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Google Colab and Virtual Simulations: Practical e-Learning Tools to Support the Teaching of Thermodynamics and to Introduce Coding to Students

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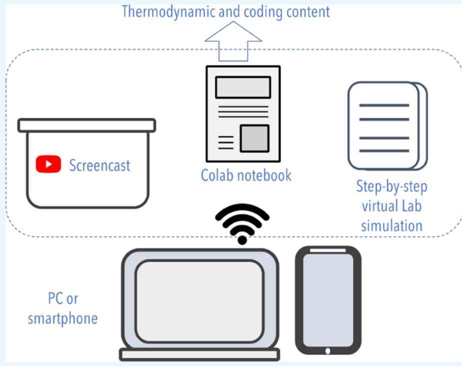
ABSTRACT: Various studies have reported the versatility and great scope of programming tools in all areas of knowledge. Coding is generally of paramount importance to chemistry students regardless of whether they intend to work with theoretical chemistry. Google Colab notebooks can introduce students to programming concepts and could be a convenient tool to assist in the chemistry teaching process. In this article, we implemented Google Colab notebooks to aid in the teaching of thermodynamics in a physical chemistry class. We presented six notebooks, covering introductory concepts of both coding and thermodynamics as a set of learning objects that can be useful in a virtual learning environment. In addition, in some of the notebooks, we included a step-by-step guide on how to run virtual lab simulations. The Colab notebooks were created for students without previous experience in programming. All of the Colab notebooks contain exercises of the activities and the solutions of the proposed exercises. Furthermore, all of the Colab notebooks can be modified and downloaded from the Github repository. Finally, we used the Python programming language and Colab because they are free and widely used by the academic community.



■ INTRODUCTION

The world of education has been affected at all levels by the COVID-19 pandemic. This situation has caused the largest disruption of education in history.[1] In the 2020 Global Education Monitoring Report, UNESCO reported that approximately 40% of the poorest countries failed to support learners at risk during the COVID-19 crisis, increasing the disparities in the learning opportunities.[2] This situation is critical for developing countries. In Latin America, taking the Human Development Index (HDI) as a reference, Colombia is in the middle at the region's score range (HDI = 0.767), while Venezuela has the lowest HDI score (0.711). On a world scale, Norway has the best HDI score (0.957).[3] Figure 1 shows a comparison of HDI values for Latin American countries. In this context, educational institutions around the world face two big barriers: (i) first-order barriers (e.g., funding, equipment, internet access) and (ii) second-order barriers (e.g., teachers' beliefs, skills, content quality).[4] Colombia joined the Organization for Economic Cooperation and Development (OECD) in 2020. In a recent report, the OECD informed that approximately 73% of principals (of schools that participated in Teaching and Learning International Survey, TALIS-2018) reported that insufficient internet access hindered the school's capacity to provide quality instruction (e.g., the average of the OECD countries participating in TALIS was 19%).[5]

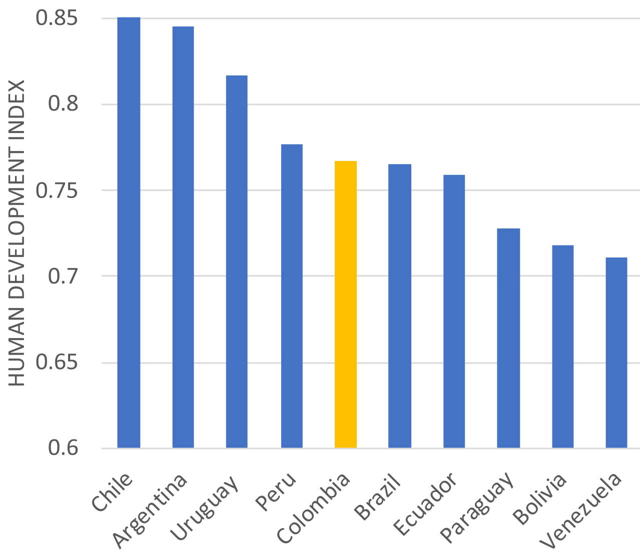


Figure 1. Human Development Index for Latin American countries.

