Objective 4 Quiz Practice Problems Solutions

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 ____.
Answers:
a. an electron collides with a sample and forms a molecular ion (radical with positve charge).
b. This molecular ion accelerates into a magnetic field.
c. The magnetic field separates particles based on mass/charge (m/z) ratio.
d. Lighter particles with a low mass/charge ratio are deflected more compared to heavier particles.
e. In a mass spectrum, relative abundance is plotted on the y axis and m/z is plotted on the x axis.
f. The molecular ion peak tells you molecular weight.

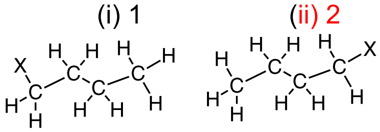
2. IR spectroscopy
a. A molecule that is exposed to IR radiation will cause the molecule to _____.
b. In an IR spectrum, ___ is plotted on the y axis and ___ is plotted on the x axis.
c. To interpret an IR spectrum, match each IR peak to a specific ______.
d. Once you identify the ___ types, then you 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.
Answers:
a. A molecule that is exposed to IR radiation will cause the molecule to vibrate.
b. In an IR spectrum, % transmittance is plotted on the y axis and energy in wavenumbers is plotted on the x axis.
c. To interpret an IR spectrum, match each IR peak to a specific bond type.
d. Once you identify the bond types, then you can match the bond types to the structure.
e. It takes more energy to stretch a O-H bond than a C-H bond. Support your answer by stating the approximate wavenumber of each bond type.
O-H bond stretches at 3300 cm^{-1}, C-H bond stretches at 3000 cm^{-1}.

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.
Answers:
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 2n + 1 (where n is the nuclear spin quantum number) states. Example: H has a nuclear spin quantum number of ½ so 2(1/2) + 1 = 2.
b. In a H NMR spectrum, intensity is plotted on the y axis and chemical shift is plotted on the x axis.
c. Downfield H NMR peaks mean H's in the compound are deshielded due to groups that withdraw electron density.
d. The number of H NMR peaks depends on the number of non-equivalent H's in the compound.
e. The intensity of each peak depends on the number of equivalent H's in the compound.
f. A peak can be split into multple peaks if H's are on adjacent carbons.

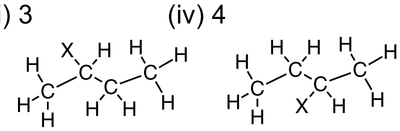
4. C NMR spectroscopy
a. The number of C NMR peaks depends on the number of ____ C's in the compound.
b. The intensity of each peak ______ on the number of ____ C's in the compound.
c. A peak _____ be split into multple peaks like in H NMR.
Answers:
a. The number of C NMR peaks depends on the number of non-equivalent C's in the compound.
b. The intensity of each peak does not on the number of equivalent C's in the compound.
c. A peak cannot 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
Answers:
a. hydrogen deficiency index (HDI) = 0.5(# of H's in alkane chain - # of H's in formula)
Use C_nH_{2n+2} to determine # of H's in alkane chain.
4 carbon alkane has 2(4) + 2 = 10 H's
So HDI of C_4H_{10} = 0.5(10 – 10) = 0
There are no pi bonds or rings in C_4H_{10}.
b. Molecular weight of C_4H_{10}. = 58 so m/z for the molecular ion peak = 58.
c. H NMR
How many non-equivalent H's?
(i) 1 (ii) 2 (iii) 3 (iv) 4



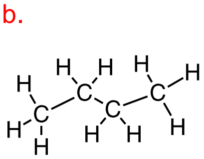
The 6 H's on C-1 and C-4 are equivalent.



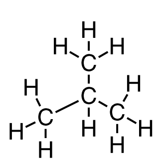
The 4 H's on C-2 and C-3 are equivalent.

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? 6:4 or 3:2
If 2 or more peaks, what is splitting?
Apply n + 1 rule where n = # of H's on adjacent carbon.
The H's on C-1 (or C-4) are split by the 2 H's on C-2 (or C-3) so 2+1 = 3 = triplet.
The H's on C-2 (or C-3) are split by the 3 H's on C-1 (or C-4) so 3+1 = 4 = quartet.
d. C NMR
How many non-equivalent C's?
(i) 1 (ii) 2 (iii) 3 (iv) 4
C-1 and C-4 are equivalent.
C-2 and C-3 are equivalent.
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.
Answers:
a. hydrogen deficiency index (HDI) = 0.5(# of H's in alkane chain - # of H's in formula)
Use C_nH_{2n+2} to determine # of H's in alkane chain.
4 carbon alkane has 2(4) + 2 = 10 H's
So HDI of C_4H_{10} = 0.5(10 – 10) = 0
There are no pi bonds or rings in C_4H_{10}.
b.



