

Calibrated Optoelectronic Instrumentation for Analyzing Absorbance of Aqueous Solutions

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ABSTRACT: Absorbance of aqueous solutions of sucrose was monitored with respect to sugar concentration using a locally calibrated optoelectronic instrumentation based on Electronic Spectroscopy (ES) technique. Sugar solutions were prepared using High Purity Laboratory Chemical (HPLC) reagent sucrose in grade-3 de-ionized water. The sucrose solution had an absorption band between 450 nm to 550 nm as measured by UV-1800 Shimadzu spectrophotometer. Transmittance of the sugar solution was measured in dark room and at room temperature using neodymium -YAG (532 nm, 30 mW) optical bench laser. Evaluation of the absorbance indicates that the absorbance increases with concentration, but with the absorbance rate higher for low concentration ($< 10\%$). Comparison with results obtained with Ordinary Cane Sugar (OCS) instead of HPLC exhibited a similar trend. The absorbance rate (ϵ) using HPLC was found to be 1.4 m^{-1} per % concentration and 0.5 m^{-1} per % concentration at low and higher concentration respectively. The value of ϵ from optoelectronic instrumentation at low concentration is higher than the calculated ϵ (0.8 m^{-1} per % concentration). This could be attributed to biological dynamics of a pure solute according to Brownian motion.

KEYWORDS: optoelectronic, electronic spectroscopy, sucrose, absorbance.

I. INTRODUCTION

Several analytical techniques have been used to determine the concentration of sugars in food samples [1 – 6]. These methods require complex pre-treatment of samples making them relatively tedious as compared to ES. Further, the organic reagents used in these pre-treatment processes are hazardous and require high cost for storage and disposal.

Electronic Spectroscopy has been used in analytical chemistry for quantitative determination of different analytes [7]. This is due to electronic transitions that are responsible for the strong absorption of the UV-Vis spectral region (200 nm – 780 nm) by biological materials [8]. ES has advantage over other techniques in that it provides a rapid, non-invasive quantitative analytical method to assess the quantity of given analyte in various aqueous samples. Tayone (2015) applied ES to determine chromium (VI) content in canned fruit juices [9], Atomic Absorption Spectroscopy (AAS) for the determination of the Chromium content in selected foods [10], Jun *et al.* (2010) used ES to quantify sucrose, fructose and glucose with respect to sugar concentration in Short – Wavelength Near-Infrared [11].

Measuring the concentration of an absorbing species in an aqueous solution is accomplished by applying Beer-Lambert's law [12]. From the result, Frank-Condon principle is used to explain the intensity of vibronic transition that simultaneously changes the vibrational and electronic quantum numbers due to absorption and emission of a photon [13]. However, ES technique currently is expensive and requires specialized skills to handle. This remains a great challenge in quantifying sugar concentration in aqueous solution at domestic level.

In this study, we demonstrate simple locally designed spectroscopic optoelectronic instrumentation and correlate its sensitivity with that of UV-1800 Shimadzu spectrophotometer as applied to measuring absorbance of sugar (sucrose) in aqueous solution against the concentration.

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II. MATERIALS AND METHODS

Optoelectronic instrumentation

Figure 1 displays a schematic illustration of the optoelectronic instrumentation set up used to measure transmittance in sugar solutions. The neodymium-YAG (532 nm, 30 mW) radiation is illuminated on the sugar solution in the quartz cell. The cell is 10 mm width centrally placed between the light source and the photo-detector. The transmitted radiation is detected by 2N3904 photo transistor. The generated photo current (i_{ph}) is processed by the LM741CN transimpedance amplifier (TIA) and the out put voltage (v_o) as a function of the transmitted light intensity is displayed on a digital voltmeter – model H27763. The instrument was zeroed to calibrate it by passing the incident radiation through a blank cell containing on the de-ionized water.

