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A Review on Multicomponent Analysis

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ABSTRACT: Origen and Characteristics of UV-VISIBLE spectrum results from the interaction of electromagnetic radiation in the UV-Visible region with molecules, ions or complexes. It forms the basis of analysis of different substances such as, inorganic, organic and biomolecules. These determinations find applications in research, industry, clinical laboratories and in the chemical analysis of environmental samples. It is therefore important to learn about the origin of the UV-VIS spectrum and its characteristics

KEY WORDS : UV Spectroscopy, Multicomponent analysis, Radiation

I. INTRODUCTION :

Spectroscopy is the study of the properties of matter through its interaction withvarious types of radiation (mainly electromagnetic radiation) of the electromagnetic spectrum.

Spectrometric Techniques : are a large group of analytical methods that are based on atomic and molecular spectroscopy. Spectrometry and spectrometric methods refer to the measurement of the intensity of radiation with a photoelectric transducer or other types of electronic device.

The UV-VIS spectrometry : It is one of the oldest instrumental techniques of analysis and is the basis for a number of ideal methods for the determination of micro and semi micro quantities of analytes in a sample. It concerns with the measurement of the consequences of interaction of Electromagnetic radiations in the UV and/or visible region with the absorbing species like, atoms, molecules or ions.

Origen and Characteristics of UV-VIS spectrum results from the interaction of electromagnetic radiation in the UV-Visible region with molecules, ions or complexes. It forms the basis of analysis of different substances such as, inorganic, organic and biomolecules. These determinations find applications in research, industry, clinical laboratories and in the chemical analysis of environmental samples. It is therefore important to learn about the origin of the UV-VIS spectrum and its characteristics.

PRINCIPLE

Basic principle of spectroscopy is **the Beer-Lambert's law**, which states that absorption of incident radiation is directly proportional to the concentration and the thickness of the material. In UV-VIS Spectroscopy, a continuum range of wavelengths from 200nm to 1100nm is used. The UV visible spectroscopy is based on the absorption of ultra violet light or visible light by chemical compounds, which results in the production of distinct spectra is based on the spectroscopy interaction between light and matter. When the,matter absorbs the light undergoes excitation de-excitation, resulting in the production of a spectrum.

Lambert's law stated that absorbance of a material is directly proportional to its thickness (path length). Much later, August Beer discovered another attenuation relation in 1852. Beer's law stated that absorbance is proportional to the concentrations of the material sample. The modern derivation of the Beer–Lambert law combines the two laws and correlates the absorbance to both the concentrations and the thickness of the material. Absorption spectra of chemical samples are generated when a beam of electromagnetic radiation is passed through a sample, and the chemical sample absorbs a portion of the photons of electromagnetic energy passing through the sample. Spectroscopy can be done for a material by having a light source, a monochromator and a photo detector, which counts the number of photons. The light source is illuminated and passed through a monochromator which separates the white light into its consecutive colours, and is passed through the material. Intensity is measured against each wavelength. As the light source is passed through the setup, incident and transmitted radiations. These measurements are used to

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calculate the transmission and absorption spectra of the material. While many modern instruments perform Beer's law calculations by simply comparing a test sample with a reference sample which have a negligible absorbance. The graphing method assumes a straight-line relationship between absorbance and concentration, which is valid only for dilute solutions.

Transmittance, $T = I/I_0$ Absorbance, $A = 2\text{-}\log(\%T)$

I –Transmitted radiation intensity I_0 – Incident radiation intensity

When the light beams are passed through a dilute sample, the absorption will be less since there is only less number of absorbing particles presented. The light beam was passed through a concentrated sample. The intensity of the transmitted beam was considerably low, which leads to violation of Beer Lambert's law.

The law thus states that for a dilute solution, A = Kcl

Where,

- A – absorbance
- K – molar absorbance coefficient
- c– molar concentration
- l - Path length

APPLICATIONS OF UV SPECTROSCOPY

- Quantitative and Qualitative analysis.
- Determination of molecular weight.
- Determination of molar absorbance coefficient.
- Determination of unknown compound.
- Detection of functional group.
- Detection of isomers and geometrical isomers.

