

# Spectroscopy Data for Undergraduate Teaching

Scott E. Van Bramer\* and Loyd D. Bastin

Cite This: *J. Chem. Educ.* 2023, 100, 3897–3902

Read Online

ACCESS |

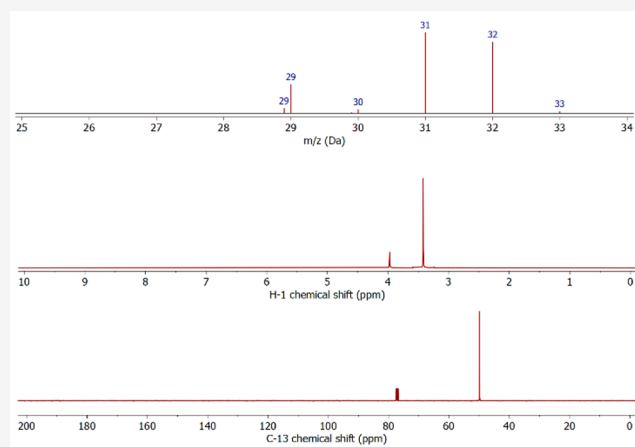
Metrics &amp; More

Article Recommendations

Supporting Information

**ABSTRACT:** This paper describes a data set of IR, MS, H-1 NMR, C-13 NMR, DEPT, and 2D NMR spectra designed for undergraduate teaching. The data files are provided as MestReNova documents containing all the available spectra for each of the 251 different compounds in the data set. The spectral data in these files can be processed, manipulated, copied, and pasted as needed by faculty to support teaching organic chemistry and instrumental analysis and for specialized courses in spectroscopy and organic synthesis. The compounds in the database were selected to provide examples for interpreting spectra and unknowns for teaching interpretation and to support teaching synthesis mechanisms. Additional MestReNova documents are provided to demonstrate how the data can be used for a variety of common undergraduate course topics—introducing IR, MS interpretation, NMR interpretation, data processing, and spectroscopy unknowns for students.

**KEYWORDS:** NMR, IR, Mass Spectrometry, Database, 2D NMR, Spectra



## INTRODUCTION

Faculty use spectroscopic techniques to teach chemical structure and function throughout the undergraduate chemistry curriculum. To do this effectively, faculty need access to spectra that support lectures, for use in student exercises and for use as unknowns. Spectra are included in organic chemistry textbooks,<sup>1–3</sup> instrumental analysis textbooks,<sup>4–6</sup> spectroscopy textbooks,<sup>7–12</sup> and specialized texts on NMR<sup>13–16</sup> and mass spectrometry.<sup>17</sup>

These books are designed to introduce spectral interpretation and often include additional example problems for students. However, the spectra in print are static images, so it is difficult for faculty to expand regions, closely examine peak shapes, change processing parameters, use in presentations, include in problem sets, and use for exams. Textbook spectra are also presented as fully processed and often cleaned up to remove solvent peaks and background. If faculty want students to acquire, process, and interpret spectra, they need experience with real data. Faculty need easy access to additional sources for spectra of unknowns and for examples to use in lectures, worksheets, and exams. At one time this was done using the print Stadler libraries of NMR and IR data that are now available by subscription through Wiley.<sup>18</sup> Additional options include the AIST Spectral Database for Organic Compounds (SDBS)<sup>19</sup> or IR, MS, C-13 NMR, and H-1 NMR spectra of commercially available compounds from Sigma-Aldrich.<sup>20</sup> All of these sources, however, present spectra as static images with

no ability to zoom or reprocess the data and do not provide consistent types of spectra.

The NIST Chemistry WebBook<sup>21</sup> is another valuable source of MS and IR spectra. These are presented as static images but may also be downloaded as JCAMP-DX files<sup>22</sup> which can be viewed in some commercial software packages or using Jmol,<sup>23</sup> an open-source program.

There are Web sites that provide practice problems for teaching spectroscopy.<sup>24</sup> These are excellent resources for students, but again they are limited to providing a single representation of most spectra or are limited to a single spectroscopic technique. Socha et al. recently published an article on [NMR-Challenge.com](https://www.nmr-challenge.com/),<sup>25</sup> another Web site that provides students with practice problems to help students develop interpretation skills.