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Table 1. Platforms that Offer Simulations under Open Access

platform	institution	description
PhET Interactive Simulations	University of Colorado	This platform offers virtual lab simulations in different science areas. It is a practical, intuitive, and interactive option to complement laboratory activities.[35,36]
Virtual-Labs ChemCollective	Carnegie Mellon University	"The ChemCollective is a collection of virtual labs, scenario-based learning activities, tutorials, and concept tests."[37]
Lab Xchange	Harvard University	"A free online platform for science education from Harvard University".[38]
MERLOT system	California State University partnering with educational institutions	This platform provides access to curated online learning and support materials, and it connects with other platforms listed in this table.[39]
Chemistry Library	U.S. Department of Education, University of California, California State, University, Carnegie Mellon University	A multi-institutional collaborative venture to develop open-access texts. It is a principal hub of the LibreText project.[40]
Classroom Resource Simulations	American Association of Chemistry Teachers	This platform provides access to resources, such as virtual labs, created and shared by teachers of chemistry.[41]

Despite the efforts made and the increasing number of people accessing the internet in Colombia, one of the challenges faced by Colombian teachers and students is to get complete internet access. This first challenge is an issue for the government to resolve in the medium term. The second challenge is up for the teachers. During the pandemic, the use of Information and Communication Technologies (ICT)-based learning methodologies increased suddenly and curriculum contents mostly had to migrate to the online format. Around the world, all teachers had to adapt quickly to be able to teach their classes online.[6−11] Chemistry teachers should ensure that ICT contents are attractive and thorough. Furthermore, they need to be creative to implement strategies to replace laboratory activities during pandemic online classes.[11] Online simulations and virtual labs emerged as an alternative solution to these challenges in chemistry teaching.[12−14] "Virtual investigation" (e.g., virtual simulation) is another type of teaching and learning tool that seems to improve students' learning.[15] The benefits of virtual simulations in teaching chemistry are no news and since long have been reported as complementary to practical chemistry exercises.[16−18] Recently, Garcia-Vedrenne et al. described strategies for a successful transition to remote learning,[19] and Kawasaki et al. explored the effectiveness and issues of remote teaching shift due to COVID-19.[20] Youmans presented an interesting report on how unique it is to teach during the COVID-19 pandemic in terms of other distance learning experiences.[21] There are many case studies on distance learning experiences in various fields of both basic and applied sciences (e.g., physics,[22] computational chemistry,[23] theoretical analysis,[24] biochemistry,[25] microbiology,[26] health,[27] mechanics[28]). Furthermore, comparative studies have been widely conducted. For instance, Rosen and Kelly presented a comparative study between traditional labs and online labs; they noted no differences in students' epistemological beliefs about the experimental content. However, the online modality offers students a choice of their preferred format regarding social interaction.[29] Humphrey carried out a study on lessons learned through listening to biology students during a transition to online learning,[30] and Marchak et al. explored "Teaching Chemistry by a Creative Approach" and reported that the online course successfully preserved the essence and the main objectives of the face-to-face course, that is, the original course was useful for remote teaching.[31] Finally, there exist thorough reviews on ICT as pedagogical tools for teaching and learning science.[32−34]

Currently, on the web, one can find different open-access platforms for science education that can be used in chemistry classes; however, not all of them are free of charge and some require a subscription. These options sometimes are expensive, hence prohibitive to traditional basic scholars and general chemistry programs. Currently, access to high-quality educational resources is a big challenge for developing countries, and ICT open access has become the best option to assist in the chemistry teaching process. Table 1 lists some platforms that offer simulations under an open-access license.

