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Technology Report

FTIR-SIS: A Fourier Transform Infrared Scientific Instrument Simulator

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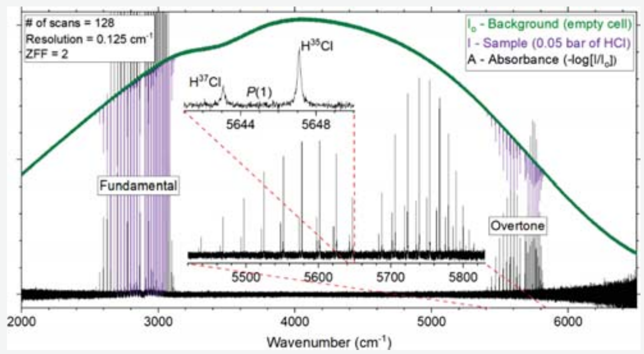
ABSTRACT: We developed a gas-phase Fourier Transform InfraRed Scientific Instrument Simulator (FTIR-SIS, https://ftir.rastonlab.org/) in response to the unavailability of one during the COVID-19 pandemic lockdown of 2020. It features an interactive interface that encourages students to explore different components of a typical FTIR, and it allows them to set up and collect realistic synthetic spectra for a wide variety of atmospherically relevant molecules (CO, HCl, O_3, HCN, etc.). This is facilitated by utilizing the HITRAN (HIgh-resolution TRANsmission molecular absorption) database and a radiative solver (RADIS, RADIative Solver for infrared spectra of molecules). Students from around the world will be able to access this SIS on any device (laptop, smartphone, etc.) and perform simulated gas-phase FTIR experiments that mimic real ones.



KEYWORDS: *Audience, Upper-Division Undergraduate, Domain, Physical Chemistry, Laboratory Instruction, Pedagogy, Computer-Based Learning, Internet, Web-Based Learning, Topic, Instrumental Methods, IR Spectroscopy, Quantum Chemistry*

■ INTRODUCTION

Upper division lab-based courses in chemistry (physical, analytical, materials, etc.) often rely heavily on the usage of instrumentation. It is no surprise then that student learning has in general suffered in these types of courses when instruction has been conducted remotely. This was abruptly realized by many (including one of the authors; P.L.R.) when switching to online learning during the COVID-19 pandemic lockdown of 2020. Providing students with data to analyze in Physical Chemistry (P-Chem) II Lab was far from ideal (P-Chem II covers quantum chemistry at James Madison University), not only because an important learning outcome was to become proficient with instrument operation but also because buy-in was impaired when students did not collect their own data. In response to this, we are developing a variety of modern scientific instrument simulators (SISs) that span many of the core spectrometers which are available in most chemistry departments. Besides their anticipated educational value during lockdown periods, we hope they will be useful to departments that might not have access to various spectrometers and also as demonstration tools (since they will show the inner workings of the instrumentation). In this report, we provide a brief overview of the first of these SISs that we have developed, i.e., a gas-phase Fourier Transform InfraRed Scientific Instrument Simulator (FTIR-SIS).

The incorporation of interactive software in chemistry education dates back to programs that were developed for the PLATO (Programmed Logic for Automatic Teaching Operations) computer-based educational system, which was initiated in 1960.[1,2] Most of these programs were developed to engage students enrolled in both general and organic chemistry[3,4] and were accessed via terminals that communicated with the mainframe. Shortly following the advent of the microprocessor and widespread incorporation of them in microcomputers (i.e., personal computers), a number of SISs were developed, including NMR,[5−7] IR,[8−10] UV−Vis,[11,12] X-ray fluorescence,[13] ESR,[14] and HPLC simulators,[15] some of which have a command line interface, while others have a visual interface that was designed to resemble that of the real instrument. Changes in computer technology over the years have necessitated the continued development of interactive software for the teaching of chemistry,[16] and accordingly, a number of SISs with more modern visual interfaces have since been developed for HPLC,[17,18] NMR spectroscopy,[19,20] Raman spectroscopy,[21] fluorescence spectroscopy,[22] UV−Vis spectroscopy,[23] and FTIR spectroscopy.[24]