Several sources of NMR data have been made available in the past but are no longer available. These sources provided original data files or FID so that the user can change processing parameters and specify which regions of the spectra to display. The first database like this was the FTNMR FID Archive at Pacific Lutheran University<sup>26</sup> which contained H-1, C-13,

Received: May 15, 2023

Revised: July 31, 2023

Published: September 11, 2023



ACS Publications

© 2023 The Authors. Published by  
American Chemical Society and Division  
of Chemical Education, Inc.

3897

<https://doi.org/10.1021/acs.jchemeduc.3c00046>  
*J. Chem. Educ.* 2023, 100, 3897–3902

APT, and DEPT NMR spectra of organic compounds in the NUTS data format. Another NMR database project was the Spectral Database for Instructors<sup>27</sup> which was hosted at the University of Minnesota. This database allowed users to share NMR data files in the original instrument file format. It included many different NMR experiments and was a rich source of data for more complex compounds.

This project meets the needs of undergraduate faculty and students by providing a single data set that includes IR, MS, <sup>1</sup>H NMR, <sup>13</sup>C NMR, DEPT, and 2D NMR data in a format that allows viewing, processing, and analysis of data that is easy to copy and paste as needed. The compounds and spectra included in the data set are selected to provide teaching examples and unknowns that are appropriate for undergraduate courses. The data set also includes 33 of the 204 compounds selected by Araneda et al.<sup>28</sup> to avoid second-order effects with benchtop NMR spectrometers. The spectra in this database were used by the authors for teaching organic chemistry, instrumental analysis, and advanced synthesis and spectroscopy courses at the undergraduate level. The complete data set is included in the [Supporting Information](#) so that it will remain available for future use.

There are several software packages available for processing NMR data but only a few programs for viewing and processing IR, MS, and NMR data. Mnova was selected for this project because it can import all the data formats used to create this database, including IR, MS, and NMR data from the Bruker, Hewlett-Packard, Shimadzu, Finnigan, and PerkinElmer instruments used by the authors. In addition, Mnova supports Windows, MAC, and Linux operating systems, so the database is not platform dependent. Mnova started as the freeware 1D NMR data processing program MestRe-C in 1996. It has developed into Mnova which is a fully featured spectroscopic data processing program. The data files can include multiple spectra from different techniques so that a single document can contain all of the data for a compound or for a lecture topic. Although the software is no longer free, Mnova is available at a significant academic discount. Faculty with a software license can easily view, process, and format data to create lectures, problem sets, and unknowns for students. With a site license, it is easy to distribute the software to students so that they can view, process, and format data.

## EXPERIMENTAL SECTION

Most compounds in the database were purchased from commercial suppliers, including Sigma-Aldrich and Fisher Scientific. Many of the esters were synthesized by undergraduate students using Fischer esterification of the corresponding carboxylic acid and alcohol in the presence of sulfuric acid as a catalyst.

IR data were acquired using a PerkinElmer Spectrum Two FTIR spectrometer with a UTAR Two diamond anvil ATR attachment (450–4000 cm<sup>-1</sup>, 4 scans, 4 cm<sup>-1</sup> resolution). Files were saved as PerkinElmer IR files and imported into Mnova.

MS data were acquired using a Hewlett-Packard 5989B mass spectrometer or a Shimadzu QP 2020 NX GC/MS. All spectra were collected using 70 eV EI, liquid samples were introduced directly using neat injection, and solids were introduced using a heated direct insertion probe. Data files were imported into Mnova, and the instrument background was subtracted. Chemical ionization spectra were collected using a Finnigan 4000 mass spectrometer with methane CI. All mass spectrometry spectra were compared with the 2011 NIST/

EPA/NIH Mass Spectral Library<sup>29</sup> to confirm sample purity and identity.

