Chem115 Fall 2023 - Ilana Berlin/Lab10: NMR Spectroscopy II: Spin-Spin Coupling/LabReport10

Jason Cody - Nov 18, 2023, 7:16 PM CST

Assignment #20 - LabReport10

You cannot edit this entry after it is graded.

Description	NMR II-Splitting
I worked in a group with	
The work for this assignment is in	My notebook

Grade **9.5 / 10**

Graded on Nov 18, 2023, 7:16 PM CST

Jason Cody - Oct 01, 2021, 10:37 AM CDT

TITLE: *(insert experimental title here. All italicized text in parentheses should be followed and then deleted throughout this template).*

Purpose: *(insert experimental purpose here).*

Reference: Kauley, L. J., *Introduction to Chemistry in the Laboratory*, 20th Ed., Lake Forest College, **2021**, Experiment xx, Appendix xx. *(Edit the experiment title and/or appendix letter; add other references, if used, following the same format).*

Observation and Data: *(Write your clear, concise, complete, past tense, passive voice description or narrative of the experiment as the experiment is performed. Complete sentences are used throughout.*
If needed, insert tables and edit the header: Table 1. Preparation of Standard Solutions.
If needed, insert figures and edit this caption below the figure: Figure 1. Beer's Law Plot of B12 Standard Solutions at λ = 520 nm. Number tables and figures in order of appearance in the report.)

Calculations: *(insert sample calculation here, if relevant. Otherwise, delete this section entirely).*

Conclusion: *(restate the quantitative values (percent error and/or CV) to indicate how well the goals of the experiment have been met; answer any questions in the experimental instructions, too).*

ReportTemplate.docx (15.5 kB)

Jason Cody - Oct 25, 2020, 11:04 AM CDT

Please insert RichText entries below the headings for the text you wish to include for each section.

Jason Cody - Oct 22, 2020, 11:38 AM CDT

Date and Title

Ilana Berlin - Nov 13, 2023, 12:08 PM CST

NMR Spectroscopy II

11/12/2023

Jason Cody - Oct 22, 2020, 11:38 AM CDT

Purpose

Jason Cody - Nov 18, 2023, 7:13 PM CST

Two unknown organic compounds will be scanned by 60 MHz proton nuclear magnetic resonance (NMR). By comparing the data from the NMR and to prediction made of 10 organic compounds (p-anisaldehyde, 4'-chloropropiophenone, 3-chloropropionic acid, 3-chloropropionitrile, diethyl malonate, ethyl acetate, 4-ethylaniline, 2-iodopropane, isopropyl acetate, and 4-isopropylbenzaldehyde) the compounds will be identified. OK, what spectral features will be predicted?

Jason Cody - Oct 22, 2020, 11:38 AM CDT

Reference

Jason Cody - Nov 18, 2023, 7:13 PM CST

(1) Kateley, L. J., *Introduction to Chemistry in the Laboratory, 20th Ed*., Lake Forest College, **2021**, Experiment 10, Appendix F.

(2) *MilliporeSigma | United States*. www.sigmaaldrich.com. https://www.sigmaaldrich.com/US/en. OK