ADVANTAGE OF UV SPECTROSCOPY

- High sensitivity.
- Require only small volume of sample.
- Linearity over wide range of concentration.
- Can be used with gradient elution.

DISVANTAGE OF UV SPECTROSCOPY

- Not linear for high concentration.
- Does not work with compounds that do not absorb light at this wavelength region.
- Requirement of high voltage for initiation.
- Generates significant heat and requires external cooling.

MULTIPLE COMPONENT ANALYSIS

In statistics, multiple component analysis is a data analysis is a data analysis technique for nominal categorical data, used to detect and represent underlying structures in a data set. It does this by representing data as points in a low-dimensional Euclidean space. The procedure thus appears to be the counterpart of the principal component analysis for categorical data. Multiple component analysis can be viewed as an extension of simple correspondence analysis in that it is applicable to large set of categorical variables. MMCA isused to represent and model datasets as "clouds" of points in a multidimensional Euclidean space; this means that it is distinctive in describing. the patterns geometrically by locating each variable/unit of analysis as a point in a low-dimensional space. The results are interpreted on the basis of the relative positions of the points and their distribution along the dimensions; as categories become more similar in distribution, the closer (distance between points)they are represented in space]. Although it is mainly used as an exploratory technique, it can be a particularly powerful one as it "uncovers" groupings of variable categories in the dimensional spaces, providing key in sights on relationships between categories(i.e.,multivariate treatment of the data through simultaneous consideration of multiple categorical variables), without needing to meet assumptions requirements such as those required in other techniques widely used to analyse categorical data (e.g.,chi-squares analysis, Fischer's exact test, G-statistics, and ratio test) . The use of MCA is, thus, particularly relevant in studies where a large amount of qualitative data is collected, often in pair with quantitative data, and where qualitative variables can become sub optimized in the data analysis. This is often the case in epidemiological and system studies where variables in the datasets may be quantitative or qualitative, temporal or no temporal and /or objective or subjective.

The spectrophotometric assay of drugs rarely involves the measurement of absorbance of samples containing only one absorbing component. The pharmaceutical analyst frequently encounters the situation where the concentration of one or more substance is required in samples known contain other absorbing substances, which potentially interfere in the assay. If the formula of the sample is known, the identity and concentration of the intereferents are known and the extent of interference in the assay may be determined.

The ability to isolate multiple absorbance curves from the total sample absorbance. This allows us to measure multiple chemical analytes simultaneously with a single analyzer, without using filters or moving parts. Photometers that offer multi-component analysis will often use crude

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techniques like rotating "chopper" filter wheels or a group of line source lamps. These solutions implement moving parts that are prone to malfunction and multiple light sources that all require replacement

METHODS OF MULTICOMPINENT ANALYSIS

- Simultaneous equation method
- Absorbance ration method
- Geometric correction method
- Orthogonal polynomial method
- Derivative spectrophotometry

SIMULTANEOUS EQUATION METHOD

If a sample contains two absorbing drugs (x and y) each of which absorbs at the lambda max of the other lambda1 and lambda2. It may be possible to determine both, the drug by the simultaneous equation method .

The information required is,

(a) The absorption of X at lambda1 and lambda 2, a_{x1} and a_{x2} respectively

(b) The absorption of Y at lambda1 and lambda2, a_{y1} and a_{y2} respectively

(c) The absorbance of the diluted sample at lambda1 and lambda2, A_1 and A_2 respectively.

Let c_x and c_y be the concentrations of X and Y respectively in the diluted sample. Two equations are constructed based upon the fact that at lambda1 and lambda2 the absorbance of the mixture is the sum of the individual absorbances of X and Y.

