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Use of UV-Vis absorption spectroscopy in the characterization of cadmium chalcogenide colloidal quantum dots

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Use of UV-Vis absorption spectroscopy in the characterization of cadmium chalcogenide colloidal quantum dots

Utilisation de la spectroscopie d'absorption dans l'UV-visible pour la caractérisation des points quantiques colloïdaux des chalcogénures de cadmium

Reference number
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Contents

Page

Foreword

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The committee responsible for this is document is ISO/TC 229, *Nanotechnologies*.

Introduction

Engineered nanoparticles of semiconductor materials with sizes down to the extent where the behaviour of electrons and holes are affected by the quantum confinement often possess unique electronic and optical properties intermediate between those of bulk semiconductors and those of discrete molecules. This normally refers to a nanoparticle diameter comparable to the Bohr radius of the exciton for the particular semiconductor material. Such nanoparticles are generally called quantum dots (QDs). A significant feature of these nanoparticles resulting from quantum confinement of charge carriers is size dependence of their electronic structure and, consequently, the excitonic absorption and emission wavelengths. Particularly, the transition energy from the valence band to the conduction band, and consequently the onset of absorption and the first excitonic transition (referred to here as first absorption peak position), is a function of the diameter of the particle (see Reference [1]).

Quantum dots commonly present sophisticated core-shell structures with a ligand shell controlling solubility and subsequent chemical functionalization. They are typically synthesized by chemical methods, with large-scale production and their size, shape, composition, and structure control capabilities. Commercially available quantum dots are mainly made from cadmium chalcogenide (CdTe, CdSe, CdS) materials. The size dependence of emission maximum, narrow emission band width, and good photostability make these engineered nanoparticles appealing in biological labelling and opto-electronics applications (see Reference [2]).

Ultraviolet-visible (UV-Vis) absorption spectroscopy has become a routine method to characterize QDs in a colloidal dispersion, by utilizing the relationship between the wavelength of the first excitonic absorption peak and the particle size that has been established after extensive photophysics research in the past, and using analytical methods for high-quality cadmium chalcogenide (CdTe, CdSe, CdS) materials of narrow size distribution. Key properties, such as average nanoparticle size and number concentration, can be approximately calculated from the measured absorption spectra. This Technical Specification intends to facilitate the use of UV-Vis spectroscopy for the characterization of quantum dot colloidal dispersions.

Use of UV-Vis absorption spectroscopy in the characterization of cadmium chalcogenide colloidal quantum dots

1 Scope

This Technical Specification provides guidelines for estimating the diameter and the number concentration of monodisperse cadmium chalcogenide (CdTe, CdSe, CdS) quantum dots (QDs) with a narrow size distribution in a colloidal dispersion using Ultraviolet-visible (UV-Vis) absorption spectroscopy.

The analysis of the spheroidal particle size is applicable to the diameter range of 3,5 nm to 9 nm for CdTe, 1 nm to 8 nm for CdSe, and 1 nm to 5,5 nm for CdS and is recommended for samples with narrow size distributions.

2 Terms, definitions, and abbreviated terms

2.1 Terms and definitions

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

2.1.1
quantum dot
QD
crystalline nanoparticle that exhibits size-dependent properties due to quantum confinement effects on the electronic states

[SOURCE: ISO/TS 27687:2008, definition 4.7]

2.1.2
quantum confinement
boundary condition resulting in phenomena when electrons and holes in a material are confined by a potential well in one dimension (quantum well), in two dimensions (quantum wire), or in three dimensions (quantum dot)

[SOURCE: ISO/IEC DTS 80004-12, definition 2.5]

2.1.3
first excitonic absorption
light absorption in quantum dots originating from the electronic transition from ground state to first excitonic excited state

2.2 Abbreviated terms

QD	quantum dot
TEM	transmission electron microscopy
TOPO	trioctylphosphine oxide
OPA	n-octylphosphonate
HDA	hexadecylamine

HWHM	half width at half maximum
FWHM	full width at half maximum
PPA	*P'*-*P'*-(di-n-octyl) pyrophosphonate
UV-Vis	ultraviolet-visible
E_{1s}	energy of first excitonic transition
I	intensity of light transmitted through a sample
I_0	intensity of incident light before it passes through the sample
A	absorbance
d	particle diameter
λ	wavelength
ε	molar extinction coefficient
c	particle number concentration
l	path length