Jason Cody - Oct 22, 2020, 11:38 AM CDT

Data and Observations

Jason Cody - Nov 18, 2023, 7:14 PM CST

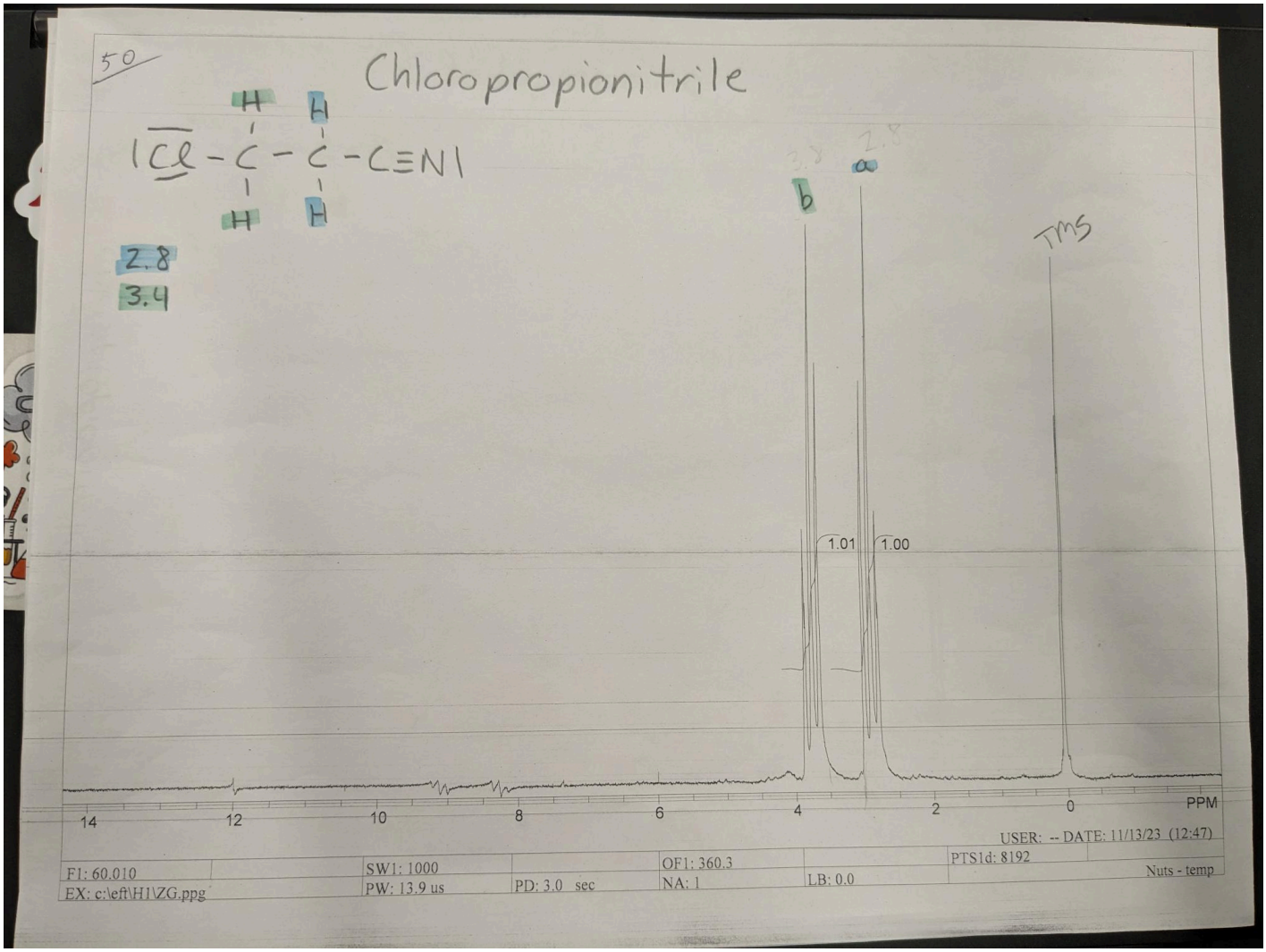


Figure 1 Sample 50 - Chloropropionitrile OK, but be careful to consider the assignment a conclusion, not data.

