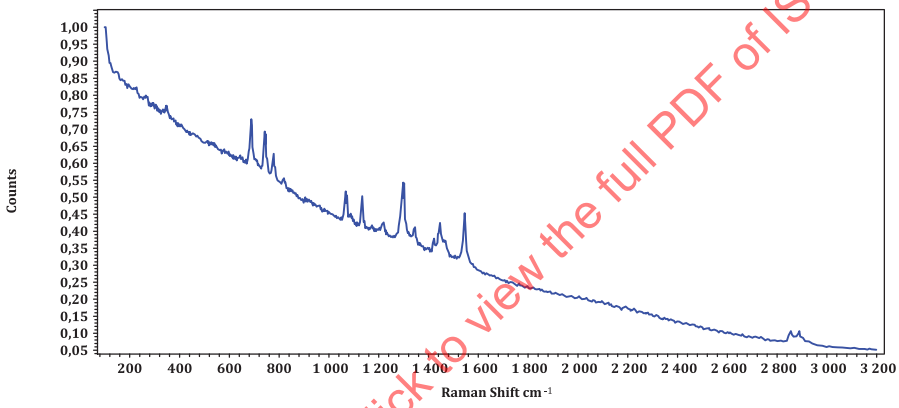
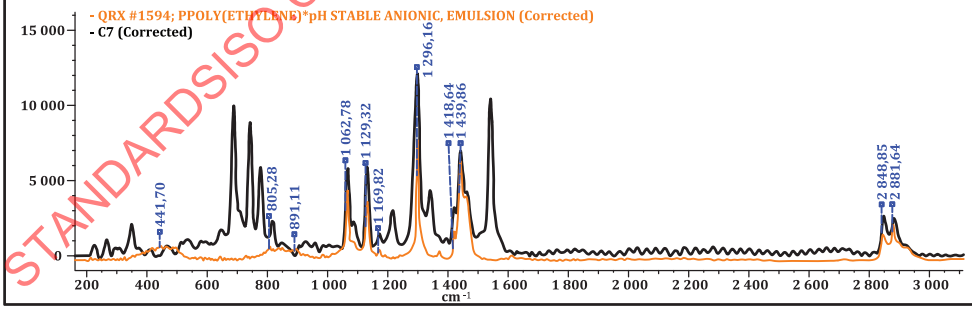
PLASTIC IDENTIFICATION TEST REPORT							
SAMPLE ID	GU-1-2						
SAMPLE TYPE	☒ GENERAL USE	☐ COLOURED	☐ MULTILAYER				
SAMPLE PREPARATION	Opaque white-coloured pellets were placed on a glass slide on the microscope stage,						
DEVICE	RM5	MANUFACTURER	EDINBURGH INSTRUMENTS				
Wavelength (nm)	Objective lens	Grating (lines/mm)	Pinhole	Slit (µm)	Laser power (%)	Exposure time (s)	Accumulations
785	10x/0,25	600	100 µm	70	100	20	3
RAMAN SPECTRUM							
							
PROCESSING	Cosmic ray removal ☒	Background correction ☐	Other: Click or tap here to enter text,				
DATABASE SEARCH	KnowltAll, Wiley						
							
MATERIAL(S) IDENTIFIED	QUALITY OF FIT						
ACRYLONITRILE-BUTADIENE-STYRENE RESINS	94,91 %						

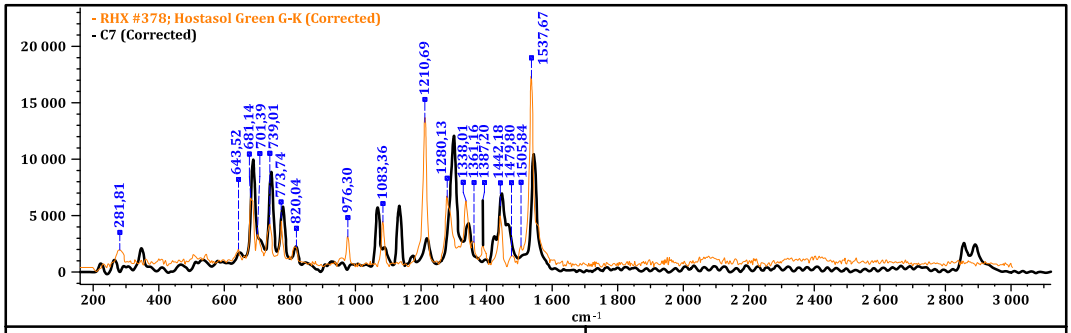
Figure C.1 — Measurement conditions and results for the identification of a general use plastics

Annex D
(informative)

Example test measurement 2

In Figure D.1, the measurement conditions and results for the identification of a coloured plastic are presented. This is a single point measurement on the surface of a sample. KnowItAll® Raman Database was used to identify the sample. In this example, two components were identified one for the plastic and the other the colourant.

