

# Spectral Zoo: Combined Spectroscopy Practice Problems for Organic Chemistry

Jennifer L. Muzyka

Centre College, 600 W. Walnut St., Danville, KY 40422

## Abstract

The Spectral Zoo is a freely accessible browser-based application designed to provide spectroscopy practice problems (IR,  $^1\text{H}$  NMR, and  $^{13}\text{C}$  NMR) for organic chemistry students. JSpecView is used to display the spectra interactively so that the user can zoom in to inspect splitting. The website does not require the use of Java, Flash, or plug-ins, so it works well even on tablets.

## Importance of spectroscopy for organic chemistry

Spectroscopy is important in the sophomore organic chemistry sequence. Since the Alexander survey was published nearly 20 years ago,<sup>1</sup> organic chemistry educators have continued to focus on this topic. Bodner explored differences between sophomore organic chemistry students and more experienced chemists as they solve combined spectral problems.<sup>2</sup> Pienta's recent eye-tracking study documented distinct gaze patterns in sophomore organic students and more experienced students as they answered questions related to  $^1\text{H}$  NMR spectra.<sup>3</sup> Pedagogical approaches used to help organic chemistry students develop their skills solving spectroscopy problems include Shultz's jigsaw approach<sup>4</sup> and Flynn's tactile strategy using sticky notes.<sup>5</sup>

Faculty members have devised various ways to introduce spectroscopy in their courses as they guide students in developing relevant skills. Chemistry instructors have described pedagogical approaches such as Kurth's synthesis spectroscopy road map problems<sup>6</sup> and Livengood's individualized homework problems.<sup>7</sup> In laboratory courses, creative approaches have been described that require students to solve combined spectral problems or that facilitate student access to spectra they generate.<sup>8-11</sup>

## Online resources for teaching/learning spectroscopy

Over ten years ago, Debska reviewed the wealth of online resources available for teaching  $^1\text{H}$  NMR spectroscopy to organic chemistry students.<sup>12</sup> While some of the resources are no longer available online,<sup>13,14</sup> alternative online books, tutorials, and other resources have been developed in their absence. Reusch and Spinney have each contributed substantial modules on spectroscopy to the LibreTexts library.<sup>15,16</sup> Wong has developed an interactive

tutorial on  $^1\text{H}$  NMR spectroscopy.<sup>17</sup> Other valuable information about spectroscopy is available at sites developed by Starkey,<sup>18</sup> Lancashire,<sup>19</sup> and the Royal Society of Chemistry.<sup>20</sup>

Enabling students' transition from spectroscopy learners to chemists who are adept at solving spectral problems would be facilitated by exposing students to a larger number of combined spectral problems. Instructors make use of the several key websites that provide spectral data ranging from images of spectra,<sup>21</sup> to JCAMP-DX IR spectra displayed in a viewer,<sup>22</sup> and even to files that can be processed to generate spectra.<sup>23,24</sup> Chalk's recently developed Open Spectral Database is a resource designed to facilitate sharing and searching spectral data, providing spectra in several formats including JCAMP-DX.<sup>25,26</sup>

Several other websites serve as resources directed at students, providing them with combined spectroscopy problems on which to practice. The most familiar of these is Merlic's WebSpectra, which uses gif images of spectra combined with cgi scripts to allow users to expand spectral regions of interest.<sup>27,28</sup> Graham's more recently reported collection which focuses on 2D NMR also uses static images of spectra.<sup>29,30</sup> Vosegaard's iSpec is a browser-based game to provide students with spectroscopy practice using images of spectra.<sup>31,32</sup> Agnello's study convincingly demonstrates that the UlgSpectra application was helpful for student learning.<sup>33</sup> Unfortunately, the Java application was difficult for students to install, required a VPN for students to access the spectra, and took students 1-2 hours to learn to use. A subset of the spectra is available for use at other institutions, but the need to download and install a Java application remains a technological barrier for many students. Several other collections are available but have not been described in journal articles.<sup>34-39</sup>

### Online resources for teaching/learning spectroscopy

The Spectral Zoo is a web-based application that provides practice problems designed to help organic chemistry students solve combined spectroscopy problems.<sup>40</sup> The website is freely accessible with a web browser (<https://tinyurl.com/speczoo>) and does not require the installation of special software, browser plug-ins, or even Java. The current iteration of the Spectral Zoo uses JSpecView<sup>41,42</sup> to display spectra interactively, so that the user can zoom into signals or determine frequency/chemical shift by placement of the cursor. This approach differs from most of the other collections available online, which display static images. There are 74 unknowns in this set, with IR and  $^1\text{H}$  NMR available for all of the compounds. For thirteen of the unknowns, the  $^{13}\text{C}$  NMR is also available. Because the site is intended for student practice rather than being a homework assignment submitted for grading, the answers are available by clicking a button.

### Using the Spectral Zoo

The website is designed to be user friendly and require no instructions other than the one presented when the page is first loaded, as shown in Figure 1.

