

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

a) $C_{10}H_{16}$ $\frac{22}{2}$	<input type="text" value="3"/>	b) $C_{17}H_{23}NO_3$ $\frac{34}{2}$ $\frac{22}{14/2}$	<input type="text" value="7"/>	c) $C_{10}H_{16}O_2$ $\frac{22}{2}$ $\frac{6}{2}$	<input type="text" value="3"/>
d) $C_8H_8O$ $\frac{18}{2}$ $\frac{19}{2}$	<input type="text" value="5"/>	e) $C_5H_9NO_2$ $\frac{12}{2}$ $\frac{8}{4/2}$	<input type="text" value="2"/>	f) $C_8H_{10}N_4O_2$ $\frac{18}{2}$ $\frac{4}{4/2}$	<input type="text" value="6"/>
g) $C_7H_{10}Cl_2$ $\frac{16}{2}$ $\frac{17}{4/2}$	<input type="text" value="2"/>	h) $C_8H_{10}ClNO$ $\frac{18}{2}$ $\frac{18}{18/2}$	<input type="text" value="4"/>	i) $C_{27}H_{46}O$ $\frac{56}{2}$ $\frac{10}{10/2}$	<input type="text" value="5"/>
j) $C_{20}H_{34}O_5$ $\frac{42}{2}$ $\frac{8}{8/2}$	<input type="text" value="4"/>	k) $C_{14}H_9Cl_5$ $\frac{30}{2}$ $\frac{14}{14/2}$	<input type="text" value="8"/>	l) $C_9H_{11}N$ $\frac{20}{2}$ $\frac{10}{10/2}$	<input type="text" value="5"/>
m) $C_{14}H_{14}N_2O$ $\frac{30}{2}$ $\frac{17}{17/2}$	<input type="text" value="9"/>	n) $C_{11}H_8ClBrO$ $\frac{24}{2}$ $\frac{18}{18/2}$	<input type="text" value="7"/>	o) $C_5H_5Br_2NO$ $\frac{12}{2}$ $\frac{6}{6/2}$	<input type="text" value="3"/>
p) $C_9H_{11}NO$ $\frac{20}{2}$ $\frac{10}{10/2}$	<input type="text" value="5"/>	q) $C_8H_{10}BrIO$ $\frac{18}{2}$ $\frac{12}{12/2}$	<input type="text" value="3"/>		

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

a)  $C_8H_xO_2$  (2 rings; 1 double bond)  $x = \boxed{12}$

$\left. \begin{array}{l} C_8H_{18} \\ - C_8H_x \end{array} \right\} \frac{(18-x)}{2} = 3$  3 dous simple math  $18-x=6$

b)  $C_7H_xN$  (2 double bonds)  $x = \boxed{13}$

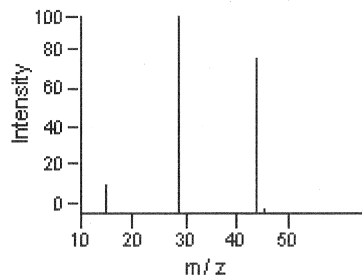
$\left. \begin{array}{l} C_7H_{16} \\ - C_7H_{x-1} \end{array} \right\} \frac{17-x}{2} = 2$   $17-x=4$   $16-(x-1)$

c)  $C_9H_xNO$  (1 ring; 3 double bonds)  $x = \boxed{13}$

$\left. \begin{array}{l} C_9H_{20} \\ - C_9H_{x-1} \end{array} \right\} \frac{21-x}{2} = 4$   $21-x=8$



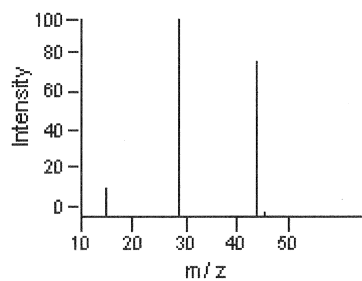
## Skill building questions:

8) Which  $m/z$  value corresponds to the base peak in the following mass spectrum?

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

Ans:

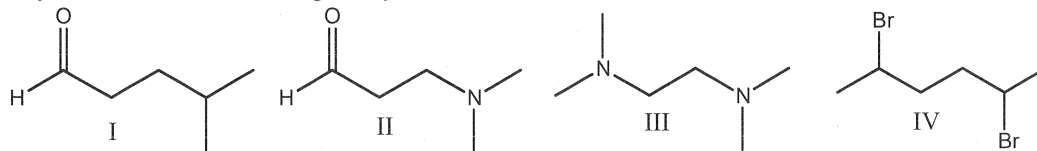
C

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

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

Ans:

B

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

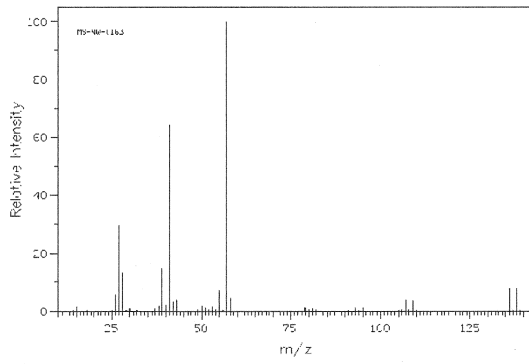
- A) I  
 B) II  
 C) III  
 D) IV  
 E) none of these

Ans:

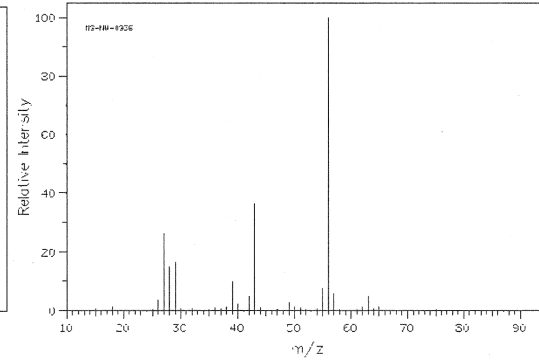
B

'odd Nitrogen Rule'

