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and

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COMMISSION ON QUANTITIES AND UNITS†

## NAMES, SYMBOLS, DEFINITIONS AND UNITS OF QUANTITIES IN OPTICAL SPECTROSCOPY

(Recommendations 1984)

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# Names, symbols, definitions and units of quantities in optical spectroscopy

## ABSTRACT

This document gives definitions and recommended names and symbols for the quantities used in the practice of optical spectroscopy (ultra violet, visible and infrared). An earlier document prepared by our two Commissions (I.5 and VII.2) was entitled "Quantities and Units in Clinical Chemistry. Optical Spectroscopy Part 1. Theoretical Outline and General Quantities (Provisional Recommendations)", IUPAC Information Bulletin 1978, No. 3, p. 241-259. That document was fully comprehensive, and it was considered that for easy reference a shorter and simplified version would be welcomed.

The arrangement follows that of the Provisional document. After a general introduction explaining the recommendations, the major part of the document is a series of sections, each devoted to one of seventeen widely used quantities in molecular spectroscopy. For each quantity there is a definition, a symbol, dimensions and name and symbol of the coherent unit in the SI system. The commonly used multiples of the coherent SI unit are listed together with the corresponding symbols. Alongside are given the commonly used non-SI units which are intended for use when reading older literature. Each section gives common synonyms and other symbols which have been used for the quantity being described, and the choice recommended is justified. Remarks are also given, where appropriate, on the interrelation of symbols.

The recommendations conclude with a summary list of the quantities described with symbols, SI units and dimensions, and a bibliography of documents referred to in the text.

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## PREFACE

This document has been based on recommendations already published by other Commissions of the International Union of Pure and Applied Chemistry (IUPAC), particularly Commission I.1 on Physicochemical Symbols, Terminology and Units (CPSTU) and Commission V.4 on Spectrochemical and other Optical Procedures for Analysis (CSOPA), as well as publications by other organizations such as the International Organization for Standardization (ISO), the International Electrotechnical Commission (IEC) and the International Commission on Illumination (CIE). Codes used in citing authorities are explained in the bibliography (§ 4). Some differences in names and definitions of the quantities have proved necessary, for instance to place some terms in a broader context than spectroscopy.

The text follows the general pattern of the document "Quantities and Units in Clinical Chemistry. Optical Spectroscopy : Part 1. Theoretical Outline and General Quantities (Provisional Recommendations) IUPAC Information Bulletin 1978 No. 3 p 241-259" (IUPAC-CQUCC, 1978). It has been produced to meet the requests for a shortened and simplified version of that document and incorporates some additions and modifications. However, in general, the earlier document provides greater detail.

## 1. INTRODUCTION

1.1 Optical spectroscopy is the study of systems by the electromagnetic radiation with which they interact or that they produce. Spectrometry is the measurement of such radiation as a means of obtaining information about the systems.

1.2 Incident radiation may be transmitted through or may interact with the system under investigation. If it interacts, one may observe absorption, reflection, refraction, polarization, scattering (diffusion) or luminescence (phosphorescence or fluorescence). Alternatively, one may also observe radiation arising by emission from the system under investigation, for instance by thermal excitation or chemiluminescence.

1.3 For incident, reflected, refracted, fluorescent, absorbed and transmitted components of radiation, symbols are modified by the subscripts *o*, *refl*, *refr*, *fl*, *abs* and *tr*, respectively.

1.4 Each section heading of the recommendations is laid out as in the example below.

Key to the layout of section headings: a. Section number. b. Name of kind of quantity. c. International symbols for quantity. d. Dimension. e. Name of coherent unit in the *Système International d'Unités*. f. International symbol of SI unit.

The subsection "Kind of quantity" begins with a definition expressed in words and symbols. It is followed by numbered remarks. The subsection "Units and values" begins with a table of unit symbols in order of decreasing magnitude with columns stating the multiples of the coherent SI unit, corresponding SI symbols, and non-SI equivalents which are commonly encountered in the literature.

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Example

4.1 <sup>a</sup>	LENGTH <sup>b</sup>	$\lambda$ <sup>c</sup>	L <sup>d</sup>
metre <sup>e</sup>		m <sup>f</sup>	

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1.5 In numerical examples requiring a decimal marker, a comma has been adopted as is preferred internationally (ISO--31.0, § C.3.2; IUPAC-CQUCC & IFCC-EPQU 1979, § 5.2.6; IUPAC-CPSTU 1979, § 4.1; IUPAP 1978, § 3.2). The full stop or period is widely used in English text and for computer work. The half-raised point is reserved for the meaning "multiplied by".

1.6 Table 1 below gives the approximate ranges of wavelength  $\lambda_0$ , and wavenumber in vacuo,  $\tilde{\nu}$ , frequency  $\nu$ , photon energy or molar energy appropriate to each of the normally distinguished parts of the electromagnetic spectrum. The values of wavelength and wavenumber apply only in media with a refractive index of 1 but are acceptably correct for routine analytical spectroscopy in air.