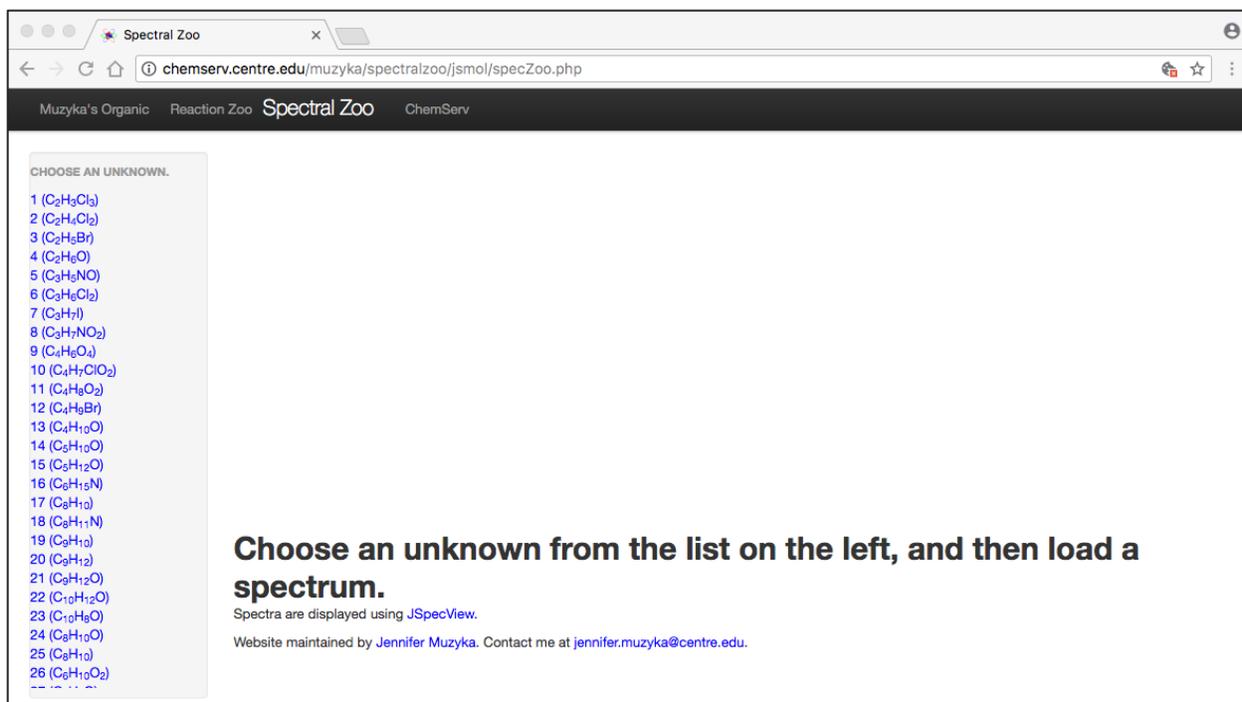


Figure 1. Spectral Zoo Opening Display

Once the user has selected an unknown, the display changes, providing links to the spectra and the structure for that unknown, as seen in Figure 2.