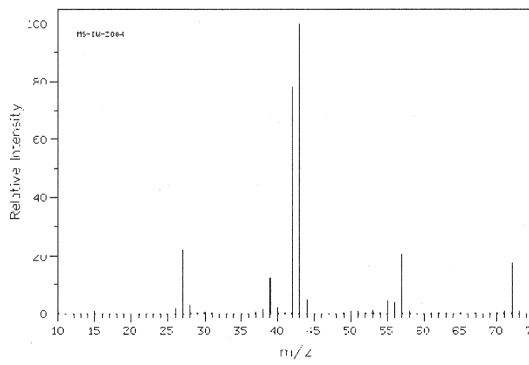
11) Which of the following mass spectra shows the presence of bromine in a compound? All spectra show the molecular ion.



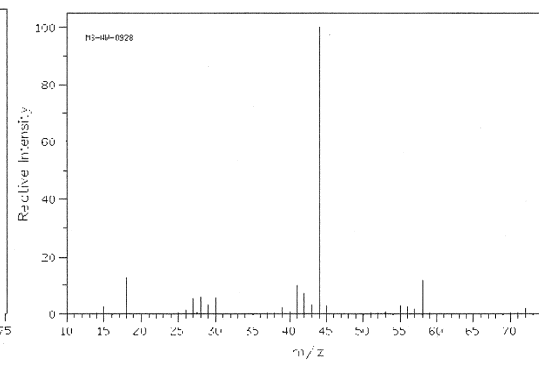
I



II



III



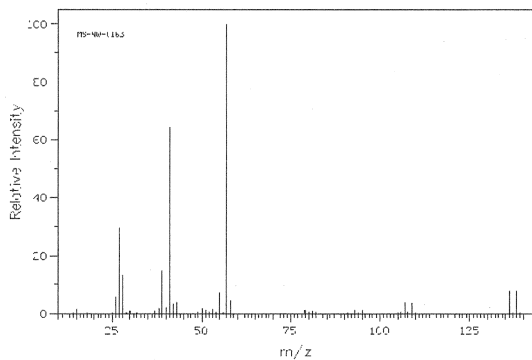
IV

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

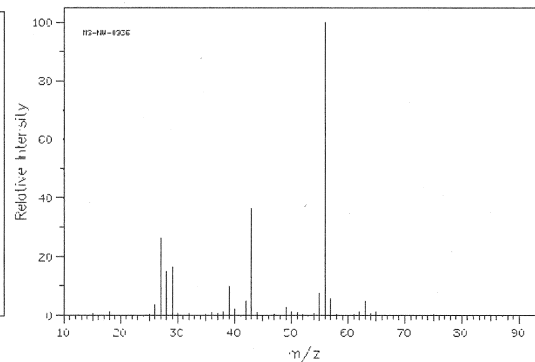
Ans:

A

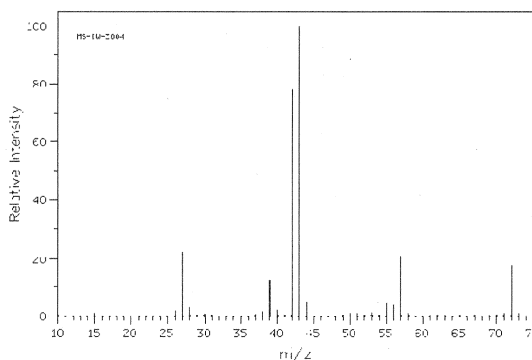
12) Which of the following mass spectra shows the presence of chlorine in a compound? All spectra show the molecular ion.



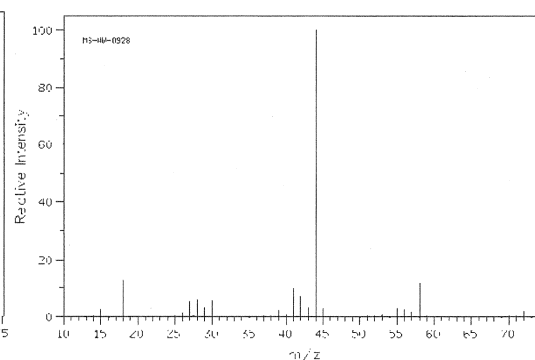
I



II



III



IV

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

Ans:

E

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:

A

$$E = h\nu ; E = \frac{hc}{\lambda}$$

$$c = \lambda\nu \rightarrow \frac{c}{\lambda} = \nu \text{ frequency}$$

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 → sun damage
- B) X-ray → lead shields needed
- C) IR → heating lamp
- D) microwave → household
- E) visible → eyes

Ans:

B

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  $\pi$  system present in a compound
- D) functional groups present in a compound
- E) all of these

Ans:

D

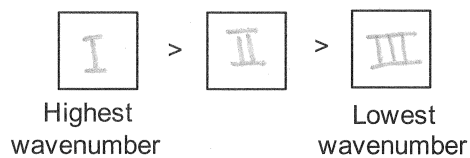
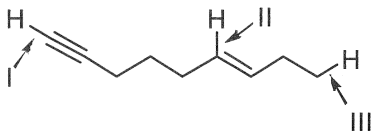
16) Which of the following vibrations are observed in IR spectroscopy?

