SLOVENSKI STANDARD
SIST EN 16981:2021

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Nadomešča:
SIST-TS CEN/TS 16981:2017

Fotokataliza - Slovar izrazov

Photocatalysis - Glossary of terms

Photokatalyse - Glossar der Begriffe

Photocatalyse - Glossaire de termes

Ta slovenski standard je istoveten z: EN 16981:2021

ICS:

01.040.25	Izdelavna tehnika (Slovarji)	Manufacturing engineering (Vocabularies)
25.220.01	Površinska obdelava in prevleke na splošno	Surface treatment and coating in general

SIST EN 16981:2021 **en,fr,de**

EUROPEAN STANDARD

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EN 16981

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ICS 01.040.25; 25.220.01

Supersedes CEN/TS 16981:2016

English Version

Photocatalysis - Glossary of terms

Photocatalyse - Glossaire de termes

Photokatalyse - Glossar der Begriffe

This European Standard was approved by CEN on 18 July 2021.

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EUROPEAN COMMITTEE FOR STANDARDIZATION
COMITÉ EUROPÉEN DE NORMALISATION
EUROPÄISCHES KOMITEE FÜR NORMUNG

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European foreword

This document (EN 16981:2021) has been prepared by Technical Committee CEN/TC 386 “Photocatalysis”, under WG 1 “Terminology”, the secretariat of which is held by AFNOR.

This European Standard shall be given the status of a national standard, either by publication of an identical text or by endorsement, at the latest by April 2022, and conflicting national standards shall be withdrawn at the latest by April 2022.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. CEN shall not be held responsible for identifying any or all such patent rights.

This document supersedes CEN/TS 16981:2016.

In comparison with the previous edition, the following technical modifications have been made:

— Change of the Scope: “The glossary lists a consistent set of definitions to be used in standards on photocatalysis for their consistency and connection with the scientific literature”.

— Change to Clause 2: Paragraphs were updated:

"Normative references and notes

There are no normative references in this document.

Most of the definitions reported in this document are a sub-set of the IUPAC definitions in *photocatalysis* and radiocatalysis [1]. Some other definitions, in particular for the *photocatalytic rate* and reactors, are taken from a dedicated work [2].

The technical specifications for the apparatus and physical values for irradiation conditions to be used in the standards are reported in a separate Technical Specification [3].

For the magnitudes implying energy or photons incident on a surface from all directions, the set of symbols recommended by the International Organization for Standardization (ISO) [4] and included in the IUPAC “Green Book”, and by the International Commission on Illumination [5] are adopted. This has been done primarily to comply with internationally agreed-upon symbols.”

— Clause 3: introductory wording and definitions were updated:

“ISO and IEC maintain a generic terminological databases for use in standardization, which could complement this dedicated Glossary, at the following addresses:

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

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

The arrangement of entries is alphabetical, and the criterion adopted by the IUPAC has been followed for the typeface used: italicized words in a definition or following it indicate a cross-reference in the Glossary.

SI units are adopted, with some exceptions, prominently in the use of the molar decadic absorption coefficient, ε, with common units dm3 mol−1 cm−1 and a mole of photons denoted as an einstein. As recently the definition of the SI units was established in terms of a set of seven defining constants, including the Avogadro number, the mole (symbol: mol) is the base unit of amount (number) of substance.

Functional dependence of a physical quantity f on a variable x is indicated by placing the variable in parentheses following the symbol for the function; e.g. $\varepsilon(\lambda)$. Differentiation of a physical quantity f with respect to a variable x is indicated by a subscript x; e.g. the typical spectral radiant power quantity $P\lambda = dP/d\lambda$. The natural logarithm is indicated with ln, and the logarithm to base 10 with log."

