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ARTICLE *in* JOURNAL OF CHEMICAL EDUCATION · AUGUST 2013

Impact Factor: 1.11 · DOI: 10.1021/ed4000124

JOURNAL OF CHEMICAL EDUCATION

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Sonified Infrared Spectra and Their Interpretation by Blind and Visually Impaired Students

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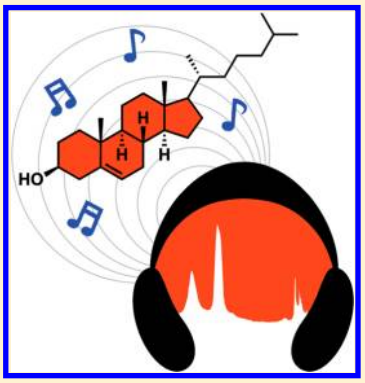
Supporting Information

ABSTRACT: To make the analysis of infrared (IR) spectra accessible to students who are blind and visually impaired (BVI), the visual information of the spectra was converted into nonspeech sounds using the open-source programs JDXview v0.2 and CSV to MIDI converter. In the sonified infrared spectra (SIRS), time is used as a spectral frequency indicator, and the range of the selected musical instrument frequencies is correlated with the intensity of the corresponding band absorptions. To simplify the identification of the absorption bands in the SIRS, seven audible distinguishable time markers were added: at the beginning, 3000, 2500, 2000, 1500, 1000 cm^{-1}, and at the end. This approach allows the fast identification of typical functional groups, or a set of frequencies related to a particular structural pattern in a molecule. By conveying IR spectral data, SIRS will aid BVI students' chemical education; SIRS can be used either for distance learning or in classroom activities.



KEYWORDS: *Second-Year Undergraduate, Chemoinformatics, Organic Chemistry, IR Spectroscopy, Computer-Based Learning, Distance Learning/Self Instruction, Minorities in Chemistry*

INTRODUCTION

According to the World Health Organization, 285 million people are visually impaired worldwide. Of these, 39 million are blind and 246 million have low vision. All must have the same educational opportunities as the general population, and particularly should have access to scientific knowledge, fundamental in modern society.[1]

Infrared (IR) spectroscopy is a simple and fast instrumental technique that provides evidence for the presence of several functional groups in a molecule. Analysis of IR spectral data is a mainstay of the undergraduate organic chemistry curriculum. However, as IR spectra information is conveyed as graphic representations, it is totally inaccessible to blind and visually impaired (BVI) students.

Over the last years, several efforts have been made to develop new, multisensory approaches to convey scientific graphical data to BVI and sighted people. DNA sequences have been transposed directly to music using nucleotides repetitions.[2] The conversion of DNA sequences to music was also accomplished using an algorithm in which the DNA nucleotide sequence made the musical top line, and the properties of the translated amino acids the bass line.[3]

In fact, one of the first approaches in the conversion of IR spectra into musical patterns was achieved using a talking laboratory instrument, with a linear presentation taking into account the variables pitch, duration, attack, waveform, loudness, and decay rate.[4] Later, the sonification of molecular vibrational spectral data from IR and Raman spectra was also accomplished.[5] This approach involves building waveforms from the molecule vibrational spectrum and the application of an algorithm to yield the auditory graph as a piece of "molecular music". The development of the Sonification Sandbox, a software program[6,7] that enables the simultaneous conversion of tabular data into nonspeech audio and visual graphs, fostered novel applications. This program was specially designed both for science education auditory research and development, and auditory display for BVI users.

