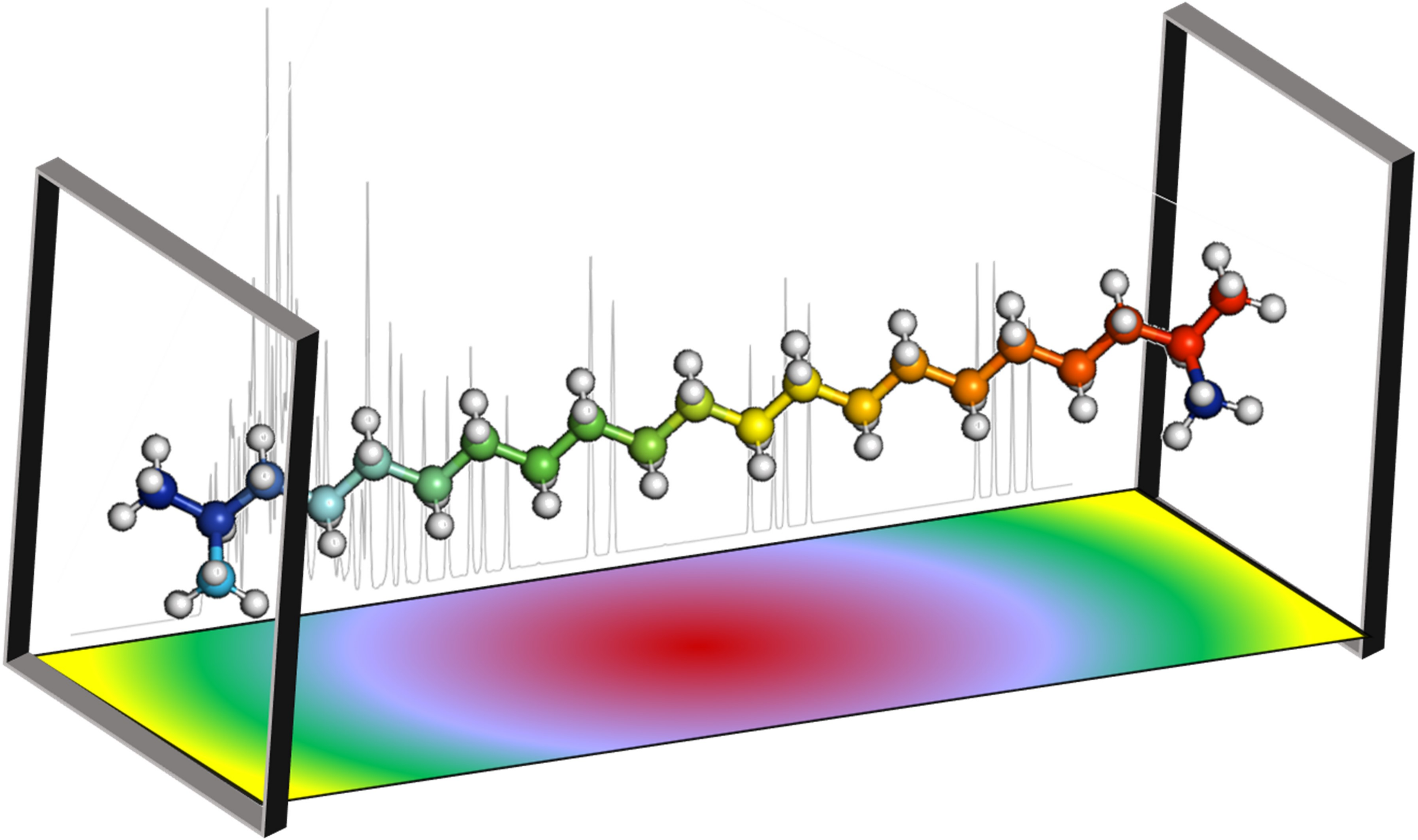


The quantum mechanical particle-in-a-box experiment- A revisit using NMR spectroscopy.

