SLOVENSKI STANDARD
SIST ISO 6286:1995

01-avgust-1995

Molekularna absorpcijska spektrometrija - Slovar - Splošno - Naprave

Molecular absorption spectrometry -- Vocabulary -- General -- Apparatus

Spectrométrie d'absorption moléculaire -- Vocabulaire -- Généralités -- Appareillage

Ta slovenski standard je istoveten z: ISO 6286:1982

ICS:

01.040.71	Kemijska tehnologija (Slovarji)	Chemical technology (Vocabularies)
71.040.50	Fizikalnokemijske analitske metode	Physicochemical methods of analysis

SIST ISO 6286:1995 en

International Standard 6286

INTERNATIONAL ORGANIZATION FOR STANDARDIZATION•МЕЖДУНАРОДНАЯ ОРГАНИЗАЦИЯ ПО СТАНДАРТИЗАЦИИ•ORGANISATION INTERNATIONALE DE NORMALISATION

Molecular absorption spectrometry — Vocabulary — General — Apparatus

Spectrométrie d'absorption moléculaire — Vocabulaire — Généralités — Appareillage

First edition — 1982-08-15

UDC 543.422 : 011.4 **Ref. No. ISO 6286-1982 (E)**

Descriptors : spectrophotometry, molecular absorption spectrophotometry, vocabulary, apparatus, generalities.

Price based on 10 pages

Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards institutes (ISO member bodies). The work of developing International Standards is carried out through ISO technical committees. Every member body interested in a subject for which a technical committee has been set up has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work.

Draft International Standards adopted by the technical committees are circulated to the member bodies for approval before their acceptance as International Standards by the ISO Council.

International Standard ISO 6286 was developed by Technical Committee ISO/TC 47, *Chemistry*, and was circulated to the member bodies in July 1980.

It has been approved by the member bodies of the following countries:

Australia	Germany, F.R.	Poland
Austria	Hungary	Portugal
Belgium	India	Romania
Brazil	Italy	South Africa, Rep. of
China	Korea, Rep. of	Switzerland
Egypt, Arab Rep. of	Mexico	USSR
France	Netherlands	

No member body expressed disapproval of the document.

Molecular absorption spectrometry — Vocabulary — General — Apparatus

1 Scope and field of application

This International Standard gives definitions of a certain number of terms, and some general information, relating to molecular absorption spectrometry of solutions, together with general data concerning the instruments used, and, in particular, specifies :

a) the terminology to be used to characterize, by description, these instruments;

b) the characteristics and qualities of an instrument, by giving a summary of the principles of certain methods of verifying them.

2 Terms, definitions, symbols, formulae and units

Molecular absorption spectrometry is a technique applicable to both qualitative and quantitative analyses and it enables measurements to be made of the concentration of a compound dissolved in a solution; it is effective in the near ultraviolet, visible and near infra-red regions, which correspond to a wavelength interval from about 180 to 1 000 nm.

The terms given in tables 1 and 2 are classified so that they are defined before their use in later definitions.

Table 1 is given for the purposes of comprehensiveness; it collates terms from the Vocabulaire international de l'éclairage (International lighting vocabulary), account of which has been taken in the choice of terms and in the drawing up of the definitions forming the subject of table 2. In table 1

— terms 1 to 8 relate to the interaction of any electromagnetic radiation of an optical nature (UV, visible, IR) with any medium observed from the outside;

— terms 9 to 11 relate to the interaction of any electromagnetic radiation of an optical nature (UV, visible, IR) with a medium with plane and parallel surfaces, which is homogeneous, isotropic, non-luminescent and non-scattering, observed from the inside.

Table 2 is in line with the scope of this International Standard and therefore concerns the interaction of a beam of monochromatic luminous radiation striking, at normal incidence, a medium consisting of a solution which is homogeneous, isotropic, non-luminescent and non-diffusing contained in an optical cell (with two plane and parallel surfaces). In table 2

— terms 14 and 15 relate to the theoretical aspect, and are a simple adaptation of terms 9 and 11 to the special case of molecular absorption spectrometry;

— terms 16 to 20 relate to actual phenomena and measurements;

— terms 21 and 22 relate to the method of expression of results.

A list of the French terms equivalent to those defined in tables 1 and 2 is given in the annex.

3 General

Molecular absorption spectrometry obeys the following laws.

3.1 Lambert-Bouguer's law

When a parallel beam of monochromatic radiation of flux Φ_0 traverses, at normal incidence, an absorbing medium with plane, parallel surfaces and which is homogeneous, isotropic, non-luminescent and non-scattering, over an optical path length b, the transmitted flux Φ_{tr} is given by the equation

$$\Phi_{tr} = \Phi_0 \, e^{-kb}$$

where

e is the base of natural logarithms;

k is a linear absorption coefficient.

This equation is derived from integration of the differential equation

$$d\Phi_{tr} = - k \, \Phi_{tr} \, dx$$

where x varies from 0 to b, $d\Phi_{tr}$ is the reduction in radiant energy flux along an infinitely small optical path length dx, and Φ_{tr} is the value of the flux at point x.