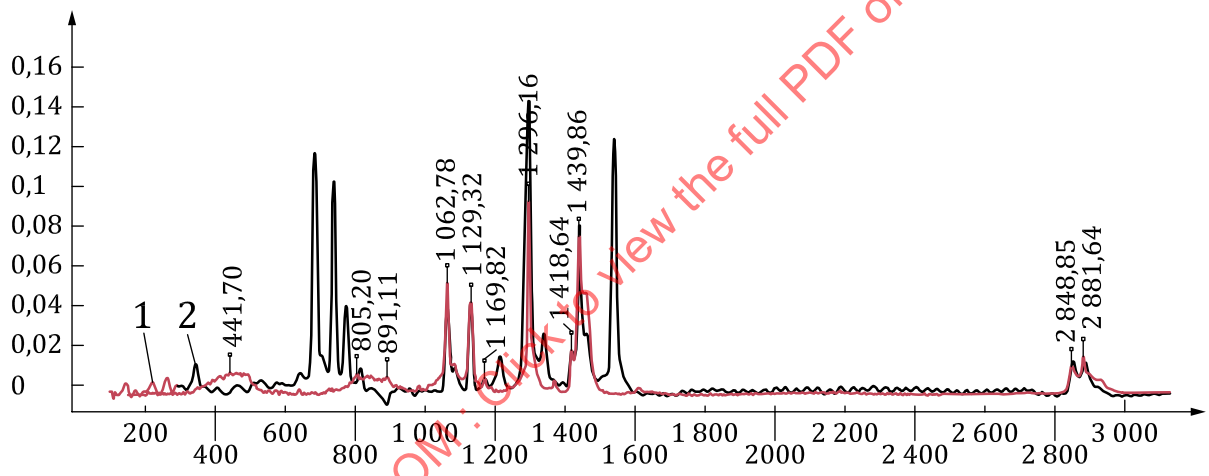
PLASTIC IDENTIFICATION TEST REPORT								
SAMPLE ID	C-7							
SAMPLE TYPE	☐ GENERAL USE	☒ COLOURED	☐ MULTILAYER					
SAMPLE PREPARATION	Dark green pellets, placed on a glass microscope slide,							
DEVICE	RM5	**MANUFACTURER**	EDINBURGH INSTRUMENTS					
Wavelength (nm)	**Objective lens**	**Grating (lines/mm)**	**Pinhole**	**Slit (µm)**	**Laser power (%)**	**Exposure time (s)**	**Accumulations**	
785	**10x/0,25**	**600**	**300 µm**	**70**	**20**	**2**	**5**	
RAMAN SPECTRUM								
								
PROCESSING	Cosmic ray removal ☐	Background correction ☒	Other: Cropped range from 850 cm^{-1}					
DATABASE SEARCH	KnowltAll, Wiley (with manual assignment)							
								



MATERIAL(S) IDENTIFIED	SCORE
Hostasol Green G-K	61,64 %
POLY(ETHYLENE)*pH STABLE ANIONIC EMULSION	60,59 %

Figure D.1 — Measurement conditions and results for the identification of a coloured plastic

The database scores were only 60 % for each component. In cases like this improvement in database match can be achieved by restricting the spectral region. For the same sample the scores of Poly(ethylene) improved to 92,90 when restricted to the peaks shown in Figure D.2.



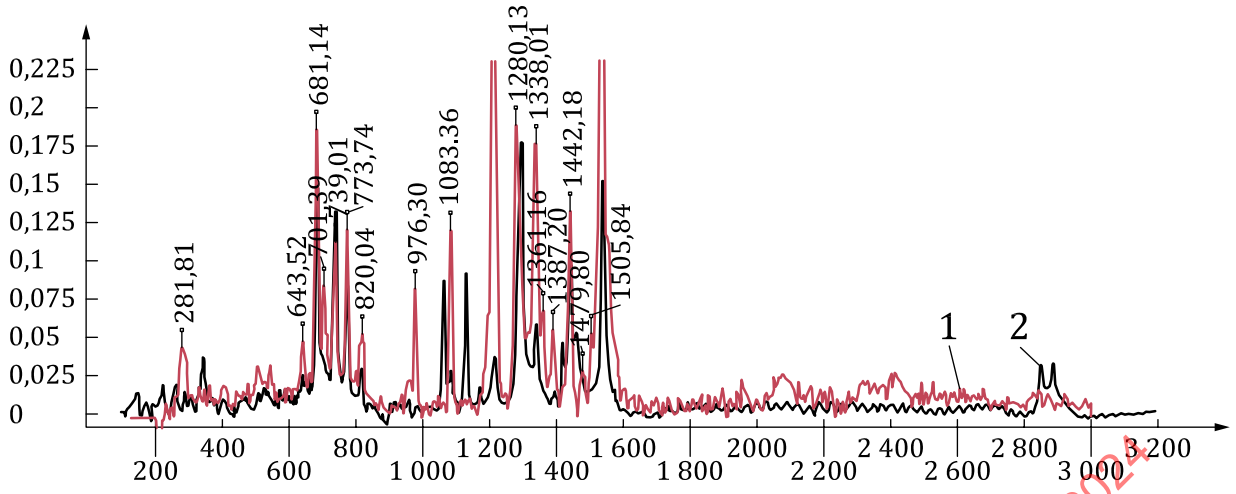
Key

1 database spectrum

2 measured spectrum

Figure D.2 — Scores of Poly(ethylene) improved to 92,90 when restricted to the peaks

Then for the colouring agent the match to Hostasol Green G-K increased to 94,05 when restricting the spectral range as shown in Figure D.3.



Key

1 database spectrum

2 measured spectrum

Figure D.3 — Colouring agent the match to Hostasol Green G-K increased to 94,05 when restricting the spectral range

This requires more expertise and prior knowledge from the analyst to identify the regions to restrict the search to. However, the identification results are the same, only the database match scores improve giving more confidence in the result.