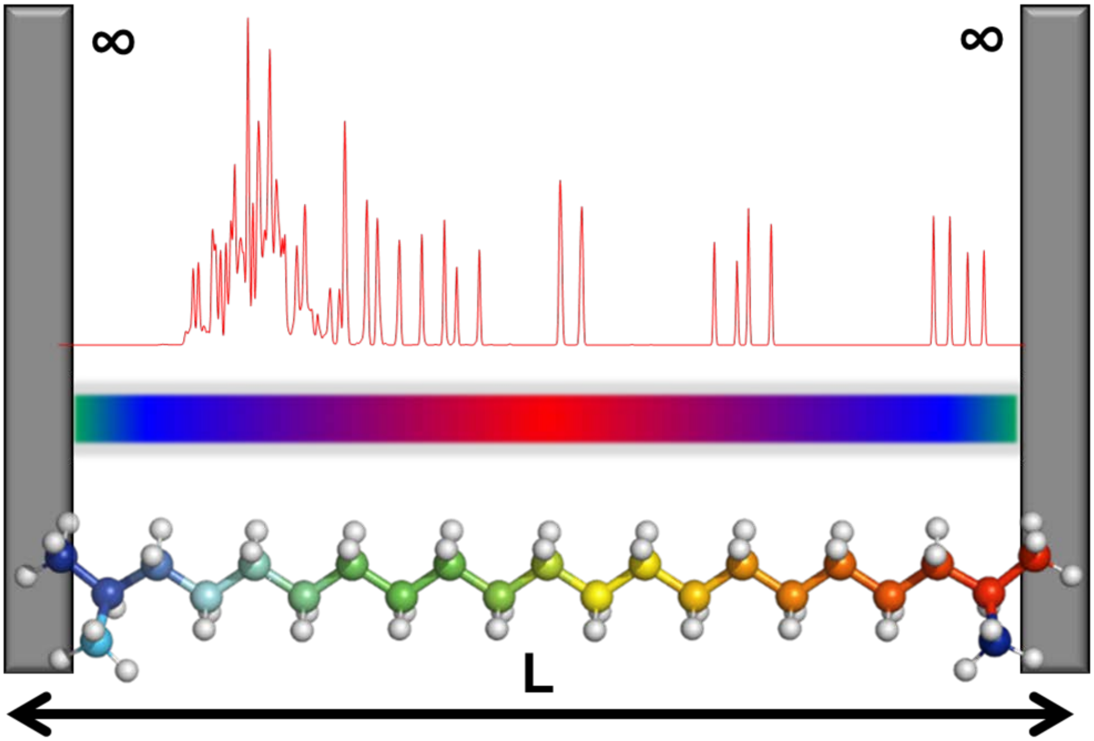
Maram Kiran[1], V. V. Krishnan[1,2,*]

[1]Department of Chemistry and Biochemistry, California State University Fresno, Fresno, California 93740; and [2]Department of Pathology and Laboratory Medicine, University of California School of Medicine, 4400 V Street, Sacramento, California 95817,

ABSTRACT

The particle-in-a-box experiment is a well-known method used to teach quantum mechanics concepts in physical chemistry labs for undergraduates. The investigation involves measuring the wavelength at maximum absorbance (λ_{max}) of electronic transitions in the UV-vis spectrum and linking it to the box length. As the electronic configurations directly influence the nuclear shielding, a computational approach to estimate the nuclear magnetic resonance (NMR) chemical shifts is shown to relate to the box length. This article revisits what Flewwelling and Laidlaw suggested over 50 years ago: NMR chemical shifts can indirectly relate to the box's length via electron density calculations. For a series of molecules (polyenylic ions) of increasing carbon chain length, the activity allows the students to develop a broader understanding of how Schrödinger's equation for a particle in a box model, electron density calculations, and NMR spectroscopy are all connected at the atomic level. Additionally, the open-ended computational procedure leverages easily accessible tools to estimate NMR chemical shifts, and this approach is suitable as a viable remote learning exercise that supplements traditional UV-vis experiments.

GRAPHICAL ABSTRACT



KEYWORDS

Upper-division undergraduate; Physical Chemistry; Computer-Based Learning; Remote learning, Particle-in-a-box, quantum mechanics, NMR Spectroscopy.

INTRODUCTION

The particle-in-a-box model is a simple yet effective way to introduce undergraduate chemistry students to the Schrödinger equation and the principles of quantum mechanics. Moreover, this model can be applied to a physical chemistry experiment called the particle-in-a-box experiment, which uses the absorption spectra of polymethine dyes to determine the length of a one-dimensional box [1, 2]. The apparent box length estimated in this exercise allows the students to relate the basics of the system's wavefunction, and the energy levels (eigenvalues) truly represent the boundary conditions of the Schrödinger equation. This topic has garnered much interest in this journal, with over 25 manuscripts discussing the particle-in-a-box model, including the system's symmetry and degeneracy [3-5], improved selection of molecules [6-9], and expanded applications of the model [10-15].

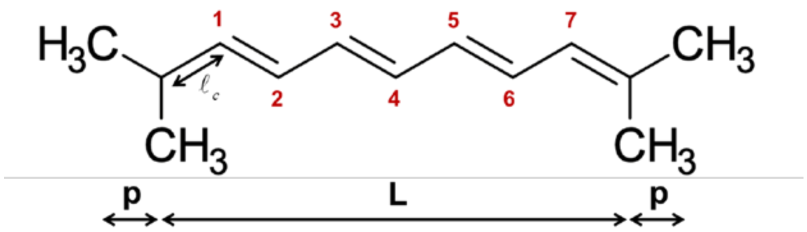


Figure 1: Theoretical estimation of the chain length. L is the calculated from the average C-C bond length and p is the penetration depth. The conjugated carbon atoms are numbered from left to right.