- A) stretching
- B) rotational
- C) bending
- D) A and B
- E) A and C

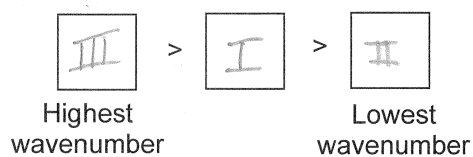
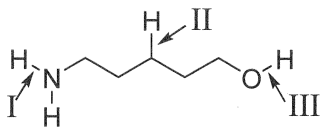
Ans:

E

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

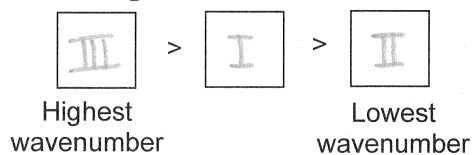
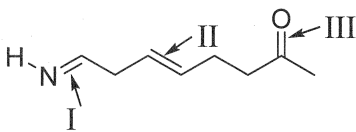


18) Rank absorption of the indicated bonds in decreasing (highest to lowest) order of wavenumber, in a dilute solution to minimize H-bonding.



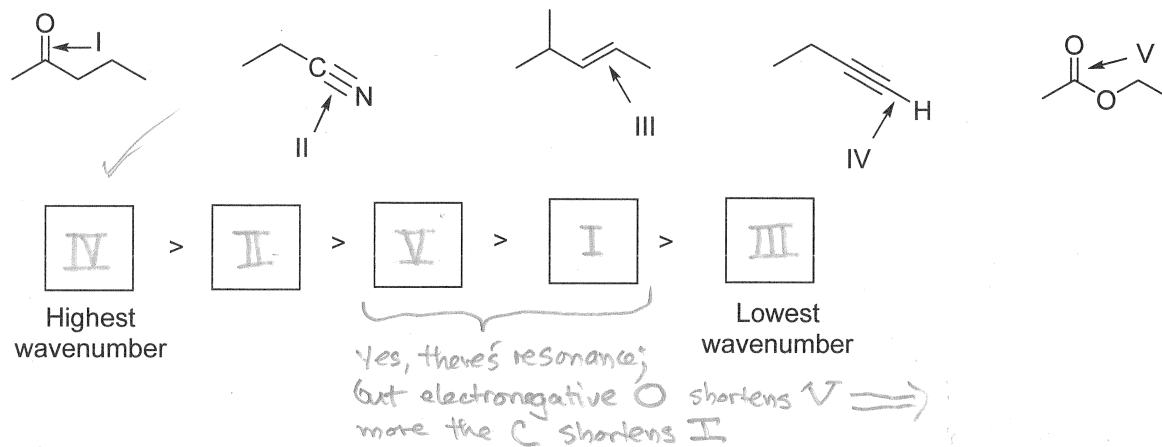
C N O  
 ↑  
 more electronegative

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



C N O  
 electro (-)  
 C=O  
 higher freq nbr

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.



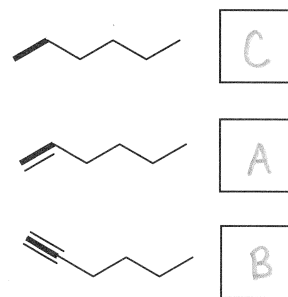
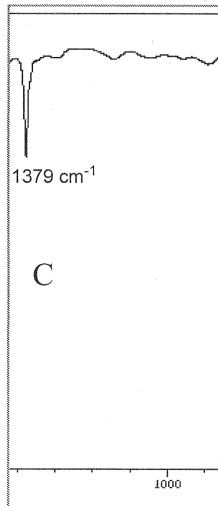
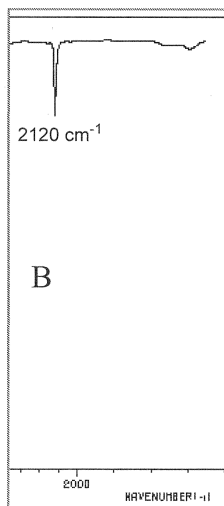
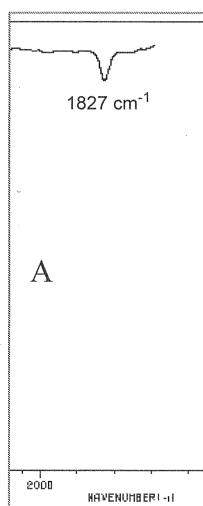
21) Which of the following are units for wavenumber in IR spectroscopy?

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

Ans:

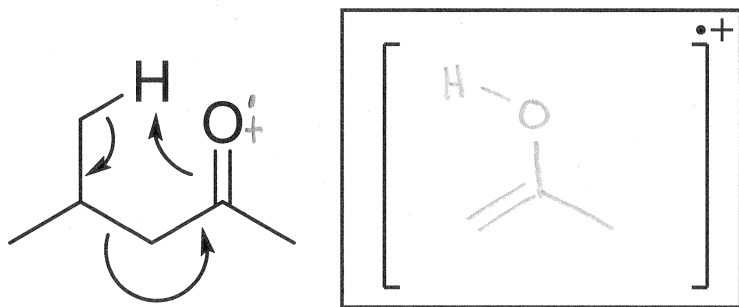
$\boxed{\text{A}}$

22) Three IR spectra of three  $\text{C}_6$  compounds with the vibrational frequency (shown) of the bond between C1 and C2. Place the letter of the spectra next to the appropriate compound.

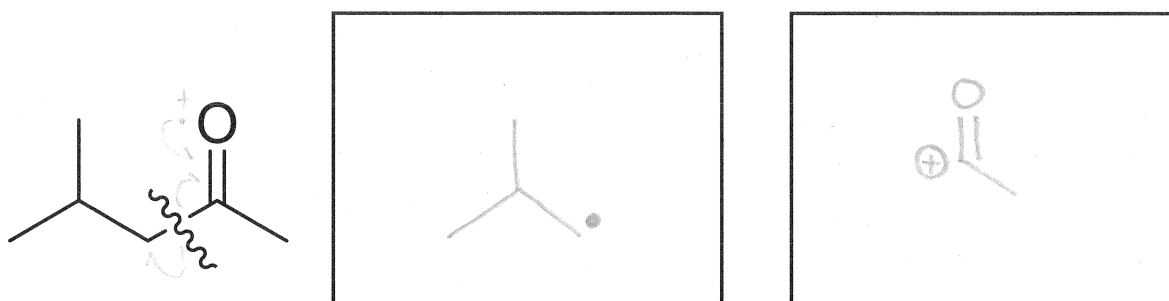




23) Draw the charged McLafferty product represented by the arrows.