TABLE 1. REGIONS OF THE ELECTROMAGNETIC SPECTRUM

Name	Approximate limiting values of ranges				
	Wavelength in vacuo, $\lambda_0$	Wavenumber in vacuo, $\tilde{\nu}$	Frequency, $\underline{\nu}$	Photon energy, $\underline{h\nu}$	Molar energy, $\underline{N_A h\nu}$
$\gamma$ -rays	10 pm	$10^9 \text{ cm}^{-1}$	30,0 EHz	$19,9 \times 10^{-15} \text{ J}$	12,0 GJ/mol
X-rays	10 nm	$10^6 \text{ cm}^{-1}$	30,0 PHz	$19,9 \times 10^{-18} \text{ J}$	12,0 MJ/mol
vacuum uv.	200 nm	$50,0 \times 10^3 \text{ cm}^{-1}$	1,50 PHz	$993 \times 10^{-21} \text{ J}$	598 kJ/mol
near uv.	380 nm	$26,3 \times 10^3 \text{ cm}^{-1}$	789 THz	$523 \times 10^{-21} \text{ J}$	315 kJ/mol
visible	780 nm	$12,8 \times 10^3 \text{ cm}^{-1}$	384 THz	$255 \times 10^{-21} \text{ J}$	153 kJ/mol
near ir.	2.5 $\mu\text{m}$	$4,00 \times 10^3 \text{ cm}^{-1}$	120 THz	$79,5 \times 10^{-21} \text{ J}$	47,9 kJ/mol
mid ir.	50 $\mu\text{m}$	$200 \text{ cm}^{-1}$	6,00 THz	$3,98 \times 10^{-21} \text{ J}$	2,40 kJ/mol
far ir.	1 mm	$10 \text{ cm}^{-1}$	300 GHz	$199 \times 10^{-24} \text{ J}$	120 J/mol
microwaves	100 mm	$0,1 \text{ cm}^{-1}$	3,00 GHz	$1,99 \times 10^{-24} \text{ J}$	1,20 J/mol
radio waves					

ir. stands for infrared and uv. for ultraviolet.  $h$  stands for the Planck constant and  $N_A$  for the Avogadro constant.

'Infrared' is a widely used alternative for what is here called 'mid infrared'. The longer wavelength limit of far infrared is sometimes placed at wavelength 0,3 mm = 300  $\mu\text{m}$   $\hat{=}$  wavenumber 33,3  $\text{cm}^{-1}$ .

An alternative commonly used, non-SI unit, for photon energy is the electronvolt, eV

$$1 \text{ eV} \approx 160,219 \times 10^{-21} \text{ J} \hat{\approx} 8 \text{ 065,6 cm}^{-1}$$

1.7 In spectroscopy, 'density' is used in at least three meanings and has therefore been avoided in recommended names :

- divided by area, for instance 'radiant flux density'
- divided by volume, for instance 'radiant energy density'
- a measure of the degree to which a sample cuts down the intensity of a beam passing through it, for instance 'optical density' or 'transmission density'.

1.8 Quantities are sometimes called 'internal' when certain boundary effects, associated for instance with reflections at cell windows, have been excluded or allowed for. They may be given the same principal symbols but should be distinguished by the subscript  $i$ .

1.9 The results of measurements are commonly expressed logarithmically and may be either 'decadic' or 'natural' (Napierian). Since the decadic group has in the past been more usual, it is treated here more fully. The base used should be specified whenever values are reported. It should be noted that the logarithmic quantities discussed in § 2.14, § 2.15, § 2.16 and § 2.17 are only usefully applicable to internal quantities (§ 1.8).

## 2. GENERAL QUANTITIES IN SPECTROMETRY

2.1 WAVELENGTH	$\lambda$	L
metre	m	

Kind of quantity

Wavelength is the distance in the direction of propagation of a regular wave,  $\lambda$ , divided by the number of cycles of the wave in that distance,  $N$ :

$$\lambda = \frac{\lambda/N}{N} \quad (1)$$

By convention, spectroscopic properties are expressed in terms of wavelength in vacuo, not the wavelength within the medium being studied. The wavelength,  $\lambda_1$ , within the medium depends on its refractive index,  $n_1$  (§ 2.4), and is related to wavelength in vacuo,  $\lambda_0$ , by the equation

$$\lambda_1/\lambda_0 = n_0/n_1 \quad (2)$$

The refractive index of a vacuum,  $n_0$ , is 1 by definition. The refractive index of air under normal laboratory conditions is very close to 1, so wavelength measured in air is sufficiently accurate for most practical purposes, except in spectral regions of strong atmospheric absorption.

Units and values of wavelength

Multiple of coherent SI unit	Symbols for SI multiples	Non-SI units
1	m	
10 <sup>-1</sup>	dm	
10 <sup>-2</sup>	cm	
10 <sup>-3</sup>	mm	
10 <sup>-6</sup>	$\mu\text{m}$	
10 <sup>-9</sup>	nm	
10 <sup>-10</sup>		Å
10 <sup>-12</sup>	pm	

Remark 1. The micrometre is appropriate for the infrared region and the nanometre for the visible and ultraviolet region of the spectrum.

