Nuclear Magnetic Ressonance III

Purpose:

- **Run H NMR on 3 unknown organic molecules samples (13,20, and 21)**
- **Analyse N NMR spectra**
  - **Determine number of signals due to number of types of H bonds**
  - **Determine chemical shift due to enviroment around H bonds**
  - **Determine ratio of area under the peak due to the ratio of H's of each type**
  - **Determine splitting due to spin-spin coupling within 3 bonds using the n+1 rule**
- **Identify unknown samples 13, 20, and 21 using NMR spectra and predictions**
- **Predict NMR Spectra based in table of H chemical shifts**
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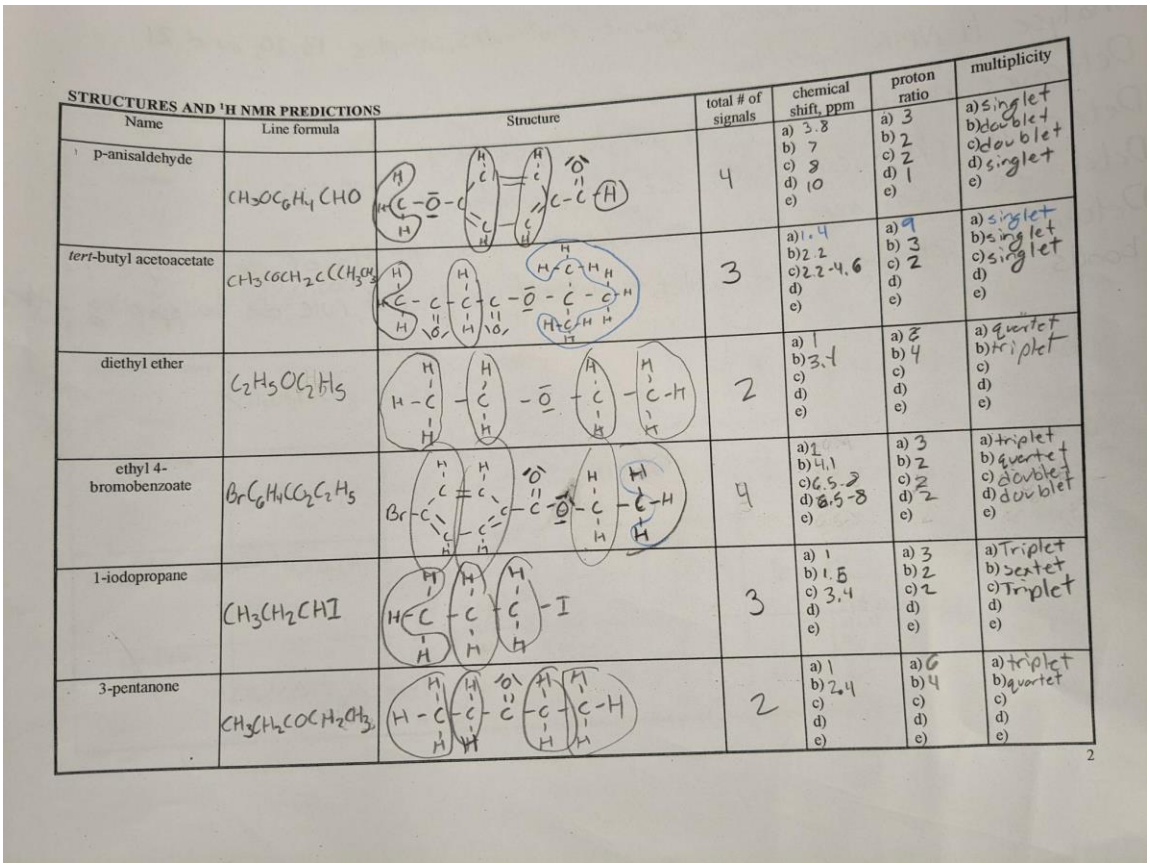
Reference:

(1) Kateley, L. J., *Introduction to Chemistry in the Laboratory*, *20th Ed.*, Lake Forest College, **2021,** Experiment NMR III, Appendix C_Spectroscopy and G_60MHzNMR**.**

