Objective 4. Determine (characterize) the structure of a compound using IR, NMR, MS.

1. In Mass spectrometry,
a. an electron collides with a sample and forms a _____.
b. This _(answer from (a)_ accelerates into a magnetic field.
c. The magnetic field separates particles based on _____ ratio.
d. Lighter particles with a low _____ ratio are deflected ____ compared to heavier particles.
e. In a mass spectrum, ___ is plotted on the y axis and ___ is plotted on the x axis.
f. The molecular ion peak tells you ____.

2. IR spectroscopy
a. A molecule that is exposed to IR radiation will cause the molecule to _____.
b. In an IR spectrum, ___ is plotted on the y axis and ___ is plotted on the x axis.
c. To interpret an IR spectrum, match each IR peak to a specific _____.
d. Once you identify the ___ types, then you can match the ____ to the structure.
e. It takes _____ energy to stretch a O-H bond than a C-H bond. Support your answer by stating the approximate wavenumber of each bond type.

3. H NMR spectroscopy
a. When a sample that has a non-zero nuclear spin quantum number is placed in a magnetic field, the nuclear spin states split into ____ states.
b. In a H NMR spectrum, ___ is plotted on the y axis and ___ is plotted on the x axis.
c. Downfield H NMR peaks mean H's in the compound are deshielded due to ____.
d. The number of H NMR peaks depends on the number of ____ H's in the compound.
e. The intensity of each peak depends on the number of ____ H's in the compound.
f. A peak can be split into multple peaks if H's are on ____ carbons.

4. C NMR spectroscopy
a. The number of C NMR peaks depends on the number of ____ C's in the compound.
b. The intensity of each peak _____ on the number of ____ C's in the compound.
c. A peak _____ be split into multple peaks like in H NMR.

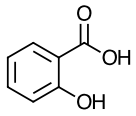
5. Consider n-butane C_4H_{10}.
a. Calculate the hydrogen deficiency index of C_4H_{10}.
b. In a mass spectrum of C_4H_{10}, what is the m/z for the molecular ion peak?
c. H NMR
How many non-equivalent H's?
(i) 1 (ii) 2 (iii) 3 (iv) 4
How many peaks in a H NMR spectrum? (i) 1 (ii) 2 (iii) 3 (iv) 4
If 2 or more peaks, what is ratio of non-equivalent H's?
If 2 or more peaks, what is splitting?
d. C NMR
How many non-equivalent C's?
(i) 1 (ii) 2 (iii) 3 (iv) 4
How many peaks in a C NMR spectrum? (i) 1 (ii) 2 (iii) 3 (iv) 4

6. C_4H_{10} has two isomers.
a. Calculate the hydrogen deficiency index of C_4H_{10}.
b. Draw the skeletal structures of the two isomers.
c. Can IR be used to identify or distinguish between these two compounds? Support your answer by stating the bond types in each compound.
d. Can H NMR be used to identify or distinguish between these two compounds? Support your answer by stating the number of non-equivalent H's and multiplicity in each compound.
e. Can C NMR be used to identify or distinguish between these two compounds? Support your answer by stating the number of non-equivalent C's in each compound.

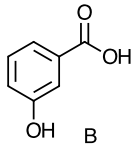
7. C_3H_6O has at least two isomers.
a. Calculate the hydrogen deficiency index of C_3H_6O.
b. Draw the skeletal structures of the two isomers.
c. Can IR be used to identify or distinguish between these two compounds? Support your answer by stating the bond types in each compound.

d. Can H NMR be used to identify or distinguish between these two compounds? Support your answer by stating the number of non-equivalent H's and multiplicity in each compound.
e. Can C NMR be used to identify or distinguish between these two compounds? Support your answer by stating the number of non-equivalent C's in each compound.

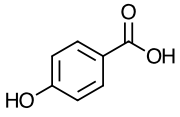
8. Structure A is salicylic acid. B and C are isomers.



A



B



C

a. State the chemical formula of salicylic acid.
b. Calculate the hydrogen deficiency index.
c. Can IR be used to identify or distinguish between these two compounds? Support your answer by stating the bond types in each compound.
d. Can H NMR be used to identify or distinguish between these two compounds? Support your answer by stating the number of non-equivalent H's and multiplicity in each compound.
e. Can C NMR be used to identify or distinguish between these two compounds? Support your answer by stating the number of non-equivalent C's in each compound.