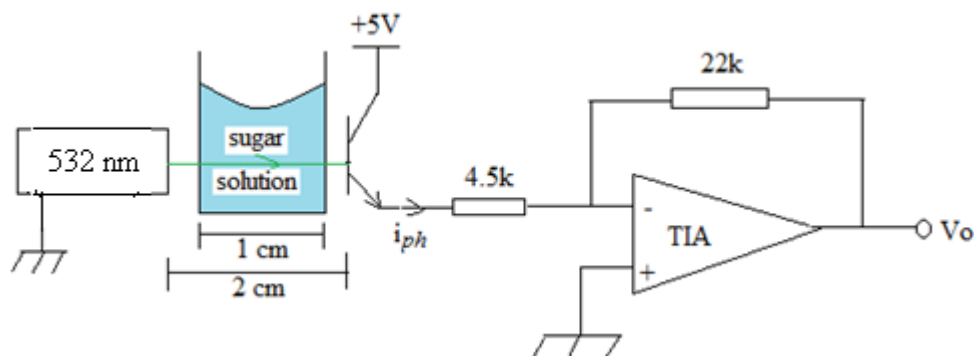


Figure 1. Schematic diagram of the calibrated instrumentation set up used for measuring transmittance of sugar in aqueous solution.

Preparation of sugar solutions

Five different aqueous sucrose solutions ranging from 0 to 60% were prepared through the procedure as outlined by Tinashe (2008) [14]. Mass of sugar is measured using an electronic balance – model XL-3100D and solutions prepared using HPLC reagent sucrose in grade-3 de-ionized water. The mixture was stirred in a glass beaker to dissolve all the sugar granules to form a homogeneous solution. To ensure equilibrium, the solution was allowed to stand for 30 minutes and checked for sedimentation. Similar procedure was applied to prepare sugar solutions using OCS.

Measurements of absorbance of sugar in aqueous solution

Since studies of aqueous samples require very thin or diluted solutions [8, 15], 10 ml of the prepared solutions was diluted in 100 ml in a volumetric flask. Absorbance of a sample solution (22.5% concentration) was scanned in spectrum mode from 190 nm to 800 nm using UV-1800 Shimadzu spectrophotometer to determine maximum wavelength absorption. The calibrated instrumentation was used to measure transmittance in sugar solutions at 532 nm using neodymium-YAG laser radiation. Transmittance of sugar solution was measured in a quartz cell against pure de-ionized water as the reference solution for all measurements and at room temperature (298 K). The absorbance of the solutions was evaluated using Beer–Lambert’s law. Reproducibility and stability of the measurement were tested. This experiment was carried out in dark room so as to eliminate detection of stray light. The sugar content of the solutions was again measured by the Shimadzu spectrophotometer at 532 nm and results compared.

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III. RESULTS AND DISCUSSION

Concentration of sucrose in aqueous solution

Five different aqueous sugar solutions of concentrations (in percentage) 0, 8.2, 22.5, 41.8, and 57.1 were prepared and used in this study. The concentration was a measure of the amount of sucrose by mass in 100 g of the aqueous solution with de-ionized water. In this case, de-ionized water, which served as the reference solution, is considered 0% concentration. The proportion of sugar in 100 g of the solution is taken as the percentage concentration.

Absorbance of sugars in aqueous solution

The absorption spectrum ranging from 190 nm to 800 nm of HPLC sucrose in aqueous solution for the 22.5% is presented in Figure 2. The absorbance initially decays exponentially from 1 to 0.0625 at 450 nm wavelength. A major absorption band is observed with the bandwidth ranging from 450 nm to 550 nm. Seven peaks are observed with the highest peak estimated at 490 nm with absorbance 0.3125.