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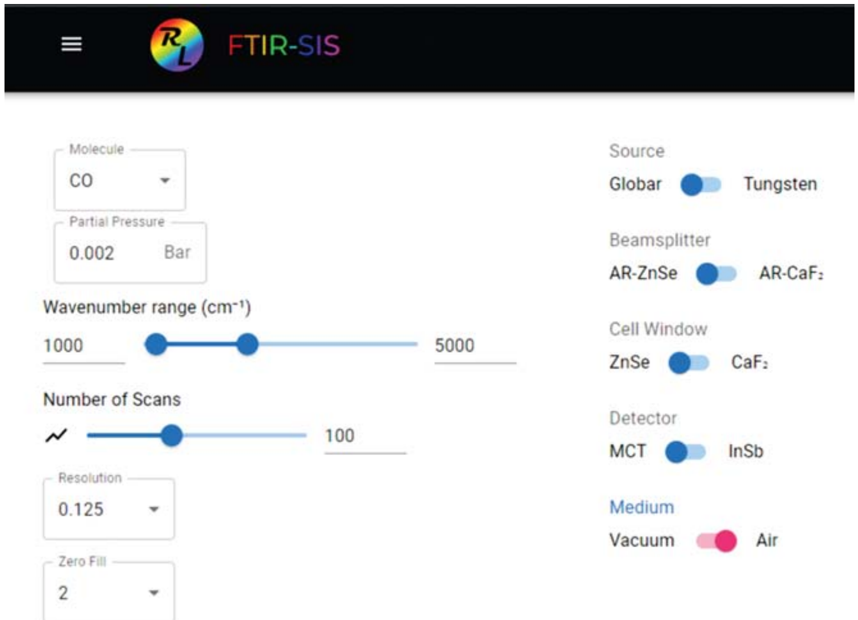

Figure 1. "Experimental Setup" window. The selected parameters are those suggested in the tutorial. The design of this window is inspired by the RADIS app (https://www.radis.app/), which is capable of generating clean (idealized) synthetic infrared spectra. This figure has been reproduced with permission from https://ftir.rastonlab.org/.

An article describing the previously developed FTIR-SIS (referred to as a virtual FTIR spectrometer) was published in 2005, where it was mentioned that spectra were utilized from a variety of sources (e.g., the National Institute of Standards and Technology (NIST) Web site) in order to simulate the spectra of a wide variety of molecules (using the Java 3D application programming interface (API)).[24] It seems that the focus was on providing students with an opportunity to learn (1) how to operate an FTIR spectrometer in an autonomous setting, enabling them to operate a real spectrometer, and (2) how peaks in vibrationally resolved spectra correlate with the normal modes of the molecule.[25] Our motivation for developing an FTIR-SIS is similar in that we would like for students to gain an intuition about instrument operation, especially how changing parameters affects the spectra. Key differences between our FTIR-SIS and that previously developed is that the one described here is capable of producing rotationally resolved spectra of gas-phase molecules and that the spectra are completely synthetic (but almost indistinguishable from real spectra).

■ THE FTIR-SIS

The FTIR-SIS was developed to be used for the experimental part of typical gas-phase FTIR laboratories. It can generate high-resolution infrared spectra for a total of 49 different atmospherically important molecules that are included in the HITRAN (HIgh-resolution TRANsmission molecular absorption) database (https://hitran.org/).[26] All of the molecules that are commonly investigated by gas-phase infrared spectroscopy in a standard undergraduate physical chemistry course are included in the database, such as hydrogen chloride,[27] carbon monoxide,[28] and carbon dioxide.[29] The generated spectra include various isotopologues and isotopomers of the selected molecule in natural (terrestrial) abundance. For example, if "CO" is selected, two fundamental bands will appear with enough averaging (*vide infra*) with an intensity ratio of 0.9865 (^{12}CO):0.0111 (^{13}CO). It should be noted that the possibility of selecting pure DCl (with natural abundance of Cl), as is often done in real (lab-based) experiments, is not currently implemented in the program and that bands corresponding to DCl are too weak (and therefore noisy) in the simulated spectra of "hydrogen chloride" to be of any practical value (the situation is better for HF/DF).

The naming we adopted for the SIS reported here draws from flight simulators, a connection which was made by a past editor of this *Journal*.[30] We wish to note that Human–Computer Interaction is particularly relevant to designing simulations that take into account more factors than physical sciences alone,[31] since it draws from the fields of computer science, ergonomics, and cognitive science. With these factors in mind, we developed the FTIR-SIS. The user interface (UI) was designed to somewhat resemble that of a real FTIR spectrometer; in order to enhance student engagement, we incorporated appealing stylistic features in the UI, beyond what is present in most FTIR control software. Its virtual nature makes for an environment that encourages experimentation with different parameters without the fear of making costly mistakes. This could enable students to gain an understanding of instrumentation while developing an intuition as to their operation. Students may therefore have an improved opportunity to develop into critically thinking research scientists who are mindful of their actions in the lab.

In the following, we provide a description of how one may navigate through the SIS by way of a tutorial example. This is followed by brief descriptions of the spectral processing that occurs, and the code that was developed (for additional details, please see the baseline code and supporting documentation which is included in ZIP files in the Supporting Information). While the software is available for general use at https://ftir.rastonlab.org/, instructions for setting up the SIS both locally (https://github.com/RastonLab/Virtual-FTIR-Spectrometer/wiki) and online (https://github.com/RastonLab/Virtual-FTIR-Functions/wiki) are available.