The following definitions were deleted:

— amalgam lamp (before 3.17),

— back electron-transfer (before 3.20)

— bioluminescence (before 3.25),

— charge-transfer (CT) absorption (before 3.35),

— charge-transfer (CT) complex (before 3.36),

— charge-transfer (CT) state (before 3.37),

— circular dichroism (CD) (before 3.43)

— charge hopping(before 3.31),

— circular dichroism (CD) (before 3.43),

— current yield see photocurrent yield(before 3.49),

— dielectric (before 3.59),

— differential quantum (before 3.60),

— diode light emitting (LED) (before 3.61),

— driving force (before 3.63),

— driving force (for electron transfer) (before 3.64),

— electron-transfer photosensitization (before 3.69),

— emissivity see emittance(before 3.73),

— excitation transfer see energy transfer (before 3.77),

— flash photolysis(before 3.85),

— FWHM(before 3.95),

— germicidal lamp(before 3.97),

— hypsochromic shift(before 3.103),

— inner-filter effect(before 3.106),

— inner-sphere electron transfer(before 3.107),

— interferometer(before 3.113),

— Lambert–Beer law (before 3.116),

— Lambert law (before 3.117),

— LED(before 3.119),

— light-emitting diode (LED) (before 3.121),

— low-pressure mercury lamp (arc) (before 3.123),

— medium-pressure mercury lamp (arc) (before 3.127),

— mercury–xenon lamp (arc) (before 3.129),

— multiphoton process(before 3.132),

— OLED (before 3.135),

— OPA (before 3.137),

— OPO (before 3.138),

— optical multichannel analyzer (OMA) (before 3.140),

— optical parametric amplification process (before 3.141),

— optical parametric oscillator (OPO) (before 3.142),

— optoacoustic spectroscopy(before 3.143),

— photo-assisted catalysis(before 3.148),

— photohydration(before 3.166),

— photon emittance(before 3.174),

— photopolymerization(before 3.185),

— quartz–iodine lamp(before 3.194),

— radiant energy fluence rate(before 3.201),

— reactor CSTR(before 3.210),

— reflection factor (before 3.214),

— reflectivity(before 3.215),

— self-absorption (before 3.219),

— self-quenching (before 3.220),

— sensitizer (before 3.221),

— sensitization (before 3.222),

— singlet oxygen (before 3.223),

— singlet state(before 3.224),

— solvent shift(before 3.226),

— spectral radiant energy, Qλ(before 3.238),

— spectral sensitization(before 3.244),

— tungsten-halogen lamp(before 3.248),

— wolfram lamp(before 3.259),

<u>The following definitions were updated:</u>

— 3.11 actinic.

— 3.12 actinism.

— 3.18 attenuance filter

— 3.28 Brewster angle

— 3.64 extinction coefficient

— 3.65 Fermi level

— 3.71 fluorescence spectrum

- 3.92 Fourier-transform spectrometer
- 3.93 Fourier-transform spectroscopy
- 3.95 mercury lamp
- 3.100 organic light-emitting device
- 3.102 phosphorescence
- 3.103 photoacoustic spectroscopy
- 3.113 photocuring
- 3.116 photodynamic effect
- 3.140 photoreaction
- 3.142 photosensitization
- 3.143 photosensitizer
- 3.145 quantum efficiency
- 3.152 radiant energy fluence
- 3.158 rate of photon absorption
- 3.159 reaction rate
- 3.160 reactor batch
- 3.163 red shift
- 3.165 RGB color model
- 3.191 UV dose

The following definitions were added:

- 3.137 photonic unit conversion
- 3.161 reactor continuous Stirred-Tank
- 3.162 reactor plug flow

Any feedback and questions on this document should be directed to the users' national standards body. A complete listing of these bodies can be found on the CEN website.

According to the CEN-CENELEC Internal Regulations, the national standards organisations of the following countries are bound to implement this European Standard: Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Republic of North Macedonia, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and the United Kingdom.

