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# Encouraging Student Engagement by Using a POGIL Framework for a Gas-Phase IR Physical Chemistry Laboratory Experiment

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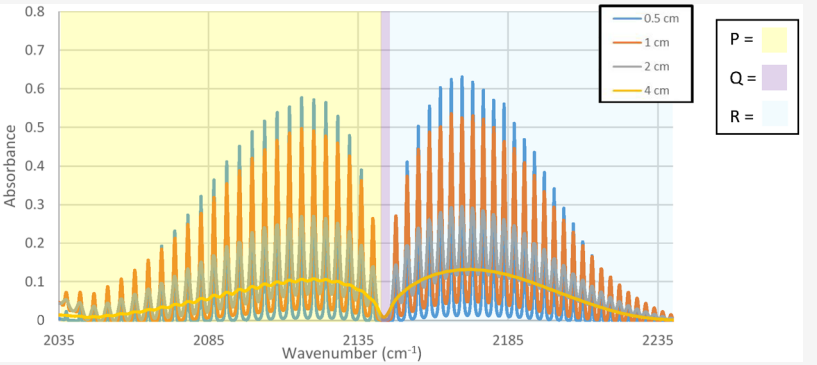


**ABSTRACT:** A version of the classic rotationally resolved infrared (IR) spectrum of a diatomic molecule experiment has been developed using the POGIL framework to more fully engage students in the collection, modeling, analysis, and interpretation of the data. An analysis of the experimental protocol reveals that the POGIL approach actively engages students in scientific practices. The student learning objectives for this laboratory experiment are to (1) develop an energy level diagram and relate that diagram to rotational−vibrational spectra; (2) identify, describe, and interpret the molecular constants that can be extracted from gas-phase IR spectra; (3) discover the impact of spectral resolution on precision of molecular constants derived from the spectral data; and (4) use data to evaluate and refine quantum mechanical models. The learning cycles, analysis of student engagement with scientific practices, and reflections from instructors are described.

**KEYWORDS:** *Upper-Division Undergraduate, Laboratory Instruction, Physical Chemistry, Inquiry-Based/Discovery Learning, IR Spectroscopy*



## INTRODUCTION

Students in a typical physical chemistry curriculum are introduced to models of molecular motion including the harmonic oscillator and rigid rotator models. Corrections to these models, such as the anharmonic oscillator and centrifugal distortion, are often also discussed as a way to refine the models and more accurately represent molecular motion. These models are then often used to interpret experimental data acquired in the laboratory to extract molecular parameters. A classic example of this pedagogy is the vibrational−rotational spectra of HCl and DCl.[1,2] In fact, the HCl/DCl experiment has been so foundational to physical chemistry curricula that it has been presented in this *Journal* many times. The first example of a rotationally resolved HCl infrared (IR) spectrum in this *Journal* along with a discussion of the theory was from Stafford et al. in 1963.[3] Since that time, papers have been published about different aspects of the HCl/DCl experiment including the following: increasing the resolution of the spectrum,[4] using computer programs or spreadsheets to analyze the data,[5−10] simulating the spectra,[11] modeling potential curves,[12,13] and connecting it with statistical mechanics.[14,15] The HCl/DCl IR experiment is so prevalent that there are many journal articles devoted to describing safe and efficient techniques to generate HCl and DCl gas in the physical chemistry laboratory.[16−24]

Of course, HCl and DCl are not the only small molecules that have been studied using IR spectroscopy in the physical chemistry laboratory. Other diatomic molecules commonly used are carbon monoxide,[12,25−27] nitric oxide,[12,27] and the hydroxyl radical (this one reported, interestingly, as an infrared emission spectrum).[28] Moving beyond diatomic molecules increases the complexity of the molecular models a bit. Nevertheless, there are reports of introducing physical chemistry students to the analysis of IR spectra of many small molecules including $CO_2$,[29] $N_2O$,[30] $NH_3$,[31] HCN/

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Table 1. Predictions, Experimental Data, and Analysis for Each Data-Think Cycle in the Main Section

| | Data-Think Cycle 1 | Data-Think Cycle 2 | Data-Think Cycle 3 |
|---|---|---|---|
| Prediction(s) | Features of an absorbance spectrum, in the range 1000−5000 $cm^{-1}$, of a diatomic gas molecule | How changing the resolution will impact the spectrum | How refinements to the model will impact a residual plot; how spectral resolution will impact the uncertainties in extracted molecular parameters |
| Experimental data collected | Gas-phase IR spectrum of a diatomic molecule at a resolution just high enough to reveal individual P- and R-branch peaks | Gas-phase IR spectrum of a diatomic molecule at a variety of resolutions, with each group responsible for collecting data at a particular resolution | Multiple linear regression of the experimental data using the refined model, with each group responsible for carrying this out on their data obtained at a particular resolution |
| Data analysis | Creation of a model energy level diagram, with labeled transitions and a corresponding spectrum | Development of several mathematical models in order to fit the data, culminating in a residual plot and a critique of the model | Determination of multiple molecular parameters, including uncertainties, with a discussion of meaning and the impact of resolution on the value and uncertainties; comparison of residual plot to predictions |

