

SI Organic Chemistry - Full Discipline Demo

Nuclear Magnetic Resonance

Final Report - Answer Guide

Institution	Science Interactive University
Session	SI Organic Chemistry - Full Discipline Demo
Course	SI Organic Chemistry - Full Discipline Demo
Instructor	Sales SI Demo

Test Your Knowledge

Match the term with the best description.

Terms to match:

- Chemical shift
- Nuclear magnetic resonance
- Spectrometry
- Spin-spin coupling

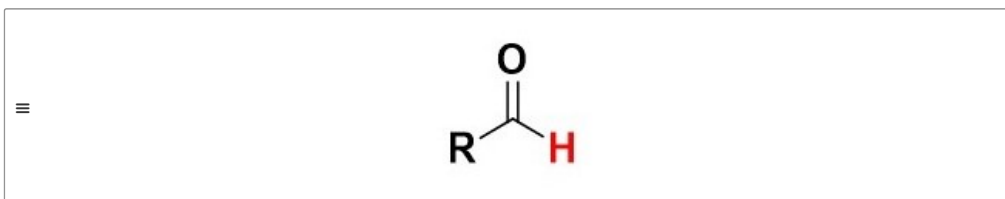
Descriptions to match with:

- 1 The absorption and release of electromagnetic radiation by a nucleus in an applied magnetic field.
- 2 A measurement of radiation interacting with matter.
- 3 Resulting interaction between two non-chemically equivalent hydrogens.
- 4 Frequency of an atom's resonance in an applied magnetic field compared to a standard.

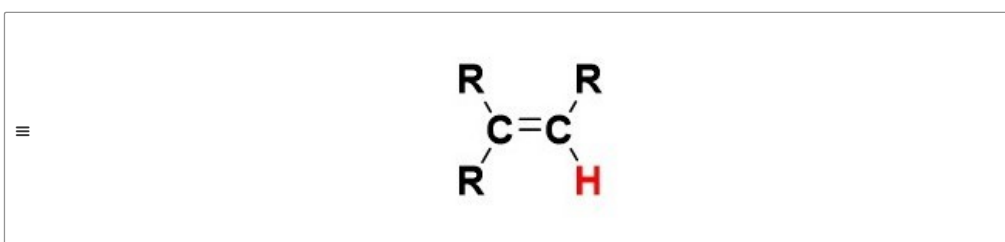
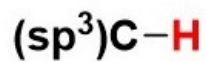
Correct answers:

- 1 Nuclear magnetic resonance 2 Spectrometry 3 Spin-spin coupling
4 Chemical shift

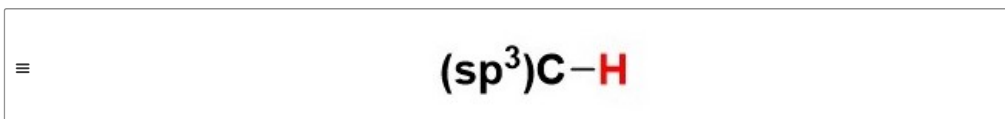
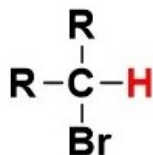
Order the hydrogens of the molecules from most shielded to most deshielded.



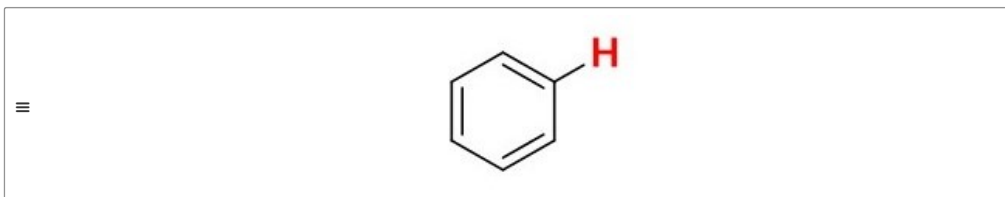
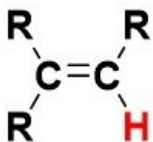
1 Correct answer:



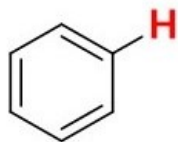
2 Correct answer:



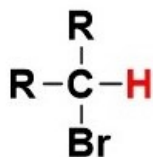
3 Correct answer:



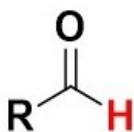
4 Correct answer:



≡



5 Correct answer:



Exploration

Energy is directly proportional to frequency in the electromagnetic spectrum.

☐ True



☐ False

An emission spectrum is detected when a sample is excited from the ground state to the excited state.

☐ True



☐ False

The isotopes ____ and ____ are NMR-active nuclei.

- ☐ ^1H ; ^{12}C
- ☐ ^2H ; ^{12}C
- ☒ ^1H ; ^{13}C ✓
- ☐ ^2H ; ^{13}C

When an atom is placed in a magnetic field, aligning with a magnetic field is higher in energy than aligning against the magnetic field.

- ☐ True
- ☒ False ✓

A ____ group is electronegative and would cause nearby protons to be shifted downfield.

- ☐ carbonyl ($\text{C}=\text{O}$)
- ☐ chloro (Cl)
- ☐ amine (N)
- ☒ All of the above ✓

The closer a proton is to an electronegative group, the more shielded it will be.

- ☐ True
- ☒ False ✓

A ring has ____ degree(s) of unsaturation.

- ☐ 0
- ☒ 1 ✓
- ☐ 2
- ☐ 3

Carbon NMR uses the ____ isotope, which is less abundant than the ^1H isotope.

- ☐ ^{12}C
- ☒ ^{13}C
- ☐ ^{14}C
- ☐ None of the above



Exercise 1

What were the common functional group patterns observed in NMR Spectra 1?

In Spectra 1 there was an ethyl and methyl group.

In the NMR Spectra 3, what was the most deshielded hydrogen's chemical shift and what functional group caused it to be that downfield?

In NMR spectra 3 the most deshielded hydrogen had a chemical shift of ~ 9.7 ppm. This hydrogen was attached to a carbonyl making it an aldehyde.

Based on the calculated degree of unsaturation for Spectra 1, what functional groups account for the unsaturation? What functional groups account for the unsaturation in Spectra 2? And in Spectra 3?

Spectra 1 has a DOU of 0 with no functional groups accounting for the unsaturation.

Spectra 2 has a DOU of 6, and the functional groups that account for them are an aromatic ring (4), a carbonyl (1) and a double bond (1).

Spectra 3 has a DOU of 1 and the functional group that accounts for the unsaturation is the aldehyde (1).

Data Table 1: Peak Assignment for NMR Spectra 1
(SAMPLE ANSWER BELOW)

Degree of Unsaturation	0	
Peak (ppm)	Integration	Multiplicity
1.8	2	pentet (p)
3.25	3	singlet (s)
3.4	2	triplet (t)
3.5	2	triplet (t)

Photo 1: Work to solve NMR Spectra 1
(SAMPLE ANSWER BELOW)