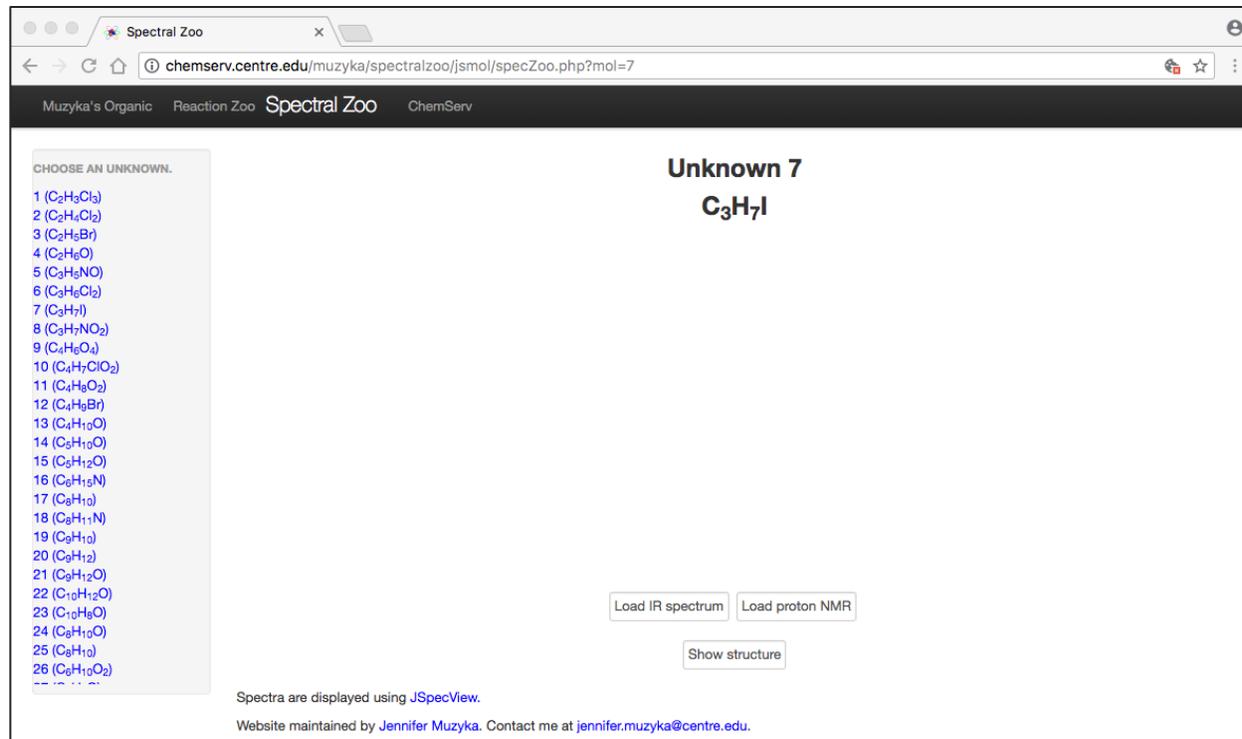


Figure 2. Spectral Zoo display after an unknown has been selected.

Figure 3 shows the application displaying the IR spectrum for unknown 7 in the JSpecView applet. The slider to the right of the spectrum allows the user to modify the vertical scale for the spectrum. The slider at the top of the spectrum allows the user to zoom in or out for the spectrum's x-axis. It is also possible to zoom in by clicking and dragging with the mouse. Several other convenient features offered by JSpecView can be accessed by right clicking on the spectrum.

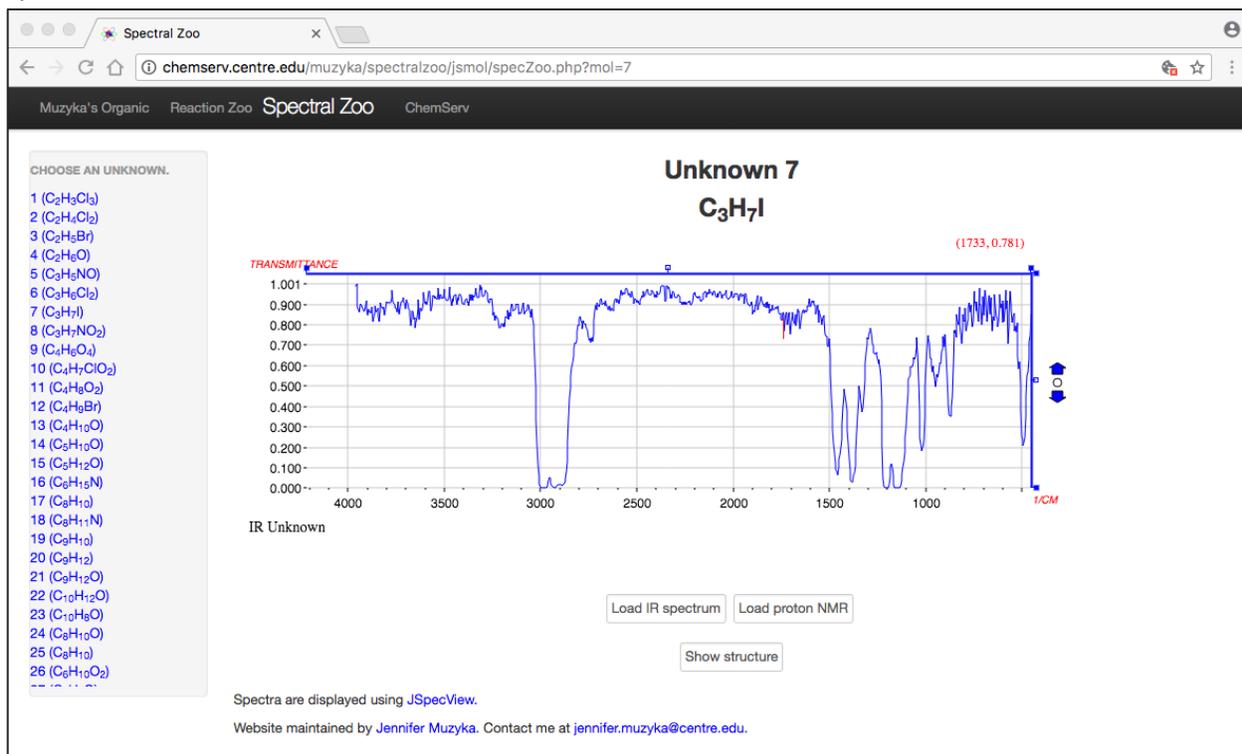


Figure 3. IR spectrum for Unknown 7 in Spectral Zoo.

