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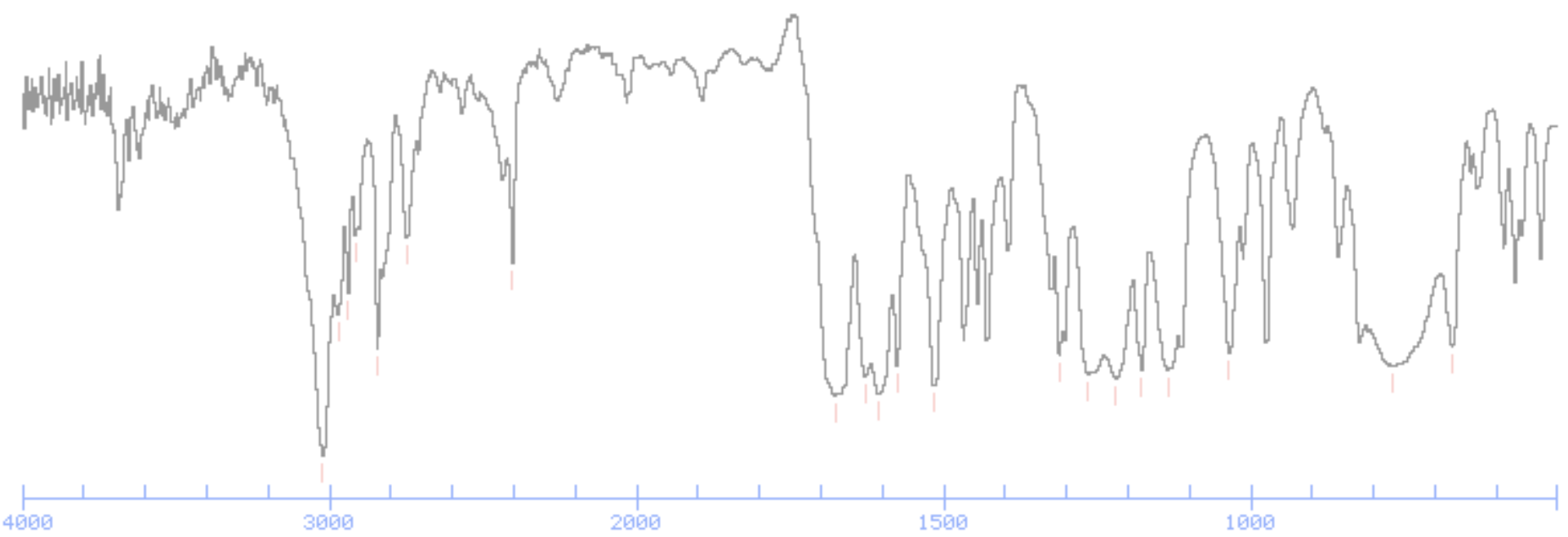


WebSpectra

An Organic Chemistry LO

Renata Everett and Grace Winschel
MELO3D Meeting, June 14, 2011
University of Michigan, Ann Arbor

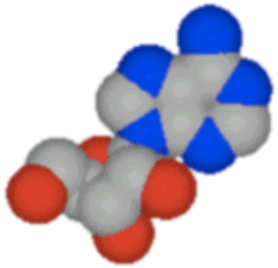
WebSpectra

- Spectroscopy is a widely used identification technique in Organic Chemistry
- Many students learning introductory spectroscopy in CH216 struggle to learn how to interpret spectra
- Website provides 1H-NMR, 13C-NMR, IR, COSY and DEPT spectra practice problems and solutions.

Website can be found at: http://www.merlot.org/merlot/viewMaterial.htm?id=88400

WebSpectra

Problems in NMR and IR Spectroscopy



Welcome to WebSpectra - This site was established to provide chemistry students with a library of spectroscopy problems. Interpretation of spectra is a technique that requires practice - this site provides ^{1}H NMR and ^{13}C NMR, DEPT, COSY and IR spectra of various compounds for students to interpret. Hopefully, these problems will provide a useful resource to better understand spectroscopy.