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Navigation

Upon navigating to https://ftir.rastonlab.org/, a welcome screen is displayed which contains the text, "Please use the navigation bar above to explore the application!". From there, a tutorial can be found in the "Help" menu which describes how to acquire spectra, find peaks, and export data for CO. In this tutorial, the user is first instructed to go to the "Experimental Setup" window, where various experimental parameters can be selected, as shown in Figure 1. Upon selecting "Collect Background Spectrum", the user is taken to the "Instrument" window (after a small amount of processing), which contains the essential elements of an FTIR spectrometer (see Figure 2).

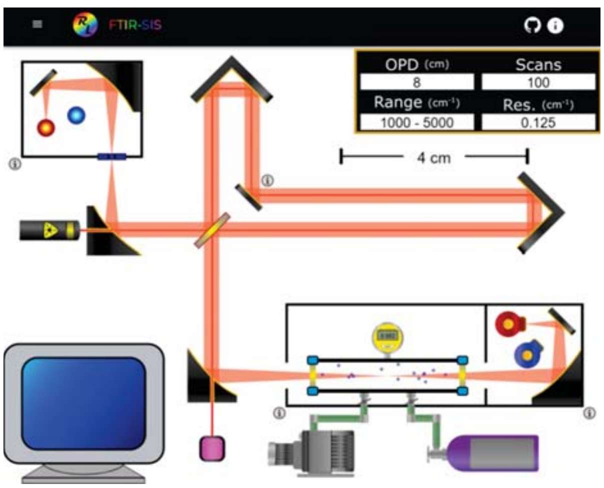

Figure 2. "Instrument" window. This state was captured shortly after initiating the acquisition of a background spectrum. The layout was designed for simplicity and was inspired by that of a Nicolet 6700 FTIR spectrometer that we disassembled for this project, in addition to a Bruker IFS 125 HR spectrometer. This figure has been reproduced with permission from https://ftir.rastonlab.org/.

The instrument immediately begins scanning the movable mirror of the interferometer (which is animated), and the progress of the scans is indicated. Acquisition of the background (and sample) spectrum using the parameters suggested in the tutorial (100 scans at a resolution of 0.125 cm^{-1}) takes about 9 min; note that a "loading spinner" indicates the scan progress.

While scanning is in progress, the user is encouraged to explore features of the SIS. They correspond to interactive objects within the schematic diagram of the FTIR spectrometer; clicking on an object within the diagram of the FTIR opens a popup window that provides a description of it. For example, the upper left box has an information icon next to the lower left corner of it; by clicking on that icon, a description of the "Source Compartment" is displayed, which includes plots of the blackbody emission spectra that is used to generate the simulated FTIR spectra (see Figure 3). As another example, by clicking on the solid red/orange/yellow circle within the Source Compartment, an image of a globar source is displayed along with the text, "Globar heating element which emits radiation corresponding to a blackbody at 1200 K. The word "globar" is ...".

After the background scans have been completed, the text "BACKGROUND SPECTRUM READY" is displayed on the computer monitor object. While this spectrum can be inspected at this point, the user is instructed (within the tutorial) to select "Collect Sample Spectrum", which will initiate the acquisition of a spectrum with the chosen sample in the gas cell (note that the solid blue circles in the sample cell represent air molecules, while the red circles represent the selected molecule). Once again, the user is encouraged to explore the FTIR spectrometer while the averaging is occurring.

After both spectra have been acquired ("SAMPLE SPECTRUM READY" will (also) be displayed on the computer monitor object), one can navigate to the "Window" menu and choose "Spectra". Here, all of the different types of spectra can be inspected, i.e., the sample spectrum (I), background spectrum (I_o), transmittance spectrum ($T = I/I_o$), and absorbance spectrum ($-\log_{10}T$). In the tutorial, the user is instructed to toggle to the "ABSORBANCE SPECTRUM" and zoom in on the (rotationally resolved) fundamental band of CO (~2000−2250 cm^{-1}), which should more-or-less be indistinguishable from a real spectrum. A particularly useful feature of FTIR-SIS is the ability to generate a list of the peaks and intensities. Using these values, one can perform analyses to determine molecular constants and the rotational temperature. Within the tutorial, the user is instructed to generate such a list in the "Find Peaks" window; see Figure 4. This peak list can be saved to the file by navigating to the "File" menu and choosing "Save" and then "Peaks Data". Note that the four different types of spectra can also be saved to a file in the "Save Data" window; they can be loaded into another program if desired, e.g., OPUS or OMNIC.