Proton NMR spectra are slightly more complex, as the user typically needs to expand regions of the spectrum to inspect splitting. With the JSpecView applet this zooming process is intuitive for users. Another complexity associated with <sup>1</sup>H NMR spectra is integration. The JSpecView applet provides an interface that allows the user to normalize the integrals based on a specific signal selected by the user. Figure 4 displays a zoomed section of interest of the <sup>1</sup>H NMR spectrum for Unknown 7. Also shown in this figure is the popup panel allowing the user to configure the integrals. Although the integration interface is intended to be intuitive, there is a video tutorial demonstrating its use which was developed by a Centre College student.<sup>43</sup>

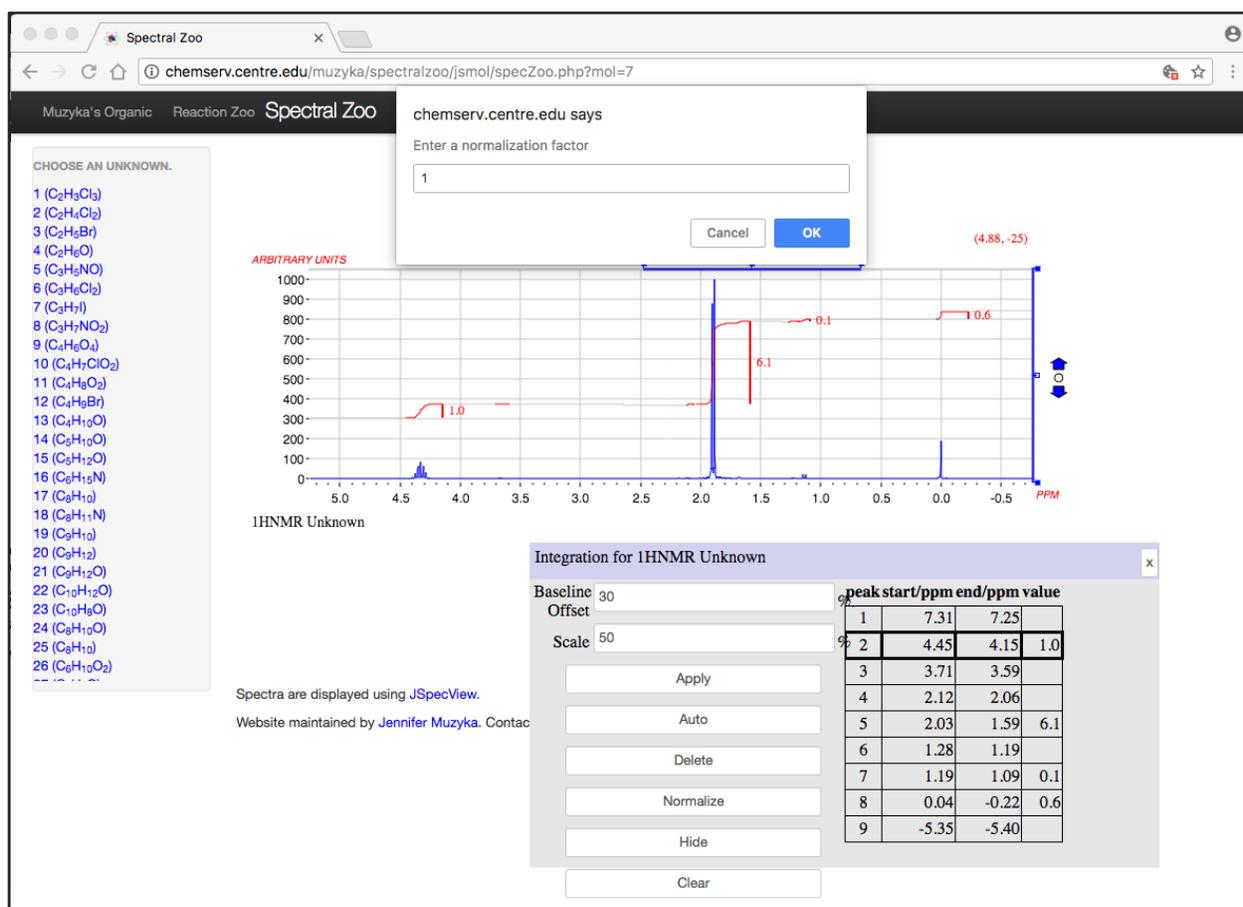


Figure 4. Proton NMR spectrum of Unknown 7 while normalizing integrals.

Figure 5 shows the popup window displaying the structure for Unknown 7, which is accessed by clicking the "Show structure" button at the bottom of the screen (See Figures 2 and 3). The Jsmol applet is used to display the structure, which means the structure may be rotated for inspection by the user.