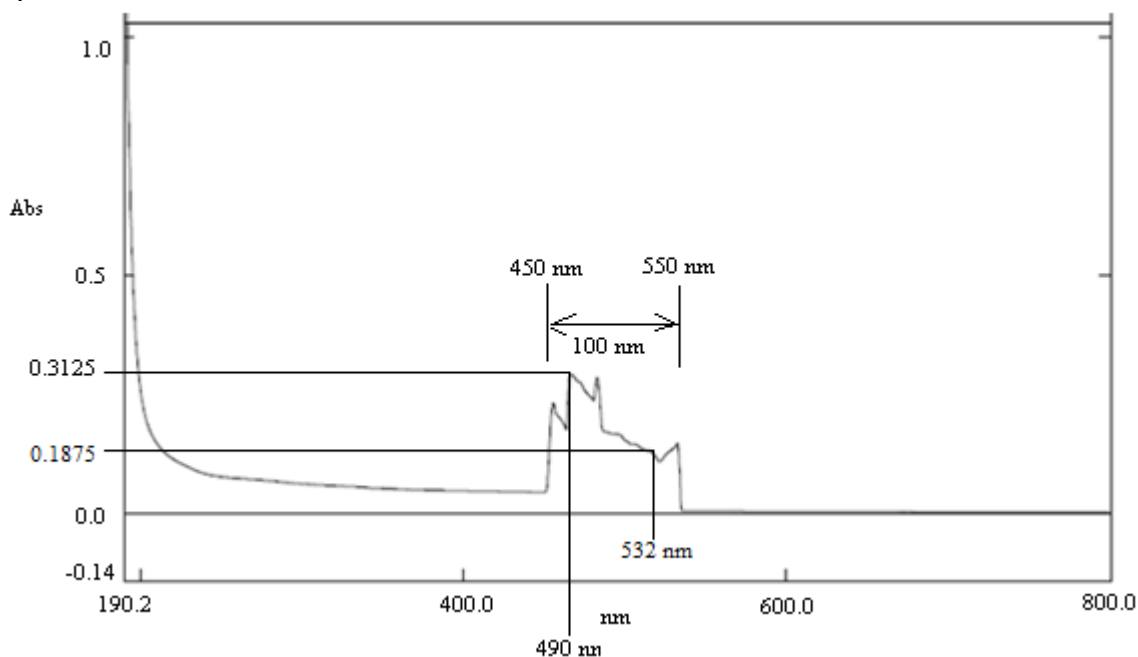


Figure 2. Absorbance spectrum of HPLC sucrose solution at 22.5%

The transmittance of the five different HPLC sucrose and OCS solutions were measured in a quartz cell using the optoelectronic instrumentation system. The absorbance was evaluated from the measured transmittance using the Beer-Lambert's law;

$$A = -\log(T) = \epsilon cb = \alpha b \dots\dots\dots 1$$

where A is the absorbance, T is the measured transmittance, ϵ is the molar absorptivity, c is the concentration, α is the absorption coefficient and b is the width of the sample solution. The value of α was extracted from the measured absorption spectrum at 532 nm (Figure 2) using Beer-Lambert's formula:

$$\alpha(w, c) = \frac{A(w, c)}{b} \dots\dots\dots 2$$

The obtained value of α was used to evaluate the value of ϵ , that was further used to calculate theoretical absorbance of the prepared sugar solution according to Beer-Lambert's law (equation 1).

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Figure 3 displays curves obtained from optoelectronic instrumentation, Shimadzu instrumentation and theoretical measurement (as given by equation 2). The experimental data points are an average of four measurements with an error of 5% as shown by the error bars. From the graph, it is observed that there is an overall increase in absorbance with concentration. The absorbance by the optoelectronic instrumentation (blue with diamond) is fairly higher than the absorbance by the Shimadzu instrumentation (red with squares). The absorbance obtained using the optoelectronic instrumentation is very sensitive at low concentration between 0 to 10%. Thereafter, the absorbance increases linearly with concentration with a fairly constant slope. For the curve obtained with the Shimadzu instrumentation increase in absorbance is fairly gradual between 0 to 20% concentrations. Beyond this, a steep slope is observed up to around 40% concentration after which the change in absorbance with concentration was not remarkable but fairly horizontal.