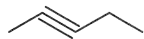
24) Draw the  $\alpha$ -cleavage products by cleavage of the bond, designated with (~~~~).



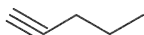
Larger uncharged  
fragment

Smaller charged  
fragment

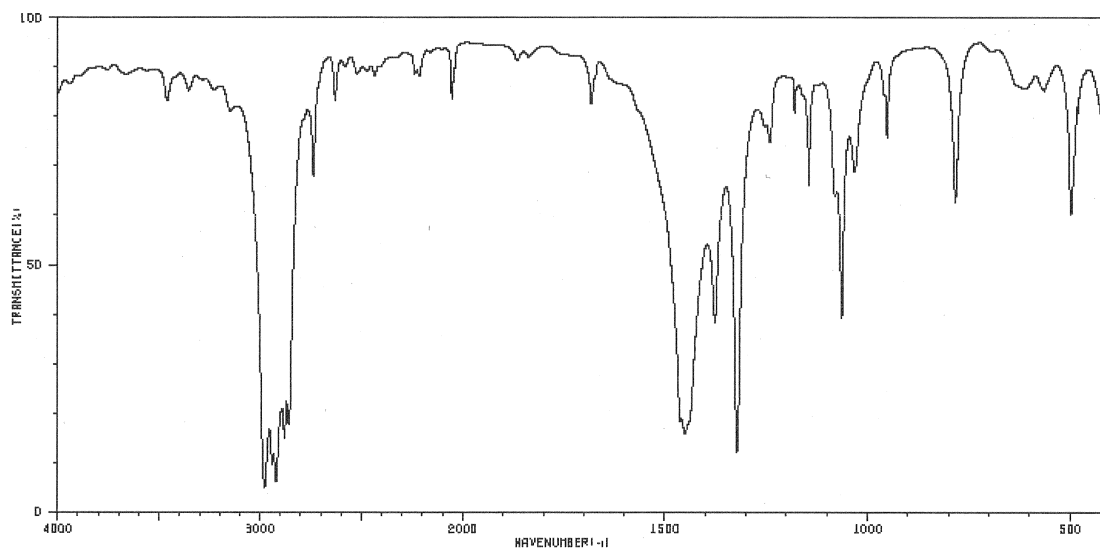
25) Match compounds A and B below to their IR spectrum. Place letter in box at right.



A

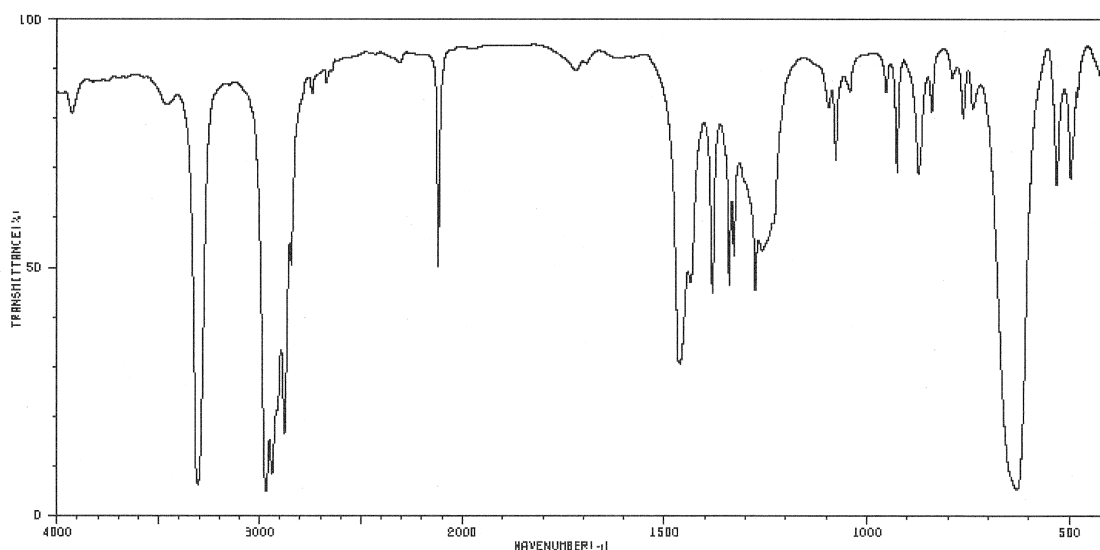


B



A

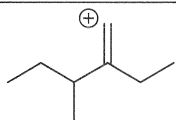
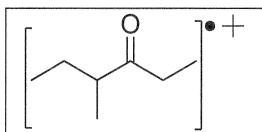
Ltr Here



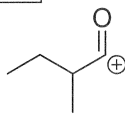
B

Ltr Here

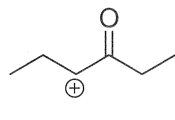
26) A feasible alpha cleavage fragment ION for each of the following molecules would be...Place letter in box.



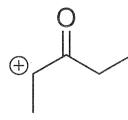
A



B



C



D

Both B and D

E

B

Letter Here

27) Match compounds A and B below to their IR spectrum. Place letter in box at right.



