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General rules for molecular  
absorptiometric analysis

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## Contents

Page

|     |                                                                            |    |
|-----|----------------------------------------------------------------------------|----|
| 1   | Scope .....                                                                | 1  |
| 2   | Normative references .....                                                 | 1  |
| 3   | Terms and definitions .....                                                | 1  |
| 4   | Apparatus .....                                                            | 4  |
| 4.1 | General requirements .....                                                 | 4  |
| 4.2 | Construction of apparatus .....                                            | 4  |
| 4.3 | Performance indication of apparatus .....                                  | 10 |
| 4.4 | Accessory devices .....                                                    | 12 |
| 4.5 | Additional functions .....                                                 | 15 |
| 5   | Operation method .....                                                     | 17 |
| 5.1 | Conditions for apparatus setting up .....                                  | 17 |
| 5.2 | Calibration of wavelength graduation and absorbance graduation .....       | 18 |
| 5.3 | Preparation of test sample .....                                           | 19 |
| 5.4 | Establishment of operational conditions for apparatus .....                | 19 |
| 5.5 | Preparation for measurement .....                                          | 21 |
| 6   | Measurement of absorbance at specified wavelength .....                    | 23 |
| 6.1 | Measurement by double beam method .....                                    | 23 |
| 6.2 | Measurement by single beam method .....                                    | 23 |
| 6.3 | Measurement of cell blank value .....                                      | 23 |
| 7   | Measurement of absorption curve in the range of specified wavelength ..... | 24 |
| 7.1 | Measurement by double beam method .....                                    | 24 |
| 7.2 | Measurement by single beam method .....                                    | 24 |
| 7.3 | Measurement of cell blank value .....                                      | 25 |
| 8   | Determination .....                                                        | 25 |
| 8.1 | General requirements .....                                                 | 25 |
| 8.2 | Pretreatment .....                                                         | 25 |
| 8.3 | Absorbance and concentration .....                                         | 25 |
| 8.4 | Method for determination .....                                             | 26 |
| 8.5 | Expression of determined value .....                                       | 29 |
| 9   | Management of quality of data (quality control) .....                      | 29 |
| 9.1 | General requirements .....                                                 | 29 |
| 9.2 | Securement of metrological traceability .....                              | 29 |
| 9.3 | Securement of reliability of analytical value .....                        | 30 |
| 9.4 | Measurement for management of quality of data .....                        | 30 |
| 9.5 | Implementation of validation of analytical method .....                    | 30 |
| 9.6 | Periodical check of apparatus performance .....                            | 31 |

9.7 Preparation of work procedure manual ..... 31

10 Safety ..... 31

11 Record of measurement results ..... 31

12 Items to be described when absorption spectrometry is adopted as an analytical method in an individual standard ..... 32

Annex A (informative) Uncertainty evaluation ..... 33

## Foreword

This Japanese Industrial Standard has been revised by the Minister of Economy, Trade and Industry through deliberations at the Japanese Industrial Standards Committee as the result of proposal for revision of Japanese Industrial Standard submitted by Japan Analytical Instruments Manufacturers' Association (JAIMA)/Japanese Standards Association (JSA) with a draft being attached, based on the provision of Article 12, paragraph (1) of the Industrial Standardization Act applied mutatis mutandis pursuant to the provision of Article 16 of the said Act. This edition replaces the previous edition (**JIS K 0115 : 2004**), which has been technically revised.

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# General rules for molecular absorptiometric analysis

## 1 Scope

This Japanese Industrial Standard specifies general rules in the case where quantitative analysis is carried out by measuring the transmittance, absorbance or reflection of light by a substance within a range from near 200 nm to near 1 100 nm of wavelength by using a spectrophotometer or a photoelectric photometer. This Standard does not apply to the methods using an atomic absorption spectrometer, a near-infrared spectrometer, infrared spectrometer or a nephelometer.

## 2 Normative references

The following standards contain provisions which, through reference in this text, constitute provisions of this Standard. The most recent editions of the standards (including amendments) indicated below shall be applied.

JIS K 0050 *General rules for chemical analysis*

JIS K 0211 *Technical terms for analytical chemistry (General part)*

JIS K 0212 *Technical terms for analytical chemistry (optical part)*

JIS K 0215 *Technical terms for analytical chemistry (Analytical instrument part)*

JIS R 3505 *Volumetric glassware*

## 3 Terms and definitions

For the purpose of this Standard, the terms and definitions given in JIS K 0211, JIS K 0212, JIS K 0215, and the following apply.