(2) Sigma Aldrich

STRUCTURES AND 1H NMR PREDICTIONS



STRUCTURES AND ^{1}H NMR PREDICTIONS

Name	Line formula	Structure	total # of signals	chemical shift, ppm	proton ratio	multiplicity
p-anisaldehyde	$CH_3OC_6H_4CHO$		4	a) 3.8 b) 7 c) 8 d) 10 e)	a) 3 b) 2 c) 2 d) 1 e)	a) singlet b) doublet c) doublet d) singlet e)
tert-butyl acetoacetate	$CH_3COCH_2C(CH_3)_3$		3	a) 1.4 b) 2.2 c) 2.2-4.6 d) e)	a) 9 b) 3 c) 2 d) e)	a) singlet b) singlet c) singlet d) e)
diethyl ether	$C_2H_5OC_2H_5$		2	a) 1 b) 3.4 c) d) e)	a) 8 b) 4 c) d) e)	a) quartet b) triplet c) d) e)
ethyl 4-bromobenzoate	$BrC_6H_4CO_2C_2H_5$		4	a) 1 b) 4.1 c) 6.5-7 d) 8.5-8 e)	a) 3 b) 2 c) 2 d) 2 e)	a) triplet b) quartet c) doublet d) doublet e)
1-iodopropane	$CH_3CH_2CH_2I$		3	a) 1 b) 1.5 c) 3.4 d) e)	a) 3 b) 2 c) 2 d) e)	a) Triplet b) sextet c) Triplet d) e)
3-pentanone	$CH_3CH_2COCH_2CH_3$		2	a) 1 b) 2.4 c) d) e)	a) 6 b) 4 c) d) e)	a) triplet b) quartet c) d) e)