At this point, the experimental part of the lab is complete, and students can begin analysis in the desired format of the instructor so that molecular constants can be determined (band origin, rotational constants, rotational temperature, etc.). This traditionally involves performing polynomial fits to the peak positions and intensities,[32] which is most applicable to the simpler molecules that can be selected (linear[27−29] and symmetric tops[33]). For more complicated molecules (asymmetric tops), third-party programs like PGOPHER[34] or SPFIT/SPCAT[35] could be used, or code could be developed in-house.[36] Learning objectives of the analysis part of the lab will therefore vary somewhat, depending on the method used (e.g., see ref 37). Learning objectives of the experimental part will also vary, depending on a number of considerations, such as the molecule that is under investigation and the parameters that students are encouraged to explore. For the tutorial example described above, the primary learning objective is to develop an understanding of how a gas-phase FTIR spectrometer works, while setting up and acquiring a high-resolution infrared spectrum.

Spectral Processing

FTIR-SIS utilizes RADIS[38] (RADIative Solver for infrared spectra of molecules) and the HITRAN[26] database in order to generate idealized synthetic sample spectra of atmospherically important molecules. As implemented here, RADIS essentially converts linelists retrieved from HITRAN into idealized spectra, accounting for both pressure (collisional) and thermal (Doppler) broadening. The spectra are then processed to make them appear similar to what would be acquired using a real spectrometer. The first step in the processing involves multiplying an idealized transmission sample spectrum, T_{ideal}, by the emission spectrum of the source (globar or tungsten), B_{source}, for which we utilized Planck's blackbody formula (see Figure 3). The resulting spectrum is then multiplied by the

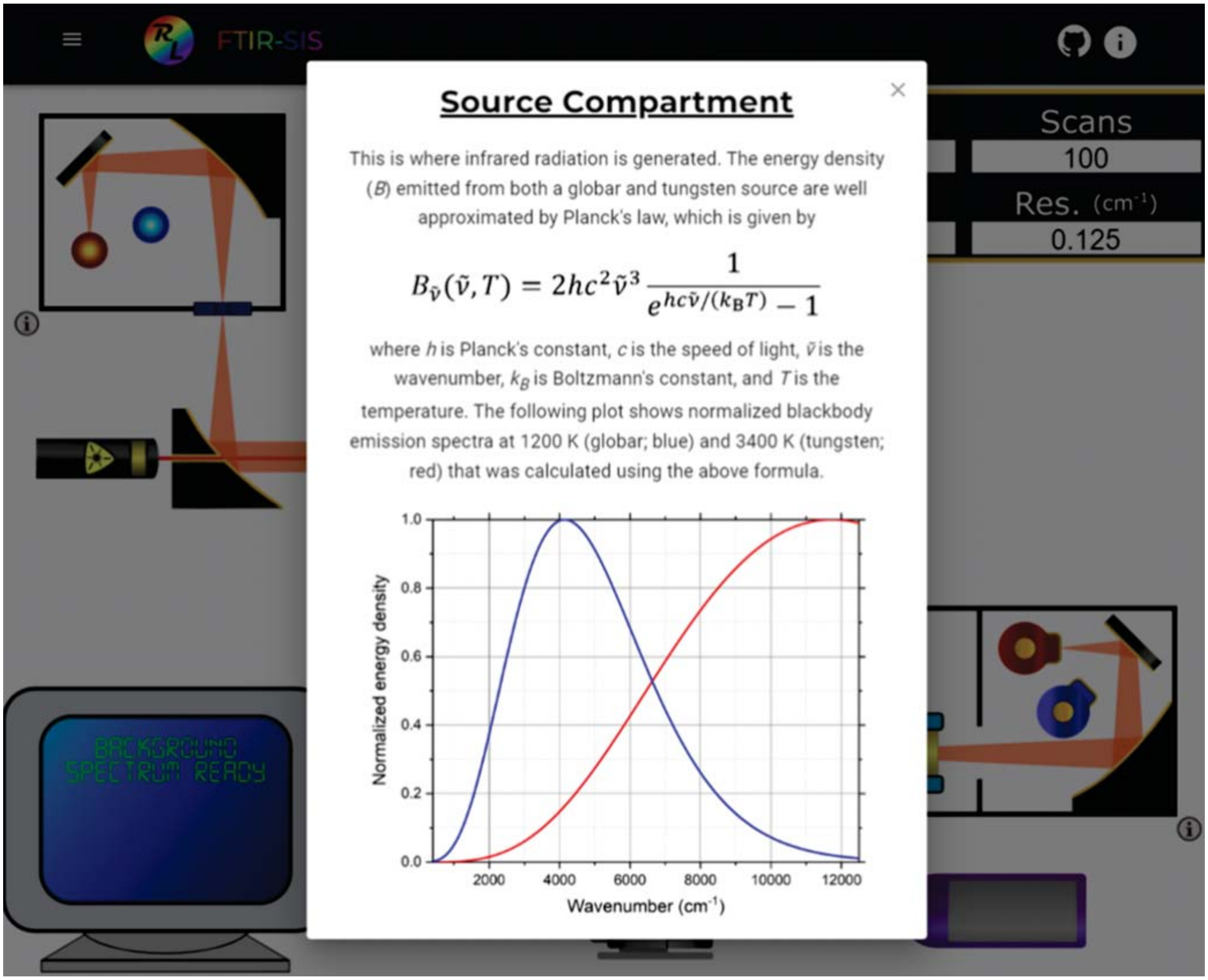

Figure 3. Popup window showing information about the Source Compartment. This figure has been reproduced with permission from https://ftir.rastonlab.org/.