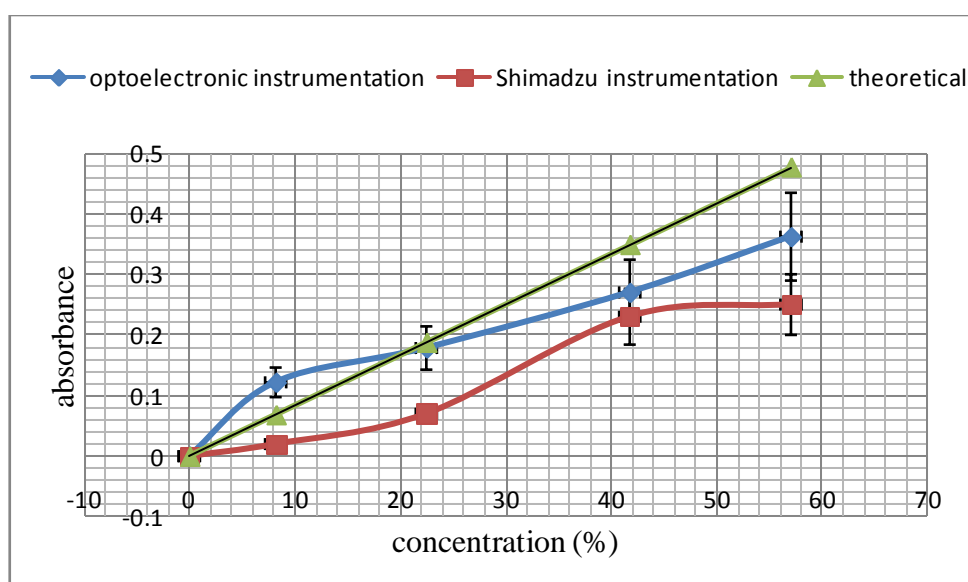


Figure 3. A comparison for the absorbance curve of HPLC sucrose in solution using the optoelectronic instrumentation and the Shimadzu instrumentation measurements

Similar procedure and analysis was carried out with OCS using the instrumentation of Figure 1 and the results are shown in Figure 4. The slope of experimental result (blue with diamond) is fairly horizontal between 0 to 10% after which it rises linearly and steeply. The theoretical slope (red with squares) is a straight line graph through the origin. Initially, the experimental absorbance is lower than the theoretical but past 20% concentration the absorbance is higher than theoretical.

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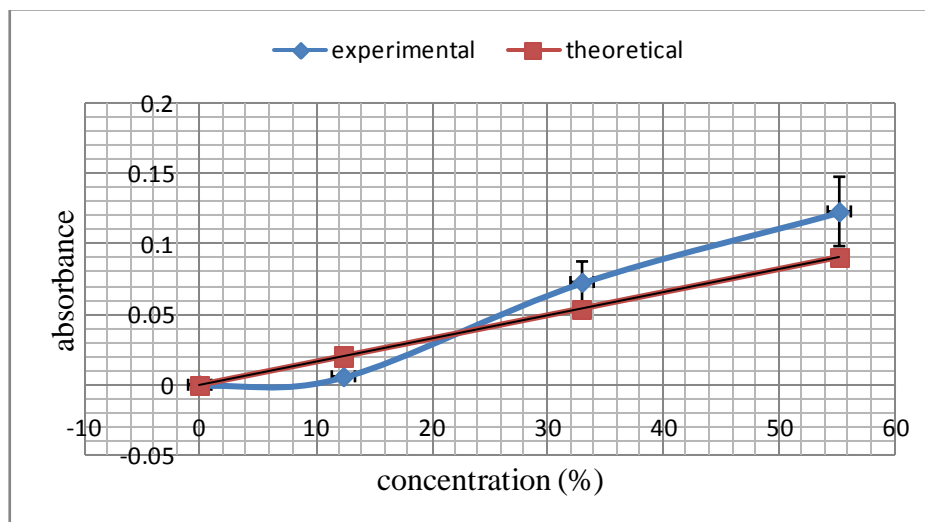


Figure 4: Standard absorbance curve for OCS in aqueous solution

The absorption band (Figure 2) occurred only in sucrose solution but was absent in pure solvent. This strong absorbance band in visible spectral region therefore, is attributed to electronic transitions due to absorption of light energy by sugar molecules. The chemical environment of each OH and CH bond in water and sugar molecules is different, so the effective absorption band is relatively wide even at the fundamental frequency [8]. The binding process between the solvent and solute changes the absorbance of the solution, hence, the amount of light energy absorbed at this wavelength will increase as the number of atoms of the selected solute in the light path increases.