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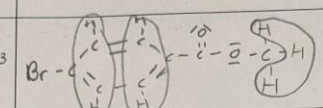
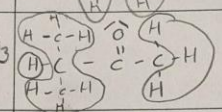
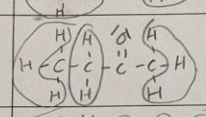
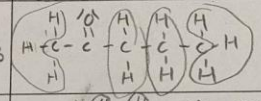
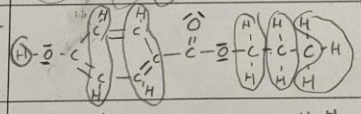
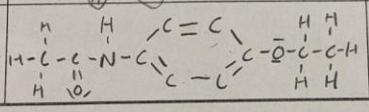
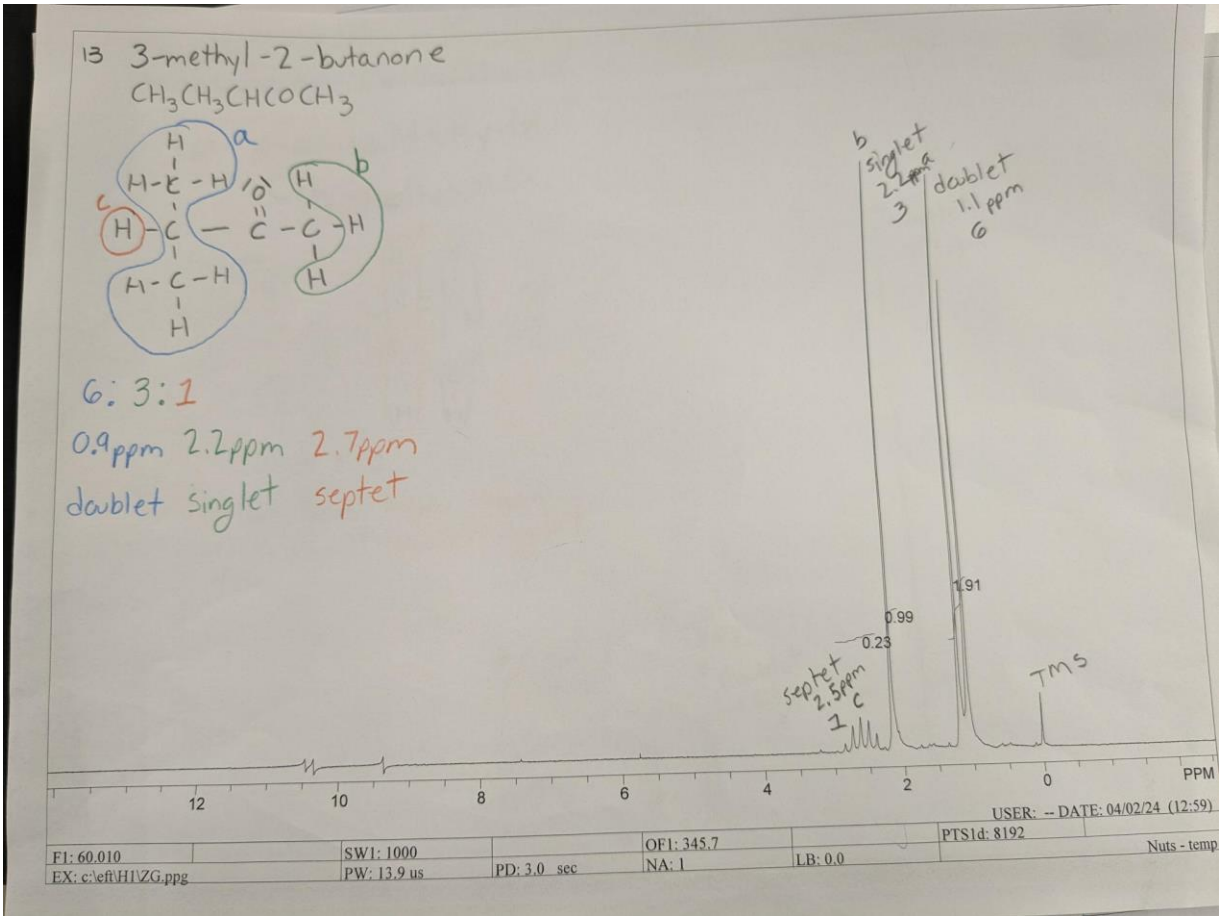
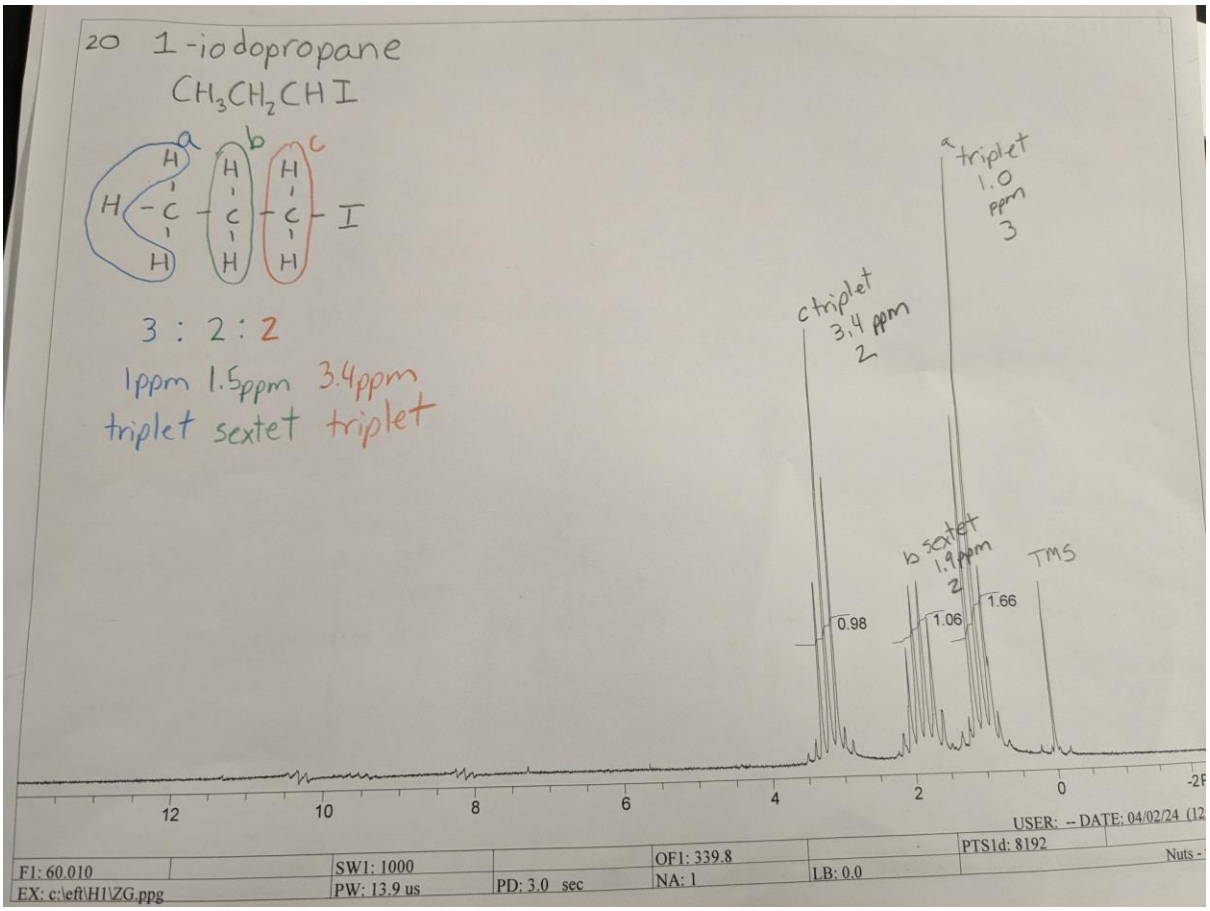
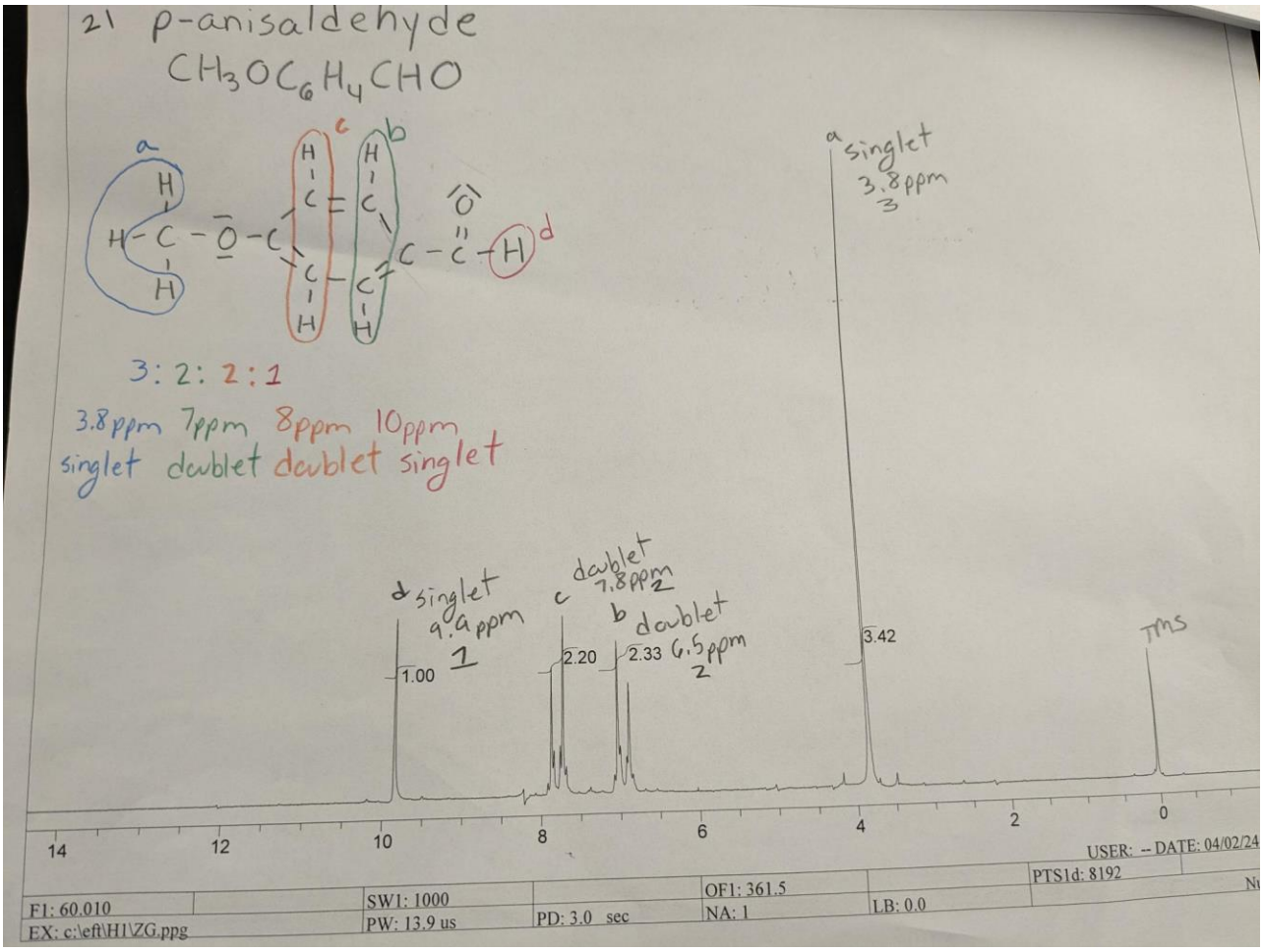
Name	Line Formula	Structure	Total # of signals	Chemical shift, ppm	Proton ratio	Multi-plicity
Methyl p-bromo-benzoate	$BrC_6H_4CO_2CH_3$		3	a) 3.7 b) 6 c) 7 d) e)	a) 3 b) 2 c) 2 d) e)	a) Singlet b) Doublet c) Doublet d) e)
