NMR Worksheet #2 – Structural Elucidation

1. Please present thy work…

Molecular Formula: $C_4H_8O_2$

#1 Degrees of unsaturation	Show your work for degrees of unsaturation:

What does *degrees of unsaturation* tell you about the molecule?

^{1}H NMR	**^{13}C NMR**
a) List data - chemical shift, integration, & splitting b) Draw a 'fragment' for each signal and/or list potential functional groups c) Draw the proposed structure with all H's drawn and labeled – ex. A, B, C, etc. d) Correlate each ^{1}H NMR signal to hydrogen(s) on the structure	a) List chemical shifts b) Draw a 'fragment' for each signal and/or list potential functional groups c) Draw the proposed structure, label all carbons, and correlate each NMR signal (ppm) to carbon(s) on the structure
Proposed structure and ^{1}H NMR assignments	Proposed structure and ^{13}C NMR assignments ^

2. Express thyself…

Molecular Formula: $C_3H_5BrO_2$

Degrees of unsaturation	Show your work for degrees of unsaturation:

What does *degrees of unsaturation* tell you about the molecule?

IR Spectroscopy – list the significant IR absorbances by **wavenumber** and potential **functional group** names with substructure or fragment. *Pro-tip: ignore the mess between 1000 – 1500 cm^{-1}.*

^{1}H NMR

a) List data - chemical shift, integration, & splitting
b) Draw a 'fragment' for each signal and/or list potential functional groups
c) Draw the proposed structure with all H's drawn and labeled – ex. A, B, C, etc.
d) Correlate each ^{1}H NMR signal to hydrogen(s) on the structure

Structure with ^{1}H NMR assignments

#2 cont'd - <u>Molecular Formula</u>: $C_3H_5BrO_2$

^{13}C NMR

a) List chemical shifts
b) Draw a 'fragment' for each signal and/or list potential functional groups
c) Draw the proposed structure, label all carbons, and correlate each NMR signal (ppm) to carbon(s) on the structure

Structure with ^{13}C NMR assignments

Totes Optional: Mass spec data notes – read up on it if you like and show fragmentation patterns

3. Work it…

Molecular Formula: $C_{10}H_{12}O$

Degrees of unsaturation	Show your work for degrees of unsaturation:

What does *degrees of unsaturation* tell you about the molecule?

IR Spectroscopy – list the significant IR absorbances by **wavenumber** and potential **functional group** names with substructure or fragment. *Pro-tip: ignore the mess between 1000 – 1500 cm^{-1}.*

^{1}H NMR

a) List data - chemical shift, integration, & splitting
b) Draw a 'fragment' for each signal and/or list potential functional groups
c) Draw the proposed structure with all H's drawn and labeled – ex. A, B, C, etc.
d) Correlate each ^{1}H NMR signal to hydrogen(s) on the structure

Structure with ^{1}H NMR assignments

#3 cont'd - Molecular Formula: $C_{10}H_{12}O$

^{13}C NMR

d) List chemical shifts
e) Draw a 'fragment' for each signal and/or list potential functional groups
f) Draw the proposed structure, label all carbons, and correlate each NMR signal (ppm) to carbon(s) on the structure

Structure with ^{13}C NMR assignments

Totes Optional: Mass spec data notes – read up on it if you like and show fragmentation patterns

4. Get after it!…

Molecular Formula: C_5H_8O

Degrees of unsaturation	Show your work for degrees of unsaturation:

What does *degrees of unsaturation* tell you about the molecule?

IR Spectroscopy – list the significant IR absorbances by **wavenumber** and potential **functional group** names with substructure or fragment. *Pro-tip: ignore the mess between 1000 – 1500 cm^{-1}.*

^{1}H NMR
a) List data - chemical shift, integration, & splitting b) Draw a 'fragment' for each signal and/or list potential functional groups c) Draw the proposed structure with all H's drawn and labeled – ex. A, B, C, etc. d) Correlate each ^{1}H NMR signal to hydrogen(s) on the structure
Structure with ^{1}H NMR assignments

#4 cont'd - Molecular Formula: C_5H_8O

^{13}C NMR

g) List chemical shifts
h) Draw a 'fragment' for each signal and/or list potential functional groups
i) Draw the proposed structure, label all carbons, and correlate each NMR signal (ppm) to carbon(s) on the structure

Structure with ^{13}C NMR assignments

Totes Optional: Mass spec data notes – read up on it if you like and show fragmentation patterns

5. Show me what'cha workin' with!...

Molecular Formula: $C_9H_{13}NO$

Degrees of unsaturation	Show your work for degrees of unsaturation:

What does *degrees of unsaturation* tell you about the molecule?

IR Spectroscopy – list the significant IR absorbances by **wavenumber** and potential **functional group** names with substructure or fragment. *Pro-tip: ignore the mess between 1000 – 1500 cm^{-1}.*

^{1}H NMR

e) List data - chemical shift, integration, & splitting
f) Draw a 'fragment' for each signal and/or list potential functional groups
g) Draw the proposed structure with all H's drawn and labeled – ex. A, B, C, etc.
h) Correlate each ^{1}H NMR signal to hydrogen(s) on the structure

Structure with ^{1}H NMR assignments

#5 cont'd - Molecular Formula: $C_9H_{13}NO$

^{13}C NMR

j) List chemical shifts
k) Draw a 'fragment' for each signal and/or list potential functional groups
l) Draw the proposed structure, label all carbons, and correlate each NMR signal (ppm) to carbon(s) on the structure

Structure with ^{13}C NMR assignments

Totes Optional: Mass spec data notes – read up on it if you like and show fragmentation patterns