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Integrating Computation and Visualization to Enhance Learning IR Spectroscopy in the General Chemistry Laboratory: Computer-Assisted Learning of IR Spectroscopy

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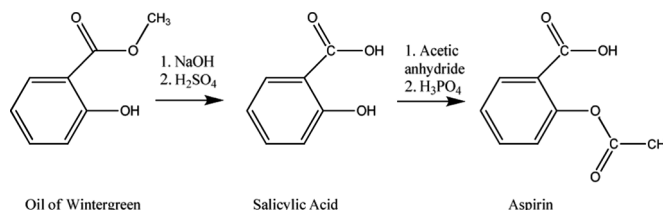
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ABSTRACT An exercise to compute and visualize the IR spectra of small organic molecules was incorporated into a general chemistry laboratory module on the synthesis of aspirin. The effectiveness of the computation–visualization component was measured by pre- and postquizzes, a survey, and correct interpretation of experimental IR spectra. The assessment results showed that the students’ conceptual understanding of IR spectroscopy was enhanced and that their ability to interpret IR spectra improved. Students learned the basics of the Scigress Explorer software package, gained invaluable introductory skills in molecular modeling and computational chemistry, and enjoyed the experience.

KEYWORDS aspirin, computation, general chemistry, hands-on learning, IR, molecular modeling, molecular properties, synthesis

INTRODUCTION

One of our students’ favorite laboratory exercises is the preparation of aspirin, a well-known pain-reliever, from oil of wintergreen, a naturally occurring substance,^[1] during the second semester of General Chemistry. The conversion involves a two-step sequential synthesis: oil of wintergreen (methyl-2-hydroxybenzoate) to salicylic acid (2-hydroxybenzoic acid) to aspirin (2-(acetyloxy)benzoic acid):



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In this 4-week laboratory module, students are also introduced to infrared (IR) spectroscopy to characterize the product aspirin and its precursors. These

compounds feature the hydroxyl (-OH) and carbonyl (C=O) functional groups that have characteristic IR absorptions around 3000 cm^{-1} and 1700 cm^{-1} , respectively. Since the absorption frequency is sensitive to the surrounding vibrations in the molecule, spectral differences are present among these compounds due to different types of -OH (phenol vs. carboxylic acid) and C=O (ester vs. carboxylic acid) functionalities. As a result, IR spectroscopy serves as a fingerprint for identifying these compounds.

Introducing IR spectroscopy in General Chemistry aids students in their 2nd-year chemistry courses.^[2,3] It also allows students in their early college years to gain experience with the modern tools chemists use to determine molecular structures. This is significant considering that more than 60% of these students usually do not take additional chemistry courses.^[2] In recent years, an increased number of general chemistry experiments exposing students to IR spectroscopy have been developed.^[1–9] However, our experience has been that establishing the correlation between the functional groups and their IR frequencies presents challenges to students, particularly when the topic is only taught in a single prelab lecture session. This is because the concept that atoms in molecules vibrate when exposed to infrared light is abstract and unobservable. Students therefore have difficulty in bridging the microscopic activities (molecular vibrations) to macroscopic behaviors (observed IR spectra). Desktop molecular modeling software such as Scigress Explorer 7.7 (Fujitsu, Bioscience, Beaverton, OR) may prove to be effective in teaching IR spectroscopy. Its split-screen feature allows students to visualize simultaneously the IR absorption frequencies and the associated vibrational modes of the functional groups. This interactive discovery-driven interface is believed to allow students to link between microscopic and macroscopic worlds, thus enhancing students' understanding of IR spectroscopy and aiding in their successful interpretation of IR spectra. Due to a wide accessibility of powerful computational tools, today's chemists increasingly rely on theory to guide their research efforts in molecular design and diagnostic applications.^[10–12] Exposing students to the use of modern computational software allows them to gain this powerful 21st-century skill.^[13,14]

In this project, we developed and integrated a Scigress Explorer activity in the aspirin laboratory module to introduce students to computational

chemistry with the goal of enhancing their learning of IR spectroscopy. At this point, students are familiar with the three-dimensional molecular structures (VSEPR theory) and orbital hybridization introduced in the first semester of the general chemistry sequence. A brief introduction to organic chemistry including common organic functional groups (alcohol, carbonyl, carboxyl, etc.) and the basics of IR spectroscopy is presented in a prelab lecture. The 4-week module includes the two-step synthesis of aspirin (weeks 1 and 2); the computation exercise (week 3); and acquisition of the IR spectra of the starting material, the intermediate product, and the final product (week 4). The goals of the module are three-fold: (a) introduce students to simple organic synthesis, (b) teach students how to acquire an IR spectrum of the starting material and products and use the results to confirm success of the synthesis, and (c) use Scigress Explorer to enhance the students' understanding of IR spectroscopy and their ability to make correct assignments to the spectrum.