Delocalized electrons in a conjugated π-system can be approximated using the particle-in-a-box model by confining its location within the walls of a one-dimensional horizontal box that spans the length of the conjugated chain, as shown in an example in **Figure 1**. To determine the experimental length of the conjugated π-system for linear carbon chain molecules like cyanine dyes [2], polyenes [6, 16], or polyynes [7, 17], the wavelength of maximum absorbance in a UV-vis spectrum (λ_{max}) is related to the lowest energy transition. This experimental length is then compared to the calculated length of the molecule from its molecular structure, as shown in Figure 1, to validate the model system. However, the model's accuracy depends on the molecules chosen [10].

During the recent pandemic, remote learning has become essential for online laboratory experiments. Although UV-vis spectroscopy is still practical and vital, this article focuses on leveraging the manifestation of the electronic environment of a nucleus as an NMR chemical shift to predict the length of a particle-in-a-box approximation. We demonstrate that the wavelength at maximum absorption, defined by the electronic states of the molecule, and the chemical shift changes, based on the nuclear states, can be related to the length of the box (i.e., the number of carbons in a molecule's carbon chain).

NMR spectroscopy is a powerful and versatile technique used in various fields, from classroom applications in chemistry to advanced research in biotechnology and medicine. In particular, the chemical shift of a nucleus depends on its electronic environment, which is vital in protein structure determination [18-20].

In measuring the electronic configuration of an atom, the electron density, determined by the λ_{max}, affects the nuclear shielding, which is measured by NMR chemical shifts. We can associate a similar relation between chemical shifts and box length by establishing a linear relationship between electron density and box length. This approach supplements traditional methods when in-person experimental access is limited. A set of polyenylic molecules with varying carbon chain lengths was used to explore this relationship. For example, we have found that the chemical shifts of protons at the 2nd and 3rd (Fig .1) carbons are sensitive to box length. This exercise covers topics such as estimating electron density, introducing absorption and NMR spectroscopy, and numerical data analysis, which are relevant to undergraduate physical chemistry laboratory requirements.

EXPERIMENTAL DETAILS

(I) Learning objectives

Target students: The target students have finished a one or two-semester lecture course in physical chemistry. Students who completed prerequisite calculus and modern physics courses, taking physical chemistry lectures and laboratory courses concurrently, can also be considered. During the course, they learned about postulates of quantum mechanics, the time-independent Schrödinger equation, model systems such as particle-in-a-box, and broader spectroscopy principles. Additionally, they have completed lecture and lab organic chemistry courses, including an introduction and basic interpretation of NMR spectroscopy.

Learning objectives:

1. Able to set up a boundary-value problem for the stationary Schrödinger equation of particle in a box model.
2. Able to derive an expression relating the eigenvalues of the Schrödinger equation and wavelength and maximum absorption (λ_{max}) to the length of the one-dimensional box.
3. Adopt a method to calculate the electron density using a Worksheet-based (e.g., Excel) or other computer programs (e.g., Mathematica/Matlab/R).
4. Use the SMILE representation of molecules (polyenylic ions) to estimate the NMR chemical shifts of a selected set of molecular configurations.
5. Describe the physical meaning of the connection to electron density and chemical shifts and how it relates to the box length of the quantum mechanical model.

(I) Molecules (polyenylic ions) (polyenylic ions) investigated

This demonstration is developed using the list of polyenylic cations suggested by Flewwelling and Laidlaw [21]: The series of molecules (cations), $(CH_3)_2C{=}CH{=}(CH{=}CH{=})_{k-2}\ C(CH_3)_2$, k=2 to 10. The molecules (polyenylic ions) are converted into the SMILES (Simplified Molecular Input Line Entry System) format to obtain the other calculations [22]. For k=2, the first molecule in the series will be $(CH_3)_2C{=}CH{=}C(CH_3)_2$ to the last in the series with k=10 as $(CH_3)_2C{=}CH{=}(CH{=}CH{=})_8C(CH_3)_2$. **Table 1** lists the molecules (polyenylic ions) and their respective SMILES format.