### 3.1

#### absorbance

numerical value obtained by taking common logarithms of a ratio of the intensity of the light which transmitted a sample to an intensity of the light before transmission

### 3.2

#### transmittance

ratio of an intensity of the light after transmission to an intensity of the light before transmission for expressing a proportion of the light which transmitted substance

### 3.3

#### percent transmission

value obtained by expressing transmittance in percentage

### 3.4

**molar absorption coefficient**

coefficient obtained by converting absorbance of a specific sample into absorbance when a cell with a concentration of analyte of 1 mol/L and optical path length of 1 cm is used

**3.5****specular reflection, regular reflection**

reflection which follows a law of optical reflection like a mirror plane

**3.6****diffuse reflection**

reflection of which the light diffuses in many directions regardless of the laws of optical reflection

**3.7****percent reflection**

ratio of an intensity of reflected light from a surface of a target substance to an intensity of reflected light from a reference substance for expressing a proportion of the light reflected on a surface of substance in percentage

**3.8****spectrometer**

apparatus in which the light from one light source is dispersed to make a slit image on one focal plane in order of wavelength and a photodetector is installed on the image plane

**3.9****monochromator**

instrument which isolates the light with a specified wavelength

**3.10****single monochromator**

monochromator with a single dispersive device such as a diffraction grating or a prism

**3.11****double monochromator**

monochromator generally composed of two single monochromators optically connected in series

**3.12****single beam**

optical method in which an optical path does not branch between the light source and the detector in a spectrophotometer or a photoelectric photometer

### 3.13

#### **double beam**

optical method which makes the light from a light source branch into the sample side and into the reference side

### 3.14

#### **optical filter**

general term of optical devices used for passing or blocking the light with a specified range of wavelength

### 3.15

#### **gelatin filter**

optical filter, made of colored gelatin film laminated between glass layers or the like, through which the light with a specified range of wavelength can be isolated

### 3.16

#### **interference filter**

optical filter through which the light with required wavelength can be isolated making use of interference of light on thin film or multilayer film

### 3.17

#### **color optical filter**

optical filter, made of colored glass, through which the light with a specified range of wavelength can be isolated

### 3.18

#### **absorption cell**

container which contains solutions, solvents, etc. in order to measure the absorption of light using them

### 3.19

#### **sample cell**

absorption cell which contains samples

### 3.20

#### **reference cell**

absorption cell which contains solvents or reference solutions

### 3.21

#### **photometer**

instrument which measures an intensity of light

### 3.22

### **light source**

portion which generates and emits a light wave (photon) in a photometric analysis instrument

### **3.23**

### **resolution**

capacity of a spectroscopy capable of separating two spectrum lines which are mutually adjacent

### **3.24**

### **dispersion**

dividing the light containing various wavelength components into the light for every wavelength component using a prism and/or a diffraction grating

### **3.25**

### **stray light**

light other than the light with a set wavelength in the light dispersed and taken out by the monochromator

### **3.26**

### **analyte**

component to be analysed in a test sample or in a sample solution

### **3.27**

### **metrological traceability**

property of a measurement result that can relate the measurement result to a reference through an unbroken documented chain of calibration in which each calibration contributes to measurement uncertainty

## **4 Apparatus**

### **4.1 General requirements**

Generally, for the photometer used for absorptiometry, there are a spectrophotometer which uses a monochromator for the wavelength selection part and a photoelectric photometer which uses an optical filter.

### **4.2 Construction of apparatus**

#### **4.2.1 General**

The photometer is generally composed of a light source part, wavelength selection part, sample part, photometry part, signal processing part, data processing part, operation part, and indication, recording and output part.

There are a wavelength pre-selection method in which the light which passes through a wavelength selection part enters into a sample and a wavelength post-selection

method in which the light from a light source passes through a sample and enters into a wavelength selection part. Examples of the composition of photometers of a wavelength pre-selection method and a wavelength post-selection method are shown in Figure 1 and Figure 2, respectively.

For the detection method, there are a method for detecting the light with a single wavelength and a method for detecting the light with multiple wavelengths simultaneously.