In addition to the skill that students can acquire and consolidate during the development of virtual labs and simulations, an important skill for all chemists is the ability to process, analyze, and visualize data.[42,43] This goal is normally achieved with the use of spreadsheets. However, when the data amount increases and so does the complexity of the task, this option becomes insufficient. In this context, computer science offers an engaging alternative toward a solution to this through the use of coding, even on a smartphone.[44] Computer science offers chemists different tools for solving problems (e.g., to formulate, to think creatively about solutions, and to express a solution clearly). Incorporating the computer science content into chemistry learning allows students to practice problem-solving skills.[45] Furthermore, due to the latest advances in digital science (e.g., cloud computing, Internet-of-Things), computer science will become an important part of chemistry laboratories.[46] Nowadays, many teachers around the world have begun introducing programming assignments as a component of their classes.[47] Coding contents can help in the chemistry teaching process, reinforcing the physical and chemical meaning of the mathematical equations studied in class, and teaching students additional skills useful in school and in their future jobs.[48] In an important report, Weiss carried out a thorough study on scientific computing aimed at chemists based on the Python programming language through Jupyter notebooks.[49] Jupyter notebooks are electronic documents designed to support interactive data processing, analysis, and visualization in an easily shared format. Jupyter notebooks utilize cloud computing to get started with coding with scant requirements. An Anaconda installer is a very popular option as a Jupyter launcher.[50] Jupyter notebooks use Python, which is a programming language used in a wide variety of applications, with the advantage of applicability to different work platforms; in addition, Python is open-access software, accessible to anyone who wishes to use it.[51] Different uses of Jupyter notebooks in chemistry have been reported in the last years; recently, Menke discussed the implementation of Jupyter notebooks in analytical chemistry classes.[43] Lafuente et al. carried out an interesting study directed to Machine Learning

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ACS Omega 2022, 7, 7421−7429

Figure 2. Scheme of six Google Colab notebooks. The figure shows the lesson title, exercises, and an estimation of the required time for each lesson; some lessons include a step-by-step guide on how to run virtual lab simulations. All notebooks contain the solutions to the proposed exercises. The Introductory Topics section covers the first three notebooks and the Special Topics section covers the last three sessions. The play icon indicates the notebooks that include screencasts. Details of each lesson in the Resource and Content section.

for Chemists through Jupyter notebooks.[52] Inside the Open Chemistry Project, Hanwell et al. presented the JupyterLab for use in Quantum chemistry, and the project was developed using Open Source Initiative.[53] Mendez et al., looking for more transparency and reporting standards in the scientific community of omics science, utilized Jupyter notebooks to generate collaborative open data science in metabolomics.[54] The potential of Jupyter notebooks in other areas is astounding (e.g., engineering, physics, mathematics). The impact of Jupyter notebooks as an interface for cloud computing has reached the high-tech companies: (i) Microsoft, with the Azure notebook;[55] (ii) Amazon, with the Segemaker notebook;[56] and (iii) Google, with Colaboratory (also known as Colab).[57] Among these, Colab is a cloud service based on Jupyter notebooks, which is a service linked to a Google Drive account, and free of charge.[58] It has all advantages of Jupyter notebooks and the power of Google (the Colab infrastructure is hosted on the Google Cloud platform). In this case, the only requirement to use Colab is guaranteed internet access and a Gmail account (additional software installation is not necessary). Colab is an interesting option to complement online activities of science teaching. Traditional physical chemistry classes (e.g., Thermodynamics, Quantum Chemistry) apply mathematics to solve different kinds of problems. Mathematical demonstrations and solving equations require the use of special software outside the scope of traditional basic scholars and general chemistry programs. In this case, the Python language is an attractive option, and Colab offers all its advantages in applying code to solve these challenges. Different courses in different universities are incorporating Google Colab as an ICT (e.g., Educational & Classroom Technologies,[59] Advanced Topics in Data Science,[60]). Recently, Baptista reported results on the use of Colab for teaching some topics of physical chemistry.[61] Another example of Colab's potential in the teaching of chemistry can be verified in the online published book "Deep Learning for Molecules and Materials", and all of the book's code (examples and exercises) is available for free on Colab.[62] Recently, Jumper et al. reported a highly accurate protein structure prediction with AlphaFold;[63] all of this code of this software is on open source at GitHub.[64] This tremendous software runs in Colabs' pipelines even from a smartphone.[65−67]

In the present study, we used the Colab and virtual labs platforms as an e-learning resource for the teaching of thermodynamics through coding and simulation activities.

■ DISCUSSION

Many students have shown difficulties in learning thermodynamics for decades, and quite a number of researchers have written about this issue and emphasized that, even after instruction, students retain significant misconceptions about thermodynamics principles.[68] In this way, interactive simulations that support multirepresentational fluency are considered critical by the chemistry education community.[69] There are various studies reporting the efforts made to overcome such deficiencies and offering suggestions of teaching approaches to enhance students' learning (e.g., the blended learning approach,[70] flipped courses,[19] gamification,[71] active learning environment,[72,73] virtual lab simulations[69,74]). All of these strategies attempt to engage students in active, constructive, and cooperative learning activities. We implemented six Google Colab notebooks to assist in the teaching of thermodynamics in a physical chemistry class, the notebooks to cover the contents related to the first law of thermodynamics.