Table 1. Molecules used to model the quantum mechanical particle-in-the box

PiB Model	*Molecule (ion)*	*SMILE-Format*	*Number of conjugated carbons (n_c)*	*Number of electrons (n_e)*	*λ_{max} (nm) Calculated*
1	$(CH_3)_2C=CH=(CH=CH=)_{k-2}\ C(CH_3)_2$ k=2	CC(C)C=C(C)C	3	2	272.34
2	$(CH_3)_2C=CH=(CH=CH=)_{k-2}\ C(CH_3)_2$ k=3	CC(C)=CC=CC(C)C	5	4	316.10
3	$(CH_3)_2C=CH=(CH=CH=)_{k-2}\ C(CH_3)_2$ k=4	CC(C)=CC=CC=CC(C)C	7	6	406.56
4	$(CH_3)_2C=CH=(CH=CH=)_{k-2}\ C(CH_3)_2$ k=5	CC(C)=CC=CC=CC=CC(C)C	9	8	503.69
5	$(CH_3)_2C=CH=(CH=CH=)_{k-2}\ C(CH_3)_2$ k=6	CC(C)=CC=CC=CC=CC=CC(C)C	11	10	603.04
6	$(CH_3)_2C=CH=(CH=CH=)_{k-2}\ C(CH_3)_2$ k=7	CC(C)=CC=CC=CC=CC=CC=CC(C)C	13	12	703.40
7	$(CH_3)_2C=CH=(CH=CH=)_{k-2}\ C(CH_3)_2$ k=8	CC(C)=CC=CC=CC=CC=CC=CC=CC(C)C	15	14	804.30
8	$(CH_3)_2C=CH=(CH=CH=)_{k-2}\ C(CH_3)_2$ k=9	CC(C)=CC=CC=CC=CC=CC=CC=CC=CC(C)C	17	16	905.53
9	$(CH_3)_2C=CH=(CH=CH=)_{k-2}\ C(CH_3)_2$ k=10	CC(C)=CC=CC=CC=CC=CC=CC=CC=CC=CC(C)C	19	18	1006.97

(III) Estimation of box length and electron density

First, the length of the molecules (polyenylic ions) is calculated using a linear chain of conjugated carbons following the methodology of Flewwelling and Laidlaw [21]. Following the geometry defined in **Figure 1,** the length of the box is defined as

$$L = \ell_C \cos(30^\circ)(n_c - 1) + 2p \ , \qquad [1]$$

where ℓ_C is the length of the conjugated carbon-carbon bond (1.437 Å, average of C-C and C=C bond length) and n_c the number of conjugated carbon-carbon bonds. The cosine of 30° is incorporated to determine the horizontal length of each conjugated carbon-carbon bond. For this exercise, the penetration length is equal to ℓ_C. The wavelength at maximum absorption using the particle-in-the-box model is then written as [21]

$$\lambda_{\max} = \frac{32 m_e c\left[\ell_C \cos 30^\circ (n-1) + p\right]^2}{h(2n-1)} \qquad [2]$$

where m_e the mass of the electron (9.11×10^{-31} kg), c velocity of light (2.99×10^{-8} m/s), h is Planck's constant (6.62×10^{-34} Js), and p is the penetration depth (1.4 Å). Equation [2] is derived in the Supporting Material.

Electron density on a carbon atom due to an electron on the m^{th} molecular orbital using the solution to the Schrödinger equation for a particle-in-the-box is given as

$$\rho = \int_{x=b}^{x=c} \psi_m^2(x)\,dx \qquad [3]$$

As there would be two electrons in each (n-1)th occupied orbital, the total electron density at a given carbon center 'r' is determined by summing the Eq.[3] over all the electrons as

$$\rho_r = 2\sum_{m=1}^{n-1}\left(\frac{2}{L}\right)\int_b^c \sin^2\left(\frac{m\pi x}{L}\right)dx \qquad [4]$$

The lower and upper limits of integration (b and c) are from the midpoints between carbon atom positions and the two carbon atoms on either side (see Fig 1). The electron density is calculated on each π electron on the chain (σ electrons are not included). The electron density given in equation [4] can be estimated straightforwardly, analytically, or numerically for each carbon center with the integration limits spanning both sides of the carbon center over the length of the chain. **Table 2** lists each carbon position's estimated λ_{max}, box length, and electron density values.

Table 2: Estimated electron densities and NMR chemical shifts

PiB Model	λ_{max} Calculated (nm)	Estimated Box Length calculated (Å)	Electron Density									Chemical Shifts of the protons (ppm)								
			C1	C2	C3	C4	C5	C6	C7	C8	C9	C1	C2	C3	C4	C5	C6	C7	C8	C9
1	272.34	4.98	4.90E-03	3.11E-02																
2	316.10	9.96	7.22E-03	4.51E-02	1.09E-01							2.48								
3	406.56	14.93	8.50E-03	5.27E-02	1.25E-01	2.04E-01						2.48	5.79							
4	503.69	19.91	9.31E-03	5.75E-02	1.35E-01	2.18E-01	2.79E-01					2.48	5.74	6.02						
5	603.04	24.89	9.87E-03	6.08E-02	1.42E-01	2.27E-01	2.87E-01	3.10E-01				2.48	5.72	6.01	6.39					
6	703.40	29.87	1.03E-02	6.31E-02	1.47E-01	2.33E-01	2.93E-01	3.14E-01	2.99E-01			2.48	5.70	5.99	6.39	6.39				
7	804.30	34.85	1.06E-02	6.49E-02	1.51E-01	2.38E-01	2.98E-01	3.17E-01	3.00E-01	2.66E-01		2.48	5.68	5.97	6.39	6.39	6.39			
8	905.53	39.82	1.08E-02	6.63E-02	1.54E-01	2.42E-01	3.01E-01	3.19E-01	3.00E-01	2.66E-01	2.37E-01	2.48	5.66	5.95	6.39	6.39	6.39	6.39		
9	1006.97	44.80	1.10E-02	6.75E-02	1.56E-01	2.45E-01	3.04E-01	3.21E-01	3.01E-01	2.66E-01	2.38E-01	2.48	5.64	5.93	6.39	6.39	6.39	6.39	6.39	