NMR data were acquired using a Bruker AVANCE 400 NMR running topspin 2.1 under CentOS 7. A small number of spectra were acquired using a Nicolet QE 300. Most compounds in the database include <sup>1</sup>H-1, <sup>13</sup>C-13, DEPT 45, DEPT 90, DEPT 135, COSY, and one or more proton–carbon correlation 2D experiments. For most compounds, an inverse gradient probe was used, and proton detected HMQC spectra were acquired for the proton–carbon correlation experiment; however, carbon detected HETCOR data are provided for some compounds. For spectra acquired with the QE 300 only, HETCOR spectra are provided for proton–carbon correlation. HMBC data are included for long-range proton–carbon correlations of most compounds in the database. For a few compounds, NOESY spectra are included to demonstrate through-space proton–proton coupling. Most NMR samples were prepared in deuterated chloroform, with TMS added as a chemical shift reference. For samples that were not soluble in chloroform, deuterated dimethyl sulfoxide or a mixture of dimethyl sulfoxide and chloroform was used. All NMR spectra were processed and checked against the structure.

## RESULTS AND DISCUSSION

The spectra in this database have been used by the authors for teaching organic chemistry, instrumental analysis, and

**Table 1. C2–C4 Compounds Available for Synthesis Problems<sup>a</sup>**

C#	Alcohol	Aldehyde/Ketone	Carboxylic Acid	Other Functional Groups
C2	ethanol	ethanal	acetic acid	acetic anhydride
C3	1-propanol	propanal	propanoic acid	propionyl chloride propionic anhydride
	2-propanol	acetone		2-bromopropane 2-propanamine
C4	1-butanol	butanal	butanoic acid	butanoic chloride butanoic anhydride
	2-butanol	2-butanone		2-bromobutane 2-butanamine
	2-methyl-1-propanol	2-methyl-propanal	2-methyl-propanoic-acid	2-methyl-1-propanamine 2-methyl-propanoic-anhydride
	2-methyl-2-propanol			<i>t</i> -butyl-amine
		crotonaldehyde	<i>trans</i> -crotonic-acid	

<sup>a</sup>A complete listing that includes C2–C8 and C10 compounds is provided in the [Supporting Information](#).

advanced synthesis and spectroscopy courses at the undergraduate level. The examples, lectures, and worksheets discussed below have been used in teaching these courses, and many of the spectra in the data set have been used as student unknowns. Faculty using this data set for teaching should be aware that spectra include solvent peaks and impurities that may surprise students who have only seen textbook spectra.

Table 2. Esters and Precursors in the Database

	Ethyl	Propyl	Butyl	2-Ethylbutyl	2-Methylpropyl	2-Methylbutyl	Hexyl	Decyl
formate	ethyl formate							
acetate	ethyl acetate	propyl acetate	butyl acetate	2-ethylbutyl acetate	2-methylpropyl acetate	2-methylbutyl acetate	hexyl acetate	decyl acetate
propanoate	ethyl propanoate			2-ethylbutyl propanoate		2-methylbutyl propanoate		decyl propanoate
butanoate	ethyl butanoate		butyl butanoate	2-ethylbutyl butanoate	2-methylpropyl butanoate	2-methylbutyl butanoate	hexyl butanoate	decyl butanoate
3-methyl butanoate	ethyl 3-methyl butanoate			2-ethylbutyl 3-methyl butanoate		2-methylbutyl 3-methyl butanoate	hexyl 3-methyl butanoate	decyl 3-methyl butanoate
heptanoate	ethyl heptanoate			2-ethylbutyl heptanoate		2-methylbutyl heptanoate		
additional esters	methyl 3-methyl butanoate methyl 2-chloro propanoate ethyl cinnamate methyl salicylate ethyl <i>trans</i> -crotonate methyl benzoate ethyl acetate							

### Full Data Set

The database consists of 2337 spectra for 251 different compounds as Mnova workbook files. Of the 247 compounds in the data set with H-1 and C-13 NMR data:

- 241 also include DEPT and 2D NMR for H–H and C–H correlation
- 204 also include the above plus IR and MS
- 180 of these include the above plus HMBC for long-range C–H correlation

The [Supporting Information](#) includes a spreadsheet file listing all of the compounds in the database and includes the chemical formula, CAS number, functional groups, and the type of spectra available for each compound. This spreadsheet also includes lists of compounds sorted by carbon count; matching molecular formulas; alcohols with possible reaction products; and lists of all aromatic, alcohol, carbonyl, alkene, nitrogen containing compounds, anhydrides, esters, ethers, and halogens. The spreadsheet file allows users to search and sort to identify data to use for creating lectures, exercises, and unknowns.