Introductory Topics. We divided the six Colab notebooks into two sections: (i) introductory topics (first three notebooks) and (ii) special topics (the last three sessions). Figure 2 shows the scheme to use the Colab notebooks. All of the notebooks have the same structure: (i) title of the lesson, (ii) objectives, (iii) introduction, (iv) Colab activities, (v) solutions of the proposed exercises, and (vi) recommended links to blogs and tutorials. Furthermore, the notebooks for sessions 3, 5, and 6 included a step-by-step guide for virtual simulation activities. Finally, we added four screencasts to explain how to use Colab notebooks and to introduce some lessons.

More detail on access to the Colab notebooks and instructions on how to replicate procedures can be found in the Resource and Content section.

The Colab notebooks are meant for chemistry students without previous knowledge of coding. Furthermore, no software installation is needed to use the notebook, which was introduced to the students in the first two lessons. These two lessons could be covered in 3 h. We considered these first two lessons (Figure 2) critical for two reasons: (i) first, it is

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ACS Omega 2022, 7, 7421−7429

necessary that students both know and learn the basic concepts of the Python language and (ii) second, programming thinking is a useful tool for learning thermodynamics. In sessions 1 and 2 we provide an introductory guide on how to apply basic concepts of coding using the Python language to solve chemistry exercises through Google Colab. In the solution of activity 2, we obtained the Lennard-Jones (L-J) potential to CCl_4. Figure 3 shows the resolution of activity 2.

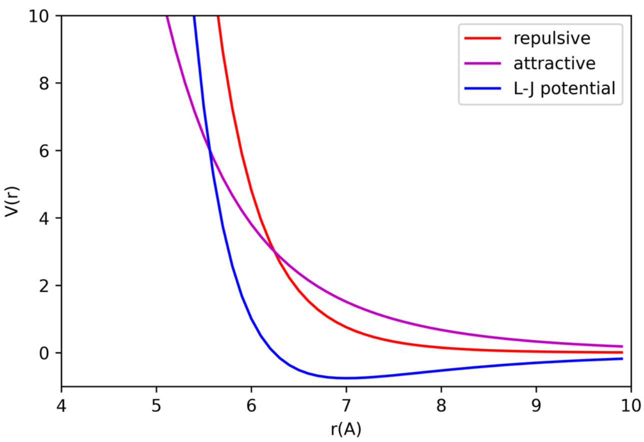

Figure 3. Lennard-Jones potential (L-J) as a function of distance (r) to CCl_4 (ε = 0.753 kcal/mol; σ = 6.24 Å). Details of coding of this exercise are given in the Colab notebook of session 2.

In session 3, we explored Charles's law for ideal gases. In this activity, we utilized the `Plotly` library to generate an interactive chart (e.g., a function of zoom, pan autoscale, toggle spike lines, and download the plot as a png file). Figure 4 shows the resolution of exercise 4 of this lesson.