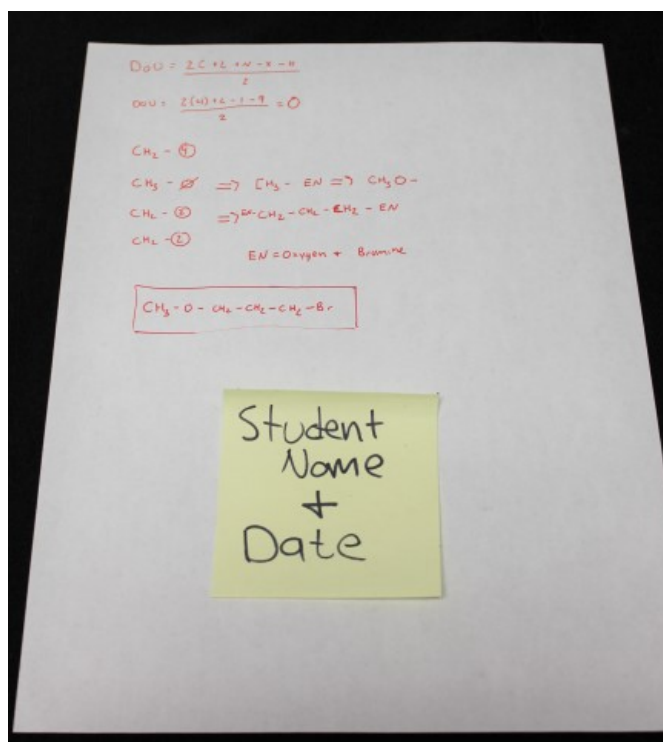
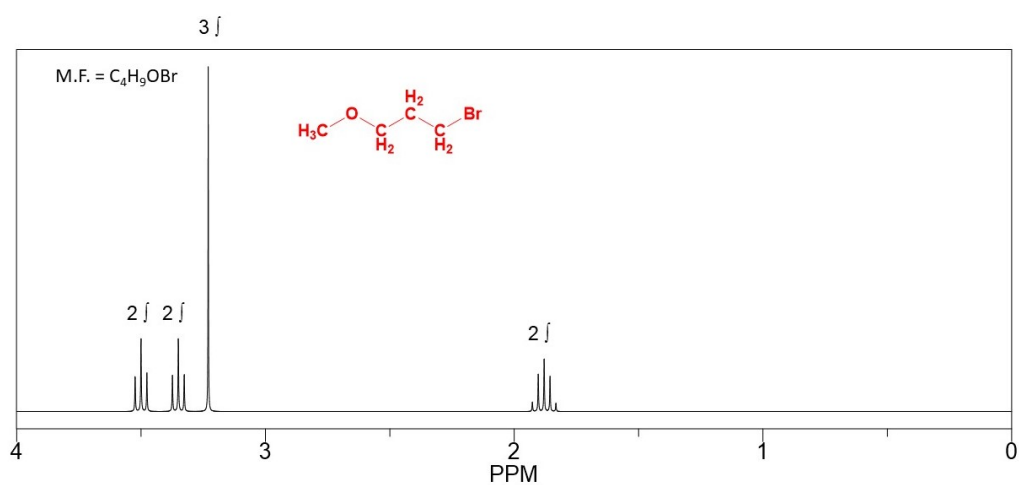


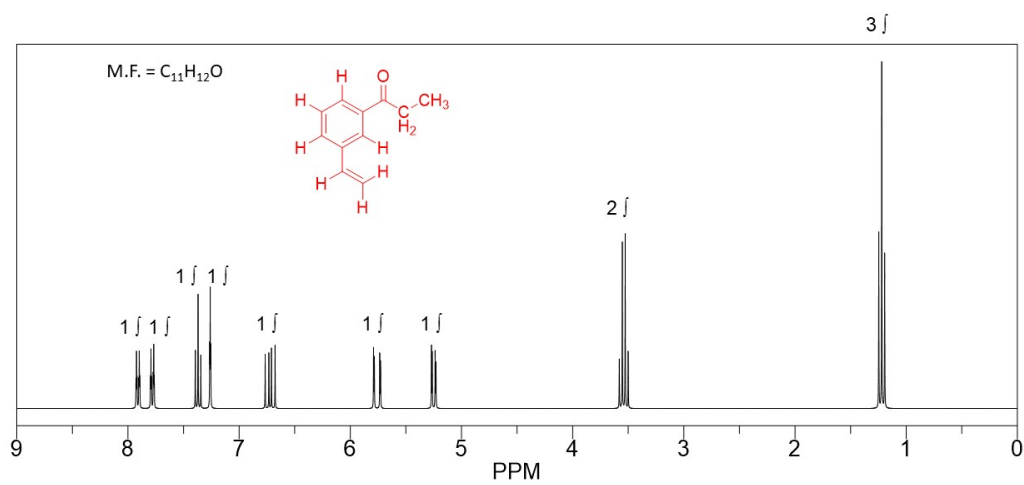
Photo 2: NMR Spectra 1 with structure
(SAMPLE ANSWER BELOW)