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2.2 WAVENUMBER IN VACUO	$\tilde{\nu}$	L <sup>-1</sup>
per metre	m <sup>-1</sup>	

Kind of quantity

Wavenumber is the number of cycles of a regular wave,  $N$ , in a given distance,  $\lambda$ , divided by that distance :

$$\tilde{\nu} = \frac{N/\lambda}{\lambda} \quad (3)$$

(IUPAC-CPSTU 1979 § 2.1.07). As with wavelength, the wavenumber used in spectrometry is that in vacuo (or in air), and not in the system being studied. It is symbolized  $\tilde{\nu}$  and is defined from frequency,  $\nu$ , and the speed of electromagnetic radiation in vacuo,  $c_0$ :-

$$\tilde{\nu} = \frac{\nu}{c_0} \quad (4)$$

From Equations 1 and 3, it follows that

$$\tilde{\nu} = 1/\lambda_0 \quad (5a)$$

Remark 1. The customary SI multiple in optical spectroscopy is  $\text{cm}^{-1}$ , equal to  $100 \text{ m}^{-1}$ .

Remark 2. The symbol  $\tilde{\nu}$  should not be written  $\bar{\nu}$  which would designate mean frequency.

Remark 3. The symbol  $\underline{\sigma}$  is used for the wavenumber in the medium being studied, but is rarely used in optical spectroscopy; in this case,

$$\underline{\sigma} = 1/\lambda \quad (5b)$$

#### Units and values of wavenumber

Multiple of coherent SI unit	Symbols for SI multiples
$10^3$	$\text{mm}^{-1}$
$10^2$	$\text{cm}^{-1}$
1	$\text{m}^{-1}$

Remark 4. Note that  $1 \text{ mm}^{-1} \equiv 10 \text{ cm}^{-1}$ ;  $1 \text{ m}^{-1} \equiv 0,01 \text{ cm}^{-1}$ .

### 2.3 FREQUENCY $\nu$ $\text{T}^{-1}$

hertz; per second  $\text{Hz} = \text{s}^{-1}$

#### Kind of quantity

Frequency in electromagnetic radiation is the number of regular waves,  $N$ , in a given time,  $t$ , divided by that time:

$$\nu = N/t \quad (6)$$

Remark 1. In contrast to wavelength, frequency is independent of the medium.

Remark 2. The frequency of electromagnetic radiation is proportional to photon energy. The latter is the product of Planck constant,  $h$ , and frequency. Frequency is also related to the speed of light,  $c$ , and to wavelength,  $\lambda$ :

$$\nu = c/\lambda \quad (7)$$

in which  $c$  and  $\lambda$  refer to the same medium.

Remark 3. For oscillatory phenomena in electronics, frequency is designated by the symbol  $f$  (IUPAC-CPSTU 1979, § 2.1.13).

#### Units and values of frequency

Multiple of coherent SI unit	Symbols for SI multiples	Non-SI symbols
$10^{15}$	PHz; $\text{fs}^{-1}$	
$10^{12}$	THz; $\text{ps}^{-1}$	
$10^9$	GHz; $\text{ns}^{-1}$	
$10^6$	MHz; $\mu\text{s}^{-1}$	Mc/s
$10^3$	kHz; $\text{ms}^{-1}$	kc/s
1	Hz; $\text{s}^{-1}$	c/s, $\text{sec}^{-1}$

Remark 4. The unit hertz (Hz) is permitted by the Conférence Générale des Poids et Mesures (CGPM) only for periodic phenomena. The unit  $\text{s}^{-1}$  and its multiples may be used for all types of phenomena but are sometimes misunderstood, for instance

$$\text{ps}^{-1} = 10^{12} \text{ s}^{-1} = \text{THz} \neq 10^{-12} \text{ s}^{-1}.$$

2.4 REFRACTIVE INDEX	$\underline{n}$	1
one	1	

Kind of quantity

For a non-absorbing medium, the refractive index of a medium is the ratio of the speed in vacuo of electromagnetic radiation ( $\underline{c}_0$ ) at a given spectral position to its speed in the medium ( $\underline{c}_1$ ):

$$\underline{n}_1 = \underline{c}_0/\underline{c}_1 \quad (8)$$

(IUPAC-CPSTU 1979 § 2.8.21.1).

Remark 1. In most regions of the spectrum the difference in refractive index of air and vacuum is negligible (§ 2.1) and hence refractive index is usually calculated as the ratio of the sine of the angle of incidence,  $\underline{\alpha}_0$ , of a beam in air to the sine of the angle of refraction within the medium,  $\underline{\alpha}_1$ :

$$\underline{n} \approx \sin \underline{\alpha}_0/\sin \underline{\alpha}_1 \quad (9)$$

Remark 2. For an absorbing material the refractive index is a complex quantity,  $\hat{\underline{n}}$ , of which  $\underline{n}$  is the real component

$$\hat{\underline{n}} = \underline{n} + i \cdot \underline{k} \quad (10)$$

where  $\underline{k}$  is the absorption index and  $i = \sqrt{-1}$ .  $\underline{k}$  is dimensionless and equal to  $\underline{\alpha}/4\pi\underline{\nu}$  where  $\underline{\alpha}$  is the linear Napierian absorption coefficient (§ 2.16, Remark 4).