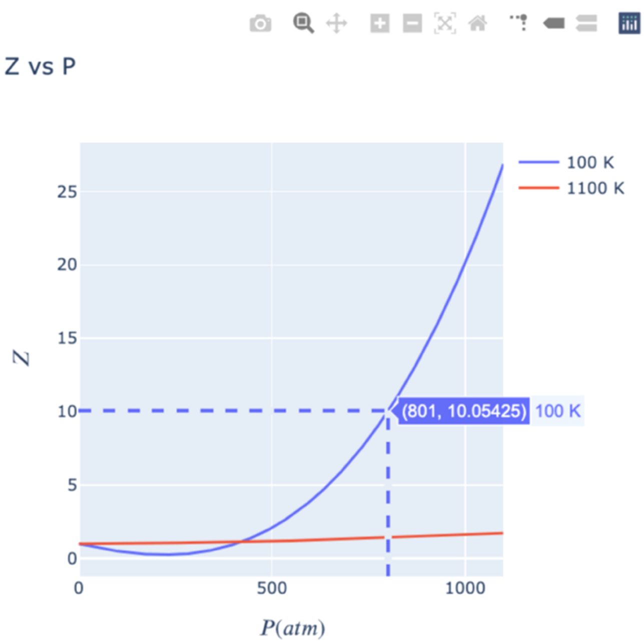

Figure 4. Screenshot of the interactive chart of solution exercise 4 in lesson 3. The compressibility factor (Z) of ethane is expressed as $Z = 1 + BP + CP^2 + DP^3$, where P is the pressure (atm) and B, C, and D are constants. Details of coding and solution of this exercise are given in the Colab notebook of session 3.

The interactive chart allowed students to interact differently (manipulating chart) with the properties of the gas. In the last part of session 3, we included a step-by-step guide for virtual lab simulation to verify Boyle's law and Charles's law for ideal gases. Virtual lab simulations are illustrative and very attractive for students. This lesson could be covered in 4 h.

Special Topics. In this section (right side of Figure 2), we presented the coding aspects useful to solve different physical chemistry problems. In these lessons, we put together math, chemistry, and coding to give students some tools to see the typical problem from other views.

The functions are essential tools in the part of python; in the Introductory topics section, we already used functions (e.g., pyplot and linregress) and, in session 4, we defined the functions. This tool is especially useful to solve thermodynamic problems. In session 4, we plotted van der Waals and Redlich Kwong equations. Figure 5 shows the resolution of activity 3 in lesson 4.

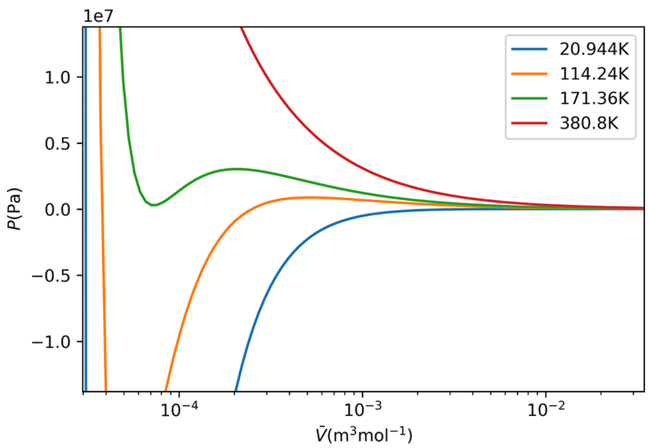

Figure 5. Redlich−Kwong equation of methane at temperature values of $0.11T_c$, 0.6 T_c, $0.9T_c$, and $2.0T_c$. In this exercise, first, we defined the function and then the parameters to plot the PV diagram at four temperatures, (T_c = critical temperature). Details of coding and solution of this exercise are given in the Colab notebook of session 4 activity 3.

Furthermore, in session 5, we presented typical PV diagrams for different thermodynamic processes, and in addition, we cover basic concepts for applying the `pandas` library. `pandas` is a library of data structures and statistical tools initially developed for quantitative finance applications.[75] Currently, the `pandas` library is a fast, powerful, flexible, and easy-to-use open-source data analysis and manipulation tool.[76] This library is useful for manipulating thermodynamic information. We used the `pandas` Python package to obtain the heat capacity $c_p(T)$ of 23 chemical substances from a dataframe. The students were shown how to import a file into a `pandas` DataFrame, how to obtain a polynomial equation, and how to calculate the enthalpy for heating one of the chemical substances. You can edit the dataframe file to add new chemical substances. Figure 6 shows the scheme to obtain the polynomial equation from dataframe. The `pandas` library allows for the treatment of large data sets in the convenient structure of dataframes and various tools for their handling;[52] this is especially useful when students manipulate large data sets.