3 Principle

3.1 General

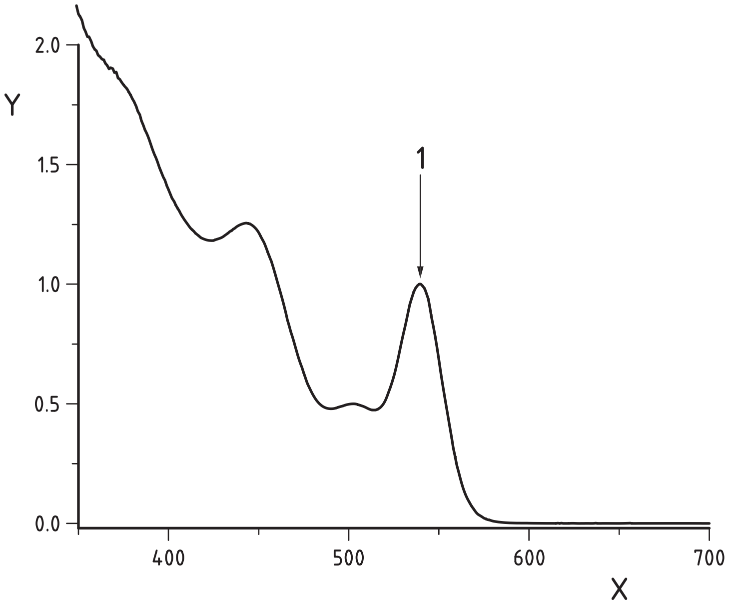
The absorption spectrum (absorbance A as a function of wavelength) of a QD colloidal sample with a narrow size distribution shows discrete peaks, due to the quantized energy levels in the quantum dots. Among these, the first excitonic absorption contains information on particle size (through the wavelength of the peak maximum), size distribution (through the peak HWHM), and concentration (through the peak intensity).

3.2 UV-Vis absorption spectroscopy

The intensity of light passing through a sample (I) is measured and compared to the intensity of incident light (I_0). The absorbance, A, is expressed as $-\log (I/I_0)$. The plot of the absorbance against wavelength for a particular compound is referred to as an absorption spectrum.[3][4]

3.3 Absorption peaks of quantum dots in the UV-Vis region

A typical optical absorption spectrum of colloidal CdSe QDs is shown in Figure 1. The lowest energy (longest wavelength) first excitonic absorption peak at 545 nm is attributed to the excitonic transition from the valence band to the conduction band.



Key

1 first excitonic absorption peak

X wavelength/nm

Y absorbance

Figure 1 — Typical optical absorption spectrum of CdSe quantum dots in a dispersion

3.4 Relation between quantum dot diameter and optical absorption peak wavelength

Chalcogenide specific relationships have been established between the nanoparticle number averaged Feret diameter, *d*, (in nm) determined mainly by TEM and the wavelength, *λ*, (in nm) of the lowest energy excitonic absorption peak in the UV-Vis absorption spectra. The relationship formulae are recommended as follows (see Reference [5]):

For CdTe:

$$d = \mathrm{A} + \mathrm{B}\lambda + \mathrm{C}\lambda^2 + \mathrm{D}\,\lambda^3 \tag{1}$$

coefficient	A	B	C	D
value with unit	−194,84 nm	10 064	$-1{,}714\,7 \times 10^{-3}$ nm^{-1}	$9{,}812\,7 \times 10^{-7}$ nm^{-2}

For CdSe:

$$d = \mathrm{A} + \mathrm{B}\,\lambda + \mathrm{C}\,\lambda^2 + \mathrm{D}\,\lambda^3 + \mathrm{E}\,\lambda^4 \tag{2}$$

coefficient	A	B	C	D	E
value with unit	41,57 nm	−0,427 7	$1{,}624\,2 \times 10^{-3}$ nm^{-1}	$-2{,}657\,5 \times 10^{-6}$ nm^{-2}	$1{,}612\,2 \times 10^{-9}$ nm^{-3}

For CdS:

$$d = \mathrm{A} + \mathrm{B}\lambda + \mathrm{C}\lambda^2 + \mathrm{D}\,\lambda^3 \tag{3}$$

coefficient	A	B	C	D
value with unit	13,29 nm	$-9{,}235\,2 \times 10^{-2}$	$1{,}955\,7 \times 10^{-4}$ nm^{-1}	$-6{,}652\,1 \times 10^{-8}$ nm^{-2}

These formulae allow the users to approximate the average size of monodisperse QD from a measured absorption spectrum. The analysis is applicable to the size range of 3,5 nm to 9 nm for CdTe, 1 nm-8 nm for CdSe, and 1 nm to 5,5 nm for CdS.

Given the approximative nature of the formulae above, and the various approximations made both in the TEM measurements and the UV-Vis measurements, the d-values determined shall be reported as: UV-Vis absorption peak equivalent QD diameter (obtained according to ISO/TS 17466).

3.5 Relation between quantum dot concentration and optical absorption peak intensities

According to the Beer-Lambert law [Formula (4)], the molar extinction coefficient ε (in the unit of L $mol^{-1}cm^{-1}$) is related to A at the first excitonic absorption peak position, with particle concentration c in mol L^{-1} and path length l in cm.

$$A = \varepsilon\, c\, l \tag{4}$$

The concentration c of QDs can be calculated if A, I, and ε are known.

Given the approximative nature of Formula (4), and the various approximations made in the UV-Vis measurements, the c-values determined shall be reported as: UV-Vis absorption peak equivalent QD concentration (obtained according to ISO/TS 17466).

