1) Calculate the degree of unsaturation (dous) for each.

a) C_{10}H_{16}  

b) C_{17}H_{23}NO_3  

c) C_{10}H_{16}O_2  

d) C_8H_8O  

e) C_3H_9NO_2  

f) C_8H_{10}N_4O_2  

g) C_7H_{10}Cl_2  

h) C_8H_{10}ClNO  

i) C_{27}H_{46}O  

j) C_{20}H_{34}O_5  

k) C_{14}H_9Cl_5  

l) C_9H_{11}N  

m) C_{14}H_{14}N_2O  

n) C_{15}H_8ClBrO  

o) C_5H_5Br_2NO  

p) C_8H_{11}NO  

q) C_8H_{10}BrI0  

2) How many (H)ydrogens are in each compound?

a) C_8H_xO_2  
\( x = \)  
(2 rings; 1 double bond)

b) C_7H_xN  
\( x = \)  
(2 double bonds)

c) C_9H_xNO  
\( x = \)  
(1 ring; 3 double bonds)
3) Draw the alpha cleavage products generated from the alcohol in an electron impact ionization mass spectrometer.

Refer to the mass spectrum of 2-methylbutane shown below to answer questions 2 – 5.

4) What peak represents $M^+$?

$m/z$

5) What peak represents the base peak?

$m/z$

6) What organic molecule fragment is lost to give the $m/z$ 57 peak? Draw the structure of the fragment.

7) What organic molecule fragment is lost to give the transition from $m/z$ 72 to $m/z$ 43? Draw the structure of the fragment.
Skill building questions:
8) Which m/z value corresponds to the base peak in the following mass spectrum?

\[ \text{Intensity} \]
\[ \text{m/z} \]

A) 45
B) 44
C) 29
D) 15
E) none of these
Ans: 

9) Which of the m/z values correspond to the molecular ion peak in the following mass spectrum?

\[ \text{Intensity} \]
\[ \text{m/z} \]

A) 45
B) 44
C) 29
D) 15
E) none of these
Ans: 

10) Which of the following compounds will have odd m/z value for the molecular ion?

A) I
B) II
C) III
D) IV
E) none of these
Ans: 

11) Which of the following mass spectra shows the presence of bromine in a compound? All spectra show the molecular ion.

A) I  
B) II  
C) III  
D) IV  
E) none of these

Ans: 

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Chapter 15: 4

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12) Which of the following mass spectra shows the presence of chlorine in a compound? All spectra show the molecular ion.

A) I
B) II
C) III
D) IV
E) none of these

Ans: [ ]

13) Which of the following about electromagnetic radiation is FALSE?
   A) frequency is directly proportional to wavelength
   B) frequency is directly proportional to energy
   C) frequency is inversely proportional to wavelength
   D) wavelength is inversely proportional to energy
   E) none of these

Ans: [ ]
14) Which of the following electromagnetic radiation has the HIGHEST energy? Remember the analogy used in class. Try to avoid seeking a table of energy values to solve this; use intuition.
   A) UV
   B) X-ray
   C) IR
   D) microwave
   E) visible
   Ans:  

15) Which of the following information is primarily obtained from infrared spectroscopy?
   A) arrangement of carbon and hydrogen atoms in a compound
   B) molecular weight of a compound
   C) conjugated π system present in a compound
   D) functional groups present in a compound
   E) all of these
   Ans:  

16) Which of the following vibrations are observed in IR spectroscopy?
   A) stretching
   B) rotational
   C) bending
   D) A and B
   E) A and C
   Ans:  

17) Rank absorption of the indicated bonds in decreasing (highest to lowest) order of wavenumber.

18) Rank absorption of the indicated bonds in decreasing (highest to lowest) order of wavenumber in a dilute solution to minimize H-bonding.

19) Rank absorption of the indicated bonds in decreasing (highest to lowest) order of wavenumber.
20) Rank absorption of the indicated bonds in decreasing (highest to lowest) order of wavenumber. Most students are inclined to need a table to determine this, try it without a table using deductive reasoning.

\[ \text{O} \quad \text{II} \quad \text{III} \quad \text{IV} \quad \text{V} \quad \text{H} \]

Highest wavenumber

Lowest wavenumber

21) Which of the following are units for wavenumber in IR spectroscopy?