3-methyl-2-butanone	$CH_3CH_3CHCOCH_3$		3	a) 0.9 b) 2.2 c) 2.7 d) e)	a) 6 b) 3 c) 1 d) e)	a) doublet b) singlet c) septet d) e)
Methyl ethyl ketone	$CH_3CH_2COCH_3$		3	a) 1 b) 2.2 c) 2.4 d) e)	a) 3 b) 3 c) 2 d) e)	a) triplet b) singlet c) quartet d) e)
2-pentanone	$CH_3COCH_2CH_2CH_3$		4	a) 0.9 b) 1.3 c) 2.2 d) 2.4 e)	a) 3 b) 2 c) 3 d) 2 e)	a) triplet b) sextet c) singlet d) triplet e)
Propyl 4-hydroxy-benzoate	$HOC_6H_4CO_2CH_2-CH_2CH_3$		6	a) 1 b) 1.3 c) 4.1 d) 4.8 e) 7	a) 3 b) 2 c) 2 d) 1 e) 2	a) triplet b) sextet c) triplet d) singlet e) doublet doublet
phenacetin	$CH_3CONHC_6H_4-OC_2H_5$		6	a) 1.4 b) 2.2 c) 3.9-4.3 d) 5 e) 7	a) 3 b) 3 c) 2 d) 1 e) 2	a) triplet b) singlet c) quartet d) singlet e) doublet doublet