At lambda1

$$A_1 = a_{x1}bc_x + a_{Y1}bc_Y \_\_\_\_\_ (1)$$

At lambda2

$$A_2 = a_{x2}bc_y \_\_\_\_\_ (2)$$

For measurements in 1cm cells, b =1

Rearrange equation (2)

$$C_Y = A_2 – a_{x2}C_x / a_{y2}$$

Substituting for c_Y in equation (1) and rearranging gives

$$C_X = A_2a_{Y1} – A_1a_{Y2} / a_{x2}\ a_{Y1} – a_{x1}\ a_{Y2} \_\_\_\_\_ (3)$$

And,

As an exercise you should derive modified equations containing a symbol (b) for pathlenth.

Criteria for obtaining maximum precision, based upon absorbance ratios, have been suggested that place limits on the relative concentrations of the components of the mixture. The criteria are that the ratios

$$A_2 / A_1 / a_{X2} / a_{X1} \text{ and } a_{Y2}/a_{Y1} / A_2/A_1$$

Should lie outside the range 0.1- 0.2 for the precise determination of Y and X respectively. These criteria are satisfied only when the lambda max of the two components are reasonably dissimilar. An additional criterion is that the two components do not interact chemically, thereby negating theintial assumption that the total absorbance is the sum of individual absorbances.

ABSORBANCE RATIO METHOD

The absorbance ratio method is a modification of the simultaneous equation procedure. It depends on the property that for a substance which obeys Beer's law at all wavelengths, the ratio of absorbances at any two wavelengths is a constant value in depend of concentration or path length.

For example, two different dilutions of the same substance give the same absorbance ratio A_1/A_2, 2.0. In the USP, this ratio is referred as Q value. The British pharmacopeia also uses a ratio of absorbances at specified wavelength in certain confirmatory tests of identity. For example cyanocobamin exhibits three lambda max at 278nm, 361nm and 550 nm. The A_{361}/A_{278} to be 1.79 +/- 0.5 and the A_{361}/A_{278} to be 1.79+/ - 0.09

In the quantitative assay of the two components in admixture by the absorbance ratio method, absorbance are measured at two wavelengths one being the lambda max of one of the component and the other being a wavelength of equal absorptivity of the two components an iso-absorptive point. The two equations are constructed as described above for the method of simultaneous equations [eqn (1) and eqn (2)]. Their treatment is somewhat different, however, and uses the relationship $a_x = a_{y1}$ at lambda 1. Assume b = 1cm.

$$A_1 = a_{x1}c_x + a_{x1}c_y \_\_\_\_\_ (5)$$

$$A_2/A_1 = a_{x2}c_x + a_{y2}c_y / a_{x1}c_x + a_{x1}c_y$$

Divide each term by $C_x + C_y$ and let $F_x = c_x/ (c_x + c_y)$ and $F_y = c_y (c_x + c_y)$. That F_x and F_y are the fractions of X and y respectively in the mixture.

$$A_2/A_1 = a_{x2}F_x + a_yF_y/ A_{x1}F_x + a_{x1}F_y$$

Let $Q_x = a_{x2}/a_{x1}$, $Q_y = a_{y2}/a_{y1}$ and $Q_m = A_2/A_1$

Therefore, $Q_m = F_x (Q_x – Q_y) + Q_y$

$$F_x = Q_m – Q_y/ Q_x - Q_y \_\_\_\_\_ (6)$$

Equation 6 gives the fraction, rather than the concentration of X (and consequently of y) in the mixture in terms of absorbance ratios. As these are independent of concentration, only approximate, rather than accurate, dilutions of X,Y and the sample mixture are required to determine $Q_{x,Qy}$ and Q_m respectively.

If the absolute concentrations of X and Y are required, rearrange eq (5) :

$$A_1 = a_{x1}(c_x + c_Y)$$

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Therefore , $C_x + C_y = A_1/a_{x1}$

From equation 6,

$C_x = Q_m - Q_y/ Q_x - Q_y . A_1 / a_{x1}$ _____ (7)

Equation 7 gives the concentration of X in terms of absorbance ratios, the absorbance of the mixture and the absorptivity of the compounds at the iso-absorptive wavelength. Accurate dilutions of the sample solution and of the standard solutions of x and y are necessary for the accurate measurement of A_1 and a_{x1} respectively.