Introduction

Photocatalysis is a very efficient advanced oxidation technique which enables the production of active species following light absorption by the photocatalyst, such as bound/free hydroxyl radicals (·OH), hydroperoxyl radicals (·OOH) and other ROS, conduction band electrons and valence band holes, capable of partly or completely mineralising/oxidising the majority of organic compounds. The most commonly used photocatalyst is titanium dioxide (TiO_2). Photocatalysts can be used in powder form or deposited as thin films on different substrates (glass fibre, fabrics, plates/sheets, etc.). The objective of standardization is to introduce test standards for evaluation of the performance of photocatalysts (including photocatalysis and photo-induced effects). These standards mainly concern tests and analysis methods, and require a common language.

A common language for standards, disclosed to a wide audience and referring only to the operational protocols and to their outcomes, is needed for a consistent set of standards and the connection with the scientific literature. This glossary will take into account existing glossary of terms and literature definitions used in *photocatalysis* and *photochemistry*. Because in *photocatalysis* numerous properties are difficult to be evaluated, in this Glossary and in related standard norms the report of properties depending on some physical-chemical properties and model parameters, like the number of active sites, the mechanisms of adsorption or kinetic mechanisms of photocatalytic reactions is avoided.

Safety statement

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

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It is understood that some of the material described in this document may have negative environmental impact. As technological advantages lead to better alternatives for these materials, they will be eliminated from this document to the possible extent.

At the end of the test, the user of this document will take care to carry out an appropriate disposal of the wastes, according to local regulation.

1 Scope

The glossary lists a consistent set of definitions to be used in standards on photocatalysis for their consistency and connection with the scientific literature.

2 Normative references and notes

There are no normative references in this document.

Most of the definitions reported in this document are a sub-set of the IUPAC definitions in *photocatalysis* and radiocatalysis [1]. Some other definitions, in particular for the *photocatalytic rate* and reactors, are taken from a dedicated work [2].

The technical specifications for the apparatus and physical values for irradiation conditions to be used in the standards are reported in a separate Technical Specification [3].

For the magnitudes implying energy or photons incident on a surface from all directions, the set of symbols recommended by the International Organization for Standardization (ISO) [4] and included in the IUPAC "Green Book", and by the International Commission on Illumination [5] are adopted. This has been done primarily to comply with internationally agreed-upon symbols.

3 Terms and definitions

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

ISO and IEC maintain a generic terminological databases for use in standardization, which could complement this dedicated Glossary, at the following addresses:

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

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

The arrangement of entries is alphabetical, and the criterion adopted by the IUPAC has been followed for the typeface used: *italicized words* in a definition or following it indicate a cross-reference in the Glossary.

SI units are adopted, with some exceptions, prominently in the use of the *molar decadic absorption coefficient*, ε, with common units $dm^3\ mol^{-1}\ cm^{-1}$ and a mole of photons denoted as an *einstein*. As recently the definition of the SI units was established in terms of a set of seven defining constants, including the Avogadro number, the mole (symbol: mol) is the base unit of amount (number) of substance.

Functional dependence of a physical quantity f on a variable x is indicated by placing the variable in parentheses following the symbol for the function; e.g. $\varepsilon(\lambda)$. Differentiation of a physical quantity f with respect to a variable x is indicated by a subscript x; e.g. the typical *spectral radiant power* quantity $P_\lambda = dP/d\lambda$. The natural logarithm is indicated with *ln*, and the logarithm to base 10 with *log*.