(IV) Estimation of chemical shifts

The SMILE format of the molecules (polyenylic ions) was used to estimate the chemical shifts of the ^{1}H and ^{13}C nuclei in the open-source platform NMRDB [23]. Therefore, only the ^{1}H chemical shifts that show a variation in the molecular chain length were used for further analysis and listed in **Table 2.** The combined calculations are easy to implement using MS Excel or programs such as R (Supporting information).

(V) Implementation in Physical Chemistry Laboratory Curriculum.

Typically, students take a physical chemistry laboratory course during their senior year after completing a semester-long quantum mechanics and spectroscopy course. During the period of remote learning, educators were faced with new challenges and limitations in their teaching methods. To address this, a laboratory exercise was developed for eleven undergraduate chemistry students at Fresno State in the spring of 2021. The activity was designed to be open-ended, with the instructor providing background information and resources without step-by-step procedures to encourage student involvement (details provided in the supporting information). First, the students were introduced to the quantum mechanical particle-in-a-box model and UV-vis-based experimental approach. Then, they were introduced to the concepts of NMR spectroscopy and posed the question: "Can NMR chemical shifts be used for spectroscopic investigation of particle-in-a-box model?"

The students worked together to create a plan for the experiment, dividing into groups to focus on specific tasks such as researching relevant articles, selecting molecules (polyenylic ions) and understanding their SMILE format, estimating electron density and wavelength, and estimating NMR chemical shifts. Using Zoom, they readily shared their computer screens and documents. Finally, a group was chosen to present an overview of the experimental methods and theoretical background to the rest of the class.

Before beginning the exercise, students were required to take a pre-lab quiz, which is included in the supporting documents. Most students will need three to four laboratory sessions, each lasting three hours, to complete the necessary tasks. Each student created an Excel worksheet summarizing the calculations, data fitting process, and overall results. Students shared their data, allowing them to combine results from replicated experiments. At the end of the exercise, all students took a post-lab quiz, also included in the supporting information. The quizzes will serve as an indicator of overall improvement in their understanding of the exercise.

After the experiment, every student submitted a formal report, evaluated with a grading guide based on the learning objectives. Based on the evaluation of a small sample size of 11 students, there was a slight improvement in the average score from 8.10 to 8.50. However, the p-value (t-test) 0.5 indicated this improvement was insignificant. Students submitted an Excel worksheet for assessment, and all reports were submitted online (implementation process described in the supporting information).

RESULTS AND OBSERVATIONS

(I) The estimated ^1H chemical shifts correlate linearly with the electron density at the carbon position.

The electron density calculated using Flewwelling and Laidlaw [21] and the estimated chemical shifts of the protons in the carbon chain show a linear correlation (**Figure 2**). Although the electron density of the first carbon showed a positive linear correlation with the box length, the estimated proton chemical shifts remain the same despite the increase in electronic density. However, the electron densities of the 2nd (Fig. 2a) and the 3rd carbons (Fig. 2b) decrease linearly with the increase of proton chemical shift, demonstrating the deshielding effect. For the ^1H on the 2nd carbon, a linear fit yields a slope of $-1.02 \pm 0.06 \times 10^{-2}$ m^{-1}/ppm, and an intercept of 0.65 ± 0.03 m^{-1}($R^2 = 0.98$), while for the ^1H on the third carbon yields a slope of $-2.15 \pm 0.30 \times 10^{-2}$ m^{-1}/ppm, and an intercept of 1.43 ±

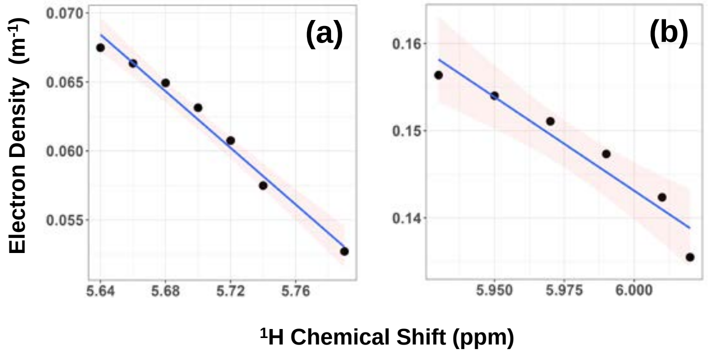


Figure 2: Correlation of chemical shifts and electron density. The plot of the proton chemical shifts at carbon positions 2 (a) and 3 (b) as a function of the estimated electron densities. The linear fit is shown as straight blue lines, and the pink bands represent the 95% confidence limit of the fits.