transmittance spectrum of the beamsplitter (antireflective coated ZnSe of CaF_2), $T_{beamsplitter}$, cell windows (ZnSe of CaF_2), $T_{cell\text{-}windows}$, detector window (ZnSe or sapphire), $T_{detector\text{-}window}$, and the detector response spectrum (for MCT of InSb), $R_{detector}$, which were all generated by fitting empirically chosen functions to experimentally measured transmittance spectra and detector response spectra (to which white noise was added, since detectors are the primary source of noise in most FTIR spectrometers). The equation used to generate the processed sample spectrum, I, is thus $I = T_{ideal} \cdot B_{source} \cdot T_{beamsplitter} \cdot T_{cell\text{-}windows} \cdot T_{detector\text{-}window} \cdot R_{detector}$. The background spectrum, I_0, is calculated by simply replacing T_{ideal} by 1. Please see the FTIR-SIS back-end code (ZIP file in Supporting Information) for further details (including line shape functions).

Computer Code

For this software development collaboration, we relied on GitHub (https://github.com/), which allowed us to track file changes over time. These tracked changes permitted multiple developers to work on the project simultaneously by contributing to a central location. GitHub also has other features for documentation and project management that we used.

The code behind the simulator is divided into two separate software stacks, a front-end and back-end. The front-end was built using React (https://react.dev/), which is an open-source JavaScript library for building UIs that uses modular "components". These components were designed to be reusable pieces of code that render various parts of the UI. The major component libraries we use are the Material UI (MUI) library (https://mui.com/) and the Plotly (data charting) library (https://plotly.com/javascript/). The overhead view of the spectrometer contains Scalable Vector Graphics (SVGs) that are animated with JavaScript. The front-end sends a request to a Flask server (https://flask.palletsprojects.com/) which hosts an API that supports three major requests: collecting background spectra, collecting sample spectra, and finding peaks of the calculated absorbance spectrum. These processes occur in the back-end, which was built using the Python programming language (https://www.python.org/), since it is the language that RADIS was written in (it is also an excellent choice due to its popularity in data science and analysis applications). The back-end is a Flask

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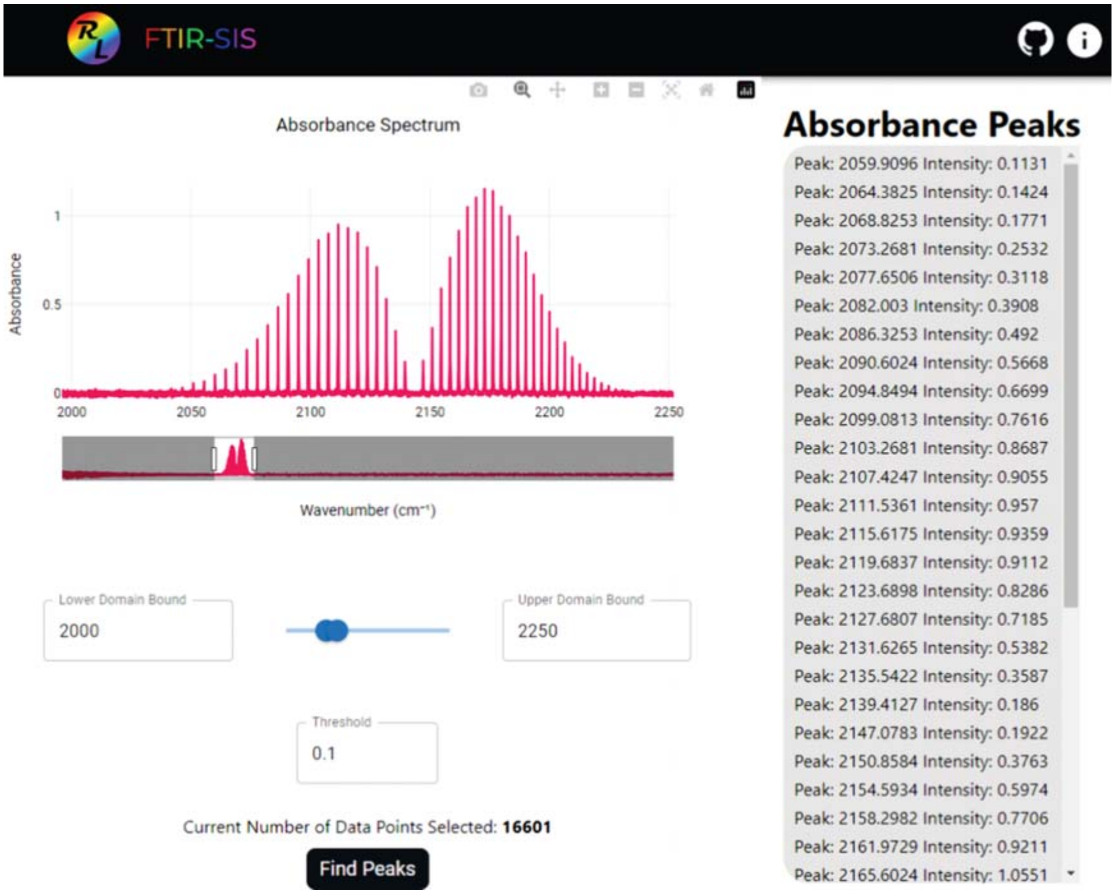