The Mnova workbook files for each compound in the database are provided in a single zip file in the [Supporting Information](#). Wherever possible identifying information is removed from the file so that instructors can easily create unknowns for students. When files are imported Mnova does preserve header information from the original data file so some identifying information may be recoverable but every effort was made to remove links and direct display of this information. Instructors can distribute the data files to students as Mnova data files that they can process and analyze, as PDF files, or as images that can be copied and pasted into other applications.

### Examples, Lectures, and Worksheets

To demonstrate how instructors can use the spectra from this data set for teaching, two example problem sets used for teaching the second semester of organic chemistry are included in the [Supporting Information](#). These problems exemplify how students can use molecular formulas, IR, H-1 NMR, and C-13 NMR to determine the structure of an unknown compound.

Additional compounds from the larger data set were selected for a variety of common undergraduate learning objectives.

These demonstrate experimental techniques, important interpretation skills, data acquisition and processing, and unknown determination strategies. These files are available in a separate zip file available in the [Supporting Information](#). A list of the compounds included in each data set is included in the [Supporting Information](#). The topics covered and a summary of the information provided are listed below.

**NMR: Introduction to Interpretation—C<sub>4</sub>H<sub>10</sub>O.** This worksheet is used to introduce how NMR is used for determining the molecular structure. It is appropriate for use in general chemistry when teaching Lewis dot structures, showing how chemists use NMR to determine the structures of different compounds. It could also be used in organic chemistry when NMR interpretation is first introduced. The worksheet includes C-13 and H-1 spectra for five different compounds with the molecular formula C<sub>4</sub>H<sub>10</sub>O. Structures are easily distinguished using the carbon spectra to determine symmetry and the integration data from the proton spectra.

**NMR: Introduction to Interpretation—C<sub>5</sub>H<sub>10</sub>O.** This worksheet uses a larger set of compounds with slightly more complex spectra to introduce how NMR is used for determining the molecular structure. It is appropriate for use in general chemistry when teaching Lewis dot structures to show how chemists use NMR to determine the structures of different compounds. It could also be used in organic chemistry to introduce NMR interpretation. The worksheet includes C-13 and H-1 spectra for eight different compounds with the molecular formula C<sub>5</sub>H<sub>10</sub>O. Distinguishing these structures requires using the carbon spectra to determine the symmetry, proton integration, and proton splitting.

**NMR: Introduction to NMR Unknown Interpretation.** This worksheet is used to teach students how to determine the structure of an unknown by using C-13 and H-1 NMR. Compounds are presented with an increasing level of complexity and show a variety of important features that are critical for using NMR to determine the structure of an unknown compound. Interpretation requires using proton integration, proton splitting, number of carbon peaks, carbon and proton chemical shift correlation tables, and carbon and proton chemical shift predictions.

**NMR: Introduction to DEPT: 2-Methyl-1-propanol.** This worksheet is used to introduce the information provided

in DEPT 45, DEPT 90, and DEPT 135 spectra. It uses 2-methyl-1-propanol as an example, showing the familiar decoupled carbon spectra acquired with the decoupler on, the coupled carbon spectrum with no decoupling, the gated decoupling spectrum which looks like the coupled carbon spectrum but also includes the NOE enhancement, and the inverse gated decoupling spectrum, which is decoupled but without NOE enhancement. These spectra show the information available in the coupling and the importance of NOE to improve the S/N level in carbon NMR. Finally the DEPT 45, DEPT 90, and DEPT 135 spectra are provided to show how these spectra provide the same information but with a large signal enhancement produced by the polarization transfer in the DEPT experiment. With these spectra, it is easy to identify quaternary, methine, methylene, and methyl carbons. The spectra can be used for a traditional lecture presentation or as a guided inquiry exercise in which students discover what information is available in each of the DEPT spectra.