0.18 m^{-1}(R^2 =0.91). The chemical shifts of the protons on the 4th,5th, and other carbons do not show a change with respect to electron density.

(II) The estimated ^{1}H chemical shifts can be used to determine the length of the one-dimensional box.

The basis of the particle-in-a-box model relies on a linear relationship between the wavelength at maximum absorption (λ_{max}) of the electrons in UV-vis to the box length of the one-dimensional well based on the eigenvalues of the Schrödinger equation of the system. As the electron densities of the carbons at the chain correlate with the nuclear chemical shifts (Fig. 1), by corollary, the chemical shifts are indirectly related to λ_{max} and box length (**Figure 3**). The chemical shifts of the protons on the 2nd carbon in the chain show a linear relation with the estimated (λ_{max}) (Fig. 2a, slope: -2.31 ± 0.19 × 10^{-4} ppm/nm; intercept: 5.86 ± 0.01 ppm; R^2=0.96) and the box length (Fig. 2c, slope: -4.66 ± 0.37 × 10^{-4} ppm/Å; intercept: 5.84 ± 0.01 ppm; R^2=0.96). The chemical shifts of the ^{1}H on the 3rd carbon is much more sensitive than the 2nd carbon yielding with respect to λ_{max} (Fig. 2b, slope: -1.84 ± 0.08 × 10^{-4} ppm/nm; intercept: 5.11 ± 0.01 ppm; R^2=0.99) and box length (Fig. 2d, slope: -3.73 ± 0.01 × 10^{-3} ppm/Å; intercept: 6.01 ± 0.01 ppm; R^2=0.99).

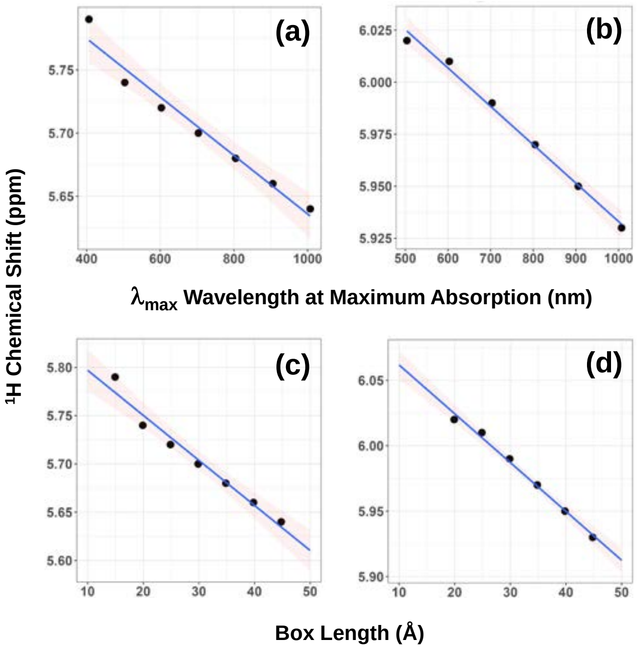


Figure 3: Correlation of chemical shifts with wavelength at maximum absorption and box length. The wavelength at maximum absorption shows a linear correlation with the estimated chemical shifts of protons at the carbon positions 2 (a) and 3 (b). Therefore, according to the particle-in-a-box model, the box length also shows a linear relation with the chemical shifts of the protons at the 2nd (c) and 3rd (d) carbons. The linear fit is shown as straight blue lines, and the pink bands represent the 95% confidence limit of the fits.

SUMMARY

In most universities, students majoring in chemistry usually take the physical chemistry laboratory course in their senior year. Typically, they would have already been introduced to NMR spectroscopy in their previous organic chemistry courses, and they are also required to complete the lecture courses in quantum mechanics and spectroscopy. This is to ensure that they have a good understanding of the concepts needed to achieve the goals of the investigation. Organic chemistry students struggle to learn and interpret NMR spectra [24-26]. However, several useful tools have been introduced and addressed pedagogical approaches for improved learning of NMR [27-32]. The exercises presented aim to help students appreciate that chemical shift in the NMR spectra is not a single fixed parameter for a local configuration (such as the ppm values of a methylene group). Instead, it represents the molecule as a whole due to the interconnected nature of the electrons, nuclei, and overall representation of the molecular dimensions. For instance, students can learn how the chemical shift of a -CH2 group changes systematically as a function of the molecular length.