Mobile learning environments are emerging as novel and highly attractive teaching strategies for both BVI and sighted students. In this regard, a QR-coded audio periodic table of the elements (QR-APTE) was recently constructed.[8]

Our research group developed NavMol,[9,10] a molecular editor that enables the processing of chemical information, commonly processed visually (e.g., through chemical drawings), by BVI users. In the Web portal MOLinsight,[11] BVI users can find useful information about available programs and a guide about the tools for specific tasks. The molecular editor NavMol (version 2.0), recently released,[12] incorporates features such as a voice synthesizer, and a clock coordinates navigation system, both of which empower the communication interface with BVI users. It also displays a conventional chemical sketch screen that allows tutoring by sighted users. Additionally, several resources for teaching chemistry to BVI students have been reported in the last years, some of them focused on laboratory

dx.doi.org/10.1021/ed4000124 | J. Chem. Educ. XXXX, XXX, XXX−XXX

adaptations,[13−15] and others focused in conveying chemical information.[8−12,16,17]

This work presents the conversion of cartographic IR data into nonspeech audio sounds, a strategy for identifying functional groups in a molecule using sonified infrared spectra (SIRS), and teaching activities for the interpretation of SIRS by BVI students. The SIRS-assisted structural identification can be useful to BVI chemists either in the classroom or in laboratory activities.

METHODS

Description of the Method

IR spectra were downloaded from the National Institute of Standards and Technology (NIST) database[18] in the JCAMP-DX format (JDX). These were then processed to tab-separated *XY* values in a TXT format using the open-source software JDXview v0.2.[19] The IR data (transmittance, T) stored in the spreadsheet was then processed in order to obtain a file in a CSV (comma separated values) format, which was subsequently converted to the SIRS.

The conversion process of the CSV data to MIDI converter[20] included the following steps:

1. Transmittance (T) was converted into $(1 - T)$.
2. Time was used as a spectral frequency indicator.
3. The range of musical instrument frequencies was correlated with the intensity of the corresponding absorption $(100 - \%T)$.
4. Seven time markers were added to the file: at the beginning, 3000, 2500, 2000, 1500, 1000 cm^{-1}, and at the end.
5. The speed was set to approximately 32 pulses per quarter note in order to obtain a SIRS with about 1 min of duration.
6. The instrument was set to marimba.

The CSV file was easily imported using the CSV to MIDI converter[20] and a MIDI file (SIRS) was automatically generated in the MIDI file format. The methodology was optimized using the IR spectrum of propanone. SIRS for 20 spectra were obtained in the optimization process of all parameters except for the parameter "instrument". A tutorial for generating SIRS is available at the MOLinsight Web portal.[21,22]

DISCUSSION

The full interpretation of an IR spectrum is difficult because of its inherent complexity. Fortunately, it is not necessary to fully interpret an IR spectrum to get useful structural information. Our goal was directly focused on enabling the audio perception of structural information by BVI students, allowing them to conceive the main features of an IR spectrum. Although this information can be made available in a nongraphical form, for example by an extensive listing of the spectral data in a table, the analysis of these data is very often a cumbersome process. Through SIRS, the student will easily have a straightforward general perception of the spectra and its most relevant data that will aid the identification of the functional groups present in the corresponding molecules. This methodology can be easily adapted to classroom or distance learning activities concerning the identification of functional groups by BVI students.

For example, in the case of the IR spectrum of butanoic acid[18] (see Figure 1), from the visual profile of the spectrum it is possible to identify a carboxylic acid functional group (COOH), owing to the presence of a strong and very broad band about 3000 cm^{-1} (vibration of the OH group, H-bonded, of the carboxylic acid), and a sharp, strong band at approximately 1700 cm^{-1} [vibration of the carbonyl group (C═O) of the carboxylic acid].

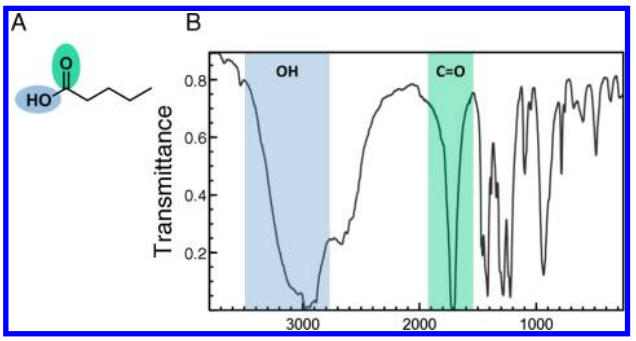


Figure 1. Butanoic acid: (A) chemical structure with highlighted functional groups; and (B) the IR spectrum highlighting typical vibration bands of the carboxylic acid. The IR spectrum of butanoic acid was taken in solution (10% in CCl_4 for 3800−1300 cm^{-1}; 10% in CS_2 for 1300−650 cm^{-1}; 10% in CCl_4 for 650−250 cm^{-1}) and was digitized by NIST from hard copy (from two segments).