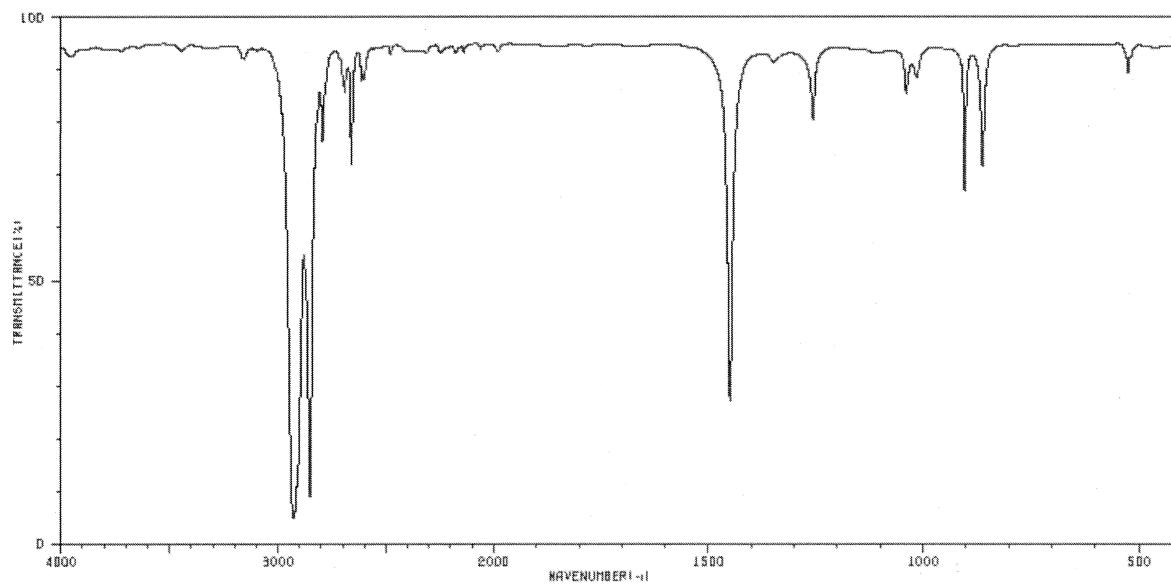
A



B

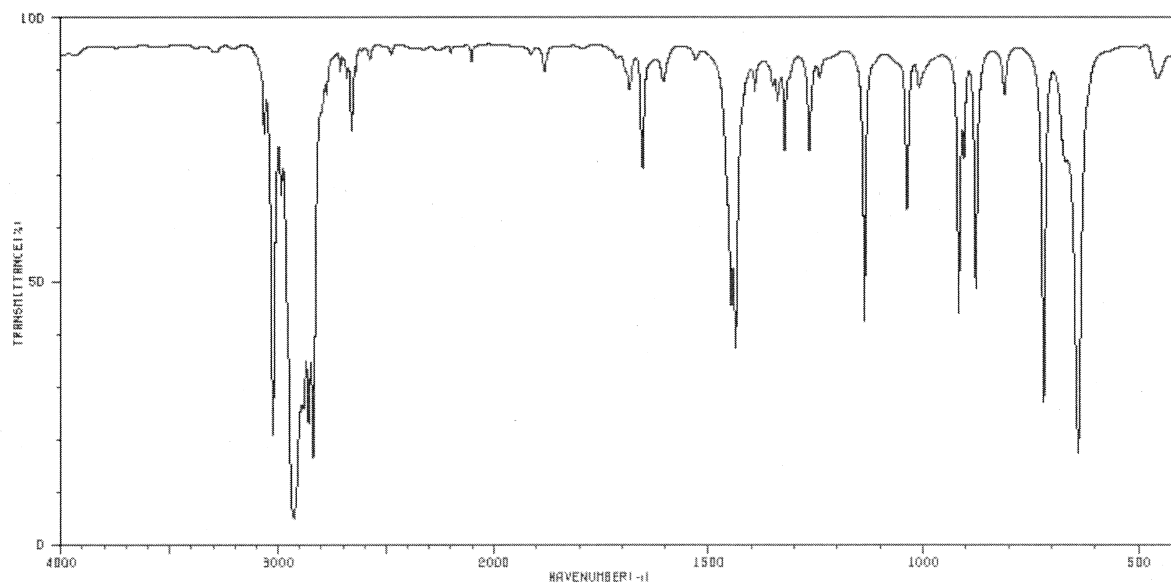
A

Ltr Here

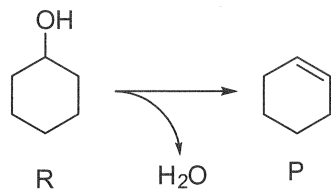


B

Ltr Here

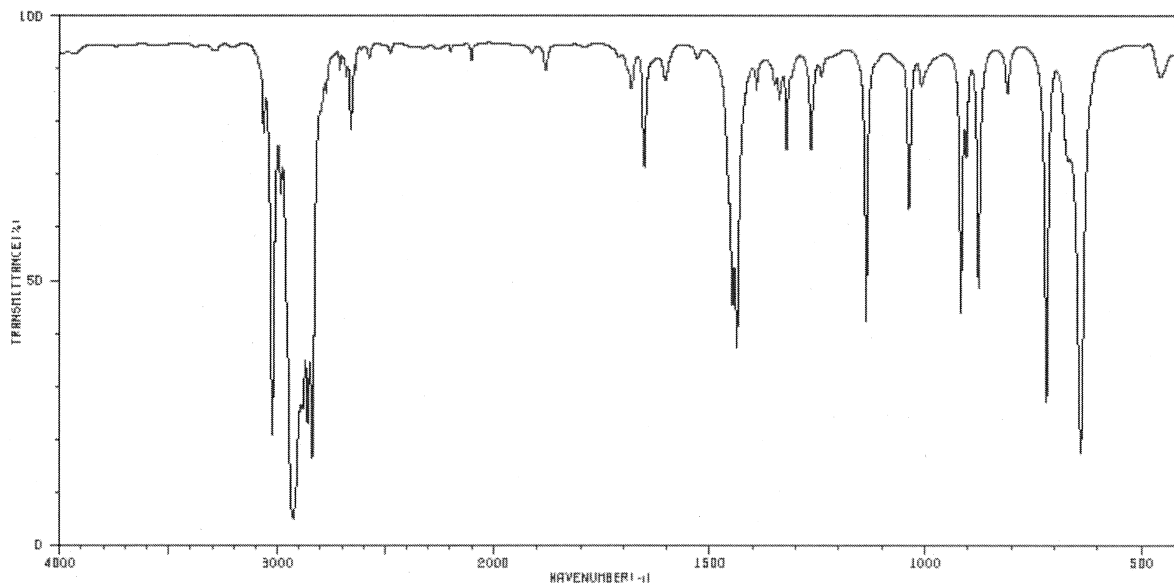


28) Identify the IR spectrum that belongs to the reactant (R) and product (P).