While the proposed exercise is valuable in expanding traditional experimental approaches, the results demonstrate some notable limitations. The procedure yields dependable results for polyenyl molecules (polyenylic ions). Still, it does not provide reliable estimates for molecules (polyenylic ions) traditionally used in UV-vis spectroscopy, such as polymethine dyes [6], when using database-derived chemical shift calculations. Though the ^{1}H and ^{13}C chemical shifts were estimated, only the ^{1}H ones tend to show linear change with the box length. To improve the accuracy of the results, more advanced methods of calculating chemical shifts could be utilized [33]. Additionally, the estimated range of ^{1}H chemical shifts is small (~0.3 ppm), and experimental demonstrations may further be complicated due to the expected J-coupling effects between the protons in low to mid-field NMR spectrometers (< 400 MHz).

A classic experiment in the physical chemistry laboratory involves demonstrating the particle-in-a-box using UV-vis spectroscopy on linear molecules (polyenylic ions) with a conjugated carbon chain. NMR-based demonstrations can be added to this exercise to enhance student learning to connect concepts infrequently linked in the traditional classroom. It is especially important for students to understand that molecules (polyenylic ions) comprise integrated systems of electrons and nuclei, and any changes in electronic configurations can influence other elements, such as protons. However, it is also worth noting the extraordinary intuition of Flewwelling and Laidlaw's findings [21] almost fifty years ago, before the age of modern NMR.

ASSOCIATED CONTENT

Supporting Information

1. Derivation of the wavelength at maximum absorption for the particle in the box model, 2. Overview of the open-ended laboratory, 3. Pre and post-lab evaluation quizzes, 4. Answer keys, and 5. R-markdown for calculations.

The Supporting Information is available on the ACS Publications website.

AUTHOR INFORMATION

Corresponding Author

*E-mail: krish@csufresno.edu

ACKNOWLEDGMENTS

The authors thank K. Montgomery and C. Her for many discussions and the students of the CHEM 111 laboratory (Spring 2021) for their participation.

REFERENCES

1. Gerkin, R.E., *A molecular spectral corroboration of elementary operator quantum mechanics.* Journal of Chemical Education, 1965. **42**(9): p. 490.10.1021/ed042p490
2. Shoemaker, DP, C.W. Garland, and J.I. Steinfeld, *Experiments in physical chemistry.* 2018: McGraw-Hill.0070570035
3. Hollingsworth, C.A., *Accidental degeneracies of the particle in a box.* Journal of Chemical Education, 1992. **69**(6): p. 516-516.10.1021/ed069p516.4
4. Manae, M.A. and A. Hazra, *Helping Students Understand the Role of Symmetry in Chemistry Using the Particle-in-a-Box Model.* Journal of Chemical Education, 2016. **93**(6): p. 1056-1060.10.1021/acs.jchemed.5b00856
5. Rogers, D.W., *SYMMETRY AND DEGENERACY - PARTICLE IN A SQUEEZED BOX.* Journal of Chemical Education, 1972. **49**(7): p. 501-&.10.1021/ed049p501
6. Anderson, B.D., *Alternative Compounds for the Particle in a Box Experiment.* Journal of Chemical Education, 1997. **74**(8): p. 985.10.1021/ed074p985
7. Henry, M., H.G. Roth, and BD. Anderson, *The Particle in a Box Redux: Improved Experimental Conditions for the Laser Synthesis of Linear Polyynes.* Journal of Chemical Education, 2012. **89**(7): p. 960-961.10.1021/ed200728k
8. Kippeny, T., L.A. Swafford, and S.J. Rosenthal, *Semiconductor nanocrystals: A powerful visual aid for introducing the particle in a box.* Journal of Chemical Education, 2002. **79**(9): p. 1094-1100.10.1021/ed079p1094
9. Rice, CV and G.A. Giffin, *Quantum dots in a polymer composite: A convenient particle-in-a-box laboratory experiment.* Journal of Chemical Education, 2008. **85**(6): p. 842-844.10.1021/ed085p842
10. Autschbach, J., *Why the Particle-in-a-Box Model Works Well for Cyanine Dyes but Not for Conjugated Polyenes.* Journal of Chemical Education, 2007. **84**(11): p. 1840.10.1021/ed084p1840
11. Blanck, H.F., *Introduction to a quantum-mechanical harmonic-oscillator using a modified particle-in-a-box problem.* Journal of Chemical Education, 1992. **69**(2): p. 98-99.10.1021/ed069p98
12. Casaubon, J.I. and G. Doggett, *Variational principle for a particle in a box.* Journal of Chemical Education, 2000. **77**(9): p. 1221-1224.10.1021/ed077p1221
13. Muha, G.M., *ON THE MOMENTUM OF A PARTICLE IN A BOX.* Journal of Chemical Education, 1984. **61**(5): p. 414-415.10.1021/ed061p414
14. Padnos, N., *Approximating harmonic oscillator by a particle in a box.* Journal of Chemical Education, 1965. **42**(11): p. 600-&.10.1021/ed042p600
15. Wimpfheimer, T., *A particle in a box laboratory experiment using everyday compounds.* J. Lab. Chem. Educ., 2015. **3**: p. 19
16. Soltzberg, L.J., *Electronic Spectra of Conjugated Systems: A Modern Update for a Classic Experiment.* Journal of Chemical Education, 2001. **78**(10): p. 1432.10.1021/ed078p1432
17. Anderson, B.D. and C.M. Gordon, *The laser synthesis of linear polyynes: The particle in a box revisited.* Journal of Chemical Education, 2008. **85**(9): p. 1279-1281.10.1021/ed085p1279
18. Berjanskii, M.V. and D.S. Wishart, *Unraveling the meaning of chemical shifts in protein NMR.* Biochim Biophys Acta Proteins Proteom, 2017. **1865**(11 Pt B): p. 1564-1576.10.1016/j.bbapap.2017.07.005
19. Mielke, S.P. and V.V. Krishnan, *Characterization of protein secondary structure from NMR chemical shifts.* Prog Nucl Magn Reson Spectrosc, 2009. **54**(3-4): p. 141-165.10.1016/j.pnmrs.2008.06.002
20. Wishart, D.S., *Interpreting protein chemical shift data.* Prog Nucl Magn Reson Spectrosc, 2011. **58**(1-2): p. 62-87.10.1016/j.pnmrs.2010.07.004
21. Flewwelling, R.B. and W.G. Laidlaw, *Calculation of NMR shift using particle in a box wave functions: An undergraduate exercise.* Journal of Chemical Education, 1969. **46**(6): p. 355.10.1021/ed046p355
22. Weininger, D., *SMILES, a chemical language and information system. 1. Introduction to methodology and encoding rules.* Journal of chemical information and computer sciences, 1988. **28**(1): p. 31-36