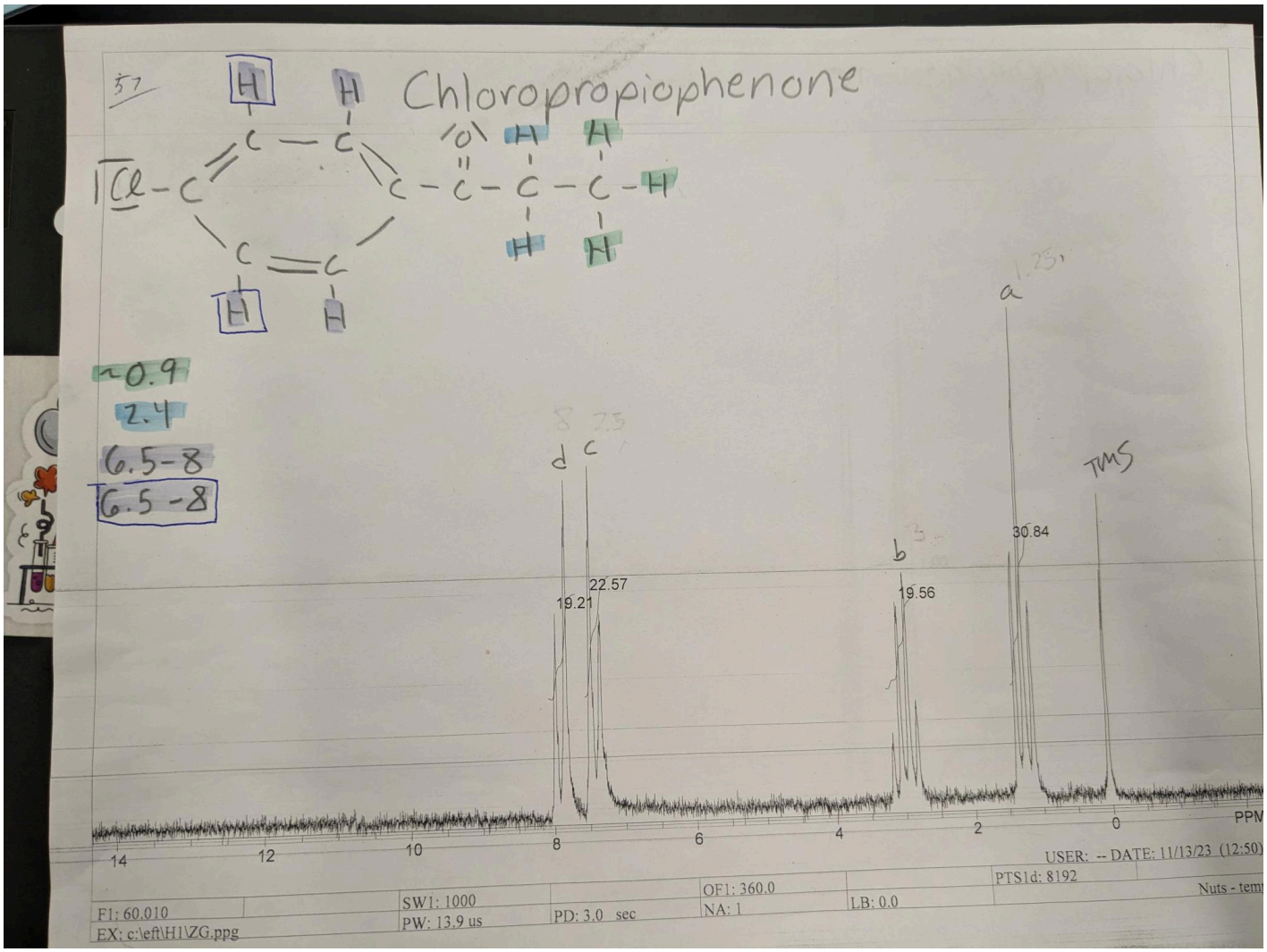


Figure 2 Sample 57 - Chloropropiophenone OK (see above)