3.5.1 Normalization of absorbance A for samples with wide size distributions

For the purpose of this Technical Specification, QDs with a size standard deviation less than 10 % are considered monodisperse. For samples with broader size distributions, it is necessary to take into consideration the resulting absorbance peak broadening and normalize the value of the absorbance A at the first excitonic absorption according to the following formula.

$$A = A_\mathrm{m}\ (\mathrm{HWHM})_\mathrm{m}/(\mathrm{HWHM})_\mathrm{ref} \tag{5}$$

where A_m is the measured absorbance, $(\mathrm{HWHM})_\mathrm{m}$ is the measured half width at the half maximum (HWHM) on the low energy side of the first exciton absorption peak and $(\mathrm{HWHM})_\mathrm{ref}$ is a reference value obtained for a corresponding high quality colloidal II/VI quantum dot, 18 nm, 14, and 11 nm for CdTe, CdSe, and CdS, respectively.[5]

3.5.2 Derivation of extinction coefficient ε from particle size

When the first excitonic absorption energy or the diameter of the QDs is known, ε can be calculated from the following formulae, as recommended in References [5] and [6]:

For CdTe:

$$\varepsilon = 10\,043\ (\mathrm{d})^{2,12} \tag{6}$$

For CdSe:

$$\varepsilon = 155\,507 + 6{,}670\,54 \times 10^{13}\exp(-E_{1s}/0{,}105\,51) \tag{7}$$

For CdS:

$$\varepsilon = 21\,536\ (\mathrm{d})^{2,3} \tag{8}$$

where d is a particle diameter (in nm), and E_{1s} is the energy of the first excitonic transition (in eV). Formulae (6) and (8) are taken from Reference [5] and Formula (7) is taken from Reference [6]. Conversion between the wavelength λ in nm and transition energy E in eV is through λ (nm) = 1240/E (eV).

4 Sample preparation

For the measurement of absorption spectra, a homogeneous and stable dispersion of QDs is needed. The solvent should be compatible with the surface chemistry of the QDs to produce a clear dispersion, while not interfering with the QDs absorption spectrum. Commercially available QDs are normally synthesized by a wet chemical organometallic reaction, and the surface of QDs is coated with organic molecules, such as TOPO, OPA, PPA, and HDA.[7] These molecules prevent aggregation and maintain dispersibility of QD. Nonpolar solvents such as hexane or chloroform should be used if the QDs are hydrophobic. If the QDs' surface chemistry was changed to become hydrophilic by performing a ligand exchange, a polar solvent such as water can be used.

In general, QD are small and are well dispersed at low concentrations in the suitable solvents. Care should be taken to ensure that a visibly transparent dispersion is obtained.

For the Beer-Lambert law to be applicable for this Technical Specification, a dilute dispersion with absorbance (A) less than 1 is necessary. When performing the dilution, care should be taken to avoid particle aggregation due to desorption of ligand molecules from the nanoparticles.

5 Measurement procedure

5.1 UV-Vis spectrometer

Use any calibrated standard spectrophotometer covering the UV to visible wavelength range. For cadmium chalcogenide QDs in the size range specified in this Technical Specification, the first excitonic absorption peak occurs in the spectral window from 250 nm to 750 nm, depending on the respective core material. The UV-Vis spectrometer should be calibrated with reference materials, such as a reference optical filter.[8]

Calibration shall be performed prior to the test and shall consist of a control of the accuracy of the wavelength and intensity scale.

5.2 Optical measurement procedure

Follow the standard procedure for the measurement of an absorption spectrum, referring to the instrument user manual. Use quartz cuvettes for the test solution sample and use an identical cuvette containing the solvent of the QDs colloidal dispersion as the reference for background subtraction. Measurements are to be performed in air at room temperature.

5.3 Recommended conditions

The following conditions are recommended:

a) The wavelength range is 250 nm to 750 nm.

b) The scan step is set to be 0,5 nm or 1 nm.

c) The spectral bandwidth is 1 nm or 2 nm.

6 Data analysis and interpretation of results

Record the wavelength and absorbance value of the absorption maximum, according to the manufacture's instruction, for the first excitonic absorption peak.

6.1 Data analysis for approximation of QD size

Using the recorded wavelength for the first excitonic absorption peak, calculate the mean diameter, *d*, using the formulae given in 3.4 within the range of their applicability.

NOTE The analysis using the formulae is applicable for the diameter range of 3,5 nm to 9 nm for CdTe, 1 nm to 8 nm for CdSe, and 1nm to 5,5 nm for CdS.

6.2 Data analysis for characterization of QD concentration

The procedure for determining the concentration of a QD specimen is as follows:

a) Determine the mean particle diameter, *d*, following the procedure specified in 6.1.

b) Calculate the molar extinction coefficient of QD dispersion, ε, from the formula given in 3.5.

c) Normalize the peak absorbance, *A*, if required, according to Formula (5) in 3.5.1.

d) Calculate the number concentration of the QD dispersion, *c*, following Beer-Lambert law [Formula (4) in 3.5].