23. Banfi, D. and L. Patiny, *www.nmrdb.org: Resurrecting and Processing NMR Spectra Online.* CHIMIA, 2008. **62**(4): p. 280.10.2533/chimia.2008.280
24. Topczewski, J.J., et al., *NMR Spectra through the Eyes of a Student: Eye Tracking Applied to NMR Items.* Journal of Chemical Education, 2017. **94**(1): p. 29-37.10.1021/acs.jchemed.6b00528
25. Connor, M.C., et al., *Developing Expertise in 1H NMR Spectral Interpretation.* The Journal of Organic Chemistry, 2021. **86**(2): p. 1385-1395.10.1021/acs.joc.0c01398
26. Connor, M.C., S.A. Finkenstaedt-Quinn, and G.V. Shultz, *Constraints on organic chemistry students' reasoning during IR and 1H NMR spectral interpretation.* Chemistry Education Research and Practice, 2019. **20**(3): p. 522-541.10.1039/C9RP00033J
27. Connor, M.C. and G.V. Shultz, *Teaching assistants' topic-specific pedagogical content knowledge in 1H NMR spectroscopy.* Chemistry Education Research and Practice, 2018. **19**(3): p. 653-669.10.1039/C7RP00204A
28. Kolonko, E.M. and K.J. Kolonko, *Introducing NMR Spectroscopy Using Guided Inquiry and Partial Structure Templating.* Journal of Chemical Education, 2019. **96**(5): p. 912-919.10.1021/acs.jchemed.8b00660
29. Balija, A.M., *1H NMR Spectroscopy Guided-Inquiry Activity Using the NMR Spectrometer: Incorporating Student-Generated Videos to Assess learning.* Journal of Chemical Education, 2020. **97**(5): p. 1387-1390.10.1021/acs.jchemed.9b00693
30. Wright, L. and M. Oliver-Hoyo, *Development and Evaluation of the H NMR MoleculAR Application.* Journal of Chemical Education, 2021. **98**(2): p. 478-488.10.1021/acs.jchemed.0c01068
31. Tan, M.J.H., et al., *Chapter 7 - Using an NMR software as an instructional tool in elucidating organic structures*, in *Technology-Enabled Blended Learning Experiences for Chemistry Education and Outreach*, F.M. Fung and C. Zimmermann, Editors. 2021, Elsevier. p. 107-114.978-0-12-822879-1
32. Socha, O., Z. Osifová, and M. Dračínský, *NMR-Challenge.com: An Interactive Website with Exercises in Solving Structures from NMR Spectra.* Journal of Chemical Education, 2023. **100**(2): p. 962-968.10.1021/acs.jchemed.2c01067
33. Jonas, E., S. Kuhn, and N. Schlörer, *Prediction of chemical shift in NMR: A review.* Magnetic Resonance in Chemistry, 2022. **60**(11): p. 1021-1031.https://doi.org/10.1002/mrc.5234