Physics 208 Report 2

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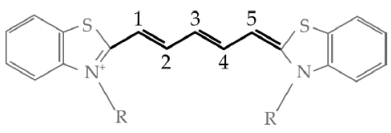
I Statement of the problem

Cyanines are a family of molecules with a central chain of carbon atoms (see fig. 1). Electrons are completely delocalized along this chain, where they are confined by end of the molecules. Cyanines are widely used as organic dyes because they can absorb and emit light at precise wavelengths, which depend on the length of this central chain.



Name	Emission wavelength	C in the chain
Kuhn V	425	3
Kuhn VI	555	5
Kuhn VII	650	7
Kuhn VIII	760	9
Kuhn IX	870	11
Kuhn X	995	13

Figure 1: Cyanine molecule (left) and the experimental data on its emission spectrum(right).

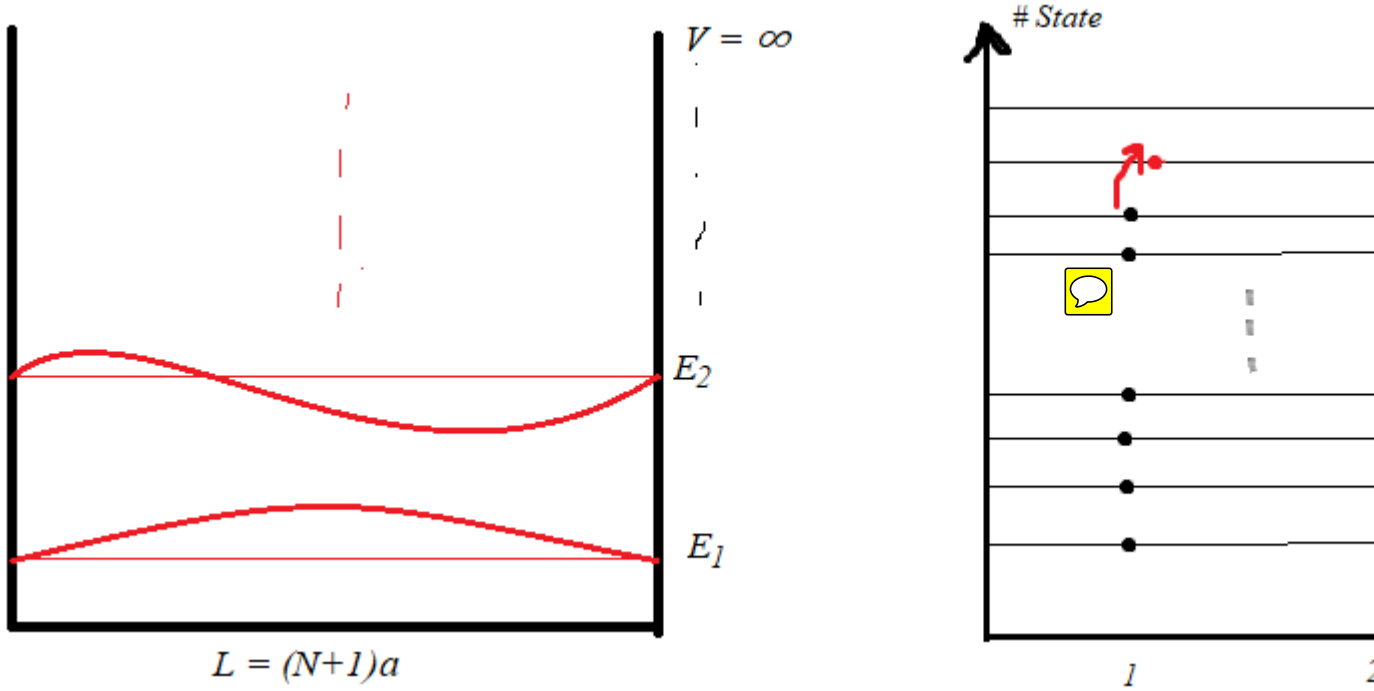


FIGURE 2: (Left) 1-D square well potential model for cyanide molecule. (Right) Delocalized electrons (black dots) are placed at states from lowest to highest. By the Pauli exclusion principle, we can place only two electrons per state. The first two probable transitions are shown with red electrons and jumps.

II Solution

II.1 Model

We describe the behavior of the electrons by the semi-quantum model. We reduce the problem to a quantum well with a width L equal to the length of the carbon chain, in which the electrons are confined. We employ the Pauli exclusion principle to motivate that there are a maximum of 2 electrons in each energy state. Thus, the energy transition depends on the number of delocalized electrons in the molecule and the number of carbons.

II.2 Variables

- a: bond length between two carbon atoms in the chain. (target variable to find)
- N: number of carbon atoms in the chain
- n: number of delocalized electrons in the chain
- λ: principal, most probable absorption/emission wavelength.

