

Author(s): MELO 3D Project Team, 2011

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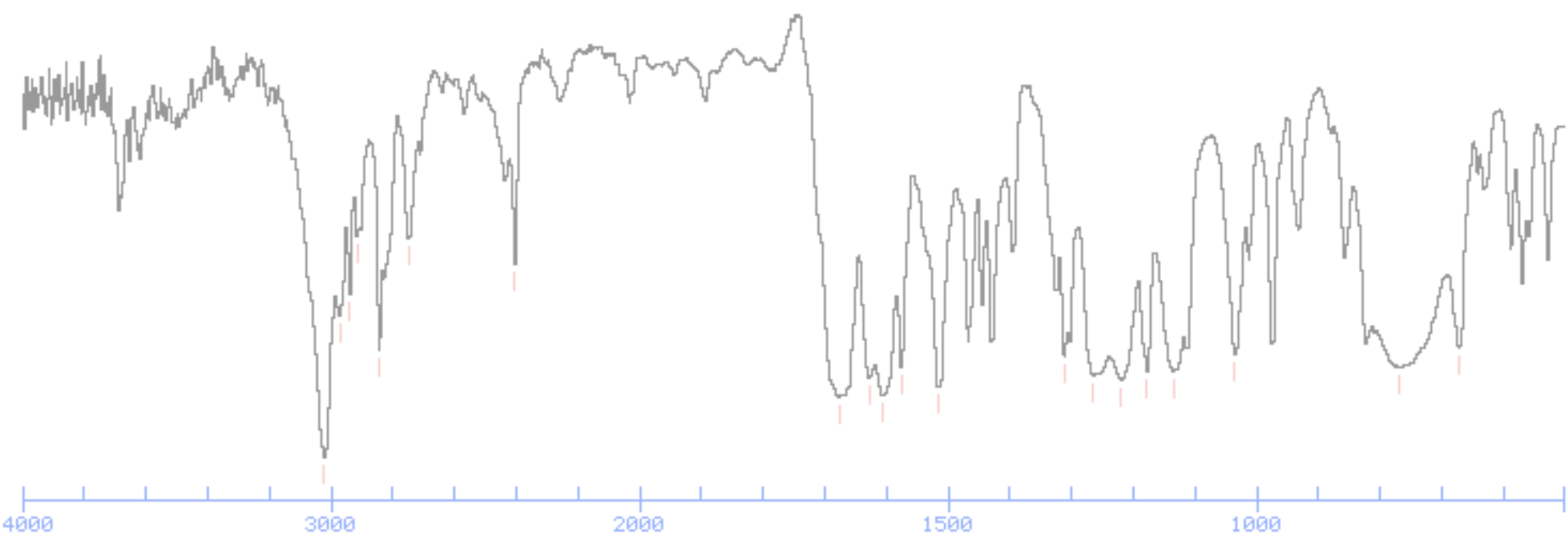
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WebSpectra

An Organic Chemistry LO

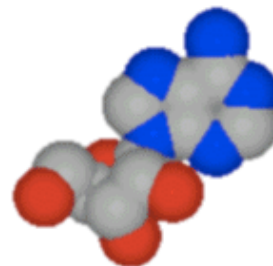
Renata Everett and Grace Winschel
MELO3D Meeting, June 14, 2011
University of Michigan, Ann Arbor

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, ^{13}C -NMR, IR, COSY and DEPT spectra practice problems and solutions.

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 ^1H 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

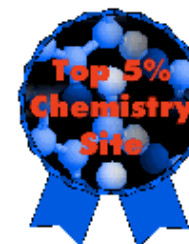


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Instructional Documents

- [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: $CDCl_3$

[\$^1H\$ NMR Spectrum](#)

[\$^{13}C\$ NMR Spectrum](#)

[View Structure Solution](#)

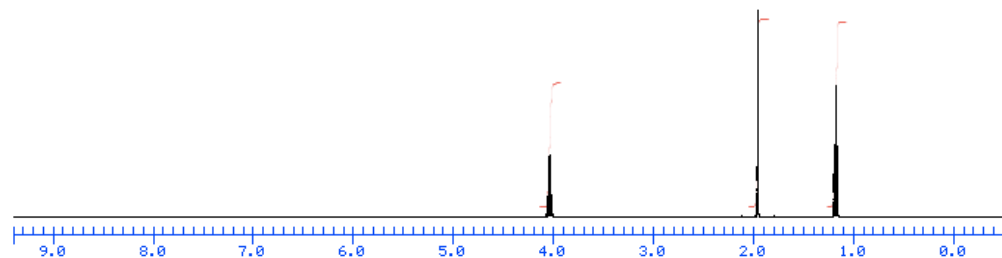
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1H NMR Spectrum - $C_4H_8O_2$

[\$^{13}C\$ NMR Spectrum](#)

[Back to Problem](#)

Peaks: 4.0665 ppm (1627.13 Hz)