**NMR: Introduction to DEPT:  $C_5H_{10}O$  Unknown.** This second worksheet for teaching DEPT interpretation is designed as an unknown for students after completing the Introduction to DEPT: 2-methyl-1-propanol example. The unknown is 2-methyl-3-buten-2-ol,  $C_5H_{10}O$ . The NIST Chemistry WebBook lists 77 matching species for this formula. Identifying the C, CH,  $CH_2$ , and  $CH_3$  carbons using DEPT and then using integration from the proton NMR to find that the methyl carbons are symmetric and not coupled allows students to quickly identify the correct structure. For students who have struggled to identify unknowns using NMR data, this example clearly shows the value of the additional information provided by DEPT spectra. Because correct phasing of the spectra is critical for interpreting DEPT spectra, the DEPT 135 spectrum is shown with the phase that results from an autophase routine. This is not the expected phasing for a DEPT 135 spectrum, and the methine and methyl carbon peaks are inverted from the expected orientation. Students should be able to identify this problem to correctly interpret the spectra. This is an opportunity to reinforce different phasing techniques that are used for data analysis so that students do not rely entirely on autophase routines.

**NMR: Introduction to 2D Lectures.** This series of worksheets is designed for introducing 2D NMR interpretation. For each compound, the H-1, C-13, DEPT, COSY, and HMQC spectra are provided. The spectra of 2-methyl-1-propanol, allyl butyl ether, and butanoic acid are provided so that students can decipher the structural information available from each of the 2D experiments. Pamoic acid is provided as an example in which students can work through the NMR data to unambiguously determine the structure of a relatively complex molecule.

1. **Example 1: 2-methyl-1-propanol.** The alcohol and methine protons overlap, and DEPT and HMQC used together clearly identify the methine proton. A proton spectrum for a sample at a different concentration shows the alcohol proton chemical shift moves so it does not overlap with the methine. An unprocessed COSY spectrum is included for demonstrating 2D processing steps that include symmetrizing and setting the F1 and F2 reference frequencies so the 2D spectrum lines up with the 1D traces.

2. **Example 2: Allyl butyl ether.** This example shows how 2D spectra allow the user to connect proton and carbon data and then use splitting and COSY to connect methyl, methylene, and methine carbons to easily determine the structure.
3. **Example 3: Butanoic acid.** This example adds HMBC to the previous spectra to demonstrate how long-range C–H coupling can show the connectivity of a quaternary carbon.
4. **Example 4: Pamoic acid.** This example shows how 2D spectra allow the unambiguous structural determination of a more complex compound. NOESY data are provided in addition to H-1, C-13, DEPT, COSY, and HETCOR. This helps distinguish between two possible arrangements for the carboxylic acid and alcohol substituents without relying on chemical shift. Predicted H-1 and C-13 spectra are provided for final confirmation of the structure.

**NMR: Data Acquisition and Processing.** These spectra are provided for teaching data acquisition parameters and data processing techniques that are important for improving the S/N and resolution of NMR spectra. The first set of spectra is for demonstrating ways to improve the S/N by increasing the number of scans during data acquisition or using apodization functions during data processing. The second set of data shows ways to improve the resolution by increasing the number of data points during data acquisition, by zero filling during data processing, or by using apodization functions during data processing.

1. S/N Enhancement—2-methyl-2-butanol C-13
  - a. Number of Scans: 4, 64, 512
  - b. Apodization: LB 1, EM
2. Resolution Enhancement—propanal
  - a. Data Points and Zero Fill; 4k, 8k, 16k, 32k (ZF)
  - b. TRAF function

**NMR Advanced Experiments.** These spectra are included to show some advanced NMR experiments that use different pulse sequences to demonstrate important data acquisition parameters. This includes a variety of decoupler experiments—decoupled, gated decoupling, inverse gated decoupling, and coupled spectra. These experiments demonstrate important concepts for understanding 2D data acquisition by showing how decoupler pulses can manipulate the spin states and demonstrate signal enhancement by NOE. There are also spectra showing selective proton decoupling and the T1 Inversion Recovery experiment for both proton and carbon. These are useful for explaining 2D data acquisition parameters and ways that pulse sequences can manipulate the spin state.