II.3 Constants

- h (Planck constant): $6.62 \cdot 10^{-34}$ kg·m^2s
- $\hbar$ (Reduced Planck constant): $1.05 \cdot 10^{-34}$ kg·m^2s

- c (Speed of light): $3 \cdot 10^8$ m/s
- m (Mass of an electron): $9.1 \cdot 10^{-31}$ kg

II.4 Derivation

The one-dimensional square well potential (see fig. 2) is the most appropriate model to describe such a phenomenon. The energy at the l-th state is

$$E_l = l^2 \frac{\pi^2 \hbar^2}{2mL^2}$$

where $L = (N+1)a$ is the width of the potential well. Then, the photon's energy must be equal to the energy of the most probable transition.

$$\Delta E = \frac{hc}{\lambda} = E_{l_1} - E_{l_2}$$

As a result of the Pauli exclusion principle and the fact that $E_l \propto l^2$, the most probable transition is $l_1 = \frac{n-1}{2}$ to $l_2 = \frac{n+1}{2}$ (see fig. 2). Then, we have

$$a = \sqrt{\frac{\lambda n h}{8mc(N+1)^2}}$$

From chemistry, we can say that there is one delocalized electron for each carbon in the chain, i.e. $N = n$. Finally, we have,

$$a = \sqrt{\frac{\lambda N h}{8mc(N+1)^2}}$$

II.5 Numerical value

As we have multiple data points given in fig. 1, we can start by a linear regression for higher precisio[illegible] Then, we modify the final result in the form,

$$\lambda = a^2 \frac{8mc}{h} \frac{(N+1)^2}{N}$$

Then, we perform a $\lambda = a^2 \cdot \frac{8mc}{h} \frac{(N+1)^2}{N} \iff y = A \cdot x$ regressio[illegible] hen we find the slope A. Finally, we deduce the numerical value of a. The results found by MATLAB are presented in Figures 3 and 4.

Finally, we found that $a = 1.62$Å. In fact, we create a confidence interval of 95% as, $a \in [1.57\text{Å}, 1.68\text{Å}]$.

II.6 Conclusion

We compare this value to the literature value. The C-C single carbon bond is generally $a_{mp} = 1.54$Å, but, the theoretical limit for these single bonds is $a_{max} = 1.80$Å (Ishigaki, Shimajiri, Takeda, Katoono, & Suzuki, 2018). We found the value with $\delta = \frac{1.62-1.54}{1.54} = 5\%$ relative error.

General model:
f(x) = a2*x
Coefficients (with 95% confidence bounds):
a2 = 2.637e-20 (2.468e-20, 2.807e-20)

Goodness of fit:
SSE: 1.008e-14
R-square: 0.9538
Adjusted R-square: 0.9538
RMSE: 4.49e-08

FIGURE 3: Numerical analysis results by MATLAB

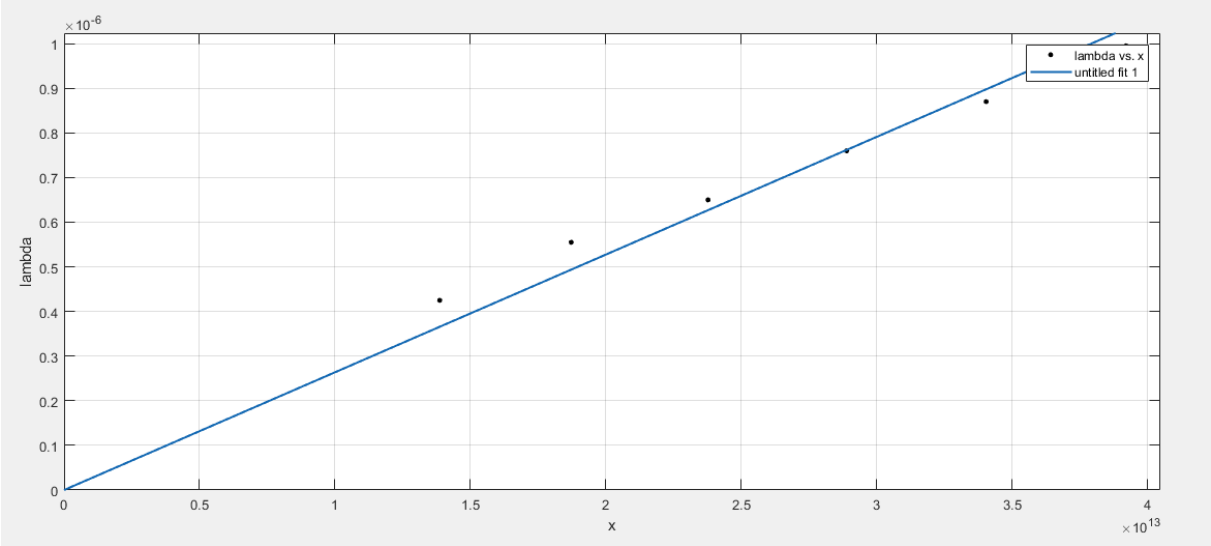


FIGURE 4: Linear regression line

References

Ishigaki, Y., Shimajiri, T., Takeda, T., Katoono, R., & Suzuki, T. (2018). Longest c–c single bond among neutral hydrocarbons with a bond length beyond 1.8 Å. *Chem*, *4*(4), 795-806. Retrieved from https://www.sciencedirect.com/science/article/pii/S2451929418300330 doi: https://doi.org/10.1016/j.chempr.2018.01.011