Figure 4. "Find Peaks" window. Note that the algorithm works best if the "Threshold" is chosen to be larger than the amplitude of the noise. This figure has been reproduced with permission from https://ftir.rastonlab.org/.

application that has been containerized, so that the application can be run on any infrastructure. We used the Kubernetes container orchestrator (https://kubernetes.io/) to manage containers, which allows for the infrastructure to scale dynamically and balance incoming traffic as demand changes.

Preliminary Implementation

The FTIR-SIS was used by students enrolled in a directed physical chemistry research class at the University of Hawai'i at Mānoa. After reading background material on molecular spectroscopy[39] and discussing basic aspects of FTIR spectroscopy,[40] students were instructed to navigate to https://ftir.rastonlab.org/ to perform the tutorial activity described above. The activity was successfully completed without guidance from an instructor. (This is important considering the SIS was developed to provide students with an autonomous learning experience, especially during lockdown.) Although quantitative assessment was not performed, from a question-and-answer session which followed, we noticed that students gained insight into the workings of an FTIR spectrometer during data acquisition, both from the animation and by clicking on various objects. We note that more insight could have been gained by increasing the data acquisition time (by increasing the number of scans and/or resolution). Following data acquisition, students analyzed the exported spectra using PGOPHER, which resulted in accurate and precise determination of the molecular constants of CO.[41]

■ SUMMARY

The FTIR-SIS presented here has been designed to engage students and help them navigate through the acquisition of simulated gas-phase spectra of a wide variety of molecules. The front-end shows the inner workings of a typical FTIR spectrometer and allows for students to select various components to learn about their functionality, and adjust instrument control parameters in a similar way to commercially available FTIR spectrometers. They can acquire background and sample spectra for a wide variety of atmospheric molecules that are available in the HITRAN database. The spectra are processed (ratioed) to give an absorbance spectrum within which peaks can be identified and exported for analysis. We anticipate that FTIR-SIS will be particularly valuable in situations when classes cannot meet in person, when necessary instrumentation is unavailable, or when samples that are particularly toxic (e.g., HCN[42]), expensive (e.g., NO[43]), or unstable (e.g., OH[44]), would like to be investigated.

■ ASSOCIATED CONTENT

Data Availability Statement

Associated material can be found on GitHub at https://github.com/RastonLab/Virtual-FTIR-Spectrometer and https://github.com/RastonLab/Virtual-FTIR-Functions.

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.3c01161.

FTIR-SIS back-end code and supporting documentation (ZIP)

FTIR-SIS front-end code and supporting documentation (ZIP)

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Author Contributions

B.S. and N.V. developed the code. R.S. set up the server infrastructure. N.V., M.S., and P.L.R. supervised and planned the project. N.V. and P.L.R. prepared the manuscript. P.L.R. conceived the project.

Notes

The authors declare no competing financial interest.

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■ REFERENCES

(1) Alpert, D.; Bitzer, D. L. Advances in Computer-based Education. *Science* **1970**, *167* (3925), 1582−1590.

(2) Smith, S. G.; Sherwood, B. A. Educational Uses of the PLATO Computer System. *Science* **1976**, *192* (4237), 344−352.

(3) Smith, S. G. Computer-Based Teaching of Chemistry. In *Computers in Chemical Education and Research*; Ludeña, E. V., Sabelli, N. H., Wahl, A. C., Eds.; Springer US: Boston, MA, 1977; pp 49−57.

(4) Smith, S. G. The use of computers in the teaching of organic chemistry. *J. Chem. Educ.* **1970**, *47* (9), 608−611.

(5) Ben-Zion, M.; Goldschmidt, Z. Simulated NMR spectrometry and shift reagents. *J. Chem. Educ.* **1977**, *54* (11), 669.