1. 2-Methyl-1-propanol
  - a. Carbon—decoupled
  - b. Carbon—coupled
  - c. Carbon—gated decoupling
  - d. Carbon—inverse gated decoupling
  - e. Attached proton
2. Pamoic acid
  - a. Selective proton decoupling
  - b. T1IR—Proton
  - c. T1IR—Carbon

**Mass Spectrometry: Introduction.** This file includes a large number of spectra to use for mass spectral interpretation. The spectra are divided into a series of different examples that



demonstrate different features commonly used for interpretation. In most cases, there are more examples than would typically be used so instructors are encouraged to select spectra they want to use for teaching. Major topics include:

- Isotope abundance using one to three chlorine atoms and two examples of brominated compounds. The examples are selected to show how useful isotope distributions are for identifying certain elements but also to show how mass spectrometry is not always useful for distinguishing isomers like 1,2-dichlorobenzene and 1,3-dichlorobenzene. Includes: benzene, chlorobenzene, bromobenzene, 1,2-dichlorobenzene, 1,3-dichlorobenzene, trichloroethene, 1-bromopropane, and 2-bromopropane.
- Linear alkanes from C5–C10 and C16. To demonstrate fragmentation, identifying molecular ions, and determining the number of carbon atoms from the C-13 isotope distribution.
- Primary alcohols from methanol to octanol. To identify molecular ions, loss of water, and  $\beta$ -cleavage formation of  $\bullet\text{CH}_2\text{OH}^{1+}$  at  $m/z$  31.
- Primary vs secondary alcohols from propanol through pentanol. To identify molecular ions, loss of water, and  $\beta$ -cleavage formation of  $\bullet\text{CH}_2\text{OH}^{1+}$  at  $m/z$  31 and other fragmentation pathways.
- Branching and fragmentation for four different butanols. To identify molecular ions, loss of water, and  $\beta$ -cleavage formation of  $\bullet\text{CH}_2\text{OH}^{1+}$  at  $m/z$  31 and other fragmentation pathways.
- Alkenes. Molecular ions, fragmentation, and rearrangement. Includes: pentane, 1-pentene, 2-pentene, hexane, and 1-hexene.
- Aldehydes from propanal to heptanal. Molecular ions, fragmentation, and McLafferty rearrangement.
- Ketones from propanone through heptanone. Molecular ions, fragmentation, and McLafferty rearrangement.
- Carboxylic acids from acetic acid to octanoic acid. Molecular ions, fragmentation, and rearrangement.
- Amines. Molecular ions using the nitrogen rule and fragmentation. Includes propyl amine and diethyl amine.
- Aromatic. Benzene shows a very high molecular ion abundance characteristic of aromatic systems at  $m/z$  78. Toluene shows a high abundance of the aromatic tropylium ion at  $m/z$  91 characteristic of benzyl compounds. Phenol shows a very high molecular ion abundance at  $m/z$  94 and a rearrangement at  $m/z$  66 caused by loss of  $\bullet\text{CO}$  through a keto–enol tautomerization.<sup>13</sup>
- Heptane, heptanal, heptanone, and heptanoic acid. Molecular ions, fragmentation, and the McLafferty rearrangement.

**Mass Spectrometry: C5 Compounds.** This set contains 22 different compounds with five carbon atoms. They include alkanes, alkenes, alcohols, aldehydes, ketones, carboxylic acids, anhydrides, and a chloride. This collection can be used for lectures or worksheets on MS interpretation and unknowns.

**Mass Spectrometry: C6 Compounds.** This set contains seven different compounds with six linear six-carbon chains. They include alkane, alkene, alcohol, aldehyde, ketone, and carboxylic acid derivatives. This collection can be used for lectures or worksheets on MS interpretation and unknowns.

**Mass Spectrometry: Chemical Ionization.** This set includes 70 eV EI and methane CI data for two compounds that demonstrate a large increase in the quasimolecular ion and a reduction in fragmentation. The EI spectrum for *n*-hexadecane shows a molecular ion abundance less than 3% and extensive fragmentation, while the methane chemical ionization spectrum shows reduced fragmentation and a  $[\text{M} - \text{H}]^{1+}$  ion with almost 30% abundance. The EI spectrum for tributylamine shows a molecular ion at  $m/z$  185 with less than 5% abundance, with almost all ions undergoing loss of  $\bullet\text{C}_4\text{H}_9$  to give  $m/z$  142. The CI spectrum for tributylamine gives a  $[\text{M} + \text{H}]^{1+}$  ion at  $m/z$  186 with an abundance of almost 50%.

**Mass Spectrometry: Interpretation Lecture.** This set includes five examples to use for teaching the interpretation of mass spectra as unknowns. It includes a table of isotope distributions and a list of common elemental compositions for several molecular ions extracted from tables available in McLafferty's *Interpretation of Mass Spectra*.<sup>10</sup> Five unknowns are given to provide an opportunity to introduce strategies for identifying molecular ions, identifying isotope distributions, identifying characteristic fragmentation patterns, and distinguishing between isomers.