The SIRS approach was developed in close interaction with a group of three BVI users having a high school science background. The test routine included the use of NavMol and SIRS tools, and was performed over one year (one task per month). For each task, the user was asked to: (i) study the organic chemistry concepts associated to the task; (ii) answer a questionnaire; and (iii) write a report. The BVI testers compared the analysis of IR data using the table form and SIRS methods and concluded that the SIRS method is a useful way to convey the spectral data. One tester commented:

> *Given the huge number of existing data on the table form in the IR tabular spectrum of butanoic acid, I consider that the sonification method implemented can be an asset to the community of people with visual impairments, because it allows [you] to summarize the spectral data into a small audio graphic, providing a more global overview of the spectrum.*

Additionally, another tester stated that the clear perception of the absorption bandwidth is a huge advantage of the SIRS approach as compared with the tabular spectral approach.

The clear and rapid perception of the absorption bandwidth corresponding to the vibration of the OH group, H-bonded, of the carboxylic acid using the SIRS of the butanoic acid allowed the unequivocal identification of the carboxylic acid functional group by BVI students, as is done using a graphical IR spectrum (Figure 1).

Table S1, given in the Supporting Information, lists the characteristic IR bands of some common functional groups and SIRS of molecules to illustrate their presence. For the successful interpretation of SIRS, an audio training is required in addition to the knowledge of rules. For this purpose, we built simulated SIRS (SSIRS) that only contain characteristic functional groups (Table 1). Our methodology can be easily adapted to classroom or distance learning activities that imply the identification of functional groups by BVI students; we present next a classroom activity.

dx.doi.org/10.1021/ed4000124 | J. Chem. Educ. XXXX, XXX, XXX−XXX

Table 1. Training Set for SIRS-Assisted Identification of Organic Compounds by BVI Students[a]

Functional Groups	MIDI Files[b]	Training Samples	Unknown Compounds
Alcohols: R-OH	SSIRS_alcohol.midi	3-Methyl-1-butanol; Cholesterol	Vanillin
Amines: R^1-NH-R^2	SSIRS_amine.midi	*N*-Allyl-isopropylamine; 2-*tert*-butyl-cyclohexylamine	2-Propylpiperidine
Imines: R-N=C	SSIRS_imine.midi	*p*-Tolualdehyde; 2,4-Dinitro-phenylhydrazone	2-Propanone phenylhydrazone
Hydrazines: R-NH-NH_2	SSIRS_hydrazine.midi	NA[c]	NA[c]
Aldehydes: R-HCO	SSIRS_aldehyde.midi	2-Propenal; Benzaldehyde	Vanillin
Ketones: R^1-CO-R^2	SSIRS_ketone.midi	Cyclohexanone; Acetophenone	Amfepramone
Carboxylic Acids: R-COOH	SSIRS_carboxyl.midi	(*E*)-Cinnamic acid; *p*-Toluoic acid	Aspirin
Esters: R^1-COO-R^2	SSIRS_ester.midi	Methyl salicylate; Ethyl butanoate	Aspirin
Amides: R^1-CON-R^2R^3	SSIRS_amide.midi	*N*,*N*-Diphenylacetamide; 2-Propenamide	Paracetamol

[a]The SSIRS files in MIDI format and the corresponding chemical structures in MDL MOLfile are available in the Supporting Information. [b]SSIRS means simulated sonified infrared spectrum. [c]Not available.