(6) Schatz, P. F. *NMR Simulator*; COMPress: Wentworth, NH, 1987.

(7) Lower, S.; Gerhold, G.; Smith, S. G.; Johnson, K. J.; Moore, J. W. Computer-assisted instruction in chemistry. *J. Chem. Educ.* **1979**, *56* (4), 219−227.

(8) Breneman, G. L. Infrared spectra simulation. *J. Chem. Educ.* **1979**, *56* (5), 340.

(9) Barrow, G. M. Computer-based studies for physical chemistry. *J. Chem. Educ.* **1980**, *57* (10), 697−702.

(10) Schatz, P. F. *IR Simulator*; COMPress: Wentworth, NH, 1987.

(11) Cavin, C. S.; Cavin, E. D.; Lagowski, J. J. Study of the efficacy of computer-simulated laboratory experiments. *J. Chem. Educ.* **1978**, *55* (9), 602−604.

(12) Kelter, P. B.; Carr, J. D. Microcomputer Simulation of a Spectronic-20 Experiment. *J. Chem. Educ.* **1980**, *57* (9), 621.

(13) Wilkins, C. L.; Klopfenstein, C. E. Simulation of NMR spectra: Computers as teaching devices. *J. Chem. Educ.* **1966**, *43* (1), 10−13.

(14) Ling, A. C. A computer program for simulating first-order electron spin resonance spectra. *J. Chem. Educ.* **1974**, *51* (3), 174.

(15) Rittenhouse, R. C. HPLC: A computer simulation of high-performance liquid chromatography. *J. Chem. Educ.* **1988**, *65* (12), 1050.

(16) Smith, S. G. From Mainframes to the Web: 1998 George C. Pimentel Award. *J. Chem. Educ.* **1998**, *75* (9), 1080−1085.

(17) Boswell, P. G.; Stoll, D. R.; Carr, P. W.; Nagel, M. L.; Vitha, M. F.; Mabbott, G. A. An Advanced, Interactive, High-Performance Liquid Chromatography Simulator and Instructor Resources. *J. Chem. Educ.* **2013**, *90* (2), 198−202.

(18) https://ispso.unige.ch/labs/fanal/practical_hplc_simulator:en (accessed March 2024).

(19) Reich, H. J. WinDNMR: Dynamic NMR Spectra for Windows. *J. Chem. Educ.* **1995**, *72* (12), 1086.

(20) http://www.vsnmr.org/ (accessed March 2024).

(21) Marlowe, J.; Tsilomelekis, G. Accessible and Interactive Learning of Spectroscopic Parameterization through Computer-Aided Training. *J. Chem. Educ.* **2020**, *97* (12), 4527−4532.

(22) Bigger, S. W.; Bigger, A. S.; Ghiggino, K. P. FluSpec: A Simulated Experiment in Fluorescence Spectroscopy. *J. Chem. Educ.* **2014**, *91* (7), 1081−1083.

(23) Papadopoulos, N.; Limniou, M.; Koklamanis, G.; Tsarouxas, A.; Roilidis, M.; Bigger, S. W. Spec UV-Vis: An Ultraviolet-Visible Spectrophotometer Simulation. *J. Chem. Educ.* **2001**, *78* (11), 1560.

(24) Bertrand, L.; Lefebvre, S.; Bernier, S.; Villiard, D.; Leblanc, M.-J.; Proulx, S. Virtual FTIR spectrometer and 3D visual display for a course in molecular spectroscopy. *SPIE* **2005**, *9664*, 96641J.

(25) We attempted to contact authors of the paper to acquire the software without success.

(26) Gordon, I. E.; Rothman, L. S.; Hargreaves, R. J.; Hashemi, R.; Karlovets, E. V.; Skinner, F. M.; Conway, E. K.; Hill, C.; Kochanov, R. V.; Tan, Y.; Wcisło, P.; Finenko, A. A.; Nelson, K.; Bernath, P. F.; Birk, M.; Boudon, V.; Campargue, A.; Chance, K. V.; Coustenis, A.; Drouin, B. J.; Flaud, J. M.; Gamache, R. R.; Hodges, J. T.; Jacquemart, D.; Mlawer, E. J.; Nikitin, A. V.; Perevalov, V. I.; Rotger, M.; Tennyson, J.; Toon, G. C.; Tran, H.; Tyuterev, V. G.; Adkins, E. M.; Baker, A.; Barbe, A.; Canè, E.; Császár, A. G.; Dudaryonok, A.; Egorov, O.; Fleisher, A. J.; Fleurbaey, H.; Foltynowicz, A.; Furtenbacher, T.; Harrison, J. J.; Hartmann, J. M.; Horneman, V. M.; Huang, X.; Karman, T.; Karns, J.; Kassi, S.; Kleiner, I.; Kofman, V.; Kwabia-Tchana, F.; Lavrentieva, N. N.; Lee, T. J.; Long, D. A.; Lukashevskaya, A. A.; Lyulin, O. M.; Makhnev, V. Y.; Matt, W.; Massie, S. T.; Melosso, M.; Mikhailenko, S. N.; Mondelain, D.; Müller, H. S. P.; Naumenko, O. V.; Perrin, A.; Polyansky, O. L.; Raddaoui, E.; Raston, P. L.; Reed, Z. D.; Rey, M.; Richard, C.; Tóbiás, R.; Sadiek, I.; Schwenke, D. W.; Starikova, E.; Sung, K.; Tamassia, F.; Tashkun, S. A.; Vander Auwera, J.; Vasilenko, I. A.; Vigasin, A. A.; Villanueva, G. L.; Vispoel, B.; Wagner, G.; Yachmenev, A.; Yurchenko, S. N. The HITRAN2020 molecular spectroscopic database. *J. Quant. Spectrosc. Radiat. Transfer* **2022**, *277*, 107949.