**Infrared Spectroscopy: Lecture.** This set includes IR spectra that demonstrate some of the most useful bands commonly used for structural interpretation using infrared spectroscopy. It includes butane with alcohol, aldehyde, ketone, carboxylic acid, and amine functional groups.

**Synthesis Problems.** Another significant feature of this data set is that it is also designed to support teaching organic synthesis. The data set includes compounds with a common carbon skeleton but different functional groups including alcohols, aldehydes or ketones, carboxylic acids, acid chlorides, halogens, amines, anhydrides, esters, and ethers. These spectra are ideal for showing changes in spectra that are characteristic of different functional groups and to accompany lectures or problem sets demonstrating chemical reactions and modification of functional groups. The topics covered and a summary of the information provided are listed below.

Table 1 shows the C2–C4 compounds available in the data set organized by a structural framework. These compounds allow faculty teaching organic chemistry to select spectra that show products and reactants for reactions to transform alcohols, aldehydes or ketones, carboxylic acids, and several other functional groups. They are organized by common carbon skeletons. A more complete listing that includes C2–C8 and some C10 compounds is included in the [Supporting Information](#).

The database also contains a set of esters with their precursors, as shown in Table 2.

**Aromatic Compounds.** Aromatic compounds in the data set include 8 halogenated aromatics, 8 benzaldehyde derivatives, 8 aniline derivatives, 5 toluene derivatives, 5 acetophenone derivatives, 4 phenol derivatives, 4 benzoic acid derivatives, 2 pyridine derivatives, 4 vanillin derivatives, and 11 other assorted aromatic compounds.

## CONCLUSION

Interpretation of IR, MS, and NMR spectra is an important part of the undergraduate chemistry curriculum. The spectra provided as [Supporting Information](#) for this paper provide a wide range of spectra for use in lectures, worksheets, and unknowns for students.

## ■ ASSOCIATED CONTENT

### ■ Supporting Information

The Supporting Information is available at <https://pubs.acs.org/doi/10.1021/acs.jchemed.3c00046>.

List of all compounds in the database by name, formula, CAS No., alternate names, and type of spectra (XLSX)

A document with links to download the complete database from figshare, google drive, or icloud (PDF, DOCX)

List of compounds included in the lecture topic database (PDF, DOCX)

Organic chemistry example problem sets (ZIP)

Spectroscopy database spectra by lecture topics (ZIP)

## ■ AUTHOR INFORMATION

### Corresponding Author

Scott E. Van Bramer — Department of Chemistry, Widener University, Chester, Pennsylvania 19013, United States;  
orcid.org/0000-0002-1029-6031; Email: [sevanbramer@widener.edu](mailto:sevanbramer@widener.edu)

### Author

Lloyd D. Bastin — Department of Chemistry, Widener University, Chester, Pennsylvania 19013, United States

Complete contact information is available at:

<https://pubs.acs.org/10.1021/acs.jchemed.3c00046>

### Notes

The authors declare no competing financial interest.

## ■ ACKNOWLEDGMENTS

Thanks to Justin Delade for synthesizing many of the esters and acquiring IR and NMR data for these compounds. And thanks to Alex Quanvie and Andrew Devany for acquiring many of the IR spectra.