MATERIALS AND METHODS

All the chemicals involved in the aspirin synthesis were used as received from Sigma–Aldrich (St. Louis, MO). IR spectra were recorded on polyethylene IR cards as neat liquid (oil of wintergreen) or thin solid films (salicylic acid and aspirin) formed by solvent evaporation. Salicylic acid and aspirin solutions were prepared by dissolving spatula-tip amounts of samples in 1 mL of ethyl acetate. To reduce costs, students prepared their own IR cards with cardboard and lightweight clear high-density polyethylene film from a grocery bag. IR spectra were collected by a Genesis II Fourier Transform Infrared Spectrometer (Mattson Instruments, Madison, WI). A total of 32 scans were used at a resolution of 4.0 cm^{-1} with a signal gain of 20. The spectrum was collected for each polyethylene substrate before the sample was scanned. Unless specified, the experimental IR spectra of the small model molecules were obtained from the built-in spectral library of the FTIR spectrophotometer, and the pertinent frequency values were provided to students.

Computational Methods

The Scigress Explorer 7.7 Software package provides nine quantum-mechanical methods for IR

spectra prediction. These include six Molecular Orbital Package (MO-G) and three Density Function Theory (DFT) methods. The DFT method is based entirely on mathematical approximations without the use of any experimental parameters. MO-G, on the other hand, is a semiempirical method that utilizes approximations from experimental data for setting initial parameter values. Different MO-G methods (e.g., AM1, PM3, PM5) vary by their model parameter set. Therefore the method best employed depends on the approximation or the parameter set that best models the specific molecular system of interest.

Several factors—such as the molecular characteristics under investigation, the accuracy desired, and the computation time (or cost)—need to be considered when selecting an appropriate or preferred computational method. In the aspirin lab, we are interested in predicting the vibrational frequencies due to the carbonyl and hydroxyl functional groups at around 1700 cm^{-1} and 3000 cm^{-1} . To compare methods for the purpose of designing the student exercise, we examined seven small molecules (ethanol, 1-propanol, 1-dodecanol, phenol, acetic acid, methyl acetate,^[15] and propyl acetate) along with oil of wintergreen, salicylic acid, and aspirin. (All the calculations were done on a Dell Latitude E6500, Intel® Core™2 Duo CPU P8400 @ 2.26 GHz, 791 MHz, 1.95 GB of RAM running Microsoft Windows XP Service Pack 3.) We found that MO-G PM5 gave good frequency predictions with errors under 10% for both functional groups. MO-G AM1 predicted the frequencies fairly well (10–20% error) for the –OH group, and MO-G PM3 predicted the frequencies fairly well (10–20% error) for the C=O group. MO-G PM3/CI gave frequency values similar to those of MO-G PM3 but took longer to compute. MO-G MNDOd predicted high values for both functionalities (by 20–35%). The DFT methods in general gave good predictions especially for C=O groups (2% error). However, they required a considerably longer computation time, particularly for large molecules with multiple configurations. For instance, using B88-LYP, the IR spectrum computation times for phenol, oil of wintergreen, and aspirin were 7 min, 35 min and 66 min, respectively. Among the three DFT methods, B88-LYP gave the best prediction. Within a given method, the calculation errors were systematic. This type of error is customarily corrected using scaling factors.^[14,16]

Scigress Explorer Student Exercise

Since computing the properties of small molecules takes significantly less time, chemists usually use small model molecules to help them select and calibrate the preferred method. They use the chosen and calibrated method to predict the properties of the compounds under investigation. The experimental results are then compared with the computed ones. The Scigress Explorer exercise, which can be completed in 1.5–2.5 hr, was designed to simulate how chemists use the computation software. There are three parts: identifying the preferred method, determining correction ratios, and computing the properties of aspirin and the precursor molecules.