For the photometry system, there are a single beam method and a double beam method.

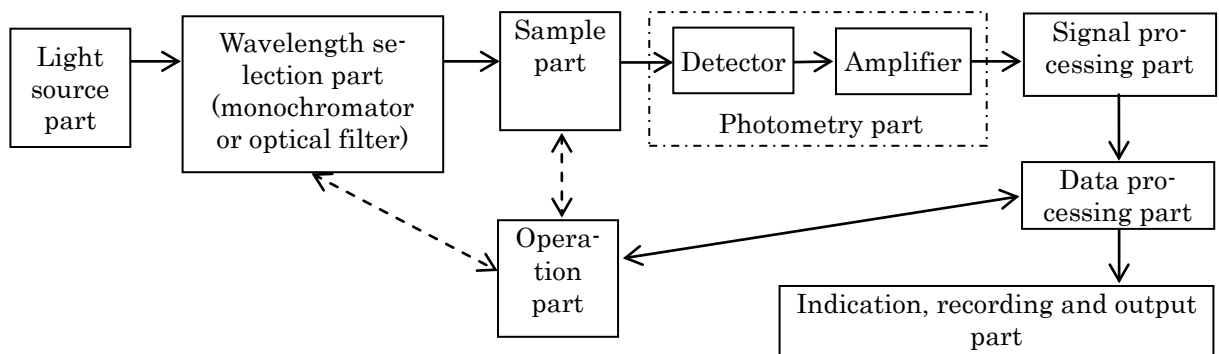


**Figure 1** Example of composition of photometer (exposing the wavelength-selected light to a sample)

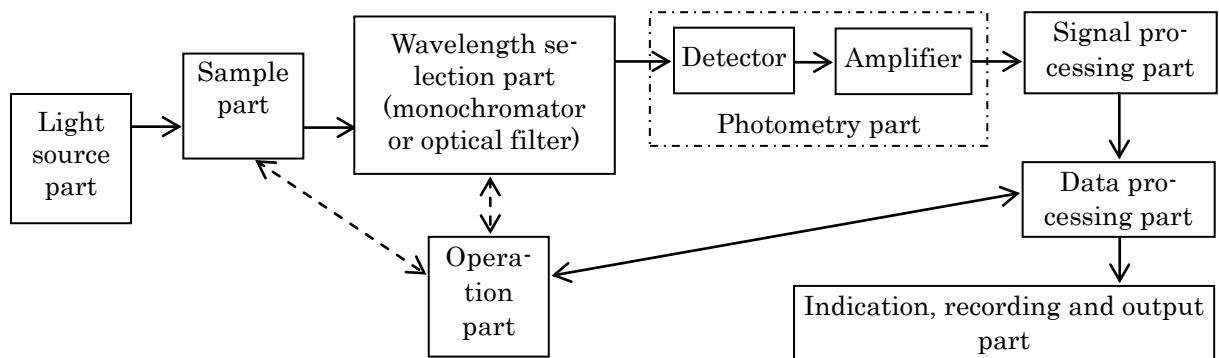


**Figure 2** Example of composition of photometer (wavelength selection of the light after exposure to a sample)

## 4.2.2 Construction of spectrophotometer

### 4.2.2.1 Light source part

The light source part shall be as follows.

a) **Emitter for light sources** The emitter for light sources shall be as follows.

1) **Tungsten lamp**, used in a long wavelength range of 320 nm or over. If lighting is

continued, the filament will evaporate and become thin gradually, the tungsten evaporated will adhere to the inner surface of a ball and it will be blackened, the light will be intercepted, radiation will decrease gradually and it will become impossible to use it eventually.

- 2) **Halogen lamp**, used in a long wavelength range of 320 nm or over. If a small amount of halogen is added and encapsulated in a gas filled lamp, it will combine with tungsten and become transparent in the low-temperature part inside the electric lamp, or it will decompose and produce tungsten in the high-temperature part. For this reason, blackening can be prevented and an electric lamp can be made small. Furthermore, it has a feature in which the reduction rate of radiation until the end of life is low.
- 3) **Deuterium lamp**, used in a wavelength range of 160 nm to 400 nm, which is a discharge lamp in which deuterium is filled up at such a degree of 0.3 kPa to 0.5 kPa.
- 4) **Xenon lamp**, used in a wavelength range of 300 nm to 800 nm, which is a discharge lamp in which light emits mainly by the excitation of xenon gas due to arc discharge.
- 5) **Light emitting diode (LED)** White LED and monochromatic LED. The white LED is used as a light source with a wavelength bandwidth. It may also be used as a light source obtained by combining several kinds of monochromatic LEDs of which the wavelength differs.
- 6) **Other light sources**, with the wavelength bandwidth of a laser excitation light source, organic electro-luminescence (OEL), organic light emitting diode (OLED), etc.