DCN,[32] $CH_3I$,[33] benzene,[34] and a collection of spherical tops.[35]

The typical physical chemistry gas-phase IR spectroscopy experiment proceeds in the following general sequential steps. First, the theory is presented to the students as an introduction to the experiment. This typically involves a presentation of the harmonic oscillator and rigid rotator models and corrections to those models to account for anharmonicity, centrifugal distortion, and vibration−rotation interactions. Sometimes the theory presented to the students goes a bit further and explains isotope effects, connection to statistical mechanics, or other specialized topics depending on the system being investigated. The introductory material also typically contains an energy level diagram and a model spectrum labeling different branches and specific transitions in each branch. Second, the students are asked to follow certain procedures to acquire quality spectra. Finally, the students are instructed to manipulate their spectral data in light of the introductory material to extract molecular parameters. This step usually involves the introduction of a spreadsheet or computer program.

While this approach allows students to experimentally determine accurate and precise molecular constants, it is a somewhat passive and rote approach. There have recently been efforts to make the chemistry laboratory a more active learning environment for students.[36] One such effort is the Process Oriented Guided Inquiry Learning—Physical Chemistry Laboratory (POGIL-PCL) group[37] where experiments are being developed and modified to make them more inquiry-based.[38] It was through this group that the authors of this paper initiated an effort to convert the standard gas-phase IR spectroscopy experiment into the POGIL-PCL format. The experiment described below is a result of several iterations of rewriting and trial testing the experiment with physical chemistry instructors and with students. In this format, students are guided to develop the appropriate equations and models themselves. For example, they develop the harmonic oscillator−rigid rotator mathematical model and then use it to develop an energy level diagram. They then use that diagram to make a prediction of what the spectrum will look like.

We believe that the experiment described below is unique and will benefit students and instructors alike. We were able to find one other paper reporting an inquiry-based version of the HCl/DCl spectrum experiment.[39] That paper describes how the experiment can be run as a "mini-project" where students are given a one-page summary of the task to perform. While that approach is admirable, it may not be accessible to many physical chemistry instructors. Our approach is to provide the students guided questions to lead them to the proper models. Students are given the ability to choose certain experimental parameters (i.e., resolution). Instructors have latitude with how the experiment is implemented because it is somewhat modular. There is a main section where the fundamental models are developed. Then, there are four optional sections covering isotope abundance (for HCl), isotope effects (for HCl/DCl), overtones, and connections to statistical mechanics. Instructors can pick and choose which optional sections they would like to use.

Converting laboratory experiments into the inquiry style has the added benefit of quite naturally incorporating more scientific practices. The National Research Council outlines eight scientific practices in their framework for K−12 science education.[40] We believe that student engagement in these practices should be a major emphasis of physical chemistry laboratory experiences. Inspired by the work of Towns et al.,[41] we used the rubrics from Cooper's group[42] to evaluate how often our experiment explicitly prompts students to engage in scientific practices. Those results are shown below after a description of the experiment. Finally, we present faculty reflections about their experiences with the experiment.

## DESCRIPTION OF THE EXPERIMENT

The traditional rovibrational gas-phase IR experiment, as shown in *Experiments in Physical Chemistry*, for example,[1] provides students with a direct application of the rotational and vibrational theory covered in a quantum mechanics course, allowing students to extract molecular parameters, such as bond length and vibrational frequency, from the spectra. However, the fitting process can be quite tedious, and students do not often reflect upon the meaning of the terms in the equations used to extract the molecular parameters. Thus, we were motivated to adopt a POGIL approach to the experiment,[38] with the goal of directly involving students in the construction of the modeling and analysis.

In the POGIL-PCL rovibrational gas-phase IR experiment, students think critically about the collection and analysis of the spectra, developing an energy diagram and refining the equations used to model the spectrum. They also consider the impact of spectral resolution on the precision of experimentally determined molecular constants. The experiment can be used with a small molecule of the instructor's choice (suitable to rovibrational IR spectroscopy, of course), such as HCl, CO, or $CO_2$, and it can be completed in two 3 h lab periods, or it can be used in a lecture-based class as a dry activity.

