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Department of Industrial Engineering

Properties and characterization of materials (mod.2)

Determination of the unknown concentration of a dye solution by UV-Vis absorption

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1. Introduction

The aim of this laboratory experience was to determine the unknown concentration of a dye solution through the evaluation of the calibration curve of the system. The uncertainty of the indirect measure was estimated using the error propagation theory (Kline-McClintock method). The UV-Vis absorption spectroscopy was performed to build the calibration curve and find the concentration.

2. Materials and Methods

A stock solution of rhodamine 6G in ethanol was used to prepare samples with different concentration through the dilution technique using 96% pure ethanol. Polystyrene cuvettes containing the samples were analysed with a Jasco V570 UV-Vis double beam absorption spectrometer with a wavelength range from 400 to 700 nm in absorbance mode.

A quantitative analysis through calibration curve was performed to determine the unknown concentration of a rhodamine 6G sample solution.

3.Experimental Results

Once all the samples were ready, they were marked with a code, corresponding to the millilitres of stock solution they contained (from 0.1 to 0.5), and immediately a preliminary consideration could be done. In fact, since the presence of rhodamine 6G caused each solution to assume a slightly pink colour, depending on the relative amount of the solute, it was possible to estimate the concentration of the unknown sample between $0.4 \cdot 10^{-7}$ M and $0.5 \cdot 10^{-7}$ M, by comparing the unknown sample with the others.

The results of the spectra acquisition are shown in Fig.1 .

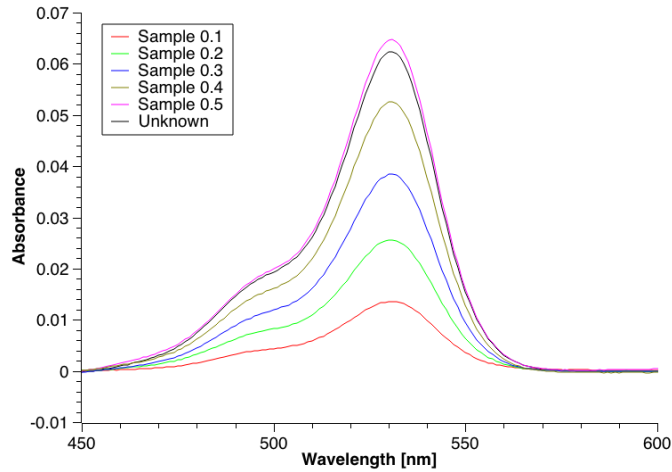


Fig.1 – Acquired spectra of the samples with different concentration.

A baseline correction was applied to the acquired spectra to highlight the region between 450 and 600 nm, in order to compare the results and to measure the peak height.

Observing the results of the experimental analysis, it was possible to see that, for each sample, the characteristic peak of rhodamine was present (at a wavelength of about $530 \text{ nm}^{[1,2]}$), with an increasing intensity according to the increasing concentration of the solute. The maximum intensity of each peak was then registered in order to build the calibration curve. For what concerns the spectrum of the unknown sample, it was possible to see that it was comprised between 0.4 and 0.5 specimens, and it was very close to the one of the 0.5 specimen. This means that the preliminary consideration (comparing the colours of the samples) was correct; furthermore, it was possible to predict a reliable result from the following quantitative analysis with the calibration curve, since the unknown concentration belonged to the concentration range studied.

4. Data Analysis

Considering the maximum absorbance for each spectrum and the relative sample concentration, a curve with the experimental points was built, and it is shown in Fig.2 .