7 Measurement uncertainty

The measurement uncertainties of the size and concentration values of QD dispersions obtained following the above optical absorption method are to be estimated according to the general method described in Reference [9] or equivalent, for which contributions from the origins listed below should be included.

a) Uncertainty associated with a potential abnormal size distribution of QDs in the sample, which cannot be accounted for by normalization of the peak maximum absorbance *A*.

b) Uncertainties associated with accuracy and precision of the formulae in 3.4 and 3.5. It is noted that these formulae are approximations recommended by some authors, and as such they have not been fully validated. Note these formulae represent a fit of experimental data, the dispersion of the data respect to the best fit, leading to dispersions of the curve parameters, A, B, C, D, and E for formulae in 3.4, should be taken into account. For the purpose of this Technical Specification, their contributions to measurement uncertainty are regarded as the biggest ones. The estimated uncertainties associated with formulae in 3.4 and 3.5 are 15 % and 50 %, respectively.

c) Uncertainties associated with the photometer calibration (accuracy of the wavelength and intensity scale) and the repeatability of the absorption measurement. For well calibrated and maintained instruments, this contribution to the overall uncertainty is small.

d) Uncertainties associated with data analysis (including determination of the peak wavelength and maximum absorbance, background subtraction, and others). For the approximation of QD sizes specified in this Technical Specification, an uncertainty of 1 nm in wavelength determination corresponds roughly with an uncertainty of 0,02 nm in QD diameter.

8 Test report

The test report shall include the following information:

a) Experimental data: peak wavelength, HWHM, and peak absorbance.

b) The results:

    (1) the mean size of the QDs including a full statement of the measurand: UV-Vis absorption peak equivalent QD diameter (obtained according to ISO/TS 17466);

   (2) the number concentration of QDs including a full statement of the measurand: UV-Vis absorption peak equivalent QD concentration (obtained according to ISO/TS 17466).

c) All information necessary for the identification of the sample tested:

   (1) the sample name;

   (2) the lot number;

   (3) the solvent/matrix used for dispersing the QDs and used as the reference.

d) The type of instrument used and measurement conditions, where applicable:

   (1) the wavelength range;

   (2) the scan step and spectral bandwidth;

   (3) temperature at which the measurement is performed.

Annex A
(informative)

Case study for determining the diameters of CdSe QDs from UV-Vis absorption spectra

A.1 General

This Annex provides an example of the approximate determination of the average diameter of CdSe QDs colloidal dispersion using UV-Vis absorption spectroscopy. Size determination using high-resolution transmission electron microscopy (HRTEM) is also given for comparison.

A.2 CdSe QD samples

Three CdSe QD samples (sample 1-3) with different size, and thus different wavelength of their first excitonic absorption peak, were analysed. CdSe QDs were dispersed in toluene (Analytical Grade) for UV-Vis absorption spectroscopy.

A.3 Instruments

UV-Vis absorption spectra were recorded on a Perkin Elmer Lambda 650 UV/Vis spectrophotometer at room temperature, with samples held in 1 cm path length quartz cuvettes. HRTEM images of CdSe QDs were taken with a FEI Tecnai G2 F20 S-TWIN TEM operating at 200 kV.

A.4 Measurement conditions for UV-Vis spectroscopy

The UV-Vis spectrometer was calibrated with a praseodymium-neodymium optical filter. Measurement conditions were set as follows:

a) Wavelength range was 250 nm to 750 nm.

b) Scan step was set as 0,5 nm.

c) The spectral bandwidth was chosen as 2 nm.

d) The background was corrected using toluene (Analytical Grade), the solvent of CdSe QDs dispersion.

A.5 Procedures for UV-Vis spectra measurement

a) An appropriate volume of the CdSe QD sample was added into a quartz cuvette with the optical path of 1 cm.

b) The cuvette was put into the instrument sample holder, and the measurement conditions were set for the UV-Vis spectrometer.

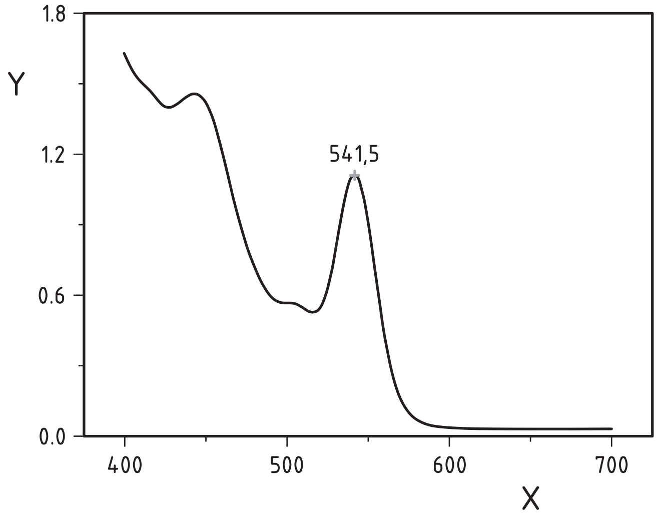
c) A scan was performed in the 250 nm to 750 nm range and the UV-Vis spectrum was recorded.

d) The wavelength of the first excitonic absorption peak was obtained either manually or by using the automatic peak search function of the spectrophotometer. Note that this measurement can also be obtained from the exported data set using a third-party software package such as Origin.