Identification of Functional Groups Using SIRS: Example of a Classroom Activity

For the successful interpretation of SIRS, an audio training is required. For this purpose, SSIRS that only contain characteristic functional groups were built (Table 1, MIDI files). After listening to each of these MIDI files, and becoming familiar with SIRS data for the corresponding functional groups, the next step is to listen to the complete SIR spectrum of the given example that contains that specific functional group (Table S1, see the Supporting Information).

All BVI testers were able to identify the characteristic IR absorption bands corresponding to the functional groups described in Table S1 (Supporting Information) in the built SSIRS that are referred to in the Table 1. However, some difficulties were reported by one of the testers with respect to grasping the absorption band intensity corresponding to a given functional group.

Taking the alcohol functional group as an example, after becoming familiar with the file, SSIRS_alcohol.midi, a student can be challenged to work through a real molecule, methanol, and listen to the file, SIRS_methanol.midi, with the goal of identifying its two characteristic IR absorption bands. After accomplishing these tasks, more complex SIR spectra of alcohols are proposed (e.g., 3-methyl-1-butanol and cholesterol), to identify again the two characteristic IR absorption bands of the alcohol functional group. We named those examples as training samples (Table 1). Before or after listening to the SIRS, the BVI students can perceive the chemical structure of the chosen molecule using NavMol 2.0 (see Figure 2 for an example). Finally, compounds containing more than one functional group are proposed (unknown compounds, Table 1): some of them are pharmaceutical or natural products.

Following the audio training described, BVI students will be capable of identifying the main functional groups that can be found in a molecule, and use SIRS to help solve the structure of unknown compounds, such as the spectrum of vanillin, also provided. A BVI student can check whether his or her answer is correct by navigating to the molecular structure of the unknown compound using NavMol 2.0. For example, if the unknown compound is vanillin, the students can easily identify the alcohol and the aldehyde groups. (See Figure 3.)

Results from the BVI testers showed that they were able to identify the main functional groups present in the unknown compounds of Table 1. Furthermore, the SIRS method can be used as an alternative method to the color tests for the detection of functional groups. For instance, after using NavMol to perceive the reactions of aldehydes or ketones with 2,4-dinitrophenylhydrazine (provided as a MDL RDFile),

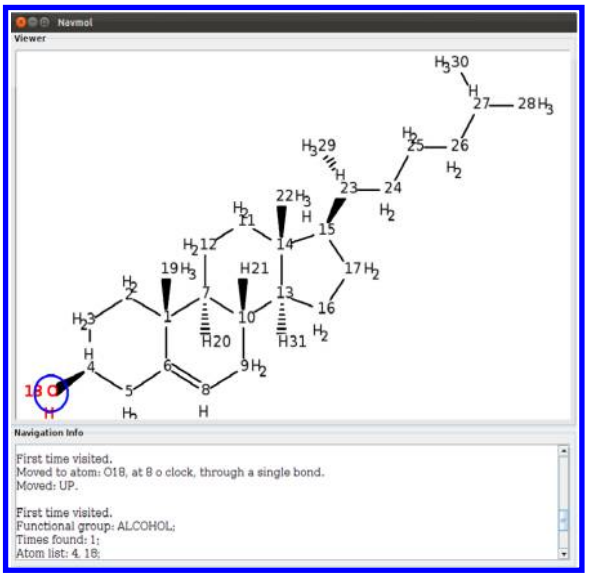


Figure 2. Snapshot of the Navmol 2.0 graphical interface showing the navigation information for the cholesterol molecule. The chemical numbering does not necessarily correspond to any systematic nomenclature, but rather to internal atom IDs assigned at the time of the structure edition.

the BVI testers were able to identify the presence of the carbonyl functional group of the reactant by listening to the SIRS of the product (e.g., *p*-tolualdehyde 2,4-dinitro-phenylhydrazone).

The testers' general opinions about the audio approach for the analysis of IR graphical information were quite positive, although they stressed that they were accustomed to more traditional approaches, such as tactile graphics, which have the advantage of requiring less training. Nevertheless, one of the testers confessed that, despite some difficulties in distinguishing the sounds, which forced her to listen to the same SIRS several times, she found this learning "very interesting, exciting, and useful".