2.5 RADIANT ENERGY	$\underline{Q}$	$L^2MT^{-2}$
joule	J	

Kind of quantity

Radiant energy,  $\underline{Q}$  (IUPAC-CPSTU 1979, § 2.8.03; GB-RS 1975, p.15) is energy propagated as electromagnetic radiation.

Units and values of radiant energy

Multiple of coherent SI unit	Symbols for SI multiples	Non-SI units
1	J	
10 <sup>-3</sup>	mJ	
10 <sup>-6</sup>	$\mu$ J	
10 <sup>-7</sup>		erg = g·cm <sup>2</sup> ·s <sup>-2</sup>

$$J = \text{kg} \cdot \text{m}^2 \cdot \text{s}^{-2} = \text{W} \cdot \text{s} = \text{N} \cdot \text{m}$$

2.6 RADIANT POWER	$\underline{P}$	$L^2MT^{-3}$
watt	W	

Kind of quantity

Radiant power is power in the form of electromagnetic radiation. It is defined (IUPAC-CPSTU 1979, § 2.2.18) as the amount of radiant energy,  $\underline{\Delta Q}$ , transferred to or from a defined system, divided by the time interval,  $\underline{\Delta t}$ :

$$\underline{P} = \underline{\Delta Q}/\underline{\Delta t} \quad (11)$$

Remark 1. An alternative name for radiant power is radiant (energy) flux (ISO--31.6. § 9.1; IUPAC-CPSTU 1979, § 2.8.04) with the associated symbol  $\Phi$  (GB-RS 1975, p.15). This symbol may be modified where necessary by the subscript e (for energy).

Remark 2. In the absence of scattering and luminescence,

$$P_0 = P_{tr} + P_{abs} + P_{refl} \quad (12)$$

#### Units and values of radiant power

Multiple of coherent SI unit	Symbols for SI multiples	Non-SI units
1	W; J·s <sup>-1</sup>	
10 <sup>-3</sup>	mW; mJ·s <sup>-1</sup>	
10 <sup>-6</sup>	μW; μJ·s <sup>-1</sup>	
10 <sup>-7</sup>		erg·s <sup>-1</sup>

$$W = J \cdot s^{-1} = kg \cdot m^2 \cdot s^{-3}$$

2.7a SPECTRAL (CONCENTRATION OF) RADIANT POWER IN TERMS OF WAVELENGTH  $\frac{P}{\lambda}$  LMT<sup>-3</sup>

watt per metre  $W \cdot m^{-1}$

#### Kind of quantity

When power  $\Delta P$  is measured over a small interval of wavelength,  $\Delta \lambda$ , the quotient

$$\frac{P}{\lambda} = \frac{\Delta P}{\Delta \lambda} \quad (13)$$

is an estimate of spectral radiant power,  $\frac{P}{\lambda}$ , at the central wavelength of the interval  $\Delta \lambda$ .

In a wavelength interval,  $\lambda_2 - \lambda_1$ , total radiant power,  $P_{1 \rightarrow 2}$  is the integral of the spectral radiant power in terms of wavelength,  $\frac{P}{\lambda}$ , over that wavelength interval :

$$P_{1 \rightarrow 2} = \int_1^2 \frac{P}{\lambda} \cdot d\lambda \quad (14)$$

Remark 1. This quantity is also called spectral density of radiant power or spectral concentration of radiant power.

Remark 2. Analogous functions, for instance in terms of wavenumber or frequency, are given in § 2.7b and § 2.7c.

#### Units and values of spectral radiant power in terms of wavelength

Multiple of coherent SI unit	Symbols for SI multiples	Non-SI units
10 <sup>10</sup>		W·Å <sup>-1</sup>
10 <sup>9</sup>	GW·m <sup>-1</sup> ; W·nm <sup>-1</sup>	
10 <sup>6</sup>	MW·m <sup>-1</sup> ; W·μm <sup>-1</sup>	
10 <sup>3</sup>	kW·m <sup>-1</sup> ; W·mm <sup>-1</sup>	
1	W·m <sup>-1</sup>	

2.7b SPECTRAL (CONCENTRATION OF) RADIANT POWER IN TERMS OF WAVENUMBER	$\frac{P}{\nu}$	$L^3MT^{-3}$
watt per reciprocal metre	$W \cdot m$	

Kind of quantity

This is the analogue of § 2.7a when the increment of power,  $\Delta P$ , is measured over a small interval of wavenumber,  $\Delta \nu$ ,

$$\frac{P}{\nu} = \frac{\Delta P}{\Delta \nu} \quad (15)$$

2.7c SPECTRAL (CONCENTRATION OF) RADIANT POWER IN TERMS OF FREQUENCY	$\frac{P}{\nu}$	$L^2MT^{-2}$
watt per hertz; watt·second	$W/Hz = W \cdot s$	