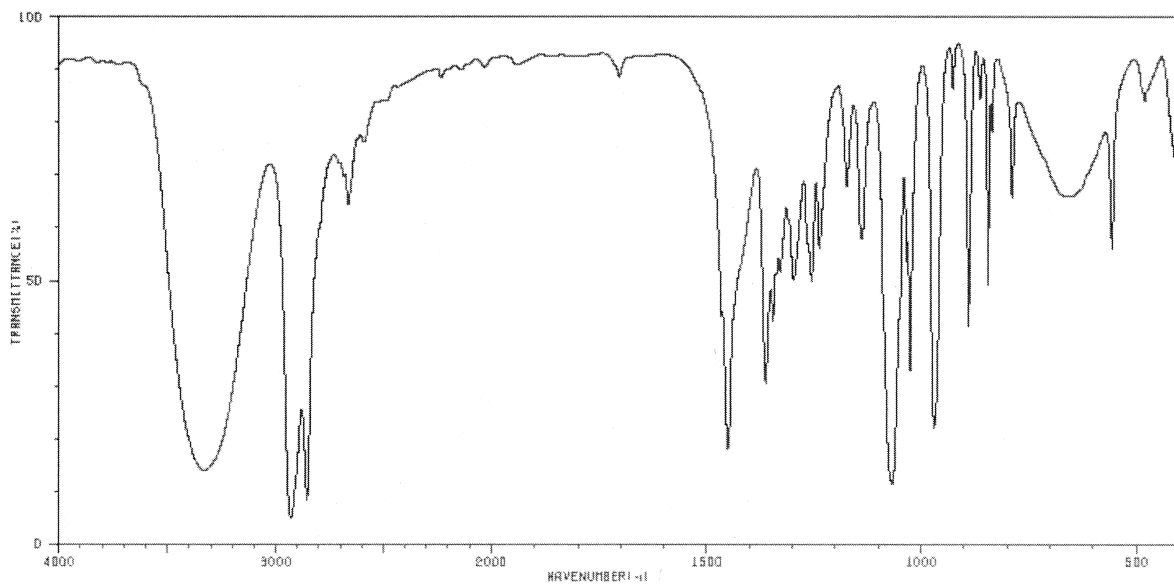
P

Ltr Here



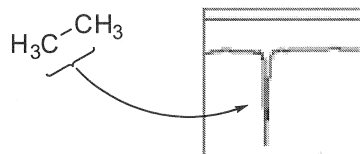
R

Ltr Here

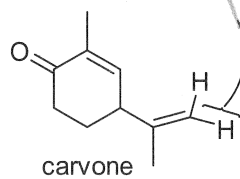
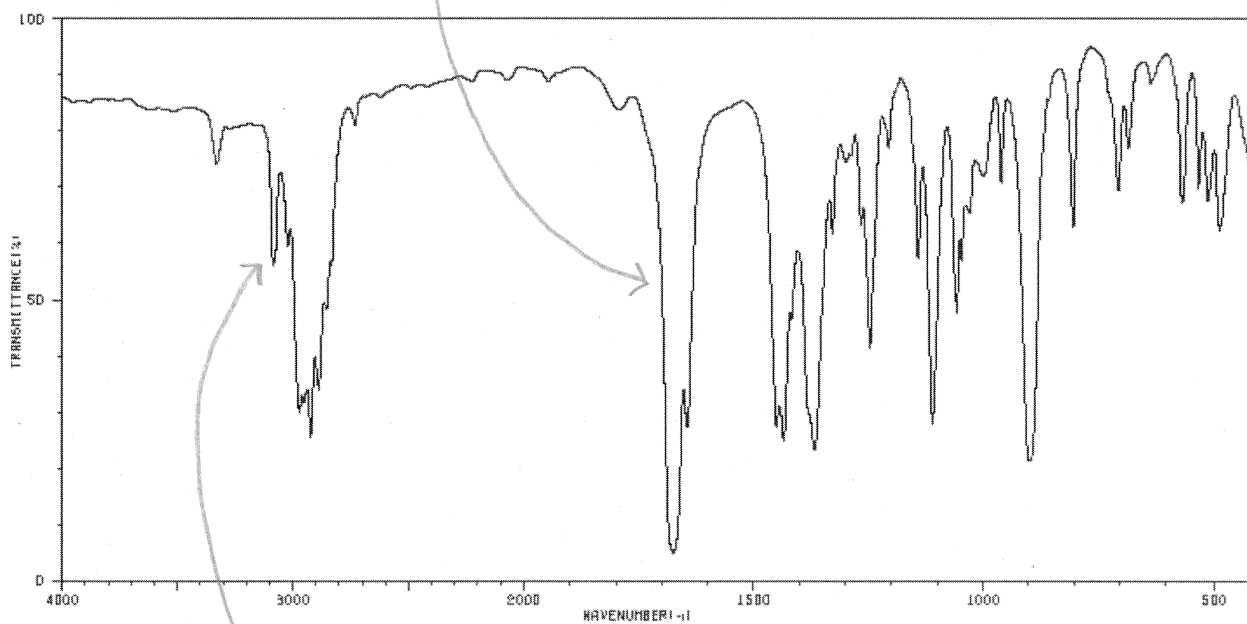
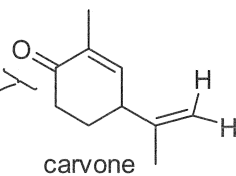


29) The IR spectrum of carvone is below, CLEARLY draw a line from the circled functional group to the IR absorbance in the spectrum. The arrow head should point at the absorbance.