Degree of Unsaturation	6	
Peak (ppm)	Integration	Multiplicity
1.25	3	triplet (t)
3.5	2	quartet (q)
5.25	1	doublet of doublets (dd)
5.75	1	doublet of doublets (dd)
6.7	1	doublet of doublets (dd)
7.3	1	singlet (s)
7.4	1	triplet (t)
7.8	1	doublet (d)
7.9	1	doublet (d)

[illegible]

Photo 4: NMR Spectra 2 with structure
(SAMPLE ANSWER BELOW)



(SAMPLE ANSWER BELOW)



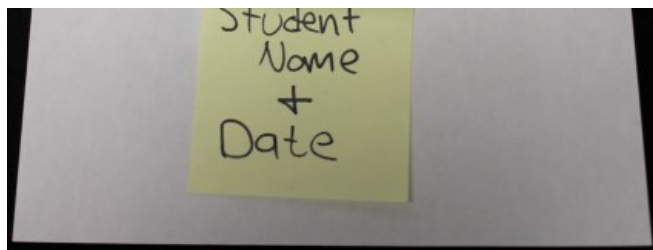
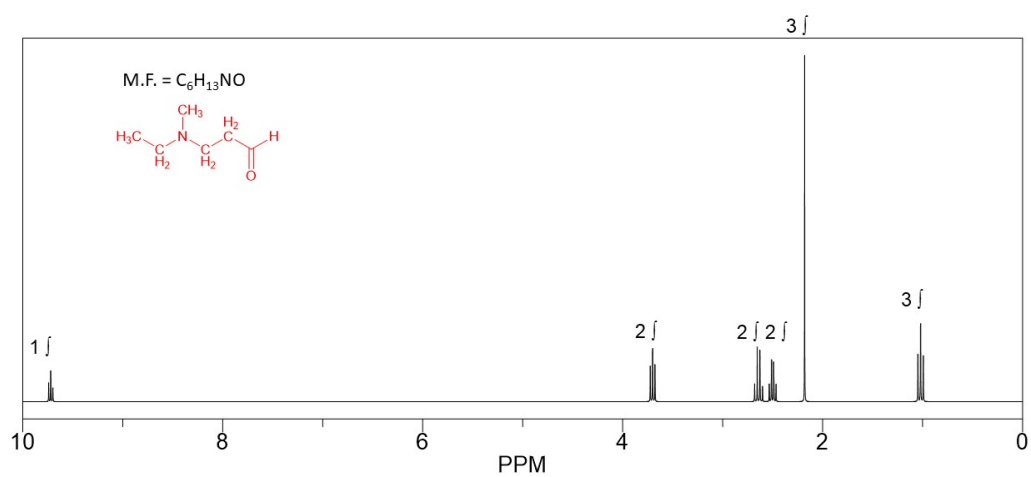


Photo 6: NMR Spectra 3 with structure
(SAMPLE ANSWER BELOW)



Exercise 2

What functional group(s) correspond to the degrees of unsaturation?

The functional groups responsible for the degrees of unsaturation are the aromatic ring (4) and the ketone (1).