The measurements were repeated three times for each sample, and the average values were calculated.

A.6 Results of UV-Vis spectra

Figures A.1 to A.3 are typical UV-Vis spectra of three CdSe QD samples (only the range 400 nm to 700 nm is shown to better identify the absorption peak).

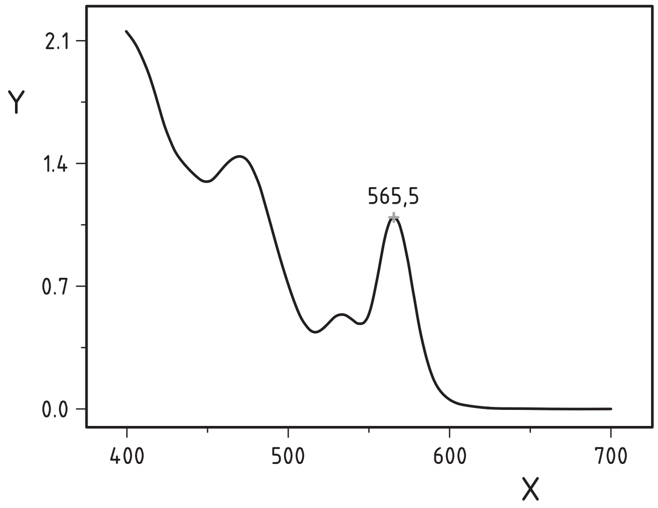


Key

X wavelength/nm

Y absorbance

Figure A.1 — Typical UV-Vis spectrum of sample 1

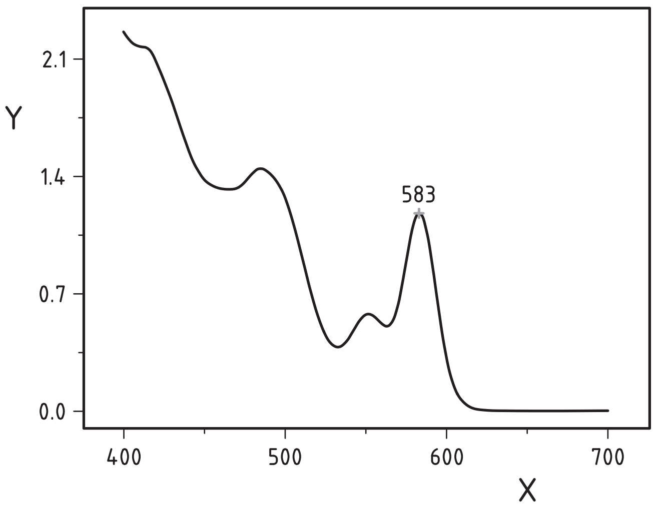


Key

X wavelength/nm

Y absorbance

Figure A.2 — Typical UV-Vis spectrum of sample 2



Key

X wavelength/nm

Y absorbance

Figure A.3 — Typical UV-Vis spectrum of sample 3

A.7 UV-Vis spectra analysis

The average diameters of the three CdSe QD samples were calculated using Formula (2) in 3.4.

A.8 Procedures for HRTEM analysis

a) One or two drops of CdSe QD samples were placed on a copper grid.

b) The grid was transferred to the sample holder, the sample holder was then inserted into the TEM according to operation instructions.

c) Images were captured according to instrument instructions.

A.9 Typical HRTEM images, image analysis and QD size statistics

Figures A.4 and A.5, Figures A.6 and A.7, and Figures A.8 and A.9 show typical HRTEM images and corresponding QD average particle diameter distribution of the three CdSe QD samples. As indicated by arrows in Figure A.4, A.6, and A.8, the long-axis and short-axis diameter of each of the particle in the images were measured. For each sample, about 1 400 particles were characterized, their average diameter distribution and its Gaussian fit were plotted, and statistically determined.

For more information about particle size analysis, ISO 13322-1:2004 can be referred to.