A) \( \text{cm}^{-1} \)
B) \( \text{cm} \)
C) \( \text{J.s}^{-1} \)
D) \( \text{mm} \)
E) none of these

Ans: 

22) Three IR spectra of three \( \text{C}_6 \) compounds with the vibrational frequency (shown) of the bond between \( \text{C}_1 \) and \( \text{C}_2 \). Place the letter of the spectra next to the appropriate compound.

\[ \text{A} \quad \text{B} \quad \text{C} \]

\[ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \quad \text{CH}_2=\text{CH}_2 \quad \text{CH}_3\text{CH}=\text{CH}_2 \]

\[ 1827 \text{ cm}^{-1} \quad 2120 \text{ cm}^{-1} \quad 1379 \text{ cm}^{-1} \]
23) Draw the *charged* McLafferty product represented by the arrows.

24) Draw the \( \alpha \)-cleavage products by cleavage of the bond, designated with ( \(- - -\) ).
25) Match compounds A and B below to their IR spectrum. Place letter in box at right.

A

B

26) A feasible alpha cleavage fragment ION for each of the following molecules would be... Place letter in box.

A

B

C

D

E

Both B and D

Letter Here
27) Match compounds A and B below to their IR spectrum. Place letter in box at right.
28) Identify the IR spectrum that belongs to the reactant (R) and product (P).
29) The IR spectrum of carvone is below, CLEARLY draw a line from the circled functional group to the IR absorbance in the spectrum. The arrow head should point at the absorbance.

For example:

![IR Spectrum of Carvone](image)

Continue the line into the spectrum
30) MATCH a structure from the list below to the following IR and/or NMR spectra.
31) MATCH a structure from the list below to the following IR and/or NMR spectra.
32) MATCH a structure from the list below to the following IR and/or NMR spectra.

A

B

C

D

E

F

Letter here
33) MATCH a structure from the list below to the following IR and/or NMR spectra.

A
\HO\H

B
\ce{C=\ce{CH2}}

C
\HO\ce{C(=\ce{O})C(=\ce{O})C}

D
\ce{PhC(=\ce{O})C(=\ce{O})C}

E
\ce{PhC(=\ce{O})C(=\ce{O})C}

F
\ce{\ce{CH3}=\ce{CH2}=\ce{CH2}=\ce{CH2}}

\begin{center}
\includegraphics[width=\textwidth]{spectrum1.png}
\end{center}
34) MATCH a structure from the list below to the following IR and/or NMR spectra.

Letter

2 peaks
35) MATCH a structure from the list below to the following IR and/or NMR spectra.

A) HO
B) H
C) O
D) O
E) H
F) H

IR Spectrum:

NMR Spectrum:

Letter here
Use the following example as a guide to answer the next set of problems

Example: (this will not be provided on the exams)

For the following pair of compounds the expected stretching absorption of the C=O bond is 1685 cm⁻¹ & 1655 cm⁻¹ respectively. Explain using both words and structural drawings.

Both compounds I and II have conjugated double bond that allows for single bond character to the carbonyl group.
- For compound II the oxygen atom allows for additional resonance structures, which results in more single bond character for the carbonyl group. This results in absorption of the carbonyl group at a lower wavenumber.

36) CIRCLE the compound that has the LOWEST wavenumber for carbonyl absorption?

37) CIRCLE the compound that has the HIGHEST wavenumber for carbonyl absorption?
38) The C—O absorption in carboxylic acids appears around 1250 cm⁻¹, whereas the C—O absorption in alcohol appears around 1050 cm⁻¹. Explain why.

![Diagram of C—O absorption in carboxylic acids and alcohol]

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39) Which of the following bonds has the weakest IR absorption?

A) C=C  
B) O—H  
C) C=O  
D) sp² C—H  
E) A and D

Ans: [ ]

40) Diluted alcohols show a _____ absorption distinctly ~3600 cm⁻¹, due to _____.

A) sharp, hydrogen bonding  
B) broad, hydrogen bonding  
C) sharp, absence of hydrogen bonding  
D) broad, absence of hydrogen bonding

Ans: [ ]

41) Concentrated alcohols show a _____ absorption in the region between 3200-3600 cm⁻¹, due to _____.

A) sharp, hydrogen bonding  
B) broad, hydrogen bonding  
C) sharp, polarity  
D) broad, polarity

Ans: [ ]
42) Match each compound to its IR spectrum below

A

B

Letter here

Letter here
43) Match each IR spectrum below to a compound.
44) Match the IR spectrum below to a compound.

45) Match the IR spectrum below to a compound.
46) Match the IR spectrum below to a compound.

![IR Spectrum Image]

1721 cm\(^{-1}\)

1731 cm\(^{-1}\)