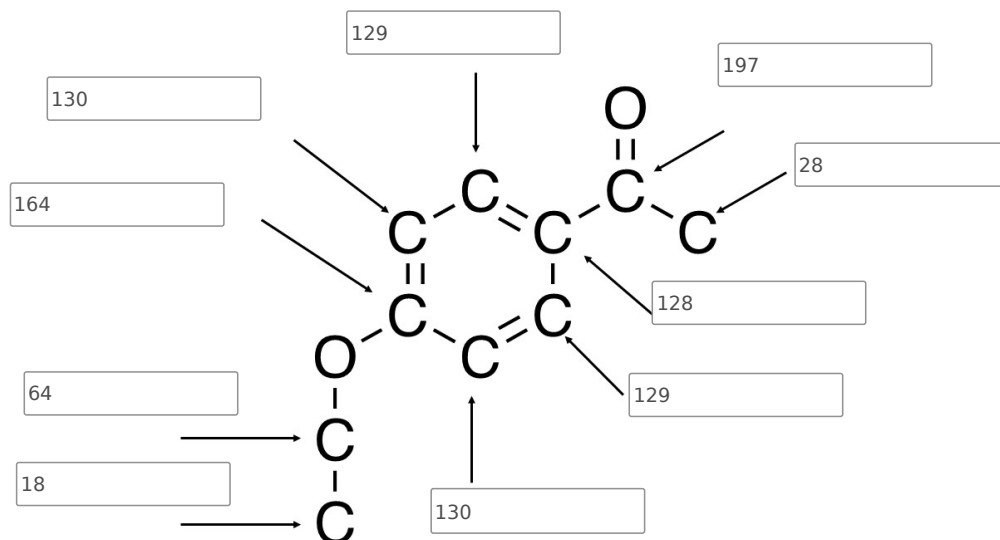
Based on the chemical shift assignment in Image Labeling 1, how many chemically equivalent carbons are in the spectra? What are their chemical shifts?

There are 2 sets of chemical equivalent carbons in the spectra. They have a chemical shift of 129 and 130 ppm.

Data Table 4: Peak Labeling of Carbon-NMR
(SAMPLE ANSWER BELOW)

Degree of Unsaturation	5
Peak	Signal (ppm)
1	18
2	28
3	64
4	127
5	129
6	130
7	165
8	197

Photo 7: Carbon-13 NMR Structure for Labeling
(SAMPLE ANSWER BELOW)



Competency Review

Nuclear magnetic resonance spectrometry uses _____ waves.

- ☐ infrared
 - ☒ radio ✓
 - ☐ X-rays
 - ☐ None of the above
-

Atoms with an odd mass number have an inherent spin.

- ☒ True ✓
 - ☐ False
-

Chemically equivalent hydrogens have the same chemical shift.

- ☒ True ✓
 - ☐ False
-

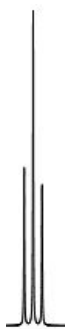
Calculating a molecule's degree of unsaturation accounts for _____ in the molecule.

- ☐ double bonds
 - ☐ triple bonds
 - ☐ rings
 - ☒ All of the above ✓
-

The functional group _____ is electronegative and causes the hydrogen to be deshielded.

- ☐ bromine
 - ☐ alkene
 - ☐ aromatic ring
 - ☒ All of the above ✓
-

The peak shown in the image below has a multiplicity of ____.