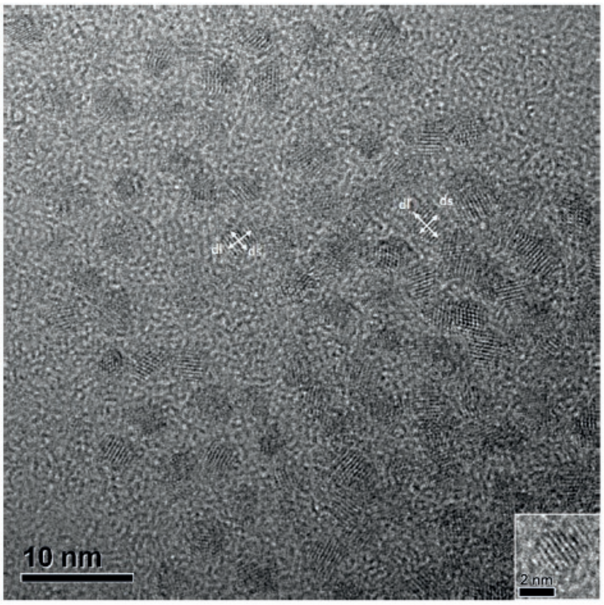
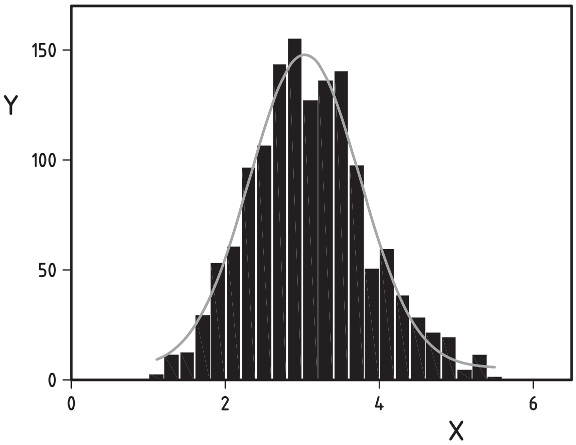


Figure A.4 — Typical HRTEM image of sample 1



Key

X d_{QD} (nm)

Y count

Figure A.5 — Diameter distribution of 1 377 particles of sample 1 (average diameter for each particle has been determined and plotted here)

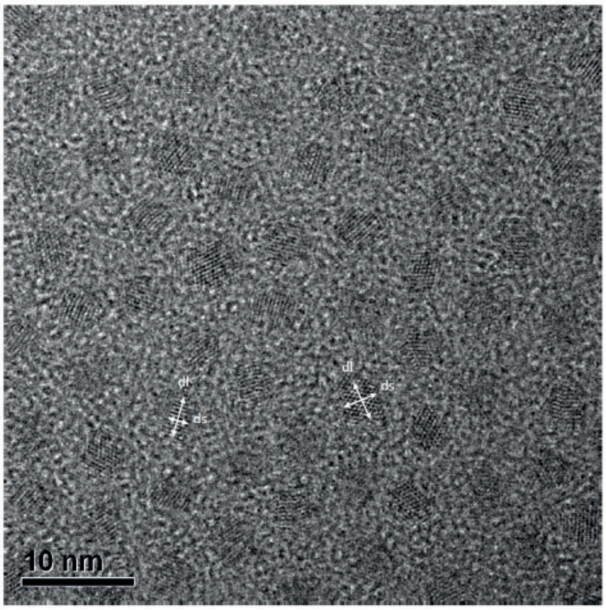
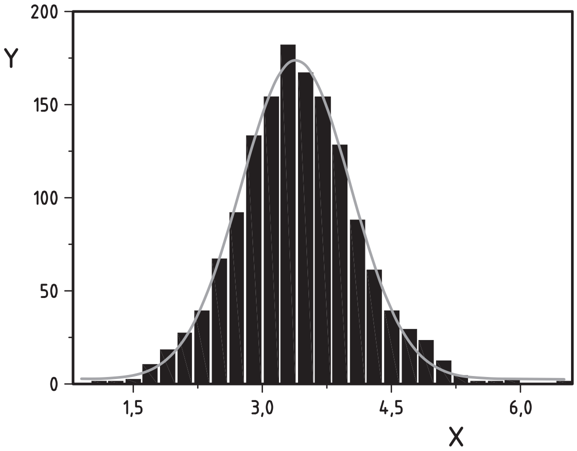


Figure A.6 — Typical HRTEM image of sample 2



Key

X d_{QD} (nm)

Y count

Figure A.7 — Diameter distribution of sample 2 on the basis of 1 436 particles (average diameter for each particle has been determined and plotted here)

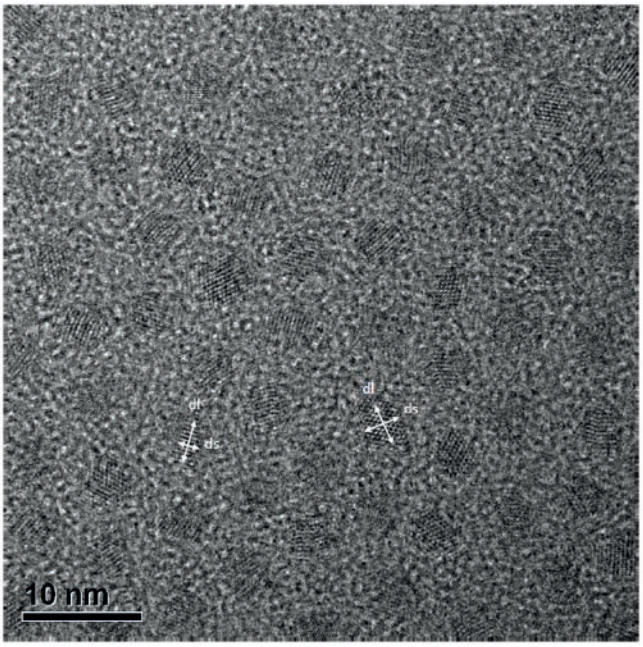
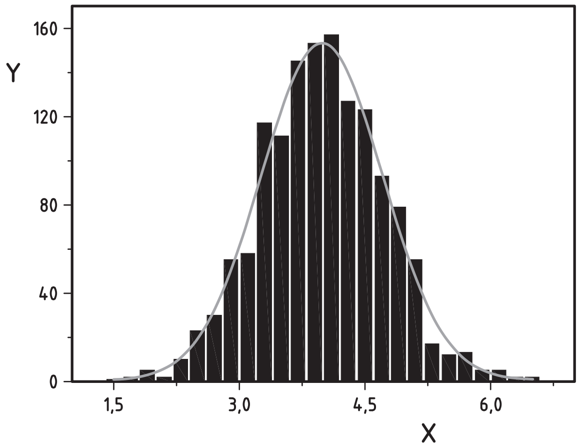