Table 1 — Summary of definitions relating to radiation and to the optical properties of matter

No.	Term	Definition	Symbol	Formula	International symbol for unit
1	incident flux[1]	Radiant (luminous) flux of the radiation striking an external surface of the medium	Φ_0		W
2	transmitted flux[1]	Radiant (luminous) flux of the radiation emerging from the medium	Φ_{tr}		W
3	transmission (CIE 45-05-65)	Passage of radiation through a medium without change of wavelength			
4	transmittance (CIE 45-20-085)	Ratio of the transmitted radiant (luminous) flux to the incident flux	τ	$\tau = \frac{\Phi_{tr}}{\Phi_0}$	
5	absorbance; transmission (optical) density (CIE 45-20-100)	Logarithm (to base ten) of the reciprocal of the transmittance	A	$A = \lg \frac{1}{\tau}$	
6	absorbed flux without phenomena other than absorption	Difference between the incident and transmitted flux	Φ_a	$\Phi_o - \Phi_{tr}$	W
7	absorption (CIE 45-05-070)	Transformation of radiant energy to a different form of energy by interaction with matter			
8	absorptance (CIE 45-20-115)	Ratio of the absorbed radiant (luminous) flux to the incident flux	a	$\frac{\Phi_a}{\Phi_0}$	
9	internal transmittance (of a homogenous non-diffusing layer) (CIE 45-20-090)	Ratio of the radiant (luminous) flux reaching the exit surface of the layer to the flux which leaves the entry surface	τ_i		
10	internal absorbance; internal transmission density (CIE 45-20-105)	Logarithm (to base ten) of the reciprocal of the internal transmittance	A_i	$A_i = \lg \frac{1}{\tau_i}$	
11	internal absorptance (of a homogenous non-diffusing layer (CIE 45-20-120)	Ratio of the radiant (luminous) flux absorbed between the entry and the exit surfaces of the layer to the flux which leaves the entry surfaces	a_i		

1) The definition or this term, used, but not defined, in the Vocabulaire international de l'éclairage (International lighting vocabulary) has been deduced from the definitions which follow it.

NOTE — The references between parentheses are those of publication CIE No. 38, *Vocabulaire internationale de l'éclairage* (TC 23) 1977.

Table 2 — Terms and definitions relating to molecular absorption spectrometry

No.	Term	Definition	Symbol	Formula	International symbol for unit
12	thickness[1]	Distance between the internal plane and parallel surfaces of an optical cell	l		mm or cm
13	optical path length[1]	Distance traversed by a light ray between the entry and exit surfaces of a solution contained in an optical cell	b		mm or cm
14	internal transmittance	Ratio of the radiant (luminous) flux reaching the exit surface of a solution contained in an optical cell, to the flux which leaves the entry surface	τ_i		
15	internal absorptance	Ratio of the radiant (luminous) flux absorbed between the entry and the exit surfaces of a solution contained in an optical cell, to the flux which leaves the entry surface	α_i		
16	reference flux	Radiant flux of the monochromatic radiation transmitted by the optical cell containing the solution used as reference and reaching the detector	Φ_r		W
17	sample flux	Radiant flux of the monochromatic radiation transmitted by the optical cell containing the solution on which the measurement is made and reaching the detector	Φ_s		W
18	percentage transmittance	The ratio, expressed as a percentage, of the sample flux to the reference flux		$100 \frac{\Phi_s}{\Phi_r}$	
19	partial internal absorbance; partial internal transmission density[2]	Fraction of the internal absorbance of a solution due to certain of its constituents. The absorbance of a solution for given experimental conditions is thus the difference between its internal absorbance and that of the solution used as reference	A_p	$\lg \frac{\Phi_r}{\Phi_s}$	
20	characteristic partial internal absorbance; characteristic partial internal transmission density[2]	The partial internal absorbance of a solution due to only one of its constituents (for example compound dissolved for analysis)	A_c	$\lg \frac{\Phi_r}{\Phi_s}$	
21	concentration	Ratio of the mass of compound dissolved to the volume of the solution According to the units used, one can differentiate 21.1 and 21.2			
21.1	mass concentration	Ratio of the mass of the compound dissolved to the volume of the solution	ϱ		kg/m^3
21.2	amount-of-substance concentration	Ratio of the amount-of-substance of compound dissolved to the volume of the solution	c		mol/l

1) Terms 12 and 13 are equivalent when the incident light ray is normal. The product of the optical path length and the refractive index of the absorbing solution is called the "chemin optique" (literally "optical path").

2) The terms "partial internal transmission density" and "characteristic partial internal transmission density" are obsolete.