- ☐ singlet
- ☐ doublet
- ☒ triplet
- ☐ None of the above

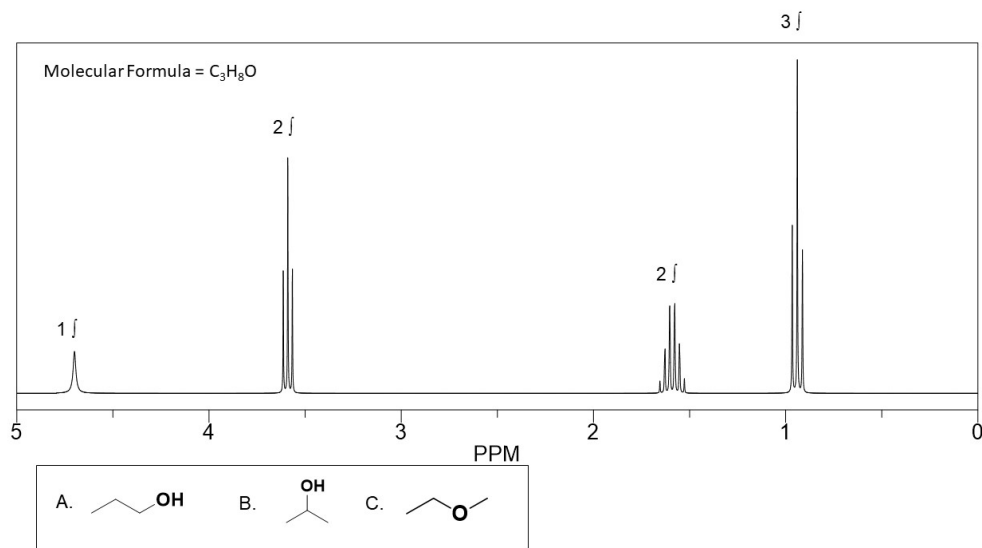
✓

The molecule represented by the formula C_5H_8O has ____ degree(s) of saturation.

- ☐ 0
- ☐ 1
- ☒ 2
- ☐ None of the above

✓

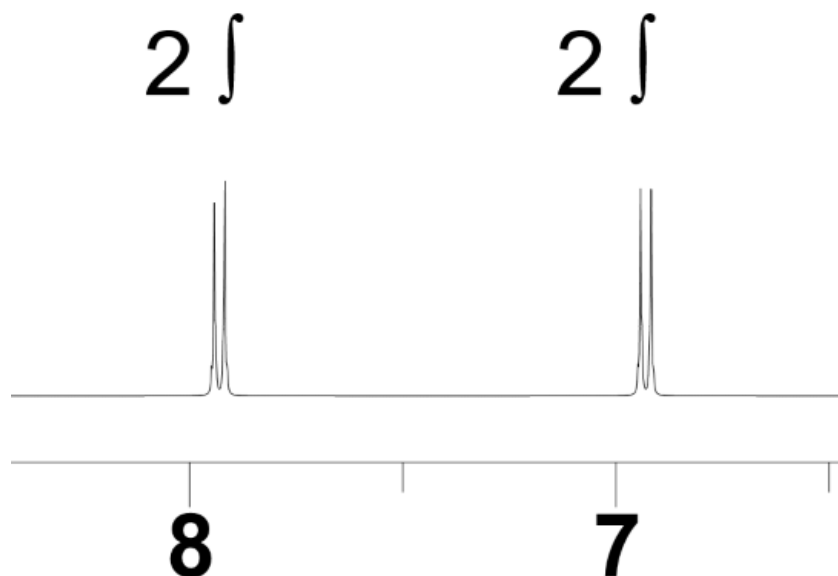
Structure ____ best matches the ^1H NMR spectra below.



- ☒ A
- ☐ B
- ☐ C
- ☐ None of the Above



What common functional group is represented by this ^1H -NMR pattern?



- ☐ doublet of doublets
- ☒ para-substituted benzene
- ☐ *tert*-butyl group
- ☐ ethyl group

✓

Extension Questions

A common technique for imaging the human body is magnetic resonance imaging (MRI). This technique uses radio waves in the same frequency as nuclear magnetic resonance. Research MRI and answer the following questions:

What atom does MRI use for imaging the body? What molecule that contains this atom is most abundant in the human body? Does an MRI detect emission or absorption of electromagnetic radiation?

(SAMPLE ANSWER BELOW)

MRI is a ^1H -NMR technique. It uses excited hydrogen atoms (also referred to as protons) and measures the release of electromagnetic energy. The molecule that is most common containing hydrogen is water (H_2O) as it makes up approximately 60% of the human body by weight. An MRI excites the water molecules and detects the emission of energy as the atoms relax.