Selecting the Preferred Computation Method

Acetic acid, a small molecule containing both carbonyl and hydroxyl functional groups, was used as the model molecule for selecting the preferred method. Using Scigress Explorer Workspace, students constructed the molecule, employed a MO-G method to compute the IR spectrum, and displayed both 3-D molecule and IR spectrum on the screen via the windows tile function. The interactive point-and-click interface allowed students to select an IR peak to visualize the associated vibration (see Fig. 1), effectively bridging the gap between the microscopic activities and the macroscopic properties. Students quickly figured out that the absorption occurring between 1700 and 2000 cm^{-1} corresponds to the C=O stretching mode and that those between 3000 and 4000 cm^{-1} correspond to the –OH stretch. The students also better grasped the criterion for absorption in the IR region, i.e., light is absorbed when the molecular vibration frequency matches that of the IR radiation.

Students then compared different methods—including MO-G AM1, MO-G PM3, MO-G PM5, and B88-LYP DFT—in terms of prediction accuracy and computation time. Typical results are shown in Table 1.

From this experience, students could see that calculations using MO-G methods were fast, taking about a fraction of a second for acetic acid. On the other hand, the DFT method took a much longer time (107.077 s) to complete even for this small

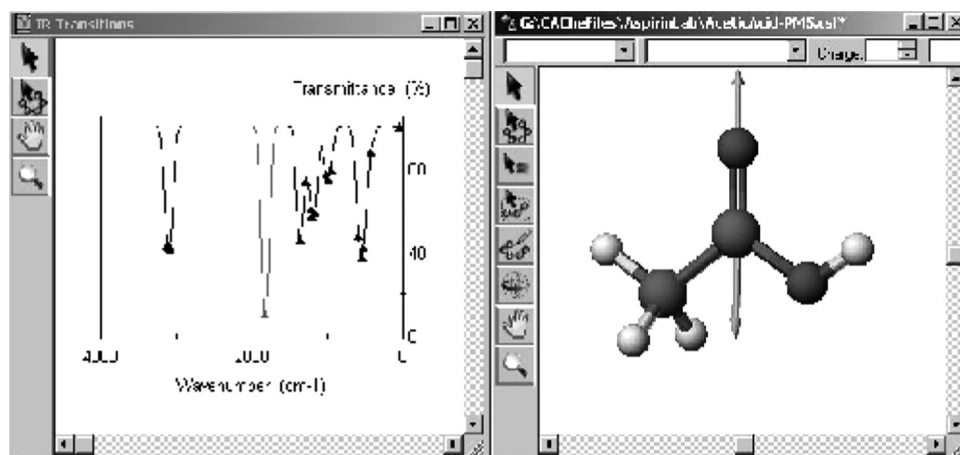


FIGURE 1 The 3-D structure (right) and the predicted IR spectrum (left) of acetic acid. The highlighted IR peak around 3400 cm^{-1} corresponds to the indicated vibration of the OH group.

molecule. Based on the lab reports, all students selected MO-G PM5 as their preferred method.

Determining the Correction Ratios

One approach to compensating for method-related systematic errors is to use different scaling factors for different vibrational modes (e.g., the C=O stretch of the carbonyl functional group).^[16] This technique requires the analysis of a set of molecules having similar vibrational modes. To simulate and simplify this approach and to develop an awareness of the effect of neighboring atoms within the molecule, students predicted the vibrational frequencies associated with carbonyl and hydroxyl groups in two additional model molecules, methyl acetate and ethanol, respectively, using MO-G PM5. The results (Table 2) showed that the frequency for the carboxylic carbonyl group (1827 cm^{-1}) was lower than that for the esteric carbonyl group (1829 cm^{-1}), and the frequency for the carboxylic hydroxyl group (3090 cm^{-1}) was lower than that for the aliphatic/phenolic hydroxyl group (3150 cm^{-1}), consistent with experiment. Using these results, students determined the value of a correction ratio, defined

as the ratio of the experimental frequency to the calculated frequency, for each vibrational mode. The correction ratio, ranging from 0.940 to 1.059 in this study, was used to approximate the scaling factor and calibrate the frequency calculation.

Predicting the IR Spectra of the Aspirin and Its Precursors

In the last part of the exercise, students built 3-D structures of oil of wintergreen, salicylic acid, and aspirin and computed the IR spectrum of each molecule using the MO-G PM5. The direct visualization and the user friendly peak-to-vibration links allowed students to see how vibrational energies of functional groups differ due to different nearby atoms in the molecules. For instance, for aspirin, there were two C=O peaks at around $1700\text{--}2000\text{ cm}^{-1}$: one at a slightly higher frequency due to the esteric C=O vibration and the other at a slightly lower frequency due to the carboxylic C=O vibration (see Table 3). To better match the experimental frequencies, students multiplied the predicted frequencies by the corresponding correction ratios.