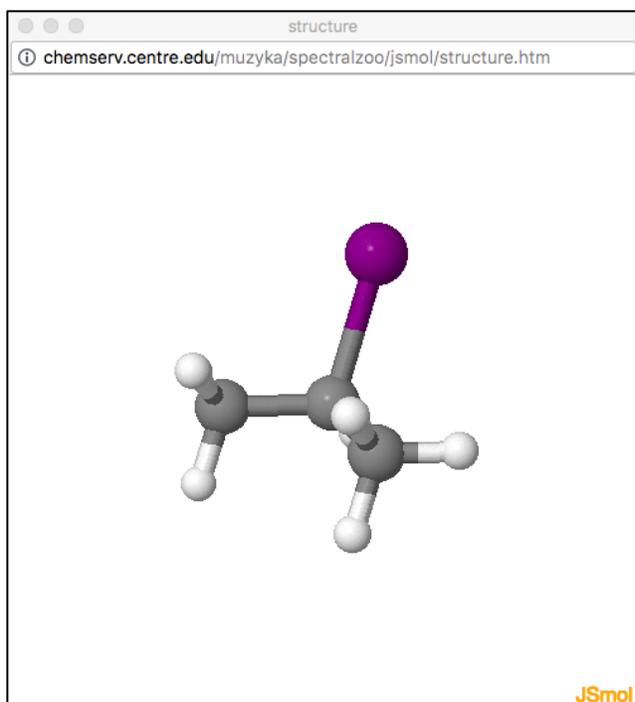


Figure 5. Structure of Unknown 7

### Student response

Students at Centre College and other institutions have been using the Spectral Zoo since 2002. Site statistics have been captured since June 2012. Unfortunately there is an 18-month gap in the data from July 2016 through the end of 2017 even though the site remained active during that time period. For the approximately five years of site statistics, there have been over 74,000 page views. This large number of page views suggests that most visitors to the site are not students in the author's classes, which typically have 17-25 students in a given section. Since the site provides answers, these users are visiting the site because they perceive it to be useful rather than it being a requirement for a course assignment. Most visitors are from North America and have been directed to the site through a link in the Sapling Learning homework system. Site statistics for the past three weeks suggest that the visitors from Sapling Learning represent 73% of visitors during this time period.

With Centre College IRB approval, pre- and post-surveys were administered to Centre College students during the 2012-13 academic year. The surveys were based on the New Traditions pre- and post-surveys for introductory chemistry.<sup>44-46</sup> Questions on the post-survey ask students to respond about the relative impact different course activities and assignments had on their learning. Additional items were added asking about the Spectral Zoo and how the website influenced student learning in the class. Thirty-two students responded to the post survey from two classes (total of 34 students) taught in separate semesters, giving a survey response rate of 94%. Responses to the Likert-scale question about how the Spectral Zoo

influenced their learning were very favorable, with 87.5% (28 students) indicating that the Spectral Zoo had a positive impact on their learning for the course. The distribution of responses is displayed graphically in Figure 6.

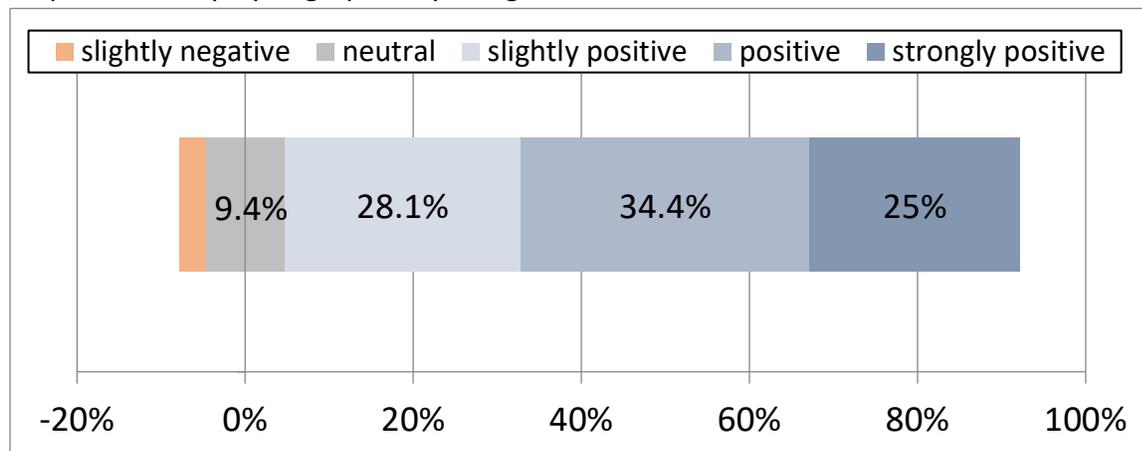


Figure 6. Distribution of student responses about Spectral Zoo effect on learning.

Most of the students (29 students, 90.6%) responded to the open-ended question, with most of the comments being positive in nature (23 students, 71.9%). Three students reported that they did not use the Spectral Zoo on their own. Two students (6.3%) expressed frustration about technical aspects of the site and one said the site was not helpful. The 2014 switch to JSpecView for display of spectra addressed student concerns about integration, as JSpecView provides integrals that can be normalized to provide numerical values. Representative student comments are provided in Table 1.