In the POGIL-PCL experimental approach, students work through several "data-think cycles".[38] Each data-think cycle begins with students answering pre-experiment questions by recalling prior knowledge, gathering information, and making predictions. Students then carry out an experimental protocol


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Table 2. Summary of the Number of Times Particular Scientific Practices (SPs) Are Prompted within the Experiment

| Asking Questions (SP1) | Developing and Using Models (SP2) | Planning Investigations (SP3) | Analyzing and Interpreting Data (SP4) | Using Mathematics and Computational Thinking (SP5) | Constructing Explanations and Engaging in Argument from Evidence (SP6 and 7) | Evaluating Information (SP8) |
|---|---|---|---|---|---|---|
| | | | | Main Experiment | | |
| 0 | 8 | 0 | 6 | 9 | 6 | 0 |
| | | | | Optional Extensions | | |
| 0 | 3 | 0 | 5 | 3 | 5 | 0 |

to collect data, followed by a series of guided questions to ensure that students think carefully about the data as they perform analyses. The experiment ends with postexperiment questions in which students are asked to apply the concepts learned.

The POGIL-PCL rovibrational gas-phase IR experiment has three data-think cycles in the main portion of the experiment Table 1. In the first data-think cycle, students predict the appearance of an absorbance spectrum, in the range of 1000−5000 $cm^{-1}$, of a diatomic gas molecule. Students then experimentally collect this spectrum at a resolution just high enough to reveal individual P- and R-branch peaks. By using that data, along with a rovibrational energy expression, students create a model energy level diagram, with labeled transitions and a corresponding spectrum.

In the second data-think cycle, students predict how changing the resolution will impact the spectrum, and then they collect experimental data for a variety of resolutions, with each group responsible for collecting data at a particular resolution. The students work through and develop several mathematical models in order to fit their data, culminating in a residual plot and a critique of the model.

In the third and final data-think cycle, students consider refinements to the model and predict how they will impact a residual plot, in addition to making a prediction about the impact of spectral resolution on the uncertainties in the extracted molecular parameters. Each group of students carries out a multiple linear regression of their experimental data using the refined model and determines the values of multiple molecular parameters, including uncertainties. The process of fitting the experimental data to the model is facilitated by an Excel template or Jupyter notebook provided to the students. Instructors have the option of customizing the template, depending on their goals and the time allotted. For example, the template can tabulate fitted molecular parameters and carry out propagation of error calculations, or these parts can be removed so that students get practice in these areas. Alternatively, other programs (i.e., IgorPro, Origin, Mathematica, etc.) could be used to carry out the fitting procedures based on the instructor's goals and familiarity with those programs. The class discusses the meaning of the molecular parameters obtained, the impact of resolution on the values and uncertainties, and how well a residual plot compares to their predictions. In the postexperiment questions, students further explain their understanding of the parameters and apply their knowledge to make predictions for another molecule and other, related experiments.

In addition, the experiment offers four optional follow-up exercises, of which an instructor could use none, any, or all. These additional sections cover the following: (1) Students consider the effect of isotope abundance of chlorine on the spectrum of HCl, with regard to frequency and intensity of peaks. (2) Students consider the effect of deliberate isotopic substitution with deuterium in HCl and calculate isotope effects. (3) Students work with data for overtone transitions of either HCl or CO to determine $\tilde{\nu}$ and $\tilde{\nu}\tilde{x}$. (4) Students carry out calculations based on statistical mechanics, modeling relative populations to compare to spectral intensities.

## EMPHASIS ON SCIENTIFIC PRACTICES

Because the POGIL approach taken in this experiment tasks students with thinking critically about data modeling and analysis, students have the opportunity to engage in many of the eight scientific practices (SPs) that have been identified by the National Research Council (NRC) in their three-dimensional framework for K−12 science education: (SP1) asking questions, (SP2) developing and using models, (SP3) planning and carrying out investigations, (SP4) analyzing and interpreting data, (SP5) using mathematics and computational thinking, (SP6) constructing explanations, (SP7) engaging in argument from evidence, and (SP8) obtaining, evaluating, and communicating information.[40]

Cooper et al. created a protocol to evaluate college science assessments to determine if the assessment measured learning in the context of the three-dimensional framework of the NRC.[42] In higher education, the Three-Dimensional Learning Assessment Protocol (3D-LAP) has been used to evaluate and design written assessments, such as ACS exam questions[43] and physics assessment tasks,[44] and examine lab activities for evidence of SPs.[41,45−50] In particular, the 3D-LAP has been used to highlight the strong presence of SPs in lab approaches designed to engage students, such as argument-driven inquiry (ADI),[49] project-based laboratories,[47] science writing heuristic (SWH),[48] and course-based undergraduate research experiences (CUREs).[50]

Rodriguez and Towns used the 3D-LAP to revise a set of pre- and postlab questions to promote students' engagement in critical thinking by including SPs, because the original set of traditional prelab and postlab questions showed very little evidence of SPs.[41] Indeed, in a comparison between two different general chemistry lab curricula, one traditional and one project-based, the project-based curriculum was found to emphasize SPs, while the traditional curriculum utilized SPs minimally.[46] It should be noted that simply looking up information or carrying out a calculation (tasks often found in traditional experiments) is not sufficient to qualify as engaging in an SP; an interpretation and/or connection to scientific concepts must also be made.