3.1
absorbance
A
logarithm to the base 10 (linear *absorbance*) of the incident (prior to *absorption*) *spectral radiant power*, P_λ^0 divided by the transmitted *spectral radiant power*, P_λ:

$$A(\lambda) = \log\left(\frac{P_\lambda^0}{P_\lambda}\right) = -\log T(\lambda)$$

Note 1 to entry: $T(\lambda)$ is the (internal) *transmittance* at the defined *wavelength*. The terms absorbancy, *extinction*, and *optical density* should not be used. When natural logarithms are used, the napierian *absorbance* is the logarithm to the base e of the incident *spectral radiant power*, P_λ^0 divided by the transmitted *spectral radiant power*, P_λ:

$$A_\mathrm{e}(\lambda) = \ln\left(\frac{P_\lambda^0}{P_\lambda}\right) = -\ln T(\lambda)$$

Note 2 to entry: These definitions suppose that all the incident *ultraviolet*, *visible*, or *infrared* radiation is either transmitted or absorbed, reflection or scattering being negligible. *Attenuance* should be used when this supposition cannot be made.

Note 3 to entry: In practice, A is the logarithm to the base 10 of the *spectral radiant power* of *ultraviolet*, *visible*, or *infrared* radiation transmitted through a reference sample divided by that transmitted through the investigated sample, both observed in identical cells.

Note 4 to entry: In common usage, A is given for a path length of 1 cm, unless otherwise specified.

Note 5 to entry: Traditionally, (spectral) *radiant intensity*, I_λ, was used instead of *spectral radiant power*, P_λ, now the accepted term.

Note 6 to entry: The *wavelength* symbol as a subscript for P and in parenthesis for T and A can be omitted. However, the *wavelength* should be specified for which the value of the particular property is reported.

Note 7 to entry: Same as internal *optical density*, which is a term not recommended.

Note 8 to entry: See also *absorption coefficient, absorptance, attenuance, Beer–Lambert law, molar absorption coefficient.*

3.2
absorbed spectral photon flux density
absorbed photon flux density
number of photons of a particular *wavelength*, per time interval (*spectral photon flux*, number basis, $q_{\mathrm{p},\lambda}$, or *spectral photon flux*, amount basis, $q_{\mathrm{n,p},\lambda}$) absorbed by a system per volume, V

Note 1 to entry: On number basis, SI unit is $\mathrm{s^{-1}\ m^{-4}}$; common unit is $\mathrm{s^{-1}\ cm^{-3}\ nm^{-1}}$. On amount basis, SI unit is $\mathrm{mol\ s^{-1}\ m^{-4}}$; common unit is *einstein* $\mathrm{s^{-1}\ cm^{-3}\ nm^{-1}}$.

Note 2 to entry: Mathematical expression: $\dfrac{q_{\mathrm{p},\lambda}^0\left[1-10^{-A(\lambda)}\right]}{V}$ on number basis, $\dfrac{q_{\mathrm{n,p},\lambda}^0\left[1-10^{-A(\lambda)}\right]}{V}$ on amount basis, where $A(\lambda)$ is the *absorbance* at *wavelength* λ and superscript 0 (zero) indicates incident photons.

Note 3 to entry: Absorbed (spectral) *photon flux* density (number basis or amount basis) is used in the denominator when calculating a differential *quantum yield* and using in the numerator the rate of change of the number, dC/dt, or the rate of change of the amount concentration, dc/dt, respectively.

Note 4 to entry: The term *rate of photon absorption* is increasingly used.

3.3
absorbed spectral radiant power density
absorbed radiant power density
spectral radiant energy per time interval (*spectral radiant power*, P_λ) absorbed by a system per volume, V

Note 1 to entry: SI unit is W m^{-4}; common unit is W cm^{-3} nm^{-1}.

Note 2 to entry: Mathematical expression: $\frac{P_\lambda^0\left[1\text{-}10^{-A(\lambda)}\right]}{V}$ where $A(\lambda)$ is the *absorbance* at *wavelength* λ and superscript 0 (zero) indicates incident *radiant power*.

3.4
absorptance
a
fraction of *ultraviolet*, *visible*, or *infrared* radiation absorbed, equal to one minus the *transmittance* (T), i.e., $(1-T)$

Note 1 to entry: The use of this obsolete term, equivalent to *absorption factor*, is not recommended.

Note 2 to entry: See also *absorbance*.