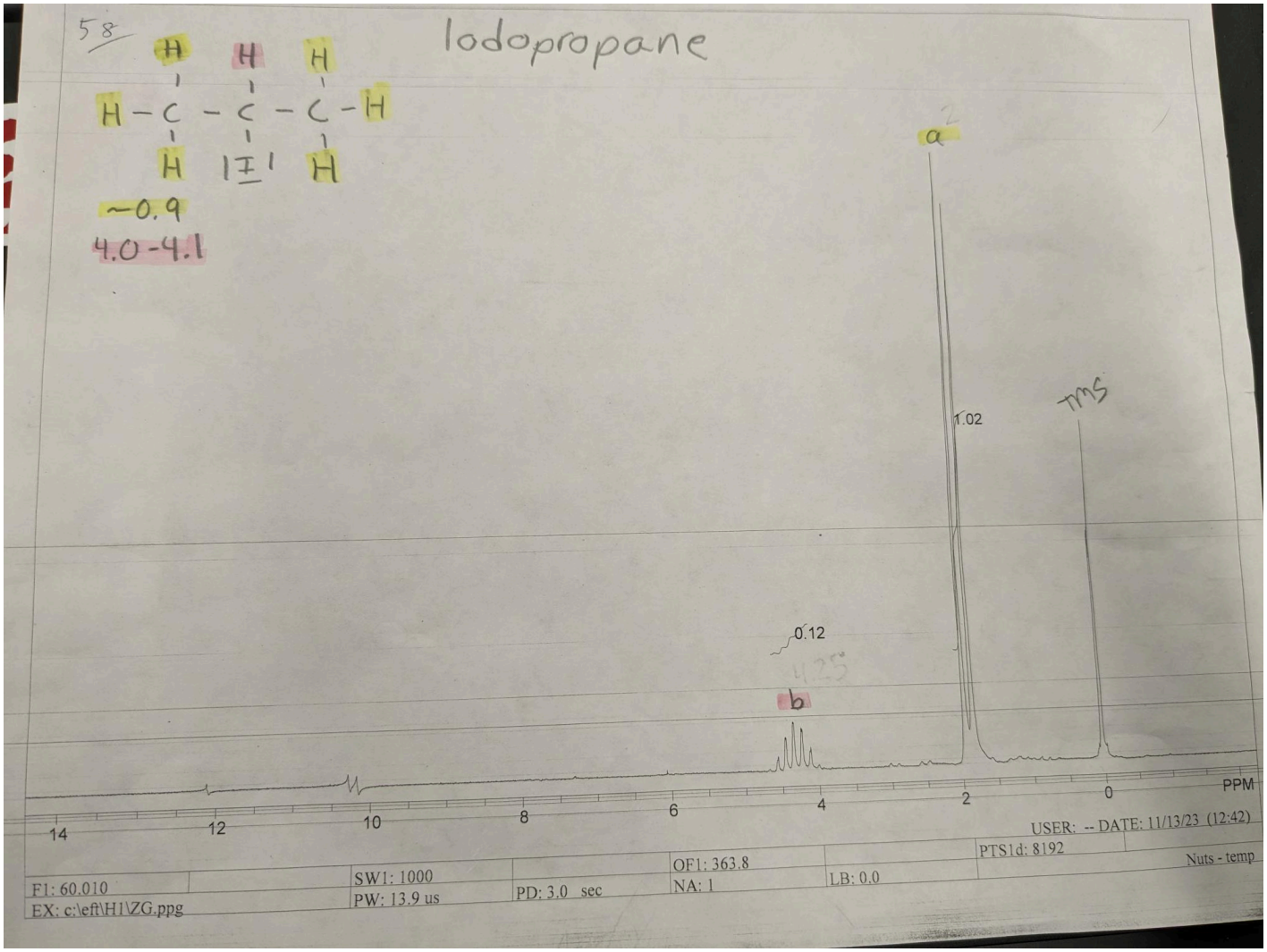


Figure 3 Sample 58 - Iodopropane OK (see above)

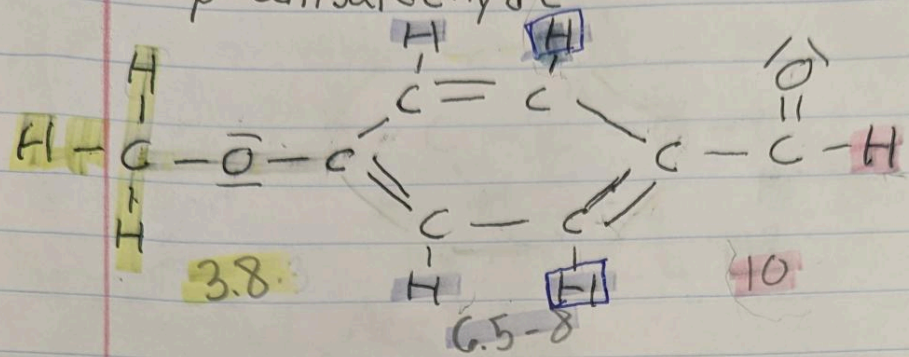
Jason Cody - Oct 22, 2020, 11:38 AM CDT

Calculations

Jason Cody - Nov 18, 2023, 7:16 PM CST

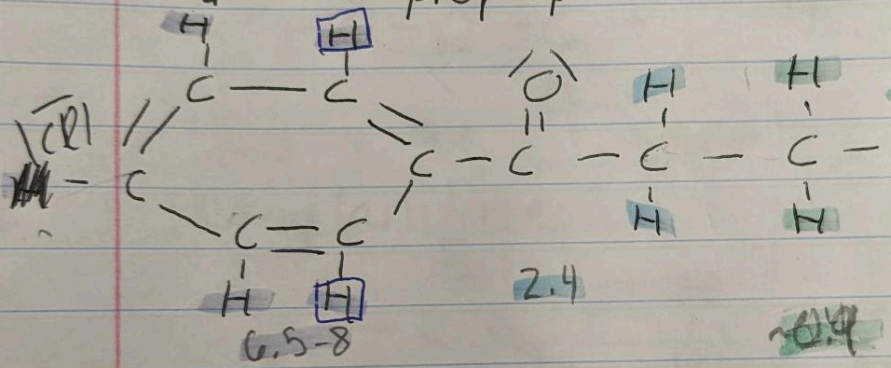
s-singlet d-doublet t-triplet
qua-quartet qui-quintet Hex-hextet hep-heptet