Figure A.8 — Typical HRTEM image of sample 3



Key

X d_{QD} (nm)

Y count

Figure A.9 — Diameter distribution of sample 3 on the basis of 1 402 particles (average diameter for each particle has been determined and plotted here)

A.10 HRTEM images analysis

Calculate the arithmetic average CdSe QD diameters, d, measured from the HRTEM images according to Formula (A.1):

$$\bar{d} = \sum \frac{\left(d_l + d_s\right)}{2n} \tag{A.1}$$

where

d_l is the long-axis diameter (in nm) of a particle, as indicated by arrows in Figures A.4, A.6, and A.8;

d_s is the short-axis diameter (in nm) of a particle, as indicated by arrows in Figures A.4, A.6, and A.8;

n is the total number of measured particles.

A.11 Size determination from UV-Vis spectra and HRTEM images

Table A.1 compares the diameters of CdSe QD samples determined from UV-Vis spectra and HRTEM images. The results obtained by the two methods are consistent. For HRTEM results, each value is expressed as the mean, plus or minus one standard deviation.

Table A.1 — Comparison of the average diameters of CdSe QDs determined from UV-Vis spectra and HRTEM images.

Sample	Sample 1	Sample 2	Sample 3
Diameter determined from UV-Vis spectra (nm)	2,88	3,40	3,92
Feret diameter determined from HRTEM images (nm)	3,07 ± 0.86	3,41 ± 0,69	3,98 ± 0,73

Annex B

(informative)

Case study for determining the number concentrations of CdSe QDs in a dispersion

B.1 General

This Annex provides an example of the approximate determination of the number concentration of monodisperse CdSe QDs in a colloidal dispersion, using UV-Vis absorption spectroscopy. Comparison of the results with those from ICP-MS analysis is also given.

B.2 CdSe QD samples

Two CdSe QD samples (sample 4-5) of different size and different concentration, and thus different wavelength and absorbance of the first excitonic absorption peak, were analysed. The CdSe QDs were dispersed in toluene (Analytical Grade) to meet the requirements of UV-Vis absorption spectroscopy.

B.3 Equipment

UV-Vis absorption spectra were recorded on a Perkin Elmer Lambda 650 UV/Vis spectrophotometer in quartz cuvette at room temperature. A Perkin Elmer NexION^{TM} 300X Inductively Coupled Plasma-Mass Spectrometer was used for the inductively coupled plasma (ICP) analysis.

B.4 Measurement conditions for UV-Vis spectroscopy

The UV-Vis spectrometer was calibrated with standard optical filter. Measurement conditions were set as follows:

a) The wavelength range was 250 nm to 750 nm.

b) The scan step was set as 0,5 nm.

c) The spectral bandwidth was chosen as 2 nm.

d) The reference is the same as dispersant of CdSe QDs dispersion, toluene (Analytical Grade).

B.5 Procedures for UV-Vis spectra measurement

a) An appropriate volume of CdSe quantum dots sample was added into a quartz cuvette with the optical path of 1cm.

b) The cuvette was put into the sample holder, and the measurement conditions were set for the UV-Vis spectrometer.

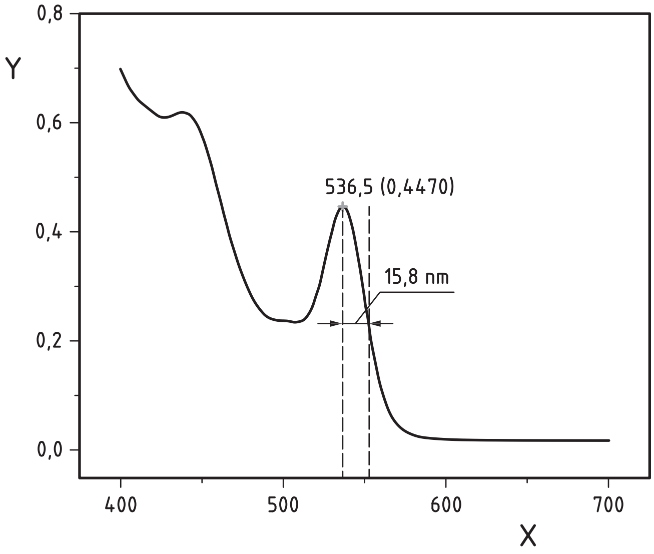
c) A scan was performed in the 250 nm to 750 nm range and the UV-Vis spectrum was recorded.

d) The wavelength of the first excitonic absorption peak was obtained either manually or by using the automatic peak search function of the spectrophotometer. Note that this measurement can also be obtained from the exported data set using a third-party software package such as Origin.