Table 1. Representative student comments about Spectral Zoo

Type of comment	Topic of comment	Percentage of comments	Representative student comment
Positive	Useful practice	53.1%	"It helped to provide a place to practice and learn from my mistakes when using NMR, IR, and interpreting data."
Positive	Helpful	18.7%	"It helped greatly learning how to do spectroscopy questions."
Neutral	Didn't use	9.4%	"Not very much. I rarely used it."
Negative	Technology	6.3%	"Spectral Zoo confused me at times because there was no clear integration. I would get halfway through a problem & then get frustrated or give up because I didn't feel like I had sufficient info to find the structure."

## Conclusions

For sixteen years students have been accessing the Spectral Zoo to gain practice analyzing spectra and solving combined spectroscopy problems. Development of the site has continued, keeping pace with changes in web technology. That development will continue into the foreseeable future. Comments from Centre College students about the site have been positive. Robust traffic to the site from visitors who are not on the Centre College campus suggests that many individuals have found this site helpful through the years.

## Technical details

The first version of the Spectral Zoo, which was based on JavaScript, was described in a presentation at the 2002 Biennial Conference on Chemical Education.<sup>47</sup> The site used MDL's Chemscape Chime plugin for the Netscape web browser to display JCAMP spectra interactively.<sup>48</sup> Unfortunately MDL had stopped development for Chime around 1998.<sup>49</sup> Further, the Chime plug-in did not have native support for integrals important for <sup>1</sup>H NMR spectra. Thus, the Spectral Zoo was updated to use a Java-based spectral viewer able to display integrals in proton NMR around 2006.<sup>10</sup> The next major update to the site was to implement a database (PHP/MySQL) to contain the information about the unknowns instead of having those details in JavaScript.<sup>50</sup> Around 2014 when security issues related to Java began to increase, the Spectral Zoo transitioned to using the JavaScript version of JSpecView which had by then been incorporated into Jmol/JSmol.<sup>51,52</sup>

The IR and NMR spectra in the Spectral Zoo are in JCAMP-DX format.<sup>53</sup> Infrared spectra for the unknowns were obtained from the National Institute of Standards and Technology in JCAMP format.<sup>22</sup> <sup>1</sup>H and <sup>13</sup>C NMR spectra were obtained from the Pacific Lutheran FID archive<sup>23</sup> and were processed with NUTS software from Acorn NMR, exported in the JCAMP-DX format.<sup>54</sup> Spectra are displayed using the JavaScript version of JSpecView applet<sup>41,42</sup> which has been incorporated into the Jmol/JSmol applet.<sup>55</sup> Structures are displayed using JSmol. The database uses MySQL with PHP as an interface. The only client-side scripting is JavaScript. The author would be happy to share her code with other instructors interested in developing their own instance of this application. Alternatively, instructors are encouraged to refer their students to the site at Centre College.

## Acknowledgments

I thank Pacific Lutheran University FTNMR FID Archive for sharing NMR data which were used in the development of the Spectral Zoo. I am particularly grateful to Robert Lancashire and Robert Hanson for helpful discussions over the years as I upgraded the site. I would like to thank Ian Kaster, who developed the Java applet used for many years to display spectra on the site and who encouraged me to convert the hard-coded JavaScript to a database format.

Thanks also to Alexander Williams, who developed the YouTube video demonstrating the use of the JSpecView integration panel.

## REFERENCES

- (1) Alexander, C. W.; Asleson, G. L.; Doig, M. T.; Heldrich, F. J. Spectroscopic Instruction in Introductory Organic Chemistry: Results of a National Survey. *J Chem Educ* **1999**, *76*, 1294–1296.
- (2) Cartrette, D. P.; Bodner, G. M. Non-Mathematical Problem Solving in Organic Chemistry. *J. Res. Sci. Teach.* **2010**, *47* (6), 643–660.
- (3) Topczewski, J. J.; Topczewski, A. M.; Tang, H.; Kendhammer, L. K.; Pienta, N. J. NMR Spectra through the Eyes of a Student: Eye Tracking Applied to NMR Items. *J. Chem. Educ.* **2017**, *94* (1), 29–37.
- (4) Winschel, G. A.; Everett, R. K.; Coppola, B. P.; Shultz, G. V.; Lonon, S. Using Jigsaw-Style Spectroscopy Problem-Solving To Elucidate Molecular Structure through Online Cooperative Learning. *J. Chem. Educ.* **2015**, 1188–1193.
- (5) Flynn, A. B. NMR Interpretation: Getting from Spectrum to Structure. *J. Chem. Educ.* **2012**, *89* (9), 1210–1212.
- (6) Kurth, L. L.; Kurth, M. J. Synthesis–Spectroscopy Roadmap Problems: Discovering Organic Chemistry. *J. Chem. Educ.* **2014**, *91* (12), 2137–2141.
- (7) Livengood, K.; Lewallen, D. W.; Leatherman, J.; Maxwell, J. L. The Use and Evaluation of Scaffolding, Student Centered-Learning, Behaviorism, and Constructivism To Teach Nuclear Magnetic Resonance and IR Spectroscopy in a Two-Semester Organic Chemistry Course. *J Chem Educ* **2012**, *89* (8), 1001–1006.
- (8) Grushow, A.; Brandolini, A. J. NMR Spectroscopy: Learned and Delivered on the Internet. *Chem Educ.* **2001**, *6*, 311–312.
- (9) Fleischer, J. M. Organic Spectroscopy - A Capstone Experience. *J Chem Educ* **2002**, *79*, 1247–1248.
- (10) Muzyka, J. L.; Kaster, I. M.; Hatcher, L. W. Making Student Acquired Spectra Available via a Web Browser. *J Chem Educ* **2007**, *84*, 1871–1872.
- (11) Chamberlain, P. H. Identification of an Alcohol with <sup>13</sup>C NMR Spectroscopy. *J. Chem. Educ.* **2013**, *90* (10), 1365–1367.
- (12) Debska, B.; Guzowska-Swider, B. Molecular Structures from 1H NMR Spectra: Education Aided by Internet Programs. *J Chem Educ* **2007**, *84*, 556–560.
- (13) Bradley, J.-C.; Lancashire, R. J.; Lang, A. S.; Williams, A. J. The Spectral Game: Leveraging Open Data and Crowdsourcing for Education. *J. Cheminformatics* **2009**, *1* (1), 9.
- (14) Kalstabakken, K. A.; Harned, A. M. Spectral Database for Instructors: A Living, Online NMR FID Database. *J. Chem. Educ.* **2013**, *90* (7), 941–943.
- (15) Reusch, W. Nuclear Magnetic Resonance Spectroscopy  
[https://chem.libretexts.org/Textbook\\_Maps/Organic\\_Chemistry/Supplemental\\_Modules](https://chem.libretexts.org/Textbook_Maps/Organic_Chemistry/Supplemental_Modules)