(27) Richards, L. W. The infrared spectra of four isotopes in HCl: A molecular structure experiment. *J. Chem. Educ.* **1966**, *43* (10), 552−554.

(28) Mina-Camilde, N.; Manzanares, I. C.; Caballero, J. F. Molecular Constants of Carbon Monoxide at v = 0, 1, 2, and 3: A Vibrational

Spectroscopy Experiment in Physical Chemistry. *J. Chem. Educ.* **1996**, *73* (8), 804−807.
(29) González-Gaitano, G.; Isasi, J. R. Analysis of the Rotational Structure of CO_2 by FTIR Spectroscopy. *Chemical Educator* **2001**, *6* (6), 362−364.
(30) Moore, J. W. About This Issue: HPLC. *J. Chem. Educ.* **1988**, *65* (12), 1051.
(31) Monk, A. *Fundamentals of Human-Computer Interaction*; Academic Press: London, 1985.
(32) Herzberg, G. *Molecular Spectra and Molecular Structure*; D. Van Nostrand Company, Inc.: New York, 1945; Vol. *II*: Infrared and Raman Spectra of Polyatomic Molecules.
(33) McNaught, I. J. Structural parameters of methyl iodide by infrared spectroscopy. *J. Chem. Educ.* **1982**, *59* (10), 879−882.
(34) Western, C. M. PGOPHER: A program for simulating rotational, vibrational and electronic spectra. *J. Quant. Spectrosc. Radiat. Transfer* **2017**, *186*, 221−242.
(35) Drouin, B. J. Practical uses of SPFIT. *J. Mol. Spectrosc.* **2017**, *340*, 1−15.
(36) Raston, P. L. Helium nanodroplet isolation spectroscopy in an undergraduate teaching laboratory. *J. Mol. Spectrosc.* **2022**, *388*, 111676.
(37) Beck, J. P.; Miller, D. M. Encouraging Student Engagement by Using a POGIL Framework for a Gas-Phase IR Physical Chemistry Laboratory Experiment. *J. Chem. Educ.* **2022**, *99* (12), 4079−4084.
(38) Pannier, E.; Laux, C. O. RADIS: A nonequilibrium line-by-line radiative code for CO_2 and HITRAN-like database species. *J. Quant. Spectrosc. Radiat. Transfer* **2019**, *222−223*, 12−25.
(39) https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Physical_Chemistry_(LibreTexts)/13%3A_Molecular_Spectroscopy (accessed February 2024).
(40) https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Spectroscopy/Vibrational_Spectroscopy/Infrared_Spectroscopy/How_an_FTIR_Spectrometer_Operates (accessed February 2024).
(41) Herzberg, G.; Rao, K. N. Rotation-Vibration Spectra of Diatomic and Simple Polyatomic Molecules with Long Absorbing Paths. II. The Spectrum of Carbon Monoxide below 1.2μ. *J. Chem. Phys.* **1949**, *17* (11), 1099−1102.
(42) Keedy, C. R. The rotational-vibrational spectra of HCN and DCN: A physical chemistry experiment. *J. Chem. Educ.* **1992**, *69* (11), A296−A298.
(43) Schor, H. H. R.; Teixeira, E. L. The Fundamental Rotational-Vibrational Band of CO and NO: Teaching the Theory of Diatomic Molecules. *J. Chem. Educ.* **1994**, *71* (9), 771−774.
(44) Henderson, G.; Ko, C.-S.; Huang, T.-C. Infrared emission spectrum of the hydroxyl radical: A novel experiment in molecular spectroscopy. *J. Chem. Educ.* **1982**, *59* (8), 683−686.

https://doi.org/10.1021/acs.jchemed.3c01161
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