Kind of quantity

This is the analogue of § 2.7a when the increment of power,  $\Delta P$ , is measured over a small frequency interval,  $\Delta \nu$ .

$$\frac{P}{\nu} = \frac{\Delta P}{\Delta \nu} \quad (16)$$

2.8a RADIANT EXITANCE	$\frac{M}{S}$	$MT^{-3}$
watt per square metre	$W \cdot m^{-2}$	

Kind of quantity

Radiant exitance is the radiant power,  $P$ , emitted by a uniform body at uniform temperature divided by the surface area,  $S$ , of that body :

$$\frac{M}{S} = \frac{P}{S} \quad (17)$$

Remark 1. Sometimes the alternative spelling, excittance, is used (e.g. IUPAC-CPSTU, 1979).

Units and values of radiant exitance

Multiple of coherent SI unit	Symbols for SI multiples	Non-SI units
1	$W \cdot m^{-2}$ ; $J \cdot m^{-2} \cdot s^{-1}$ ; $kg \cdot s^{-3}$	
$10^{-3}$	$mW \cdot m^{-2}$	$erg \cdot cm^{-2} \cdot s^{-1}$
$10^{-6}$	$\mu W \cdot m^{-2}$	

Remark 2. The term 'spectral brightness' is used to describe power per area per wavenumber, i.e.  $W \cdot cm^{-2} \cdot (cm^{-1})^{-1} = W \cdot cm^{-1}$ , and may be confused with radiant power density.

Remark 3. Spectral radiant exitance is defined analogously to the quantities in § 2.7.

2.8b IRRADIANCE,  $E$ , is the analogue of radiant exitance except that it refers to radiation received and not radiation emitted.

See also § 2.8a, Remark 2.

2.9 TRANSMITTANCE; TRANSMISSION FACTOR	$\tau$	1
one	1	

Kind of quantity

Transmittance or transmission factor is radiant power transmitted by a system,  $P_{tr}$ , in the direction of a parallel beam, divided by the incident radiant power,  $P_0$  :

$$\tau = P_{tr}/P_0 \quad (18)$$

(IUPAC-CPSTU 1979, § 2.8.11).

Remark 1. The symbol  $\underline{\tau}$  is an alternative to  $\tau$  (IUPAC-CPSTU, 1979).

Remark 2. The term 'transmission' was formerly used but is not now recommended.

Remark 3. As recommended in § 1.8, the symbol  $\tau_i$  is used for internal transmittance.

Remark 4. The value of  $\tau$  at a particular position in the spectrum can be denoted  $\tau(\lambda)$ ,  $\tau(\tilde{\nu})$  or  $\tau(\underline{\nu})$ . For sufficiently narrow intervals of spectra these three quantities are equal.

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2.10 ABSORPTANCE; ABSORPTION FACTOR	$\alpha$	1
one	1	

Kind of quantity

Absorptance or absorption factor is radiant power absorbed by a system,  $P_{abs}$ , divided by the incident radiant power,  $P_0$  :

$$\alpha = P_{abs}/P_0 \quad (19)$$

(IUPAC-CPSTU, 1979, § 2.8.09).

Remark 1. The fraction of incident radiant power lost from a parallel beam during passage through a sample cannot be called absorptance or absorption factor if the decrease be partly due to other factors such as scattering or reflection. Only when the losses are entirely due to absorption can Equation 12 be simplified and transposed :

$$P_{abs} = P_0 - P_{tr} \quad (20)$$

By combining Equations 19 and 20,

$$\alpha = (P_0 - P_{tr})/P_0 \quad (21)$$

so that then

$$\alpha = 1 - \tau \quad (22)$$

Remark 2. As recommended in § 1.8, the symbol  $\alpha_i$  is used for internal absorptance.

Remark 3. Absorptance or absorption factor can be qualified as applying to a particular position in the spectrum, e.g.  $\alpha(\lambda)$ ,  $\alpha(\tilde{\nu})$  or  $\alpha(\underline{\nu})$ .

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2.11 (SPECULAR) REFLECTANCE; REFLECTION FACTOR	$\rho$	1
one	1	

Kind of quantity

Specular reflectance or reflection factor is radiant power specularly reflected from the surfaces of a system,  $P_{refl}$ , divided by the incident radiant power,  $P_0$  :

$$\rho = P_{refl}/P_0 \quad (23)$$

(IUPAC-CPSTU 1979, § 2.8.10).

Remark 1. If scattering and luminescence are absent, the sum of transmittance, absorptance and reflectance at a given spectral position is 1 :

$$\tau + \alpha + \rho = 1 \quad (24)$$

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2.12	EMITTANCE	$\underline{\epsilon}$	1
	one	1	

#### Kind of quantity

The emittance of a sample is the radiant exitance of the sample,  $M$ , divided by the radiant exitance of a black body,  $M_B$ , at the same temperature.

$$\underline{\epsilon} = M/M_B \quad (25)$$

Remark 1. The term 'emittance' seems preferable to the alternative widely-used 'emissivity' (IUPAP, 1978, § 7.6; GB-RS, 1975, § 2.10 f) because the latter term is often reserved for radiant power divided by volume and by solid angle (IUPAC-CSOPA, 1969).