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ACS Omega 2022, 7, 7421−7429

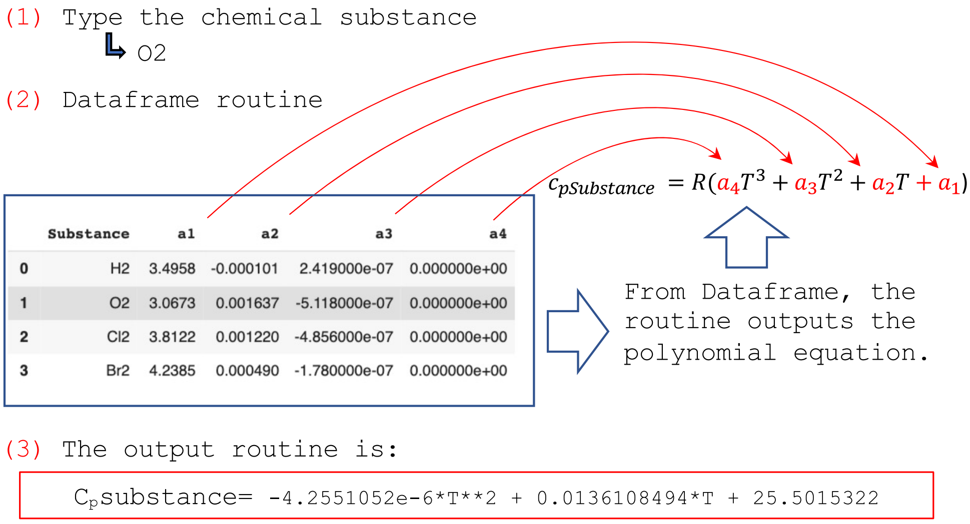

Figure 6. Process scheme to obtain the $c_p(T)$ equation in the Colab notebook of session 5: (1) one types one of the 23 chemical compounds listed in the dataframe, (2) routine execute, and (3) output routine is the $c_p(T)$ equation. Details of coding and solution of this exercise are given in the Colab notebook of session 5 activity 4.

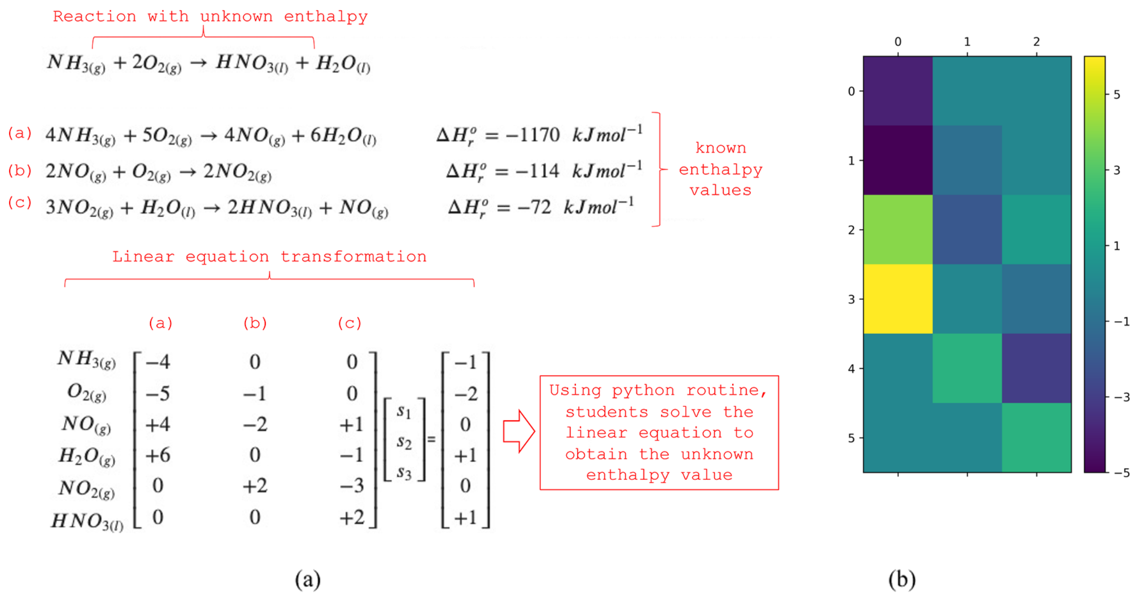

Figure 7. (a) Screenshot of the Colab notebook of session 6 explaining the matrix method: (i) we create the matrix (from reaction with known enthalpy values), (ii) we create the linear equation, and (iii) we obtain the unknown enthalpy value using the python routine. (b) Two-dimensional matrix representation using color scales with the matshow()function after applying the matrix method resolution to determine the reaction enthalpy of the reaction: $NH_{3(g)} + 2O_{2(g)} \rightarrow NHO_{3(l)} + H_2O_{(l)}$. Details of coding and solution of this exercise are given in the Colab notebook of session 6.