This method has been used for the assay of trimethoprim and sulphamethoxazole in co-trimetamol Tablets.

GEOMETRIC CORRECTION METHOD

A number of mathematical correction procedures have been developed which reduce or eliminate the background irrelevant absorption that may be present in samples of biological origin. The simplest of these procedures is the three point geometric procedure, which may be applied if the irrelevant absorption is linear at the three wavelengths selected, consider an absorption spectrum comprising the spectrum of analyte and that of the background absorbances B_1, B_2 and B_3 are linear, then the corrected absorbance A_1 , A_2 and A_3 of the sample solution at lambda 1, lambda 2 and lambda 3 respectively.

Let vD and wD be the absorbance of the drug alone in the sample solution at lambda 1 and lambda 3 respectively, that is v and w are the absorbance ratios and WD/D receptively.

Therefore, $B_1 = A_1 - VD$, $B_2 = A_2 - D$ and $B_3 = A_3 - wD$

Let y and z be the wavelength intervals (lamda 1 – lambda 2) and (lambda 3 – lambda 2) respectively.

Then ,

$B_1-B_3/B_2-B_3 = y+z /z$

$D = y (A_2 - A_3) + z (A_2 - A_3) / y(1-w) + z(1- v)$

This is a general equation which may be applied in any situation where A_1, A_2 and A_3 of the sample, the wavelength intervals y and z and the absorbance ratios v and w are known. The values of v and w are determined experimentally using a solution of the drug only. The concentration of the drug is calculated from the corrected absorbance D using any of the normal procedures

Two special circumstances allow further simplification of the general equation.

$D = y (A_2 - A_3) + z (A_2 - A_1) /(y+z) (1-r)$

II. CONCLUSION

UV-Visible spectroscopy is good for finding concentration or molar absorptivity of of biological macromolecule, organic molecule, transition metal, conjugated organic compound.. However, we need to make sure about pH of system and solvent before taking sample analysis. Using this spectroscopy, we find molar absorptivity or extinction coefficient of 2.9*10^-6 mol/L concentration Liquid seldibrdge chromophore for maximum absorption at given wavelength.

In statistics, multiple correspondence analysis is a data analysis technique for nominal categorical data, used to detect and represent underlyimg structures in a data set. It does this by representing data as points in a low-dimensional Euclidean space. MCA can be viewed as an extension of simple correspondace analysis in that it is applicable to a large set of categorical variables.

REFERENCE

[1]. Principles of instrumental analysis, skoog, 6th edition 2007.2. Modern Analytical Chemistry, D. Harvey, 2000.3. Spectrochemical analysis

[2]. Perkampus, H.H., 2013.UV-VIS Spectroscopy and its Applications.Springer Science & Business Media.

[3]. Gupta, Kumar and Sharma, Pragathi Prakashan Meerat-(1983)-Elements of Spectroscopy,6 th edition

[4]. Brown, J.Q., Vishwanath, K., Palmer, G.M. and Ramanujam, N., 2009. Advances in quantitative UV–visible spectroscopy for clinical and pre-clinical application in cancer.

[5]. Giusti, M.M. and Wrolstad, R.E., 2001. Characterization and measurement of anthocyanins by UV- visible spectroscopy.

[6]. Platt, U. and Stutz, J., 2008. Differential absorption spectroscopy. In Differential Optical Absorption Spectroscopy(pp. 135-174). Springer, Berlin, Heidelberg.

[7]. BV, D.C. and HYDRAULICS, D., 1962. Absorption spectroscopy.

[8]. Ajoy Ghatak, Tata Mc Grow Hill, (2009)-Textbook of Optics.

[9]. White, Tata Mc Graw Hill NY 1983-Atomic spectra.

[10]. C. Scott, S. Chand Co, (1998)-Introduction to optics and optical and imaging