TABLE 1 Comparison of Experimental and Calculated IR Frequencies for Acetic Acid Using Various Methods

Acetic acid	Exptl., cm^{-1}	MO-G AM1		MO-G PM3		MO-G PM5		B88-LYP DFT	
		cm^{-1}	Error	cm^{-1}	Error	cm^{-1}	Error	cm^{-1}	Error
C=O	1717	2088	22%	1981	15%	1827	6%	1747	2%
OH	3056	3431	12%	3853	26%	3090	1%	3540	16%
Cmpt. Time, s		0.172		0.235		0.187		107.077	

Cmpt. = computing; Exptl. = experimental IR frequency.

TABLE 2 Experimental and Calculated Vibrational Frequencies of Carbonyl and Hydroxyl Functional Groups Using MO-G PM5

Variable	Acetic acid (carboxylic)			Ethanol* (aliphatic/phenolic)			Methyl acetate (esteric)		
	Exptl, cm ⁻¹	Calcd, cm ⁻¹	Ratio	Exptl, cm ⁻¹	Calcd, cm ⁻¹	Ratio	Exptl, cm ⁻¹	Calcd, cm ⁻¹	Ratio
C=O	1717	1827	0.940	–	–	–	1748	1829	0.956
OH	3056	3090	0.989	3342	3156	1.059	–	–	–

Exptl. = experimental IR frequency; Calcd = calculated IR frequency.

*The correction ratios for the hydroxyl groups in ethanol and phenol are 1.059 and 1.071, respectively. To simplify the student lab procedure, the correction ratio for the aliphatic hydroxyl group is used to approximate that for phenolic hydroxyl group.

Obtaining the Experimental IR Spectra

In the first two lab periods of the module, students prepared salicylic acid and converted it to aspirin. In the 4th week, they recorded the experimental IR spectra of each including the starting material of oil of wintergreen. Led by the computational results obtained in the 3rd week, students looked for the characteristic C=O and –OH absorptions in the experimental IR spectra and decided whether each synthetic step was successful (see Table 3). The error calculation showed that the predicted values (after correction) and the experimental values agreed well, with errors ranging from 1.0% to 3.8%. The average errors were 2% for both vibrational modes.

Learning Assessment Outcome

Although IR spectroscopy and organic functional groups may go well with the unit on bonding and molecular geometry in the general chemistry curriculum, they are often not integrated in the lecture portion of the course due to time constraints. As a result, students had little background in either area before the aspirin lab. Their learning gain in IR spectroscopy as a result of this lab was evaluated by

pre- and postquizzes, a student survey, and the correct interpretation of experimental IR spectra. The same quiz was administered three different times, but is identified as prequiz, postquiz-1 and postquiz-2 based on when it was administered. Quiz questions in mixed formats of a multiple choice, true/false, and fill-in-the-blank forms were designed and implemented. The assessed areas included the information that IR spectra reveal, the criteria for IR absorption, the characteristic vibrational frequencies of C=O and OH functional groups, the effect of environment (vibrations of neighboring atoms in the molecule) on frequency, and the students' ability to interpret their experimental spectra. Two classes, referred to as Class A (18 students) and Class B (10 students), participated in the learning-assessment process. The prequiz was administered to students in both classes at the very beginning of the lab period in the 3rd week. The laboratory instructor then presented a 20–30 min lecture on the basics of IR spectroscopy and organic functional groups relevant to the experiment. Following the prelab lecture, the same quiz (referred to as "postquiz-1") was administered only to the students in Class B to assess learning gained from the prelab instruction. Students in both Class A and Class B then

TABLE 3 Experimental and Calculated IR Absorptions Using MO-G PM5 for the Listed Molecules

Variable	Oil of wintergreen		Salicylic acid			Aspirin		
	Esteric C=O	Phenolic OH	Carboxylic C=O	Phenolic OH	Carboxylic OH	Esteric C=O	Carboxylic C=O	Carboxylic OH
Cmpt. Time, s	1.469		1.016			2.125		
Calcd., cm ⁻¹	1825	3109	1824	3107	3091	1846	1819	3088
Corr. Ratio	0.956	1.059	0.940	1.059	0.989	0.956	0.940	0.989
Corrd., cm ⁻¹	1745	3292	1715	3290	3057	1765	1710	3054
Exptl., cm ⁻¹	1681	3188	1669	3238	3017	1754	1693	2971
Error	3.8%	3.3%	2.8%	1.6%	1.3%	1.6%	1.0%	2.8%

Cmpt. = computing; Calcd. = calculated IR frequency; Corr. = correction; Corrd. = corrected IR frequency; Exptl. = experimental IR frequency.

participated in the 1.5–2.5-hr Scigress Explorer exercise. After the students completed the Scigress exercise, the same quiz (referred to as “postquiz-2”) was administered to both classes to measure the net learning gain in IR spectroscopy resulting from both the prelab lecture and the computational exercise.