In the last part of session 5, we included a step-by-step guide for virtual lab simulation to calculate the neutralization enthalpy reaction. These two lessons could be covered in 6 h.

Finally, session 6 (Hess's law—matrices) was the last Colab notebook. In this session, resorting to a procedure previously reported and used by Khalil, we calculated the enthalpy of reactions by a matrix method. Conventional thermochemistry problems involving the determination of unknown reaction enthalpy values, applying Hess's law, are based on the properties of algebraic equations. Sometimes, the resolution methodology relies on trial and error. However, depending on the number of chemical reactions, the complexity of the problem can increase significantly, making the work tedious. Khalil reported an alternative methodology using linear algebra for solving these problems.[77] The students stressed that such a method was fast and easy to implement for the solution of these typical problems in thermodynamics. In addition, at the end of session 6, we made use of the `Matplotlib` library and the `matshow()` function to plot the matrix obtained while solving the problems. Figure 7 shows the resolution of activity 2 of this lesson. Conventionally, the physical chemistry texts do not present the resolution of their exercises, leaving a conceptual gap regarding the resolution of problems. In this case, linear algebra and python routines give the student an extra tool to apply a numerical method to the resolution of typical problems in physical chemistry. Furthermore, in view of such visual analogies, this can be the key to making students

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ACS Omega 2022, 7, 7421−7429

understand an abstract concept more easily, as these visualization options create a special impact on students.[78]

To introduce coding to chemistry students may be a challenge at first; however, as soon as they learn the basic concepts thereof and all of the possibilities of this kind of knowledge, their perception and attitude toward this topic could change. Programming is not commonly included in the curriculum of chemistry undergraduate programs; however, due to current scientific and industrial requirements, such programs have seen the need to adapt to these rapidly changing sectors.[79] The platform of Colab notebooks is very intuitive, making its implementation and learning unchallenging. The implementation of the Colab platform as an e-learning resource in the teaching of thermodynamics could be a useful tool to the students. Although an increased use of ICT is associated with various health issues (e.g., physical, psychosocial, and mental outcomes),[80,81] when judiciously applied, ICT can have a positive effect on students' learning performance in the classroom.[80,82] The use of such digital technology has a positive impact on the teaching of chemistry. The use of computer codes in e-learning enables students to solve complex problems in all areas of chemistry and has the potential to equip them for the field of chemistry with additional and very useful digital skills for their future.[47,83]

■ CONCLUSIONS

We presented six Colab notebooks as an e-learning resource to aid in the teaching of thermodynamics in a physical chemistry class for undergraduates. We covered introductory topics of thermodynamics and coding. Three of the Colab notebooks included a step-by-step guide for a virtual lab simulation as a supplement in the e-learning process. All of the Colab notebooks contain exercises of the activities and the solutions of the proposed exercises. All of the six Colab notebooks are available for free at the Github repository, and anyone can download or save the notebooks in their own Google Drive account or their own PC, or even on a smartphone, without any additional software installation. The Colab notebooks are meant for chemistry students without previous knowledge of coding. Although the six Colab notebooks can be perfectly run in the current version, readers can edit them to modify or add information they consider necessary. We estimate that the students can cover all contents of the Colab notebooks in 17 h. Finally, the six Colab notebooks can be useful for students and teachers during virtual learning.

■ RESOURCE AND CONTENT

Resource. We presented six notebooks covering introductory concepts of both coding and thermodynamics. We used Google Colab notebooks[57] to assist in the teaching of thermodynamics in a physical chemistry class for undergraduates. Throughout the sessions, different links connect the students with diverse contents so they can review concepts that are new to them or access content they wish to recall. In some notebooks, we included a step-by-step guide for virtual lab simulation using the PhET[36] and ChemColletive[37] platforms to assist in the e-learning process of teaching thermodynamics. All of the Colab notebooks are available in English and Spanish at Github.[84]We added four screencasts to explain how to use Colab notebooks and to introduce some lessons. The first screencast can be watched through this link: introductory screencast ▶.