For example:

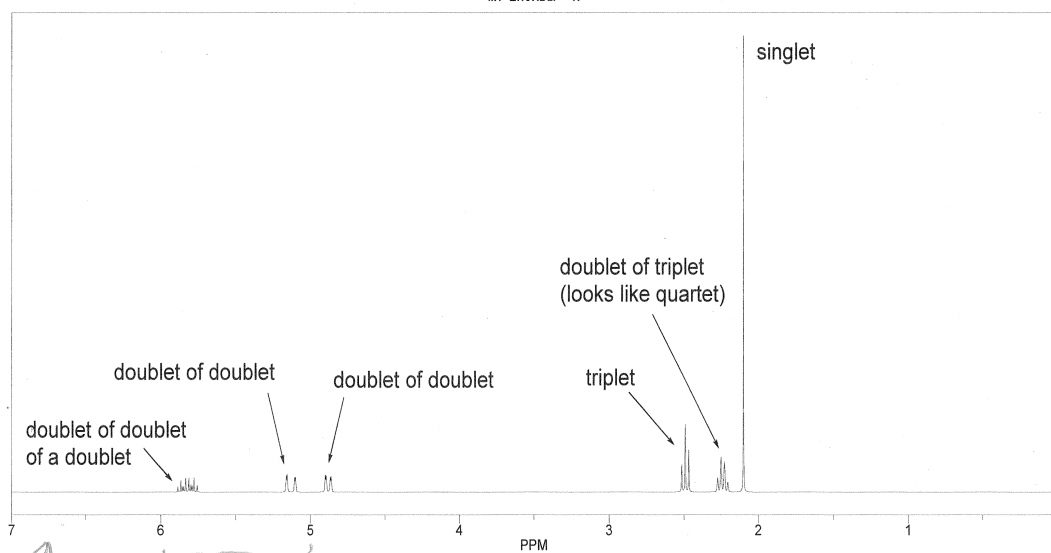
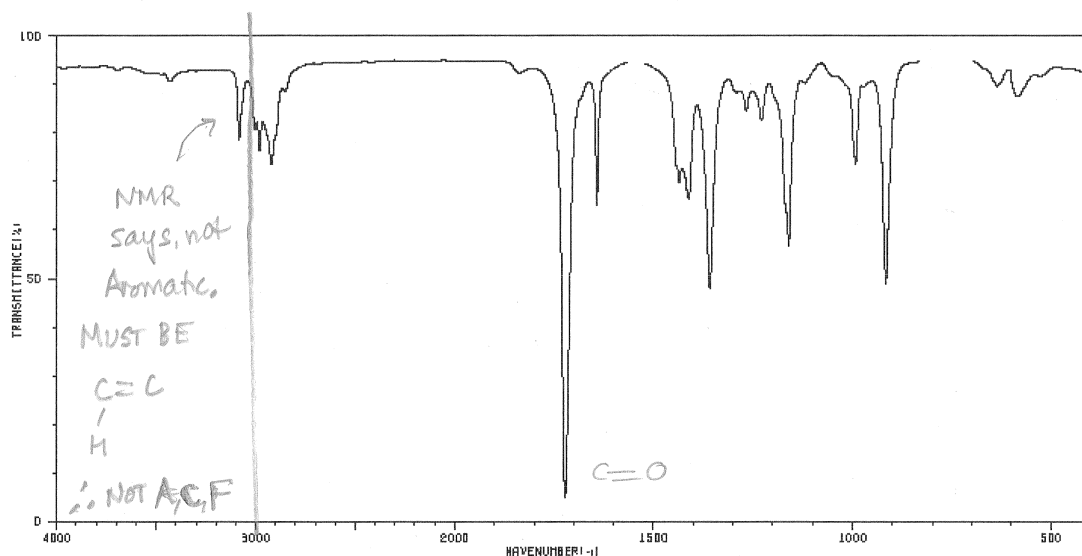
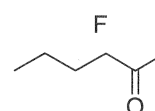
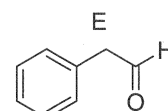
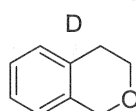
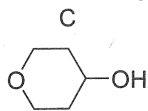
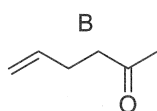
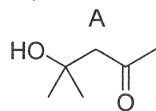


Continue the line into the spectrum



Continue the line into the spectrum

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

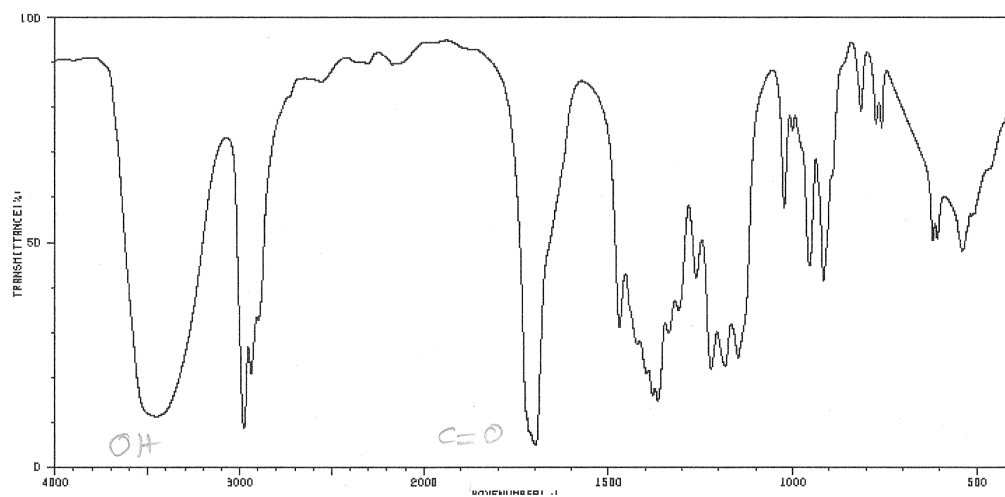
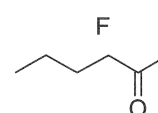
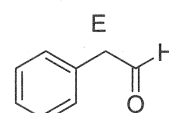
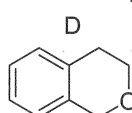
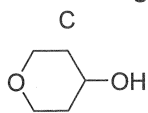
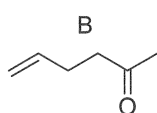
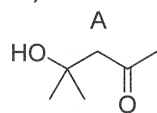