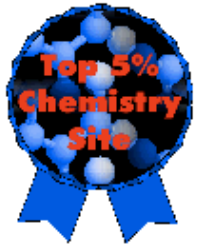
This project is supported by Cambridge Isotope Laboratories and the UCLA Department of Chemistry and Biochemistry.

Project Director Professor Craig A. Merlic
NMR Facility Contributor Dr. Jane Strouse

Instructional Documents

- Solving Spectral Problems
- Overview of NMR Spectroscopy
- Notes on NMR Solvents
- Types of NMR Spectra
- Introduction to IR Spectra
- Table of IR Absorptions

Awards



Why This is a Great LO:

- Drill and Practice
- Instruction manual provided
- Range of difficulty levels
- Solutions provided
- Helpful links to other spectroscopy tools and information

Beginning Problem #1

$C_4H_8O_2$
NMR Solvent: $CDCl_3$

[^{1}H NMR Spectrum]
[^{13}C NMR Spectrum]

[View Structure Solution]

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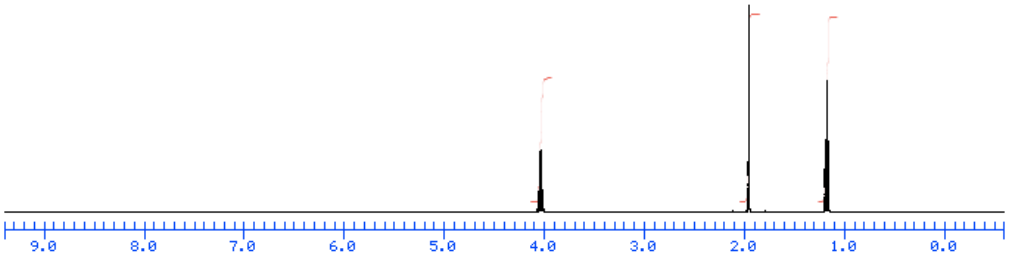
^{1}H NMR Spectrum - $C_4H_8O_2$

[^{13}C NMR Spectrum]
[Back to Problem]

Peaks: 4.0665 ppm (1627.13 Hz) Zoom to Peak



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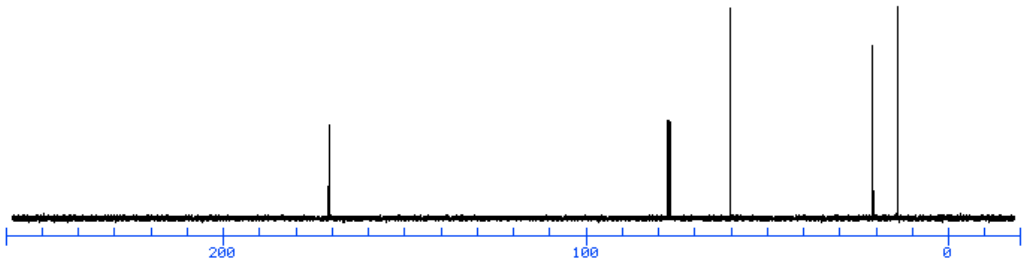
^{13}C NMR Spectrum - $C_4H_8O_2$

[^{1}H NMR Spectrum]
[Back to Problem]

Peaks: 170.939 ppm Zoom to Peak



Zoom to range: to ppm Zoom

Spectrum may be magnified 16X by clicking on peaks of interest

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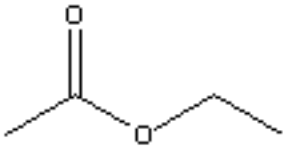
ethyl acetate
ethyl ethanoate