1 p-anisaldehyde



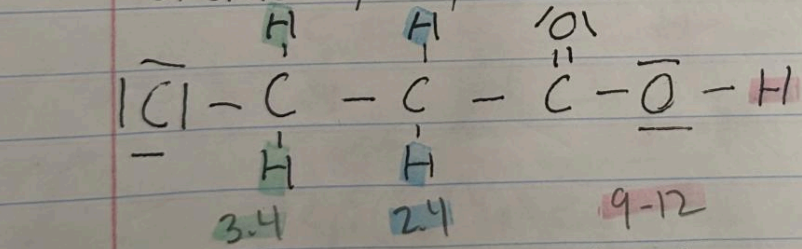
4
a b c d
s d s
3.8 6.5 8 10
3 : 2 : 2 : 1

2. β-chloropropiophenone



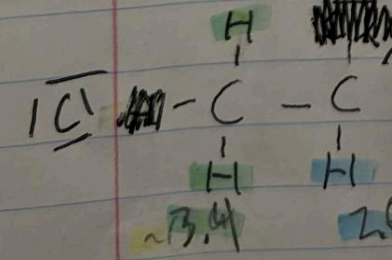
4
a b c d
qua t d
2.4 3.9 6.5-8
2 : 2 : 2 : 2

3. chloropropionic acid



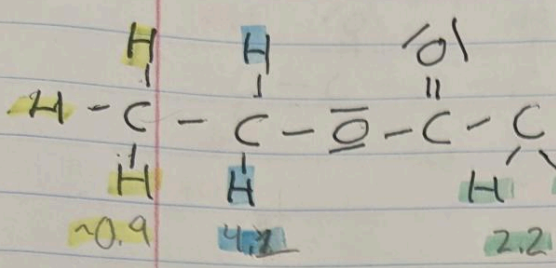
3
a b c
t t s
2.4 3.4 9-12
2 : 2 : 1

4 chloropropionitrile



2
a b
t t
2.8 3.4
2 : 2

5. Diethyl Malonate



3

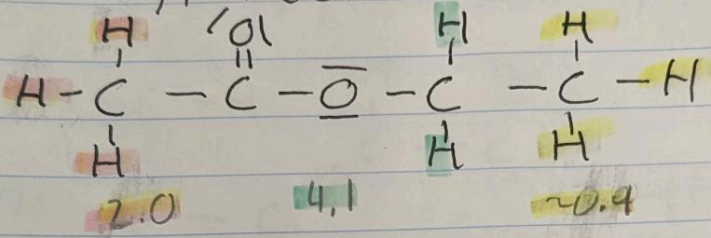
a b c

t s qua

0.9 2.2 4.1

6 : 2 : 4

6. Ethyl Acetate



3

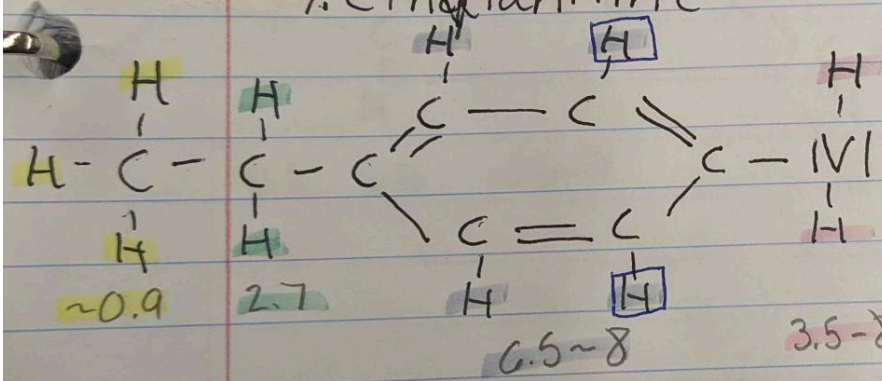
a b c

t s qua

0.9 2.0 4.1

3 : 3 : 2

7. ethylaniline



5

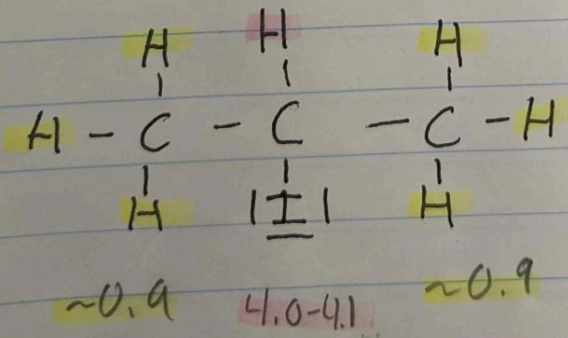
a b c d e

t qua s d

0.9 2.7 3.5-8 6.5-8

3 : 2 : 2 : 2 : 2

8. Iodopropane



2

a b

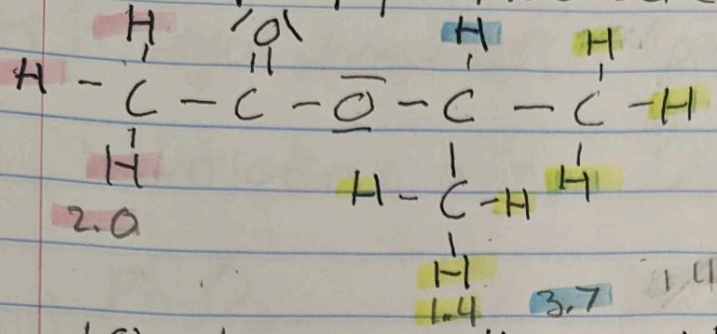
s hep

0.9 4.0-4.1

6 : 1

OK, but diethyl malonate needs the 2.2+1.1=3.3ppm calculation (there's a COO group on both sides of the central CH2 group).