Remark 2. According to Kirchhoff's radiation law, the emittance is equal to the absorptance (§ 2.10) :

$$\underline{\epsilon} = \underline{\alpha} \quad (26)$$

for any wavelength (wavenumber or frequency) or direction of observation. From Equation 24 it follows that for an opaque sample ( $\tau = 0$ )

$$\underline{\epsilon} = \underline{\alpha} = 1 - \rho \quad (27)$$

Remark 3. As with other radiation quantities (§ 2.7, § 2.10) emittance varies with wavelength (wavenumber or frequency) and values at a particular position in the spectrum are denoted by  $\underline{\epsilon}(\lambda)$ ,  $\underline{\epsilon}(\nu)$ , or  $\underline{\epsilon}(\nu)$ .

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2.13	(DECADIC) ATTENUANCE (see note 1)	$\underline{D}$	1
	one	1	

#### Kind of quantity

Attenuance is the negative decadic logarithm of transmittance of a parallel beam through a uniform sample :

$$\underline{D} = -\lg \tau \quad (28)$$

Remark 1. Attenuance applies without specification of the cause of the reduction of transmittance of the sample, e.g. due to absorption, or scattering. The alternative term 'transmission density' is used. 'Optical density' has also been used, but this is discouraged because of confusion between internal losses due solely to absorption, which are related to absorbance (§ 2.15), and internal losses due to both absorption and scattering.

Remark 2. This quantity is only of practical use if  $\tau$  refers to an internal measurement. As recommended in § 1.8, internal attenuance can be symbolized by  $\underline{D}_i$ .

Remark 3. For a sample that scatters radiation, some of the radiation emerges from the sample in directions other than that of the original beam. How much of this radiation reaches the detector depends upon the geometry of the optical system used for the collection of radiation.

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Note 1: The term 'attenuance' and its symbol,  $\underline{D}$ , are tentative.

2.14 LINEAR (DECADIC) ATTENUATION COEFFICIENT;  $\underline{m}$   $L^{-1}$   
per metre  $m^{-1}$

Linear attenuation coefficient is the attenuation (§ 2.13) divided by the pathlength,  $\underline{l}$ , of a parallel beam through a sample of uniform properties.

$$\underline{m} = -(\lg \underline{\tau})/\underline{l} = \underline{D}/\underline{l} \quad (29a)$$

Remark 1. It should be noted that this quantity is only of practical use if  $\underline{\tau}$  refers to an internal quantity (§ 1.8; § 1.9).

Remark 2. The Napierian analogue is more commonly used and has the symbol  $\underline{\mu}$ .

$$\underline{\mu} = -(\ln \underline{\tau})/\underline{l} \quad (29b)$$

2.15 (DECADIC) ABSORBANCE  $\underline{A}$  1  
one 1

#### Kind of quantity

Decadic absorbance is the negative decadic logarithm of one minus absorbance as measured on a uniform sample :

$$\underline{A} = -\lg (1 - \underline{\alpha}) \quad (30a)$$

When  $\underline{\alpha} = 1 - \underline{\tau}$  (Equation 22), then

$$\underline{A} = -\lg \underline{\tau} = \lg (1/\underline{\tau}) = \lg (P_0/P_{tr}) \quad (31)$$

The term 'absorbance' applies only to the decrease in radiant power due entirely to absorption, i.e. it is that part of internal attenuation due to absorption.

Remark 1. This quantity is only of practical use if  $\underline{\tau}$  refers to an internal measurement (§ 1.8; § 1.9).

Remark 2. 'Optical density' has also been used but this is discouraged because it now has other meanings.

Remark 3. In the analysis of solutions, values are measured with reference to those from the pure solvent or a reference solution (IUPAC-CPSTU 1979, p.13, Footn. 7).

Remark 4. Napierian absorbance is analogously defined :

$$\underline{B} = -\ln (1 - \underline{\alpha}) \quad (30b)$$

2.16 LINEAR (DECADIC) ABSORPTION COEFFICIENT;  $\underline{a}$   $L^{-1}$   
per metre  $m^{-1}$

#### Kind of quantity

Linear (decadic) absorption coefficient is decadic absorbance,  $\underline{A}$ , divided by the pathlength,  $\underline{l}$ , of a parallel beam within a uniform sample :

$$\underline{a} = \underline{A}/\underline{l} \quad (32a)$$

(IUPAC-CPSTU 1979, § 2.8.14.1; GB-RS 1975, p.15). The term applies only if the decrease in radiant power is due to absorption, i.e. it is that part of the internal linear attenuation coefficient due to absorption.

Remark 1. If the cause of loss of power is undefined the quantity is linear (decadic) attenuation coefficient (§ 2.14).