The results of applying the protocol[42] to the POGIL-PCL gas-phase IR experiment are shown in Table 2. For this process, the authors first coded the questions independently using the 3D-LAP and then came to a consensus on the coding. Some series of related questions were grouped together, and some questions/question series were assigned to multiple SPs. Examples of experiment questions that address particular SPs are shown in Table 3. It was found that, because


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Table 3. Examples of Questions That Address Particular SPs

| | Example Experimental Prompts | Scientific Practices |
|---|---|---|
| 21a. | In Model 1, does the J represent the rotational quantum number of the lower state or upper state of the transition? Explain your reasoning. | SP2 – Developing and using models<br>SP5 – Using mathematics and computational thinking |
| b. | Show mathematically how Equation 1 is used to develop Model 1. | |
| c. | Use sentences and diagrams to describe how Model 1 and Equation 1 relate to your energy diagram. | |
| d. | Derive an expression analogous to Model 1 for the R branch transitions where $\Delta v = +1$ and $\Delta J = +1$. Call this Model 2. | |
| 24. | Fit your data to Model 3 to determine $\tilde{\nu}$ and $\tilde{B}$. Record your results with appropriate uncertainties in your lab book. Also add your results for $\tilde{\nu}$ and $\tilde{B}$ to a combined class spreadsheet. | SP4 – Analyzing and interpreting data<br>SP5 – Using mathematics and computational thinking |
| 25. | Create a residual plot for your data. It is ideal to have residuals which are normally distributed. They should look random with no obvious trends. | |
| a. | Are your residuals normally distributed? | |
| b. | What does this suggest about Model 3 with respect to your data? | |
| 26. | What are the limitations of Model 3? | |
| 27. | What assumptions have been made in Model 3? | |
| 40. | Create a residual plot based on the fit of your data with Model 4. How does this residual plot compare to the plot in question 23? Which model appears to do a better job fitting the data? | SP2 – Developing and using models<br>SP4 – Analyzing and interpreting data<br>SP5 – Using mathematics and computational thinking |
| 44. | A ro-vibrational spectrum for $I_2$ does not exist. Explain why and propose an explanation for how we have standard values for all the parameters $\tilde{\nu}, \tilde{B}, \tilde{D}$ and $\tilde{\alpha}$ found in Model 4 for this molecule. | SP6&7 – Constructing explanations and engaging in argument from evidence |

the model used in this experiment is mathematical in nature, several questions/question series satisfied both SP2 and SP5. Throughout the experiment, SP2, SP4, SP5, SP6, and SP7 were used, with students having the opportunity to work through each SP several times. Although we did find some evidence for elements of SPs 1, 3, and 8, we applied the rubric rigorously and concluded that all of the criteria were not fully met for these SPs.

This analysis of SPs is not to suggest that students do not or cannot engage in SPs in the more traditional versions of this experiment. Many of the references provided in the Introduction section of this paper include suggestions for engaging students. The extent to which students engage in SPs will likely vary greatly on the basis of instructor facilitation. The unique approach of our experimental protocol is that the SPs are quite naturally built in. Using this version of the gas-phase IR experiment, instructors can be assured that students will be engaging in SPs.

## INSTRUCTOR FEEDBACK AND REFLECTIONS

Feedback from others who have used the experiment suggests that this version of the experiment more fully engages students in the collection, modeling, analysis, and interpretation of rovibrational spectra, compared to the more traditional approach to this classic physical chemistry experiment. Students are typically surprised at the large number of rotational peaks, as they are used to interpreting IR spectra with only a single peak per vibration. Another exciting aspect of the experiment is that students can gain an appreciation and understanding of how resolution impacts what we visually observe and can extract from a spectrum. The Excel template for fitting IR spectra seems to help students proceed through the data analysis without getting overwhelmed or bogged down, allowing them to focus on modeling and interpretation. In our experience, this has led to a more enjoyable laboratory experience for both the students and the instructors.

## ASSOCIATED CONTENT

### Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.2c00314.

Student handbook (PDF, DOCX)

Complete table showing the SPs identified in each question/question-series and the instructor handbook (PDF, DOCX)



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Excel template with sample data (XLSX)
Jupyter notebook template (ZIP)

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### Notes

The authors declare no competing financial interest.

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