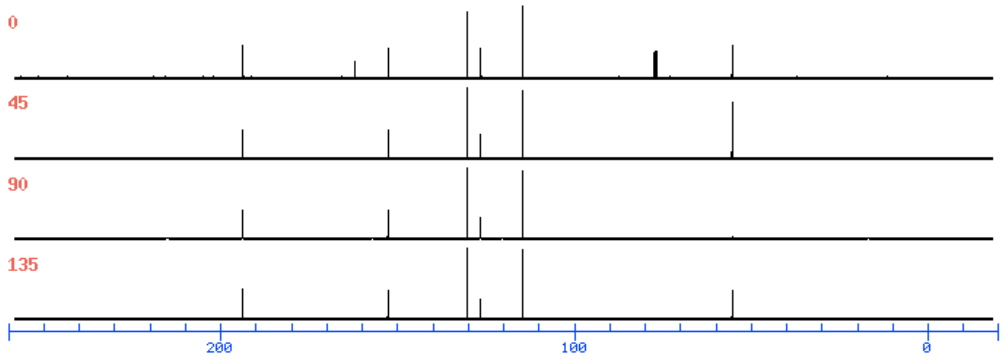
What Needs Improvement:

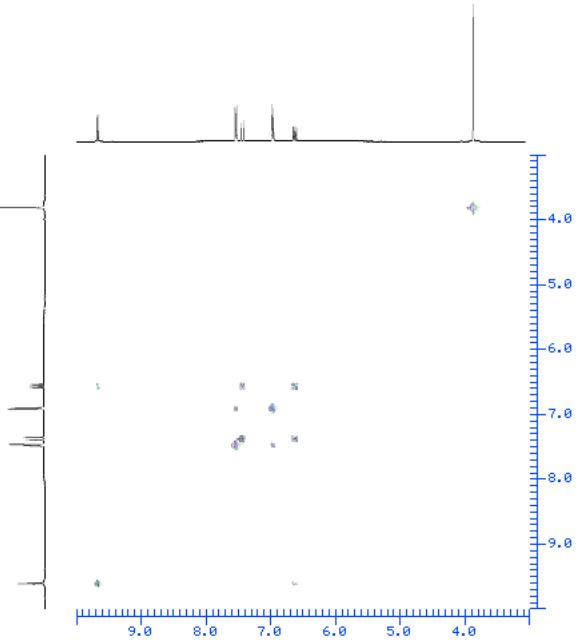
- Some problems are too advanced for the undergraduate coursework at Michigan
  - Needs a slightly modified wrapper
- Limited amount of problems
- Unsightly

DEPT Spectra - $C_{10}H_{10}O_2$

IR Spectrum
^{1}H NMR Spectrum
^{13}C NMR Spectrum
COSY Spectrum
Back to Problem

Peaks: 193.697 ppm Zoom to Peak





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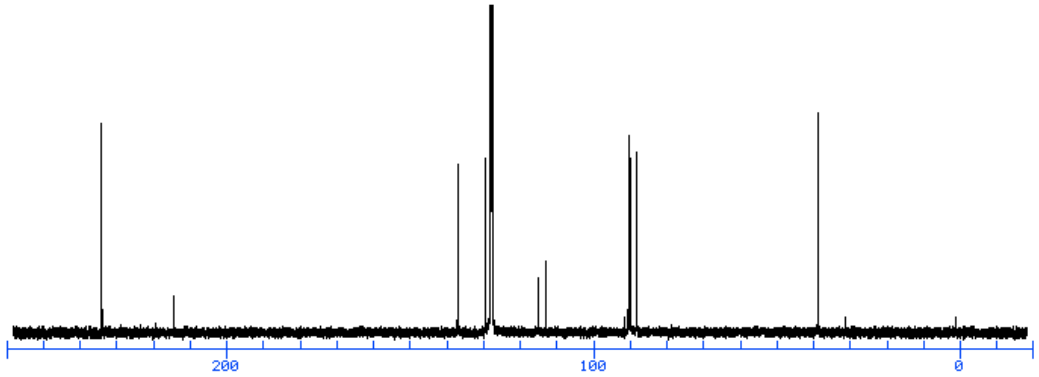
^{13}C NMR Spectrum - $C_{12}H_8CrO_3$

^{1}H NMR Spectrum
Back to Problem

Peaks: 234.104 ppm Zoom to Peak



Zoom to range: to ppm Zoom

Spectrum may be magnified 16X by clicking on peaks of interest

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