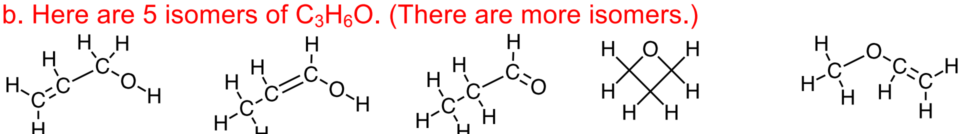
n-butane



isobutane

c. IR cannot be used to identify or distinguish between n-butane and isobutane because these two compounds have the same bond types (C-C and C-H).
d. H NMR can be used to identify or distinguish between n-butane and isobutane.
n-butane has 2 non-equivalent H's in 6:4 ratio. 6 H's on C-1 and C-4 are split by the 2 H's on C-2 or C-3 into a triplet. 4 H's on C-2 and C-3 are split by the 3 H's on C-1 or C-4 into a quartet.
isobutane has 2 non-equivalent H's in 9:1 ratio. 9 H's on C-1, C-3, and C branch are split by the 1 H's on C-2 into a doublet. 1 H's on C-2 are split by the 9 H's on C-1, C-3, and C branch into a 10 smaller peaks.
e. C NMR cannot be used to identify or distinguish between these two compounds. Both compounds have two non-equivalent C's.

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.
Answers:
a. hydrogen deficiency index (HDI) = 0.5(# of H's in alkane chain - # of H's in formula)
Ignore O in chemical formula.
Use C_nH_{2n+2} to determine # of H's in alkane chain.
3 carbon alkane has 2(3) + 2 = 8 H's
So HDI of C_3H_6O = 0.5(8 – 6) = 1
There is 1 pi bonds or rings in C_3H_6O.
b. Here are 5 isomers of C_3H_6O. (There are more isomers.)



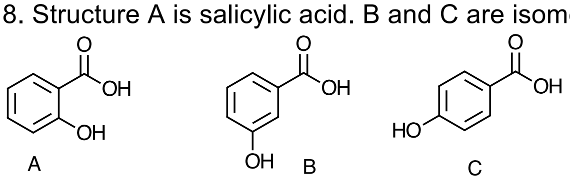
A B C D E

c. Compare Compounds A and B: IR cannot be used to identify or distinguish between A and B because these two compounds have the same bond types (C-C, C=C, C-H, C-O, O-H).
Compare Compounds B and C: IR can be used to identify or distinguish between B and C because these two compounds have different bond types (B has C-C, C=C, C-H, C-O, and O-H bond types and C has C-C, C-H, and C=O bond types).
d. Compare Compounds A and B:
H NMR can be used to identify or distinguish between A and B.
Compound A has 4 non-equivalent H's in 2:1:2:1 ratio. The H NMR spectrum of A shows 4 peaks.
1 H on O is not split (due to H bonding) by the 2 H's on C-1 ==> singlet.
2 H's on C-1 (C bonded to O) are split by the 1 H on C-2 into a doublet (ignore the H bonded to O).
1 H on C-2 are split by the 2 H's on C-1 into a triplet AND the 2 H's on C-3 into a triplet ==> complex splitting pattern of a triplet on top of a triplet.
2 H's on C-3 are split by the 1 H on C-2 into a doublet.

Compound B has 4 non-equivalent H's in 3:1:1:1 ratio. The H NMR spectrum of B shows 4 peaks.
1 H on O is not split (due to H bonding) by the 2 H's on C-1 ==> singlet.
1 H on C-1 (C bonded to O) is split by the 1 H on C-2 into a doublet (ignore the H bonded to O).
1 H on C-2 are split by the 1 H on C-1 into a doublet AND the 3 H's on C-3 into a quartet ==> complex splitting pattern of a doublet on top of a quartet or quartet on top of a doublet.
3 H's on C-3 are split by the 1 H on C-2 into a doublet.

e. C NMR cannot be used to identify or distinguish between A and B.
A has 3 non-equivalent C's. The C NMR spectrum of A shows 3 peaks.
B has 3 non-equivalent C's. The C NMR spectrum of B shows 3 peaks.

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.

Answers:

a. The chemical formula of salicylic acid is $C_7H_6O_3$.

b. hydrogen deficiency index (HDI) = 0.5(# of H's in alkane chain - # of H's in formula)
Ignore O in chemical formula.
Use C_nH_{2n+2} to determine # of H's in alkane chain.
7 carbon alkane has 2(7) + 2 = 16 H's
So HDI of $C_7H_6O_3$ = 0.5(16 – 6) = 5
There is 5 pi bonds or 5 rings or a combination of 5 rings/pi bonds in $C_7H_6O_3$.
Salicylic acid has 1 ring and 4 pi bonds.

c. IR cannot be used to identify or distinguish between A and B and C because these 3 compounds have the same bond types (C-C, C=C, C-H, C-O, C=O, O-H).

d. H NMR can be used to identify or distinguish between A and C or B and C but not A and B.
A has 6 non-equivalent H's. The H NMR spectrum of A shows 6 peaks.
B has 6 non-equivalent H's. The H NMR spectrum of B shows 6 peaks.
In Compound C, C-1 is the ring C bonded to the acid group. C has 4 non-equivalent H's in 2 (C-2 and C-6):2 (C-3 and C-5):1 (C-4):1 (H bonded to O) ratio. The H NMR spectrum of C shows 4 peaks.

e. C NMR can be used to identify or distinguish between A and C or B and C but not A and B.
A has 7 non-equivalent C's. The C NMR spectrum of A shows 7 peaks.
B has 7 non-equivalent C's. The C NMR spectrum of B shows 7 peaks.
C has 4 non-equivalent C's (C-2 and C-6 are equivalent, C-3 and C-5 are equivalent). The C NMR spectrum of C shows 4 peaks.