- \_(Organic\_Chemistry)/Spectroscopy/Nuclear\_Magnetic\_Resonance\_Spectroscopy (accessed Jul 5, 2018).
- (16) Spinney, R. Spectroscopy [https://chem.libretexts.org/Under\\_Construction/Core\\_Construction/Spinney/Spectroscopy](https://chem.libretexts.org/Under_Construction/Core_Construction/Spinney/Spectroscopy) (accessed Jul 15, 2018).
  - (17) Wong, Y.-L. 1H NMR Spectroscopy Tutorial <http://www.wfu.edu/~ylwong/chem/nmr/h1/> (accessed Jul 5, 2018).
  - (18) Starkey, L. Spectroscopy Handouts <https://www.cpp.edu/~lsstarkey/courses/NMR/index.html> (accessed Jul 17, 2018).
  - (19) Lancashire, R. J. Spectroscopy Problems <http://wwwchem.uwimona.edu.jm/spectra/specindex.html> (accessed Jul 15, 2018).
  - (20) Royal Society of Chemistry (Great Britain). SpectraSchool <http://spectraschool.rsc.org> (accessed Jul 17, 2018).
  - (21) AIST:RIO-DB Spectral Database for Organic Compounds,SDBS [http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre\\_index.cgi?lang=eng](http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng) (accessed Apr 17, 2011).
  - (22) NIST/EPA Gas-Phase Infrared Database JCAMP Format <https://www.nist.gov/srd/nist-standard-reference-database-35> (accessed Jul 19, 2018).
  - (23) PLU. The FTNMR Free Induction Decay Archive [http://www.chem.plu.edu/fid\\_archive/fid\\_archive.html](http://www.chem.plu.edu/fid_archive/fid_archive.html).
  - (24) Van Bramer, S. NMR at Widener University [science.widener.edu/svb/nmr/nmr.html](http://science.widener.edu/svb/nmr/nmr.html) (accessed Jul 5, 2018).
  - (25) Chalk, S. J. The Open Spectral Database: An Open Platform for Sharing and Searching Spectral Data. *J. Cheminformatics* **2016**, *8* (1).
  - (26) Chalk, S. J. The Open Spectral Database <http://osdb.info> (accessed Jul 28, 2018).
  - (27) Merlic, C. A.; Fam, B. C. WebSpectra: Problems in NMR and IR spectroscopy <https://webspectra.chem.ucla.edu/> (accessed Jul 5, 2018).
  - (28) Merlic, C. G.; Fam, B. C.; Miller, M. M. WebSpectra: Online NMR and IR Spectra for Students. *J Chem Educ* **2001**, *78*, 118–120.
  - (29) Graham, K. J.; McIntee, E. J.; Schaller, C. P. Web-Based 2D NMR Spectroscopy Practice Problems. *J. Chem. Educ.* **2016**, *93* (8), 1483–1485.
  - (30) Graham, K. J.; Schaller, C. P.; McIntee, E. J. Structure and Reactivity: Nuclear Magnetic Resonance Spectroscopy, NMR15 <http://tinyurl.com/CSBSJU-2DNMR> (accessed Jul 18, 2018).
  - (31) Vosegaard, T. ISpec: A Web-Based Activity for Spectroscopy Teaching. *J. Chem. Educ.* **2018**, *95* (1), 97–103.
  - (32) Vosegaard, T. iSpec overview <http://www.ispec.dk> (accessed Jul 18, 2018).
  - (33) Agnello, A.; Carré, C.; Billen, R.; Leyh, B.; De Pauw, E.; Damblon, C. ULg Spectra: An Interactive Software Tool To Improve Undergraduate Students' Structural Analysis Skills. *J. Chem. Educ.* **2018**, *95* (2), 276–280.