The measurement was repeated three times for each sample.

B.6 Example results of UV-Vis spectra

Figures B.1 and B.2 show typical UV-Vis spectra of two CdSe QD samples. The spectrum between 400 nm and 700 nm has been shown to better identify the absorption peak. The HWHM of sample 4 and 5 are 15,8 nm and 15,5 nm. Normalization was performed according to 3.5.1.

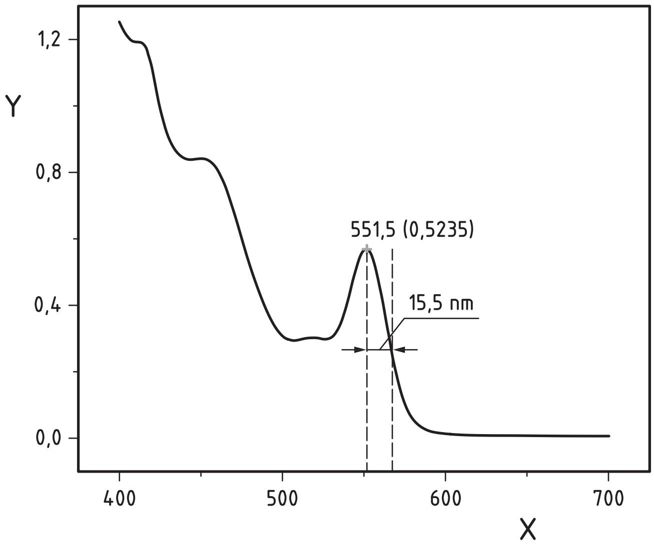


Key

X wavelength/nm

Y absorption

Figure B.1 — Typical UV-Vis spectrum of sample 4



Key

X wavelength/nm

Y absorption

Figure B.2 — Typical UV-Vis spectrum of sample 5

B.7 UV-Vis spectra analysis

The CdSe QD concentrations were calculated according to Formulae (4) and (7) in 3.5.

The transition energy E_{1S} (in eV) was converted from wavelength λ (in nm) of the absorption peak through the relationship λ (nm) = 1240/E_{1S} (eV). The ε values for samples 4 and 5 are calculated as 175 900 L mol^{-1} cm^{-1} and 192 600 L mol^{-1} cm^{-1} respectively.

B.8 Sample pretreatment procedures for ICP-MS analysis

a) CdSe QDs sample with known absorbance was put into a beaker.

b) Aqua regia was added into the beaker to digest the sample.

c) The solution was concentrated.

d) The resulting sample was transferred into a volumetric flask and adjusted to constant volume using dilute HNO_3.

e) Five working standard solutions of Cd were prepared from primary standard solutions.

B.9 ICP-MS analysis

A standard curve was obtained on the instrument with five working standard solutions (multi-point linear fitting) before measuring the samples. The data are corrected in terms of standardization blanks, 2 % HNO_3 solution. The peak intensities of the elemental signals of ICP-MS were used for quantitative online analysis. Measurements were repeated three times for each sample.

The obtained atomic Cd number concentrations were converted into the nanoparticles number concentrations by dividing by the number of Cd atoms in one nanoparticle, assuming that the nanoparticles have the same density as its bulk material (5,81 g/cm^3). The sizes of CdSe QDs were determined using UV-Vis spectra following the procedures in A.7, to be 2,80 and 3,07 nm, respectively. The volumes of nanoparticles were calculated assuming spheroidal shape. The number of Cd atoms in one nanoparticle for samples 4 and 5 are 210 and 280, respectively.

B.10 Comparison of results obtained by UV-Vis spectra and ICP-MS analysis

Table B.1 compares the number concentrations of CdSe QD samples determined by the UV-Vis method described in this Technical Specification, and ICP-MS analysis. The results obtained using the two methods are consistent: the measured values agree within their respective uncertainties estimated in Clause 7. Each value is expressed as the mean plus or minus one standard deviation of three independent determinations.

Table B.1 — Comparison of the number concentrations of CdSe QDs determined from UV-Vis spectra and by ICP-MS analysis.

Sample	Sample 4	Sample 5
concentrations determined from UV-Vis spectra (×10^{-6} mol L^{-1})	2,87 ± 0,01	3,01 ± 0,01
concentrations determined by ICP-MS analysis (×10^{-6} mol L^{-1})	2,51 ± 0,07	2,83 ± 0,03

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