Figure 2 shows the assessment results. A gain or g-factor, defined by Equation 1, was used to measure students’ learning gain:

$$\text{Gain(g - factor)} = \frac{\text{Postquizscore} - \text{Prequizscore}}{\text{Maximumpossiblescore} - \text{Prequizscore}} \quad (1)$$

The maximum possible score for this quiz was 7. After completing both the prelab lecture and the computation exercise, the average quiz score increased from 2.4 ± 1.0 to 4.6 ± 1.7 for Class A and from 2.5 ± 1.1 to 5.5 ± 1.2 for Class B, corresponding

to net learning gain values of 0.48 and 0.68, respectively. Note that for these classes, the score distributions for the same types of score sets (prequiz or postquiz-2) were similar in shape and had the same mode (2 for the prequiz score sets and 5 for the postquiz-2 score sets), suggesting similar learning outcomes from both classes. The results from Class B showed that the prelab lecture on the basics of IR spectroscopy contributed significantly to students’ learning (with a g-factor of 0.45) and that the Scigress Explorer exercise effectively enhanced this learning (g-factor increased from 0.45 to 0.68). For comparison, note that for courses taught by a traditional didactic lecture, the overall gain in conceptual understanding is g-factor = 0.25, while more interactive courses (those engaging students in heads-on and often hands-on activities that yield immediate feedback) have gain values ranging from 0.36 to 0.68.^[17] So the g-factors we obtained were comparable to learning gains in interactive courses. Although only a small data sample was used, these results indicate that our approach of utilizing prelab lecture combined with computation and visualization successfully increases student learning in IR spectroscopy.

In an attempt to investigate the role of computation and visualization in contributing to student learning in IR spectroscopy, we examined the student answers on the quiz from Class B question by question (Fig. 3). The results from the prequiz and postquiz-1 show that the students’ conceptual understanding—especially in the areas of what

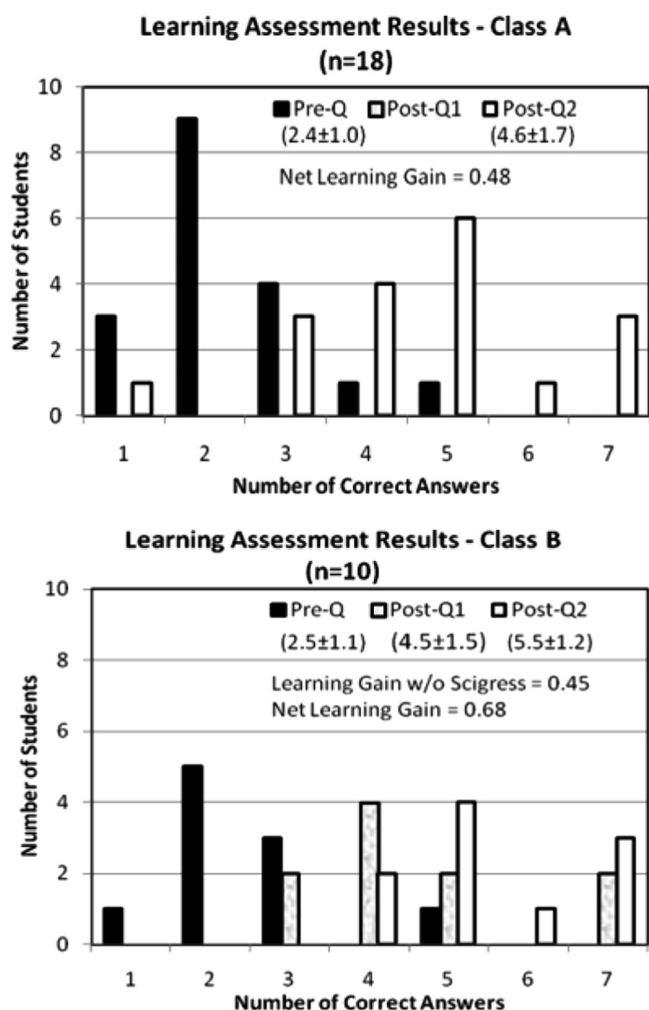


FIGURE 2 The learning assessment results.