The correlation between the sugar content in aqueous solution and absorbance (Figure 3) show that the overall absorbance was highest for optoelectronic instrumentation measurements as compared to the measurements by the Shimadzu instrumentation. This demonstrates that the sensitivity of this instrumentation is relatively high. The absorbance feature as displayed on the curve by the Shimadzu instrumentation can be attributed to fundamental deviations due to limitations of Beer–Lambert's law at low and high concentrations [7, 16].

Comparing the absorbance curve by the optoelectronic instrumentation to the theoretical (Figure 3), the rate of absorbance at low concentration is relatively higher than at higher concentration. This high absorbance rate at low concentration can be associated with the kinetic behaviour of the solute in the mixture. According to Brownian motion, at low concentration the association between solute molecules would be limited and resulting in random orientation of solute molecules. This would lead to the light beam through the solution being attenuated by both molecular absorption and scattering [17]. Adding more solute would imply more solute-solute association resulting in the solute molecules aligning to form a solution's crystal structure [18]. The scattering experienced at lower concentration is therefore minimized and the rate of absorbance slightly drops and stabilizes.

The rate of absorbance by OCS is fairly low and below the theoretical value at low concentration up to 12% (Figure 4). Above 22%, the rate of absorbance steadily increases with concentration above the theoretical. According to quantum Brownian motion theory, this feature may be attributed to the chemical impurities resulting from the procedure involved in processing of OCS for consumption. At low concentration, the sucrose molecule is limited (bound) in its random motion by these processing chemical impurities. Both the chemical impurity and the quantum solute are confined in an optical harmonic trap so that the impurity motion resembles the dynamics of a damped quantum harmonic oscillator. This limited randomness of the sucrose molecule that would have otherwise scattered the radiation results into high transmittance. Additional OCS in the solvent causes the chemical impurities to interact with solvent to produce different absorption characteristics. According to Tinashé [14], this would lead into a significant increase in

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refractive index that shifts the transmitted radiation off the detection point. The low detection thus, is registered as high absorbance by the instrumentation.

By comparing the absorbance rate (ϵ) using HPLC, we found ϵ to be 1.4 m^{-1} per % concentration and 0.5 m^{-1} per % concentration at low and higher concentration respectively. The value of ϵ from optoelectronic instrumentation at low concentration is higher than the calculated ϵ (0.8 m^{-1} per % concentration). Whereas at high concentration the experimental ϵ is lower than the theoretical. This has been attributed to the biological dynamics of a pure solute according to Brownian motion. The value of ϵ at high concentration (within the range studied) lies in the range of the other sugar families with general formula $\text{C}_n\text{H}_{2n}\text{O}_n$ [19]. These high correlations further demonstrate the high accuracy and robustness of the optoelectronic instrumentation.

IV. CONCLUSION

A simple optoelectronic instrumentation based on ES has been calibrated and used to obtain correlation of absorbance versus concentration of sucrose in solution. Absorbance was evaluated from transmitted neodymium YAG (532 nm) radiation and plotted against concentration. Evaluation of the absorbance indicates that the absorbance increases with concentration, but with the absorbance rate higher for low concentration ($< 10\%$). Comparison with results obtained with Ordinary Cane Sugar (OCS) instead of HPLC exhibited a similar trend. The absorbance rate (ϵ) using HPLC was found to be 1.4 m^{-1} per % concentration and 0.5 m^{-1} per % concentration at low and higher concentration, respectively. The value of ϵ from optoelectronic instrumentation at low concentration is higher than the calculated ϵ (0.8 m^{-1} per % concentration). This is attributed to biological dynamics of a pure solute according to Brownian motion.

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