NMR SPECTRA


13 3-methyl-2-butanone
$CH_3CH_2CHCOCH_3$
a
b
c
6:3:1
0.9ppm 2.2ppm 2.7ppm
doublet singlet septet
b
singlet
2.2ppm
3
doublet
1.1 ppm
6
1.91
0.99
0.23
septet
2.5ppm
c
1
TMS
12
10
8
6
4
2
0
PPM
USER: -- DATE: 04/02/24 (12:59)
F1: 60.010
EX: c:\eft\H1\ZG.ppg
SW1: 1000
PW: 13.9 us
PD: 3.0 sec
OF1: 345.7
NA: 1
LB: 0.0
PTS1d: 8192
Nuts - temp


20 1-iodopropane
CH_3CH_2CHI
a
b
c
3 : 2 : 2
1ppm 1.5ppm 3.4ppm
triplet sextet triplet
a triplet 1.0 ppm 3
c triplet 3.4 ppm 2
b sextet 1.9ppm 2
TMS
0.98
1.06
1.66
12
10
8
6
4
2
0
USER: -- DATE: 04/02/24
F1: 60.010
EX: c:\eft\H1\ZG.ppg
SW1: 1000
PW: 13.9 us
PD: 3.0 sec
OF1: 339.8
NA: 1
LB: 0.0
PTS1d: 8192
Nuts -



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).*