9. Isopropyl Acetate



3

a b c

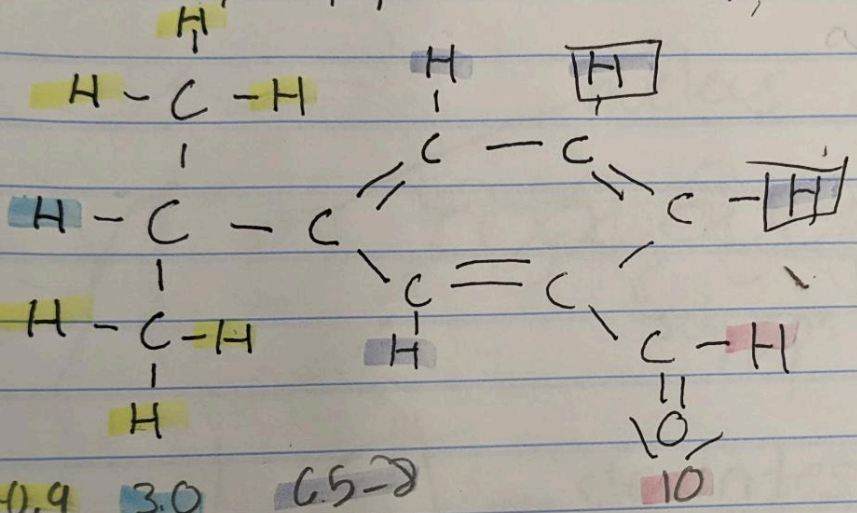
~~d~~ s ~~hep~~

1 H 2.0 3 H

6 : 3 : ~~1~~

2.0 1.4 3.7

10 Isopropylbenzaldehyde



5

a b c d e

d hep d s

0.9 3.0 6.5-8 10

6 : 1 : 2 : 2 : 1

~0.9 3.0 6.5-8 10

Jason Cody - Oct 22, 2020, 11:38 AM CDT

Conclusions

Ilana Berlin - Nov 13, 2023, 3:42 PM CST

NMR spectroscopy revealed that sample 50 was chloropropionitrile, sample 57 was chloropropiophenone, and sample 58 was iodopropane. The proton ratios, multiplicity, and chemical shifts matched the values predicted from the Lewis structures. NMR spectroscopy shows the chemical shift (with reference to tetramethylsilane $Si(CH_3)_4$) on the y-axis and it shows the proton ratios on the x-axis. The number of peaks in a small area represents the multiplicity of the protons (resulting from spin-spin splitting).