In the spectrophotometer, when the deuterium lamp or xenon lamp is an emitter for light sources, the emission line may be used for wavelength calibration.

- b) **Power source for lighting**, having a function to turn on a light source and to keep the light source radiation constant or at a constant frequency.
- c) **Light condensing system**, composed of a light condensing mirror, light condensing lens, etc.
- d) **Light guiding system**, composed of a relay lens, relay mirror, light guide plate, waveguide, optical fibre, etc.

#### 4.2.2.2 Wavelength selection part

Generally, in the spectrophotometer, the wavelength selection part is composed with one or more monochromators and two or more optical filters combined. The monochromator is a part which takes only the light of specified wavelength out of the continuous light emitted from a light source. For the dispersion of light, the optical dispersive device of a prism or a diffraction grating is used. In the apparatus which covers a wide wavelength range, the wavelength selection part may be equipped with two or more optical dispersive devices. Examples are a double monochromator in which two

monochromators are arranged in series for the purpose of reducing stray light, and a dual wavelength spectrophotometer in which two monochromators are arranged in parallel for the purpose of measuring two wavelengths.

#### 4.2.2.3 Sample part

The sample part shall be as follows.

- a) **General** The sample part shall have a function in which in the case of the double beam method, the test sample and the reference sample are fixed in optical path, and in the case of the single beam method, either the test sample or the reference sample is fixed in optical path, and shall be composed of an absorption cell, absorption-cell holder, etc. In the case of the double beam method, e.g. a beam splitter which splits a beam of light into two may be arranged.
- b) **Absorption cell**, for keeping the optical path length of the test sample such as gas and liquid constant, which consists of a material that has high transmissibility in the range of the measuring wavelength and that is not affected by the test sample. Examples of types of absorption cell are a square cell, cylinder cell, micro cell and flow cell. The square cell is also called cuvette. Normally, the square cell of 10 mm in optical path length shall be used. For the sample of which absorbance is small, the long optical path cell with a large optical path length is effective. For the volatile sample such as a gaseous sample, the cell with stopper shall be used. When the sample amount is small, the micro cell shall be used, but when the effective optical path width of the cell is smaller than actual luminous flux width, a mask which intercepts excessive luminous flux shall be attached in front of the cell. For the analyser in which the concentration change is measured while flowing a sample, a flow cell shall be used.
- c) **Absorption-cell holder**, for fixing an absorption cell placed in optical path, which has a structure to keep the optical path length of a test sample constant. Some absorption-cell holders can hold two or more absorption cells and have a mechanism to switch them.

#### 4.2.2.4 Photometry part

The photometry part shall be as follows.

- a) **Composition** The photometry part is composed of a detector and amplifier. In the double beam method, the photometry part may have a mechanism to switch optical paths.
- b) **Detector**, which is a photoelectric transducer to convert the light intensity of incident light into the electric signal proportional to the intensity. There are a phototube, photomultiplier tube, photodiode, photocell, photoconductive cell, etc. Some spectrophotometer are equipped with an array detector, two-dimensional image sensor, etc. as a detector which simultaneously detects the light in two or more wavelengths. Some spectrophotometers which covers a wide wavelength range are equipped with two or more detectors of which the sensitivity wavelength bands differ. The details of these detectors are given as follows.

- 1) **Phototube**, which is a diode tube in which the cathode which receives light and emits electrons and the anode which receives electrons are enclosed in a glass tube. The photoelectric current proportional to the amount of light received is obtained and the wavelength sensitivity characteristics differ according to the type and the window material of a photoelectric surface.
- 2) **Photomultiplier tube**, in which a dynode with a function that amplifies electrons between the cathode and the anode of a phototube is attached, and photoelectrons emitted from the photoelectric surface (cathode) are amplified millions of times. The amplification factor can be considerably changed by controlling the voltage applied to the dynode, and weak light can also be detected.