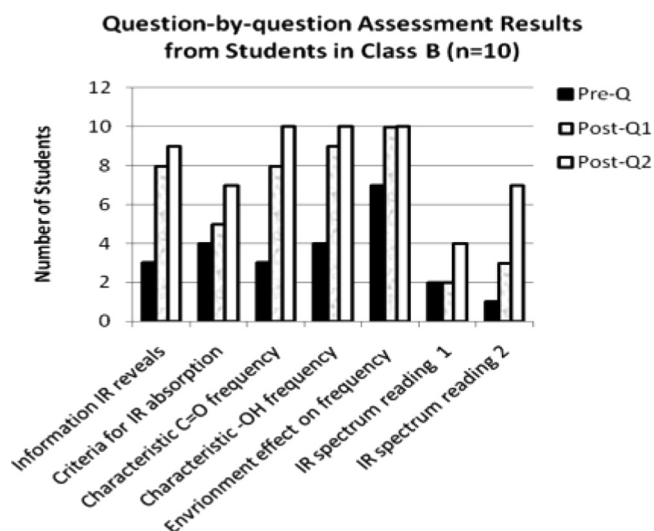


FIGURE 3 Question-by-question assessment results from students in Class B.

information IR spectroscopy offers and the characteristic frequency ranges of carbonyl and hydroxyl vibrational modes—was greatly increased as a result of the prelab lecture. Only very slight improvement was shown for questions relating to interpreting IR spectra. A comparison of the results for postquiz-1 and postquiz-2 shows that the computation and visualization exercise further improved students' understanding in all areas. Most significantly we had evidence showing that the Scigress Explorer exercise was especially effective in improving students' ability to apply the new skills to interpreting IR spectra, as reflected by a significant improvement on the quiz questions related to reading the IR spectrum. This improvement was also reflected in the lab reports where students draw the chemical structure of each of the three molecules (oil of wintergreen, salicylic acid, and aspirin) on the corresponding IR spectrum. To demonstrate that they isolated the correct product, students draw arrows matching the hydroxyl and carbonyl functional groups in each structure to the characteristic vibrational frequencies. In the past, without the Scigress Explorer component, at most 10% of the students gave *perfect* identification of and assignment to the distinctive peaks in all three IR spectra. With the Scigress Explorer component, for a survey group of 25 students, this number increased to 48%.

The students' response to survey questions revealed that students were positive about this learning experience and our approach. They enjoyed using the modern computational chemistry software for IR spectrum prediction and agreed that the computational exercise enhanced their understanding of IR spectroscopy. In a current survey of 24 students, more than 67% indicated that the computational exercise helped them see how chemists actually use the software for the purpose of predicting properties or directing their research. Two of the student comments reveal that our goals were met:

This experience helped me see how the atoms are bonded, how absorption occurs when the vibrational energy (of bonded atoms) matches that of IR radiation, and how this absorption shows in the IR spectrum.

What I learned from this lab is that if there are no peaks in a range, then the chemical groups associated with the peaks are not in the compound. You can use this to check your product in an experiment and see if you got what you

intended to get. The lab helped me better understand the experimental results and the purpose of IR spectroscopy.

CONCLUSION

We developed a Scigress Explorer exercise on IR spectroscopy and integrated it into a popular General Chemistry lab. Enhanced student learning in IR spectroscopy was measured by pre- and post-quizzes, a student survey, and correct interpretation of experimental IR spectra. The results of the assessment suggest that the prelab lecture effectively contributed to students' conceptual understanding of IR spectroscopy and that the interactive point-and-click computation–visualization activity furthered this learning. The greatest advantage of utilizing the computation–visualization exercise may lie in its effectiveness in improving students' ability to apply their conceptual learning of molecular vibrations and IR absorptions to the interpretation of IR spectra, as demonstrated by a clear improvement on the related quiz questions and the IR assignments of the experimental spectra. The Scigress Explorer package (or similar software) is therefore a powerful teaching tool that enhances students' ability to utilize IR spectroscopy and interpret the spectral results, thus uncovering the molecular structural information. The students' responses to survey questions also showed that they enjoyed the computational component and found it effective for helping them to see how chemists utilize the computer technology to aid or guide their work. Although these results were based on a small data sample, they show that incorporating a computation and visualization component in the aspirin lab enhanced student learning of IR spectroscopy. Moreover, the experience allowed students to learn the basic features and tools of modern chemistry software and to gain valuable skills in molecular modeling and computational chemistry in their early undergraduate curriculum.

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