Table 2 (*concluded*)

No.	Term	Definition	Symbol	Formula	International symbol for unit
22	characteristic partial internal absorbance coefficient	Characteristic absorbance per unit thickness and per unit concentration of the dissolved compound under consideration NOTE — By extension, and in general, the concentration used is often that of the element or molecule being determined. According to the units used, one can differentiate 22.1 and 22.2			
22.1	specific mass absorbance coefficient	Absorbance coefficient for which the thickness is usually expressed in centimetres and the concentration in grams of compound dissolved in one litre of solution	a	$\frac{A_c}{l\rho}$	$cm^{-1} \cdot g^{-1} \cdot l$
22.2	specific molar absorbance coefficient[1)]	Absorbance coefficient for which the thickness is usually expressed in centimetres and the concentration in moles of compound dissolved in one litre of solution	ε	$\frac{A_c}{lc}$	$cm^{-1} \cdot mol^{-1} \cdot l$ or $m^2 \cdot mol^{-1}$

1) Specific molar absorbance coefficient is often called "molar absorptivity"

NOTE — The units employed to express concentration and thickness should be specified, as also should the wavelength for the determination, the temperature of the solutions and, if possible, the width of the pass band. As the absorbance due to a compound depends upon the state of that compound in solution, its absorbance coefficient is only completely defined if the nature of the solvent and the physico-chemical properties of the solution are specified.

For terms 18, 19, 20 and 22, it is recommended that one of the two following typographical arrangements be used :

a)

t		solvent
	x	
λ		subscript or unit

which allows specification of :

— the temperature t, in degrees Celsius;

— the measurement wavelength λ, in nanometres;

— the nature of the solvent;

— the value x of the term in question with its subscript or unit, if necessary.

Example :

For specific mass absorbance coefficient

20		H_2O
	2 200	
540		$cm^{-1} \cdot g^{-1} \cdot l$

b)

x subscript or unit at t °C, λ nanometres, solvent

Example :

For specific mass absorbance coefficient

2 200 $cm^{-1} \cdot g^{-1} \cdot l$ at 20 °C, 540 nm, in aqueous solution

3.2 Beer's law

The radiant flux of a beam of parallel monochromatic radiation decreases exponentially as the concentration of the absorbing compound increases, all other factors being constant :

$$\Phi_{tr} = \Phi_0 \, e^{-k_m \varrho}$$

or

$$\Phi = \Phi_0 \, e^{-k_\varepsilon c}$$

where

Φ_0 is the incident flux;

Φ_{tr} is the transmitted flux;

e is the base of natural logarithms;

k_m and k_ε are absorption coefficients which are constant for given experimental conditions;

ϱ is the mass concentration;

c is the amount of substance concentration.

3.3 Additive nature of the laws of Lambert-Bouguer and Beer

When a beam of parallel monochromatic radiation traverses, at normal incidence, an absorbing medium with plane, parallel surfaces and which is homogeneous, isotropic, non-luminescent, and non-scattering, and consists of a solution of n dissolved compounds which do not react with one another, the total absorbance is equal to the sum of the n characteristic absorbances.

3.4 General law

The laws of Lambert-Bouguer and Beer can be expressed by a single equation :

$$\Phi_{tr} = \Phi_0 \, 10^{-ab\varrho}$$

or

$$\Phi_{tr} = \Phi_0 \, 10^{-\varepsilon bc}$$

where

a is the specific mass absorbance coefficient which is constant for given experimental conditions;

b is the optical path length;

ε is the specific molar absorbance coefficient which is constant for given experimental conditions;

Φ_0, Φ_{tr}, ϱ and c have the same meanings as in 3.2.

In practice, absorbances are generally measured so that the characteristic absorbance of the dissolved compound under consideration can be obtained by applying the additive law (see 3.3) in the form

$$A_2 - A_1 = A_c = ab\varrho = \varepsilon bc$$

where

A_1 is the absorbance of solution 1;

A_2 is the absorbance of solution 2;

A_c is the characteristic absorbance of the dissolved compound under consideration;

a, b, c, ε and ϱ have the same meanings as in 3.2 and in the previous equation.

4 Apparatus

Sub-clause 4.1 is intended to facilitate understanding of the objectives mentioned in clause 1 and which are detailed in 4.2 and 4.3.

4.1 Components of molecular absorption spectrometers

The components which make up molecular absorption spectrometers, i.e. instruments designed for the determination of absorbance or percentage transmittance, are intended to assure the three following functions :

a) production of a beam of radiation of a selected band of wavelengths and control of the bandwidth;

b) introduction of the solution to be examined into the beam of radiation;

c) measurement.

To the three fundamental units assuring these three functions, one must add various associated devices (collimators, lenses, fixed or rotating mirrors, diaphragms, slits, etc.) which define the beam appropriately in space and direct it onto the various parts of these units.

A wavelength scale system, the graduations of which may correspond to wavelength (nm) or to wave number (cm^{-1}), completes the instrument.

4.1.1 Devices for the production of a beam of radiation

The beam of radiation is characterized by its spectral composition, its intensity, its configuration and its direction in space; consequently, its production involves a source of radiation, a selector of the wavelengths emitted, and various complementary devices.

The spectral characteristics of an instrument are not directly related to any one of these parts but result from their association.