Remark 2. The alternative symbol  $K$  is used (IUPAC-CPSTU 1979, § 2.8.14.1) but has the disadvantage that it is also used for luminous efficacy (IUPAP, 1978, § 7.6; GB-RS, 1975, p.15).

Remark 3. Partial linear absorption coefficients due to several species, such as components B, C ... N can be symbolized  $a_B$  (or  $a(B)$ ),  $a_C$  ...  $a_N$  and, according to theory, are additive as long as the components do not interact. The modifiers A and R are reserved for solvent (or medium) and for a reference component, respectively (IUPAC-CPSTU, 1979, A.I.9; IUPAC-CSOPA, 1972, § 6.2.2).

Remark 4. Linear Napierian absorption coefficient,  $\alpha$ , is defined analogously

$$\alpha = B/l \quad (32b)$$

Note that the symbol  $\alpha$  (IUPAC-CPSTU 1979, § 2.8.14.2) is also used for absorptance (IUPAC-CPSTU 1979 § 2.8.09); see § 2.10.

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2.17 MOLAR (LINEAR) (DECADIC) ABSORPTION COEFFICIENT; MOLAR (DECADIC) ABSORPTIVITY; ABSORBANCE CROSS-SECTION PER MOLE

$\epsilon$   $L^2N^{-1}$

square metre per mole

$m^2 \cdot mol^{-1}$

#### Kind of quantity

Molar linear (decadic) absorption coefficient is the linear (decadic) absorption coefficient due to a component divided by the amount of substance concentration,  $c$ , of that component in moles :

$$\epsilon = a/c = A/c \cdot l \quad (33a)$$

(IUPAC-CPSTU 1979, § 2.8.17.1). The term applies only if the reduction in transmittance is due to absorption.

Remark 1. Other uses of the term 'absorptivity' are absorptance per unit length (IUPAC-CPSTU 1979, § 2.8.17.1, footn. 4), or as for molar absorptivity when the concentration term is given in terms of mass rather than moles. The former usage is not recommended.

Remark 2. The term 'absorbance cross-section per mole' is more common in the literature of physics.

Remark 3. Molar (linear) Napierian absorption coefficient is analogously defined :

$$\kappa = \alpha/c \quad (33b)$$

(IUPAC-CPSTU 1979, § 2.8.17.2).

Remark 4. Absorption bands have a finite width and it is sometimes preferable to express intensity in terms of band area rather than the value at the peakheight. Band area is the integrated molar (linear) Napierian absorption coefficient and is evaluated as

$$\underline{A} = \int_{\text{band}} \kappa(\tilde{\nu}) d\tilde{\nu} \quad (34)$$

It has the dimensions of  $LN^{-1}$  (SI unit  $m \cdot mol^{-1}$ ); unfortunately it has previously been given the same symbol as decadic absorbance.

An alternative integration

$$\Gamma = \int_{\text{band}} (\kappa(\tilde{\nu})/\tilde{\nu}) d\tilde{\nu} \approx \underline{A}/\tilde{\nu}_0 \quad (35)$$

has the dimensions  $L^2N^{-1}$  (SI unit  $m^2 \cdot mol^{-1}$ ).  $\tilde{\nu}_0$  is the wavenumber of the band centre and the approximation in equation (35) only applies if the band is relatively narrow. This quantity is used because it is directly related to a molecular property, the transition moment for the band in question.

The decadic equivalences of  $\underline{A}$  and  $\Gamma$  are rarely used.

Units and values of molar linear absorption coefficient

Multiple of coherent SI unit	Symbols for SI multiples	Non-SI units
10 <sup>2</sup>	dm <sup>2</sup> ·mol <sup>-1</sup>	L·mmol <sup>-1</sup> ·cm <sup>-1</sup>
1	m <sup>2</sup> ·mol <sup>-1</sup>	
10 <sup>-1</sup>	cm <sup>2</sup> ·mmol <sup>-1</sup>	L·mol <sup>-1</sup> ·cm <sup>-1</sup>
10 <sup>-3</sup>	m <sup>2</sup> ·kmol <sup>-1</sup>	L·mol <sup>-1</sup> ·m <sup>-1</sup>
10 <sup>-4</sup>	cm <sup>2</sup> ·mol <sup>-1</sup>	mL·mol <sup>-1</sup> ·cm <sup>-1</sup>

Remark 5. In the column of non-SI units above, L stands for litre.

Remark 6. The term 'extinction coefficient' is commonly used for this quantity as expressed in the units L·mol<sup>-1</sup>·cm<sup>-1</sup> (dm<sup>3</sup>·mol<sup>-1</sup>·cm<sup>-1</sup>).

Remark 7. An amount of substance concentration expressed in mol/L is converted to the coherent unit mol·m<sup>-3</sup> by multiplying the numerical value by 1 000

$$\text{e.g. } 1 \text{ m}^2 \cdot \text{mol}^{-1} = 1\,000 (\text{mol/L})^{-1} \cdot \text{m}^{-1}$$

Published values in the traditional unit of (moles/litre)/cm of the molar absorption coefficient must be divided by 10 in the conversion to the coherent SI unit m<sup>2</sup>·mol<sup>-1</sup>.