- (34) Houser-Archield, N. Organic Chemistry 201 Exercises in Proton NMR <http://academic.pgcc.edu/~nhousera/NMREX/> (accessed Jul 18, 2018).
- (35) Spinney, R. Structure Determination <https://undergrad-ed.chemistry.ohio-state.edu/csd/> (accessed Jul 15, 2018).
- (36) Hunt, I. Interactive Spectroscopy <http://www.chem.ucalgary.ca/courses/351/WebContent/spectroscopy/index.html> (accessed Jul 16, 2018).
- (37) Dessens, S. IR and NMR Introductory Practice Problems [http://learning.hccs.edu/faculty/steven.dessens/notes\\_and\\_practice/chem\\_2425/practice-problems/ir-nmr-problems/view](http://learning.hccs.edu/faculty/steven.dessens/notes_and_practice/chem_2425/practice-problems/ir-nmr-problems/view) (accessed Jul 18, 2018).
- (38) Nowick, J. S. Problems from Previous Years' Exams <https://www.chem.uci.edu/~jsnowick/organicspectroscopy/index.html> (accessed Jul 18, 2018).
- (39) Smith, B. D.; Boggess, B.; Zajicek, J. Organic Structure Elucidation: A Workbook of Unknowns <https://www3.nd.edu/~smithgrp/structure/workbook.html> (accessed Jul 5, 2018).
- (40) Muzyka, J. Spectral Zoo <http://chemserv.centre.edu/muzyka/spectralzoo> (accessed Jul 18, 2018).
- (41) Lancashire, R. J. The JSpecView Project: An Open Source Java Viewer and Converter for JCAMP-DX, and XML Spectral Data Files. *Chem. Cent. J.* **2007**, 1 (1), 31.
- (42) Lancashire, R. J. JSpecView Applet Specification <http://jspecview.sourceforge.net>.
- (43) Williams, A. NMR-integralsPrinting <https://www.youtube.com/watch?v=3QMGs6zTDFI> (accessed Jul 26, 2018).
- (44) Landis, C. R.; Peace, G. E.; Scharberg, M. A.; Branz, S.; Spencer, J. N.; Ricci, R. W.; Zumdahl, S. A.; Shaw, D. The New Traditions Consortium: Shifting from a Faculty-Centered Paradigm to a Student-Centered Paradigm. *J Chem Ed* **1998**, 75, 741–744.
- (45) Moore, J.; Kosciuk, S. Tools - New Traditions: Introductory Chemistry Beginning-of-semester Survey <http://archive.wceruw.org/cl1/flag/tools/attitude/ntchempr.htm> (accessed Jul 19, 2018).
- (46) Moore, J.; Kosciuk, S. Tools - New Traditions: Introductory Chemistry End-of semester Survey <http://archive.wceruw.org/cl1/flag/tools/attitude/ntchempo.htm> (accessed Jul 19, 2018).
- (47) Muzyka, J. Spectroscopic Unknowns for Organic Chemistry Students Using Chime and JCAMP; Bellingham, WA, 2002.
- (48) MDL Chime [https://en.wikipedia.org/wiki/MDL\\_Chime](https://en.wikipedia.org/wiki/MDL_Chime) (accessed Jul 18, 2018).
- (49) Martz, E. Version History of MDL Chime <https://www.umass.edu/microbio/chime/chimvers.htm> (accessed Jul 18, 2018).
- (50) Kaster, I.; Munday, G. S.; Foster, M.; Hernandez, D. Web-Based Practice Problems for Organic Chemistry; Bloomington, IN, 2008.

- (51) Hanson, R. M.; Prilusky, J.; Nakane, T.; Sussman, J. L. JSmol and the Next-Generation Web-Based Representation of 3D Molecular Structure as Applied to Proteopedia. *Isr. J. Chem.* **2013**, *53* (3–4), 207–216.
- (52) Muzyka, J. Web-Based Learning Tools for Organic Chemistry; Grand Rapids, MI, 2014.
- (53) IUPAC Committee on Printed and Electronic Publications, subcommittee on Electronic Data Standards (JCAMP-DX). Homepage of IUPAC CPEP Subcommittee on Electronic Data Standards [www.jcamp-dx.org](http://www.jcamp-dx.org) (accessed Jul 15, 2018).
- (54) Acorn NMR <http://www.acornnmr.com/> (accessed Jul 19, 2018).
- (55) Jmol: an open-source Java viewer for chemical structures in 3D <http://jmol.sourceforge.net> (accessed Jul 27, 2018).