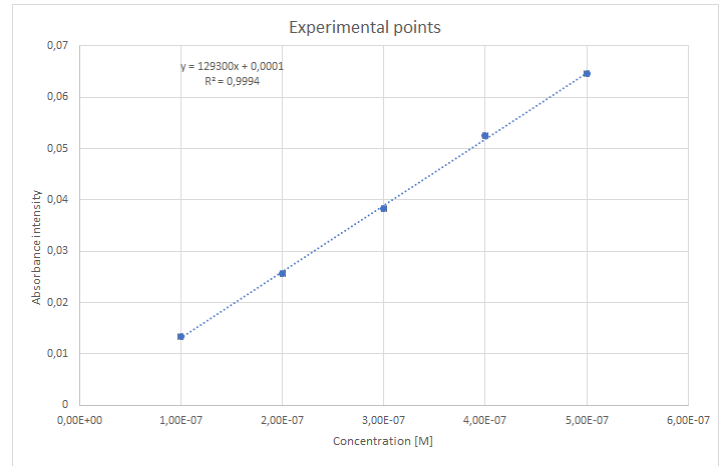


Fig.2 – Experimental points considering the maximum absorbance for every spectrum and the relative sample concentration.

The linear fitting of the data showed an intercept of about 0.00015 and therefore it was necessary to correct the curve to have 0 absorbance at 0 concentration of rhodamine 6G. The final calibration curve is reported in Fig.3 together with the sample of unknown concentration.

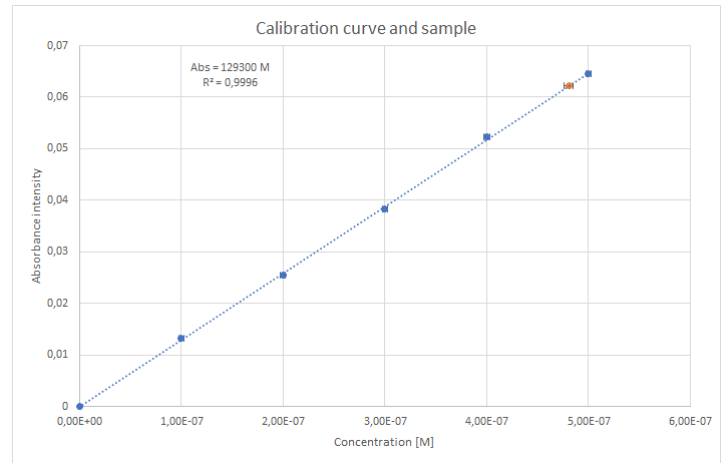


Fig.3 – Calibration curve and sample.

The measurement of the unknown concentration was done indirectly by utilizing the Lambert-Beer law:

$$A = \epsilon lc \quad (1)$$

The angular coefficient of the calibration curve represents the product of the absorption coefficient (ϵ) and the optical path length (l).

The uncertainty was obtained by implementing the error propagation theory for an indirect measurement dependent on a generic number of independent variables:

$$\sigma = \sqrt{\left(\frac{\partial f}{\partial x_1}\right)^2 \sigma_1^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 \sigma_2^2 + \dots + \left(\frac{\partial f}{\partial x_n}\right)^2 \sigma_n^2} \quad (2)$$

The absorbance intensity has been considered a perfect measurement as an approximation. The only variable contributing to the error was thus the standard deviation of the slope of the linear regression (K):

$$\sigma_c = \sqrt{\left(\frac{\partial c}{\partial K}\right)^2 \sigma_K^2} \quad (3)$$

The standard deviation of the slope was calculated with the following formula:

$$\sigma_K = \frac{\sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n-2}}}{\left\{ \sum_{i=1}^n (x_i - \bar{x})^2 \right\}^{\frac{1}{2}}} \quad (4)$$

The sample concentration and standard deviation are reported in Table 1:

Table 1. – Calculated sample concentration.

Sample concentration [M]	Standard Deviation [M]
4.81 E-07	4.54 E-09

5. Conclusions

A sample of dye solution of rhodamine 6G and ethanol was analysed through UV-Vis spectroscopy in absorbance mode to determine the concentration. The absorbance peak of the unknown sample was confronted with a calibration curve obtained by 5 standard solutions. The result obtained was 481 ± 4.54 [pM]. The result was visually corroborated by confronting the colour of the sample solution with that the standard solutions.

References

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- [2] H. Kitching, A. J. Kenyon, I. P. Parkin, 2014, The interaction of gold and silver nanoparticles with a range of anionic and cationic dyes., Physical Chemistry Chemical Physics 16, p. 6050-6059.