3.5
absorption
absorption of electromagnetic radiation
transfer of energy from an electromagnetic field to a material or a molecular entity

Note 1 to entry: In a semiclassical fashion, this transfer of energy can be described as being due to an interaction of the electric field of the wave with an oscillating electric dipole moment set up in the material or molecular entity. This dipole moment is the result of the perturbation by the outside field, and its oscillation *frequency* ν is given by the difference ΔE of the energies of the lower and upper state in the absorbing material or molecular entity, $\Delta E = h\nu$. When the *frequency* of the oscillating dipole moment and the *frequency* of the field agree, a resonance occurs and energy can flow from the field into the material or molecule (an *absorption* occurs).

Note 2 to entry: When energy flows from the material or molecule to the field, stimulated light *emission* occurs.

Note 3 to entry: The oscillating electric dipole moment produced in the material or molecular entity has an amplitude and direction determined by a vector M_{if}, known as the electric transition (dipole) moment. The amplitude of this moment is the transition moment between the initial (i) and final states (f).

3.6
absorption coefficient
a(λ), α(λ)
absorbance, *A*(λ), divided by the optical pathlength, *l*:

$$a(\lambda)=\frac{A(\lambda)}{l}=\left(\frac{1}{l}\right)\log\left(\frac{P_\lambda^0}{P_\lambda}\right)$$

where a is the linear decadic *absorption coefficient* and

P_λ^0 and P_λ are, respectively, the incident and transmitted *spectral radiant power*.

When napierian logarithms are used

$$\alpha(\lambda)=a(\lambda)\ln 10=\left(\frac{1}{l}\right)\ln\left(\frac{P_\lambda^0}{P_\lambda}\right)$$

where α is the linear napierian *absorption coefficient.*

Note 1 to entry: Since *absorbance* is a dimensionless quantity, the coherent SI unit for a and α is m^{-1}; the common unit is cm^{-1}.

Note 2 to entry: See also *absorptivity, molar absorption coefficient.*

3.7
absorption cross-section
σ
linear napierian *absorption coefficient*, $\alpha(\lambda)$, divided by the number of molecular entities contained in a volume of the absorbing medium along the *ultraviolet*, *visible*, or *infrared* radiation path:

$$\sigma(\lambda)=\frac{\alpha(\lambda)}{C}=\frac{1}{C\cdot l}\ln\left(\frac{P_\lambda^0}{P_\lambda}\right)$$

where

C is the number concentration of molecular entities (number per volume), l is the optical pathlength, and P_λ^0 and P_λ are, respectively, the incident and transmitted *spectral radiant power.*

Note 1 to entry: SI unit is m^2, common unit is cm^2.

Note 2 to entry: The relation between the *absorption cross-section* and the *molar* (*decadic*) *absorption coefficient,* $\varepsilon(\lambda)$, is $\alpha(\lambda) = \ln 10\ \varepsilon(\lambda)/N_A$ with N_A the Avogadro constant. A conversion formula in common units is:

$$\sigma(\lambda)/\mathrm{cm}^2 = (3{,}8236 \times 10^{-21}/\mathrm{mol})\quad [\varepsilon(\lambda)/\ \mathrm{mol}^{-1}\ \mathrm{dm}^3\ \mathrm{cm}^{-1}]$$

Note 3 to entry: See also *attenuance*, *Beer–Lambert law*.

3.8
absorption factor
fraction of *ultraviolet*, *visible*, or *infrared* radiation absorbed by a system

$$f(\lambda) = 1 - T(\lambda) = 1 - 10^{-A(\lambda)}$$

with

$T(\lambda)$ the *transmittance* and $A(\lambda)$ the *absorbance* at a particular *wavelength* λ.

Note 1 to entry: This term is preferred to *absorptance*.

Note 2 to entry: The *wavelength* symbol can be omitted for f, T, and A. The *wavelength* should be specified for which the value of the particular property is reported.