Session 1 and Session 2: Introduction. Previous knowledge of coding concepts is not required. In the first session, we presented basic concepts of coding in Python (e.g., description of the Colab platform, types of variables in computer science, first commands, some functions, and routines), and then we used the math library to perform some numerical calculations. Finally, we used the library NumPy to perform some exercises with arrays, and the students were then tasked with finding the HCl solution concentration from a list of titration data. In the second session, we used the `math` library to perform some typical statistical calculations. Then, we used the `Matplotlib` library to obtain a graphic data representation of the Lennard-Jones potential for some species. Finally, we used the `scipy.stats` library to perform linear regression and obtain a calibration equation. The students were then tasked with finding a concentration from a calibrating curve. The screencast of the first lesson can be watched through this link: screencast session 1 ▶.

Session 3: Ideal Gases. Using the `scipy.stats` and `Matplotlib` libraries, the students are tasked with finding the absolute temperature on the Celsius scale, assuming ideal gas behavior. We used the `Plotly` library to obtain an interactive chart. In the final activity, the students were tasked with plotting the compressibility factor (Z) vs pressure at two different temperatures. In this activity, we utilized the `Plotly` library to generate an interactive chart. In activity 6 of this third Colab notebook (the Virtual Lab Simulation section), we included a step-by-step guide to verify Boyle's law and Charles's law for ideal gases. Analysis and plotting data can be solved using the Colab notebook.

Session 4: Equation of State (EoS). In session 4, we presented basic concepts for the use of functions in Python. Then, we explored the general form of the analytic equation of state (EoS). The general equation was presented and reduced to its most simple version (the van der Waals equation). We plotted a PV diagram using the van der Waals equation for six different temperatures of methane. The students were tasked with plotting a PV diagram for CCl_4 applying the van der Waals equation. In the second activity, the students were tasked with plotting a PV diagram for methane using the Redlich Kwong equation.

Session 5: First Law of Thermodynamics. In session 5, we presented typical PV diagrams for two gas expansion processes. In the first activity, we plotted a PV diagram for both reversible and irreversible expansions. The students were tasked with plotting a PV diagram for three different temperatures. In the second activity, we plotted the PV diagram for an adiabatic reversible expansion showing isotherm curves. In the third activity, we used the polynomial equation to describe the specific heat capacity $c_p(T)$ as a function of temperature. We used the `SymPy` library to define temperature as a "symbolic" variable, obtaining the $c_p(T)$ for a specific substance, and the students were then tasked with finding the heat transfer (at constant pressure) regarding some substances listed during the explanation in class. In the fourth activity, we presented basic concepts of the `pandas` library, and then we used this library to exemplify the manipulation of a dataframe containing the coefficients of the polynomial equation to describe the specific heat capacity $c_p(T)$ of 23 chemical substances. Subsequently, we presented a routine to obtain the polynomial equation of any of the 23 chemical substances in the dataframe. The students were tasked with plotting $c_p(T)$ vs

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ACS Omega 2022, 7, 7421−7429

T in a range of 300−1500 K for one substance of the dataframe. Finally, in the Virtual Lab Simulation section, we included a step-by-step guide to explore different ways of energy conversion and heat transfer. In the second part of it, we included a step-by-step guide to determine the heat of the neutralization reaction between HCl and NaOH. The screencast of this lesson can be watched through this link: screencast lesson 5.

Session 6: Hess's Law. In session 6, resorting to a procedure previously reported and used by Khalil, we calculated the enthalpy of reactions by a matrix method.[77] In this Colab notebook, we showed the technical aspects necessary to obtain a matrix from chemical equations, and we used the `NumPy` library to introduce the matrix code, and the `linalg.lstqs()` function to solve the equation. Then, the students were tasked with calculating the enthalpy of some reactions through the matrix method. In the final activity, we utilized the `Matplotlib` library and the `matshow()` function to plot the matrix form of the chemical reaction with colormaps—this is an attractive way to present this type of information. The students were tasked with plotting the colormaps of the matrix for the chemical reactions. In the Virtual Lab Simulation section, we utilized the ChemCollective platform to verify Hess's law for the determination of the heat of the neutralization reaction in various steps.

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Notes

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