## ■ REFERENCES

- (1) Karty, J. *Organic Chemistry: Principles and Mechanisms*, 3rd ed.; W.W. Norton & Company: New York, 2022.
- (2) Wade, L.; Simek, J. *Organic Chemistry*, 9th ed.; Pearson: 2020.
- (3) McMurry, J. *Organic Chemistry*, 9th ed.; Cengage Learning: 2016.
- (4) Skoog, D. A.; Holler, F. J.; Crouch, S. R. *Principles of Instrumental Analysis*, 7th ed.; Cengage: 2017.
- (5) Robinson, J. W.; Skelly Frame, E. M.; Frame, G. M. *Undergraduate Instrumental Analysis*, 7th ed.; CRC Press: 2014.
- (6) Granger, R. M.; Yochum, H. M.; Granger, J. N.; Sienerth, K. D. *Instrumental Analysis: Revised ed.*; Oxford University Press: 2017.
- (7) Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L. *Spectrometric Identification of Organic Compounds*, 8th ed.; Wiley: 2014.
- (8) Pavia, D. L.; Lampman, G. M.; Kriz, G. S.; Vyvyan, J. A. *Introduction to Spectroscopy*, 5th ed.; Cengage: 2014.
- (9) Pretsch, E.; Bühlmann, P.; Badertscher, M. *Structure Determination of Organic Compounds: Tables of Spectral Data*, 5th ed.; Springer: 2020.
- (10) Field, L. D.; Li, H. L.; Magill, A. M. *Organic Structures from Spectra*, 6th ed.; Wiley: 2020.
- (11) Taber, D. F. *Organic Spectroscopic Structure Determination: A Problem-Based Learning Approach*, 1st ed.; Oxford University Press: 2007.
- (12) Lambert, J. B.; Gronert, S.; Shurvell, H. F.; Lightner, D. C.; Cooks, R. G. *Organic Structural Spectroscopy*, 2nd ed.; Pearson: 2010.
- (13) Breitmaier, E. *Structure Elucidation by NMR in Organic Chemistry: A Practical Guide*, 3rd ed.; Wiley: 2002.
- (14) Sanders, J. K.; Hunter, B. K. *Modern NMR Spectroscopy: A Guide for Chemists*, 2nd ed.; Oxford University Press: 1993.
- (15) Lambert, J. B.; Mazzola, E. P.; Ridge, C. D. *Nuclear Magnetic Resonance Spectroscopy: An Introduction to Principles, Applications, and Experimental Methods*, 2nd ed.; Wiley: 2019.
- (16) Abraham, R. J.; Fischer, J.; Loftus, P. *Introduction to NMR Spectroscopy*; Wiley: 1992.
- (17) McLafferty, F. W.; Tureek, F. *Interpretation of Mass Spectra*, 4th ed.; University Science Books: 1993.
- (18) Spectral Databases — Wiley Science Solutions. <https://sciencesolutions.wiley.com/spectral-databases/> (accessed October 1, 2022).
- (19) AIST: Spectral Database for Organic Compounds SDBS. <https://sdb.sdb.aist.go.jp> (accessed October 1, 2022).
- (20) Aldrich SpectralViewer, FT-IR and FT-NMR library. [www.sigmaaldrich.com](http://www.sigmaaldrich.com) (accessed October 1, 2022).
- (21) NIST Chemistry WebBook. <https://webbook.nist.gov/chemistry/> (accessed October 1, 2022).
- (22) JCAMP-DX — International Union of Pure and Applied Chemistry (IUPAC). <https://iupac.org/what-we-do/digital-standards/jcamp-dx/> (accessed October 1, 2022).
- (23) Jmol download. SourceForge.net. <https://sourceforge.net/projects/jmol/> (accessed October 1, 2022).
- (24) Graham, K. J.; McIntee, E. J.; Schaller, C. P. Web-Based 2D NMR Spectroscopy Practice Problems. *J. Chem. Educ.* **2016**, 93 (8), 1483–1485.
- (25) Socha, O.; Osifova, Z.; Dracinsky, M. NMR-Challenge.com: An Interactive Website with Exercises in Solving Structures from NMR Spectra. *J. Chem. Educ.* **2023**, 100, 962.
- (26) Fryhle, C. B.; Waldow, D. A.; Bock, J. C. The FT-NMR Free Induction Decay Archive. *J. Chem. Educ.* **1997**, 74 (4), 442.
- (27) Kalstabakken, K. A.; Harned, A. M. Spectral Database for Instructors: A Living, Online NMR FID Database. *J. Chem. Educ.* **2013**, 90 (7), 941–943.
- (28) Araneda, J. F.; Mendonça, T. M.; Hui, P.; Leclerc, M. C.; Ma, J.; Maier, A. F.; Riegel, S. D. Incorporating Benchtop NMR Spectrometers in the Undergraduate Lab: Understanding Resolution and Circumventing Second-Order Effects. *J. Chem. Educ.* **2021**, 98 (4), 1227–1232.
- (29) NIST Mass Spectral Search Program for the NIST/EPA/NIH Mass Spectral Library, Version 2.0 g, build May 19, 2011.