CONCLUSIONS

SIRS can be easily constructed using open-source software (JDXview v0.2 and CSV to MIDI converter) and experimental IR data. The interpretation of IR spectra using this tool enables classroom activities in which BVI students can identify the functional groups in a given organic compound. This audio approach can be a valuable alternative to the more conventional approaches, such as tactile graphs or tabular data. In fact, the process can be more straightforward and intuitive, is

dx.doi.org/10.1021/ed4000124 | J. Chem. Educ. XXXX, XXX, XXX−XXX

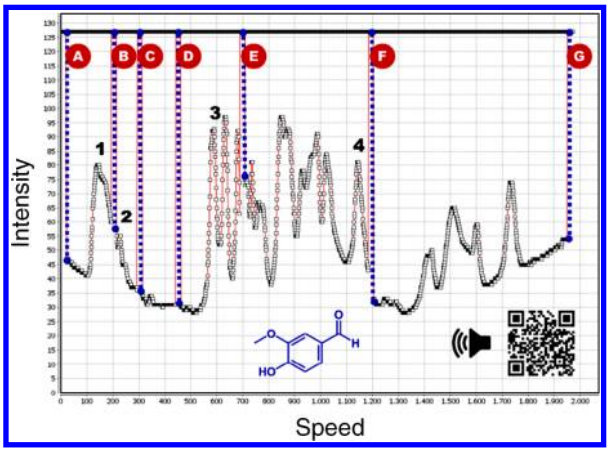


Figure 3. Identification of vanillin: visual graph generated from the CSV file sonified with Sandbox 6.1.7. Seven time markers were placed: (A) at the beginning; (B) 3000 cm^{-1}; (C) 2500 cm^{-1}; (D) 2000 cm^{-1}; (E) 1500 cm^{-1}; (F) 1000 cm^{-1}; (G) and at the end. Band assignments were made as follows: (1) O−H stretching; (2) C−H aldehyde; (3) C═O aldehyde; (4) C−O stretching. The inset shows the chemical structure of vanillin and the QR code for the vanillin SIR. The QR code can be scanned with a smart phone with a QR code reader (e.g., i-nigma) to listen to the vanillin SIR (MP3 file). The CSV file sonification of vanillin was done through the IR spectra of vanillin recorded in micrometers. The listening total time of the SIRS of vanillin is 31 s (1975 pulses).

inexpensive, and can be directly used in organic chemistry laboratory classes, for example, to identify products of an organic synthesis. It is important to acknowledge that this type of learning, as a new approach to convey graphical data, is not familiar to BVI students. The process requires extra training and concentration for the identification of all the functional groups present in a given SIRS. However, we are deeply convinced that the audio assignment of IR spectra has a strong potential to become a user-friendly, valuable tool to teach IR spectroscopy to BVI students, either in a routine classroom activity or in distance learning courses, allowing also a higher degree of independence and autonomy. Applications of the sonification process to other spectroscopic or spectrometric data, as well as evaluations of their predictive abilities in the characterization of organic compounds, will be an interesting challenge in a future work.

■ ASSOCIATED CONTENT

Supporting Information

Table of characteristic IR absorption bands of common functional groups; SIRS and SSIRS files in MIDI format; chemical structures in MDL MOLfile. This material is available via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

We thank Fundação para a Ciência e a Tecnologia (Lisbon, Portugal) and FEDER for financial support through the project CHEM4ALL (RIPD/APD/109547/2009), including the post-doctoral fellowships granted to three of us (J.C.P.S., R.P.S.F., and V.D.B.B.), and financial assistance to the blind and visually impaired testers managed by The Portuguese Association of Blind and Partially Sighted (ACAPO). We also express our gratitude to REQUIMTE and CQFB for research infrastructures and to FCT/UNL Library for the extensive use of the refreshable Braille display. This work was funded by Portuguese national funds via FCT Fundação para a Ciência e a Tecnologia (Lisboa, Portugal) under Project PEst-C/EQB/LA0006/2011.

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