

Conjugated Dyes

Ilana Berlin

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1 Introduction

1.1 Purpose

Determine the length of the box in the Particle in a Box model for polycyanine dyes using the wavelengths of max absorbance collected from UV-vis spectroscopy.

1.2 References

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Shoemaker, D. P.; Garland, C. W.; Nibler, J. W. *Experiments in Physical Chemistry, 6th edition*. p. 378, **1996**, The McGraw-Hill Companies.

Wiser, D.; *Conjugated Dyes: The Particle in A Box Experiment*; Lake Forest College: Lake Forest, IL, **2025**; pp 1-3.

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Vernier Software & Technology Version 4.12 Vernier Software & Technology. 2023

1.3 Safety Information

1,1'-diethyl-2,2'-cyanine iodide
Acute Toxicity
<ul style="list-style-type: none">• Clean contact area and contact medical professional• Keep containers tightly closed in a dry, cool and well-ventilated place.• Wear eye protection and gloves, keep in well ventilated area.
1,1'-diethyl-2,2'-carbocyanine iodide
Acute Toxicity
<ul style="list-style-type: none">• Clean contact area and contact medical professional• Keep containers tightly closed in a dry, cool and well-ventilated place.• Wear eye protection and gloves, keep in well ventilated area.
1,1'-diethyl-2,2'-dicarbocyanine iodide
Acute toxicity, Skin irritation, Eye irritation
<ul style="list-style-type: none">• Clean contact area with water• Tightly closed. Dry. Light sensitive.• Use gloves and eye protection in a well ventilated space
Methanol
Flammable, Acute toxicity, Health Hazard
<ul style="list-style-type: none">• Rinse with water for at least 15 minutes• Store in a well-ventilated place. Keep container tightly closed• Wear personal protective equipment/face protection. Do not breathe mist/vapors/spray.

2 Methods

Absorbance spectra were collected by S10895 Vernier SpectroVis Plus using Vernier Spectral Analysis Version 4.12. A cuvette with a path length of 1cm was used. One cuvet was filled with methanol. This cuvette was used as a blank. One cuvette was prepared for each polycyanine dye (Fig 1). The cuvette of 1,1'-diethyl-2,2'-cyanine iodide was diluted by a factor of 4. The solution in this cuvette was a pale pink-red color. The cuvette of 1,1'-diethyl-2,2'-carbocyanine iodide was diluted by a factor of 4. The solution in this cuvette was a royal blue color. The cuvette of 1,1'-diethyl-2,2'-dicarbocyanine iodide was diluted by a factor of 8. The solution in this cuvette was a teal color.

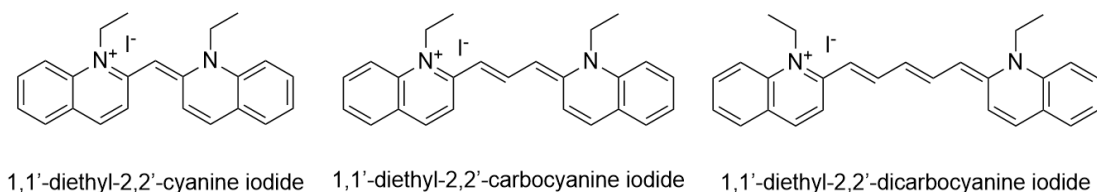


Figure 1: The chemical structure of the three polycyanine dyes used in this experiment.

3 Results/Data

The pink cyanine dye had a peak at 523.6nm. The blue carbocyanine dye had two peaks at 606.0nm and 707.5nm. The teal dicarbocyanine dye had a peak at 707.5nm (Table 1). The second peak of the carbocyanine dye matched the peak of the dicarbocyanine dye (Fig. 2). We suspect that the sample was contaminated.

Table 1: P value and wavelength of max absorbance of polycyanine dyes used in this experiment

Sample	p	$\lambda_{max}(nm)$
1	1	523.6
2	3	606.0
3	5	707.5

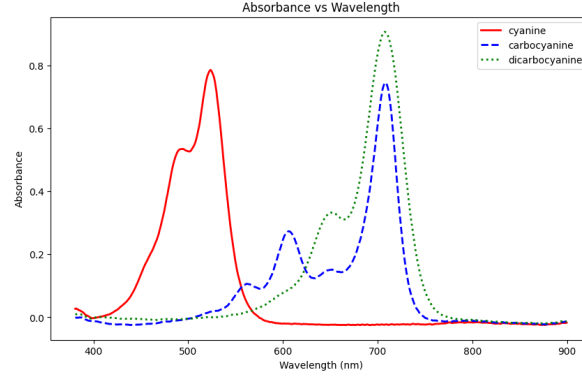


Figure 2: Wavelength vs Absorbance data collected from Vernier UV-vis spectrometer.

The relationship between λ_{max} and the number of π bonds in the carbon bridge (p) was related by the particle in a box equation by Shoemaker 1996 (Fig. 3).

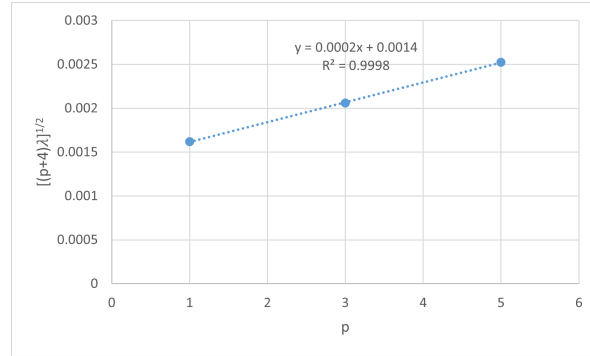


Figure 3: Linear fit of variables used to estimate box length.

The equation for the slope was rearranged to find

$$l = \sqrt{\frac{s^2 h}{8m_e c}} = 1.101\text{nm} \quad (1)$$

and the equation for the y-intercept was rearranged to find

$$\alpha = \frac{i}{\sqrt{\frac{8m_e c l^2}{h}}} - 3 = -2.300 \quad (2)$$

4 Conclusion

The length of a C-C bond within symmetrical polycyanine dyes was calculated to be 1.101nm, with a percent error of 21% when compared to a literature value of 1.40nm from Moog, 1991. Some error is

expected as the bond distance changes as the length of the bridge changes and the bonds are shared across more atoms. As previously stated, the sample of 1,1'-diethyl-2,2'-carbocyanine iodide appears to have been contaminated with 1,1'-diethyl-2,2'-dicarbocyanine iodide which may have affected accuracy.