**NOTE** Since the wavelength sensitivity characteristics change due to the heterogeneity of a photoelectric surface, and the incidence efficiency of photoelectrons which come out from the photoelectric surface to the dynode changes according to the position of a photoelectric surface, care should be taken in performing the measurement of the sample with a high refractive index and the sample with polarization properties.

- 3) **Photodiode**, which is a detector using the photoelectric effect in which electromotive force is generated when exposed to light. The silicon photo diode using a silicon semiconductor is widely prevalent.
  - 4) **Photocell**, which is a photodiode obtained by covering the semiconductor with metal coating such as selenium or copper (II) oxide.
  - 5) **Photoconductive cell**, which is a photodetector using the phenomenon in which a resistance value changes when exposed to light. It is characterized by the use of cadmium sulfide, lead sulfide, etc. and the high sensitivity in the near-infrared region.
  - 6) **Array detector**, which is a detector in which photodiodes or charge coupled devices (CCDs) are arranged in an array in the wavelength dispersion direction.
  - 7) **Two-dimensional image sensor**, which is a detector in which photodiodes or CCDs are arranged in two dimensions.
- c) **Amplifier**, which amplifies the electric signal from a detector to the magnitude which is easy to process in the subsequent signal processing part. Other types of amplifiers are, for example, an amplifier in which current output is converted into voltage and a lock-in amplifier in which the amount of change is amplified.

#### 4.2.2.5 Signal processing part

Two methods of signal processing are an analog processing method and a digital processing method in which the numeric operation etc. are performed after digital conversion. The signal obtained in the photometry part shall be separated as a required signal by analog signal processing, and the analog signal shall be converted into the digital signal which can be processed in the data processing part. The signal from the photometry part contains the offset current of the amplifier due to the dark current etc. derived from a detector. The signal processing part shall have a function to adjust

the signal to zero (offset adjustment function) when light is intercepted thoroughly. It may also have a function to adjust the signal which passes through the reference cell to 100 % (gain adjustment function). Signal processing also includes noise reduction processing, smoothing processing, etc.

#### 4.2.2.6 Data processing part

The data processing part shall be as follows.

- a) **Composition** In the data processing part, data conversion, etc. are performed. In the spectrophotometer, spectrum analysis, etc. are included.
- b) **Data conversion**, such as percent transmission, percent reflection, absorbance conversion, concentration conversion, Kubelka-Munk transformation and differential transform. Other processing functions are the preparation of working curve and statistical operation.
- c) **Spectral analysis** Functions are spectrum four arithmetic operations, smoothing processing, differential processing, baseline correction, preparation of working curve, peak wavelength detection, spectrum data retrieval, etc. Some have arithmetic functions such as multivariate analysis and statistical processing.

#### 4.2.2.7 Operation part

The operation part determines, for example, the type of processing performed in the data processing part and the type of data treated in the indication, recording and output part by operating a photometer.

#### 4.2.2.8 Indication, recording and output part

The indication, recording and output part is composed of, for example, an indicator such as a display, recording medium which records and stores data and printer which prints data on forms, etc. The data of measuring wavelength <sup>1)</sup>, percent transmission, percent reflection, absorbance, concentration, etc. are displayed in an indicator, stored in a recording medium as necessary and outputted to a form using a printer or other devices. In the spectrophotometer, for example, the relationship diagram (spectroscopy data) between the wavelength <sup>1)</sup> and percent transmission, percent reflection, absorbance, etc. is displayed on an indicator, stored in a recording medium as necessary and outputted to a form using a printer. Some have an external output function.

Note <sup>1)</sup> Instead of wavelength (nm), wave number ( $\text{cm}^{-1}$ ), energy (eV), frequency (Hz), etc. may be used.

### 4.2.3 Apparatus composition of photoelectric photometer

#### 4.2.3.1 Light source part

The light source part shall be as follows.

- a) **Emitter for light sources** The emitter for light sources of a photoelectric photometer shall be as specified in 4.2.2.1 a) and shall be as follows.
  - 1) **Monochromatic LED** The monochromatic LED shall be used as a light source of specified wavelength range.