## 3. LIST OF MAIN (DECADIC) QUANTITIES

SECTION	QUANTITY	SYMBOLS AND RELATION TO OTHER QUANTITIES	COHERENT SI UNIT	DIMENSION
2.1	Wavelength	$\lambda = \frac{c}{\nu}$ $\lambda_1 = \frac{\lambda_0}{n_1}$	m	L
2.2	Wavenumber in vacuo	$\nu = \frac{c}{\lambda} = 1/\lambda_0$	m <sup>-1</sup>	L <sup>-1</sup>
2.3	Frequency	$\nu = \frac{N}{t} = \frac{c}{\lambda}$	Hz	T <sup>-1</sup>
2.4	Refractive index	$n = \frac{c_0}{c_1}$	1	1
2.5	Radiant energy	$Q$	J	L <sup>2</sup> M T <sup>-2</sup>
2.6	Radiant power	$P$ or $\phi = \frac{\Delta Q}{\Delta t}$	W	L <sup>2</sup> M T <sup>-3</sup>
2.8a	Radiant exitance	$M = \frac{P}{S}$	W·m <sup>-2</sup>	MT <sup>-3</sup>
2.8b	Irradiance	$E = \frac{P}{S}$	W·m <sup>-2</sup>	MT <sup>-3</sup>
2.9	Transmittance; transmission factor	$\tau, T = \frac{P_{tr}}{P_0}$	1	1
2.10	Absorptance; absorption factor	$\alpha = \frac{P_{abs}}{P_0}$	1	1
2.11	(Specular) reflectance; reflection factor	$\rho = \frac{P_{refl}}{P_0}$	1	1
2.12	Emittance	$\epsilon = \frac{M}{M_B}$	1	1
2.13	Attenuance	$D = -\lg \tau$	1	1
2.14	Linear attenuation coefficient	$m = \frac{D}{\lambda}$	m <sup>-1</sup>	L <sup>-1</sup>
2.15	Absorbance	$A = -\lg (1 - \alpha)$	1	1
2.16	Linear absorption coefficient	$a = \frac{A}{\lambda}$	m <sup>-1</sup>	L <sup>-1</sup>
2.17	Molar (linear) absorption coefficient; molar absorptivity; absorbance cross-section per mole.	$\epsilon = \frac{a}{c}$	m <sup>2</sup> ·mol <sup>-1</sup>	L <sup>2</sup> N <sup>-1</sup>

NOTE : In 2.3 and 2.4 'c' stands for velocity of electromagnetic radiation, in 2.17 for amount of substance concentration in moles.

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## APPENDIX A

Descriptive names of spectroscopic quantities

Response to the provisional recommendation (IUPAC-CQUCC/IFCC-EPQU 1979) indicated a wide diversity of opinion about the best names for spectroscopic quantities. For instance, certain current national recommendations conflict to various degrees with the IUPAC Manual.

Various Commissions have proposed words to describe the component terms in the mathematical definitions of quantities. A system of nomenclature based on this idea has been developed by the Commission on Quantities and Units in Clinical Chemistry and the International Federation of Clinical Chemistry, Expert Panel on Quantities and Units, as a joint recommendation (Nomenclature of derived quantities, in press).

The Commission (VII.2) concluded that words like 'number', 'length' and 'area' should be used in a descriptive nomenclature only when those terms occurred in the numerator of the definition, and that new words were needed to describe 'divided by number, length or area' since existing words such as 'numeric', 'linear' and 'areal' could not be restricted to those meanings. The adjectival ending -ic had no existing usage for two of these three words. For number (of entities), a suitable adjective was entitic. By this convention, for instance, 'areic number' means number of entities divided by area and 'entitic area' means area divided by number of entities.

Among the words proposed are the following that are new to the English language:

- entitic: divided by number of entities
- lineic: divided by length
- areic: divided by area

If these words are approved by IUPAC, the kinds of quantity treated in this recommendation may then alternatively be described by the expressions on the right in the following list. This alternative nomenclature is for the moment provisional.

2.1	wavelength	entitic length of waves
2.2	wavenumber	lineic number of waves
2.3	frequency	number rate of waves
2.5	radiant energy	energy of radiation
2.6	radiant power	energy rate of radiation
2.7	spectral radiant power	differential quotient of energy rate of radiation
2.7a	- in terms of wavelength	- by entitic length of waves
2.7b	- in terms of wavenumber	- by lineic number of waves
2.7c	- in terms of frequency	- by number rate of waves
2.8a	radiant exitance	areic energy rate of radiation emitted
2.8b	irradiance	areic energy rate of radiation received
2.9 - 2.11		fraction of areic energy rate of radiation
2.9	transmittance	- transmitted
2.10	absorptance	- absorbed
2.11	reflectance	- reflected
2.12	emittance	emitted areic energy rate of radiation relative to that of a black body at the same temperature
2.14	linear attenuation coefficient	lineic attenuation
2.16	linear absorption coefficient	lineic absorbance
2.17	molar (linear) absorption coefficient	molar area absorbance