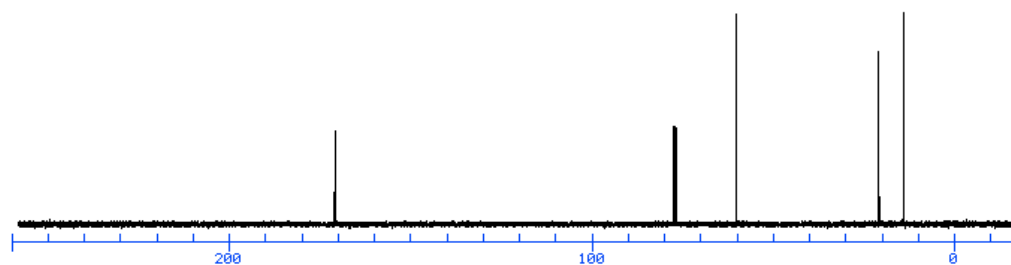
^{13}C NMR Spectrum - $C_4H_8O_2$

[\$^1H\$ NMR Spectrum](#)

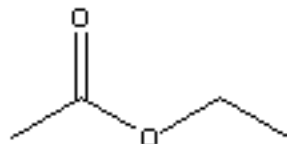
[Back to Problem](#)

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Peaks: 170.939 ppm



ethyl acetate
ethyl ethanoate



Zoom to range: to ppm

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

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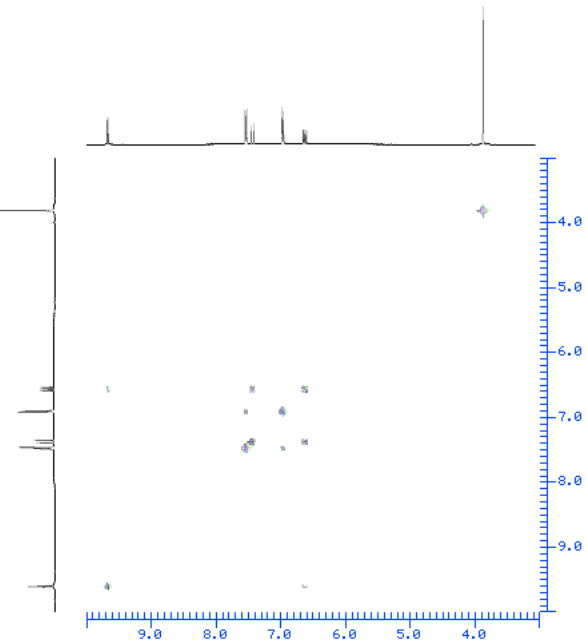
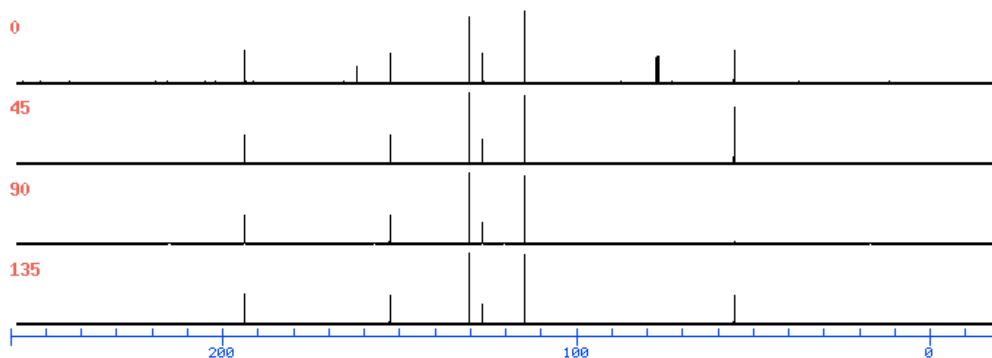
What Needs Improvement:

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

DEPT Spectra - C₁₀H₁₀O₂

[IR Spectrum](#)
[¹H NMR Spectrum](#)
[¹³C NMR Spectrum](#)
[COSY Spectrum](#)
[Back to Problem](#)

Peaks:

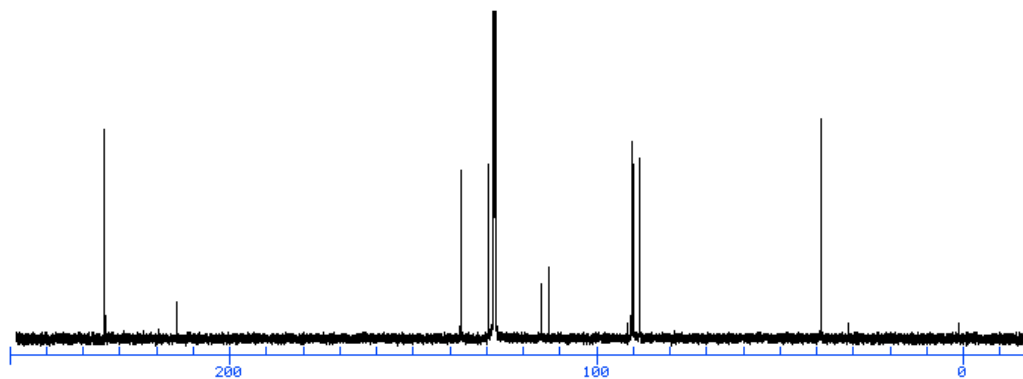


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¹³C NMR Spectrum - C₁₂H₈CrO₃ [¹H NMR Spectrum](#) [Back to Problem](#)

Peaks:



Zoom to range: to ppm

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

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