Note 3 to entry: For $A(\lambda) << 1/\ln 10$, $f(\lambda)$ approximately $A(\lambda)\ \ln 10$.

3.9
absorption spectrum
plot of the *absorption coefficient* against a quantity related to *photon* energy, such as *frequency* ν, *wavenumber* $\tilde{\nu}$, or *wavelength* λ

Note 1 to entry: The plot of the *absorbance* against a quantity related to *photon* energy is discouraged, unless the actual concentration of the species is unknown.

3.10
absorptivity
absorptance divided by the optical pathlength

Note 1 to entry: The unit length shall be specified.

Note 2 to entry: The use of this obsolete term is not recommended.

Note 3 to entry: For very low *attenuance*, i.e. for $A(\lambda) << 1/\ln 10$, it approximates the linear *absorption coefficient*, within the approximation $[1 - 10^{-A(\lambda)}]$ approximately $A(\lambda)\ \ln 10$.

3.11
actinic
chemical changes produced by radiant energy especially in the *visible* and *ultraviolet* parts of the spectrum

Note 1 to entry: Applied to, resulting from, or referred to *actinism.*

3.12
actinism
chemical changes on living and nonliving materials caused by optical radiation especially in the *visible* and *ultraviolet* parts of the spectrum

3.13
actinometer
chemical system for the determination of the number of *photons* integrally or per time interval absorbed into the defined space of a chemical reactor

Note 1 to entry: This name is commonly applied to systems used in the *ultraviolet* and *visible wavelength* ranges.

Note 2 to entry: For example, solutions of potassium oxalatoferrate(III), $K_3[Fe(C_2O_4)_3]$ (among other systems) can be used as a chemical *actinometer*. Bolometers, thermopiles, and photodiodes are physical devices giving a reading of the radiation impinging on them that can be correlated to the number of photons detected as well as to the number of photons entering the chemical reactor. Detailed information on chemical actinometers and measuring systems can be found in CEN/TS 16599:2014.

Note 3 to entry: See also *spectral sensitivity.*

3.14
action spectrum
plot of a relative biological or chemical photoresponse ($=\Delta y$) per number of incident (prior to *absorption*) *photons*, vs. *wavelength*, or energy of radiation, or *frequency* or *wavenumber*

Note 1 to entry: This form of presentation is frequently used in the studies of biological or solid-state systems, where the nature of the absorbing species is unknown.

Note 2 to entry: It is advisable to ensure that the *fluence* dependence of the photoresponse is the same (e.g. linear) for all the *wavelengths* studied.

Note 3 to entry: The *action spectrum* is sometimes called *spectral responsivity* or sensitivity spectrum. The precise *action spectrum* is a plot of the spectral (*photon* or quantum) effectiveness. By contrast, a plot of the biological or chemical change or response per absorbed *photon* (quantum efficiency) vs. *wavelength* is the *efficiency spectrum*.

Note 4 to entry: In cases where the *fluence* dependence of the photoresponse is not linear (as is often the case in biological photoresponses), a plot of the photoresponse vs. *fluence* should be made at several *wavelengths* and a standard response should be chosen. A plot of the inverse of the "standard response" level vs. *wavelength* is then the *action spectrum* of the photoresponse.

Note 5 to entry: See also *excitation spectrum*, *efficiency spectrum*.

3.15
AM 0 sunlight
solar *irradiance* in space just above the atmosphere of the earth on a plane perpendicular to the direction of the sun (air mass, AM, zero)

Note 1 to entry: Also called extraterrestrial *irradiance*.

Note 2 to entry: See also *AM 1 sunlight.*

3.16
AM 1 sunlight
solar *irradiance* at sea level, i.e., traversing the atmosphere, when the direction of the sun is perpendicular to the surface of the earth

Note 1 to entry: Also called terrestrial global *irradiance*.

Note 2 to entry: See also *AM 0 sunlight.*