B

Letter here

no aromatics  
∴ NOT D, E

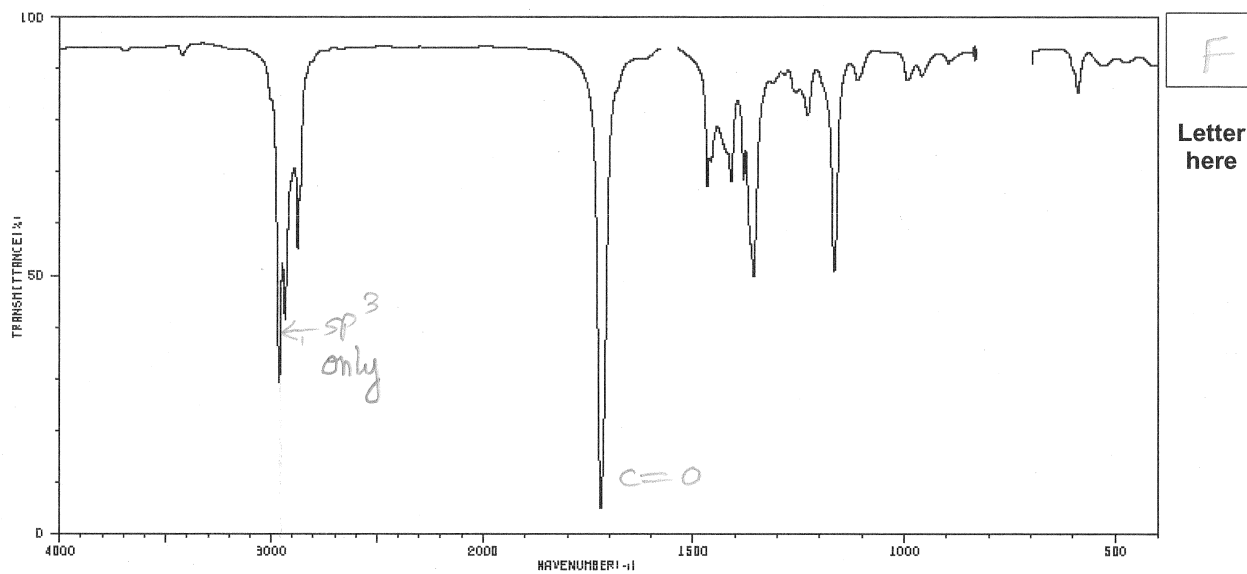
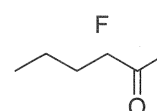
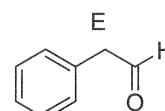
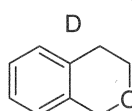
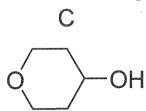
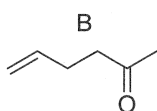
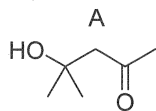
31) MATCH a structure from the list below to the following IR and/or NMR spectra.



A

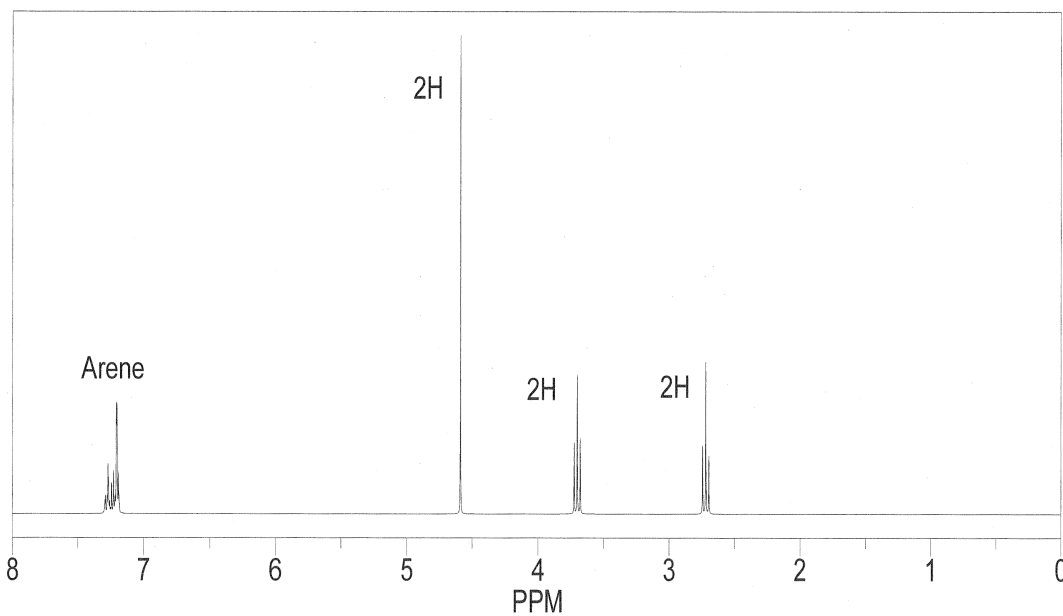
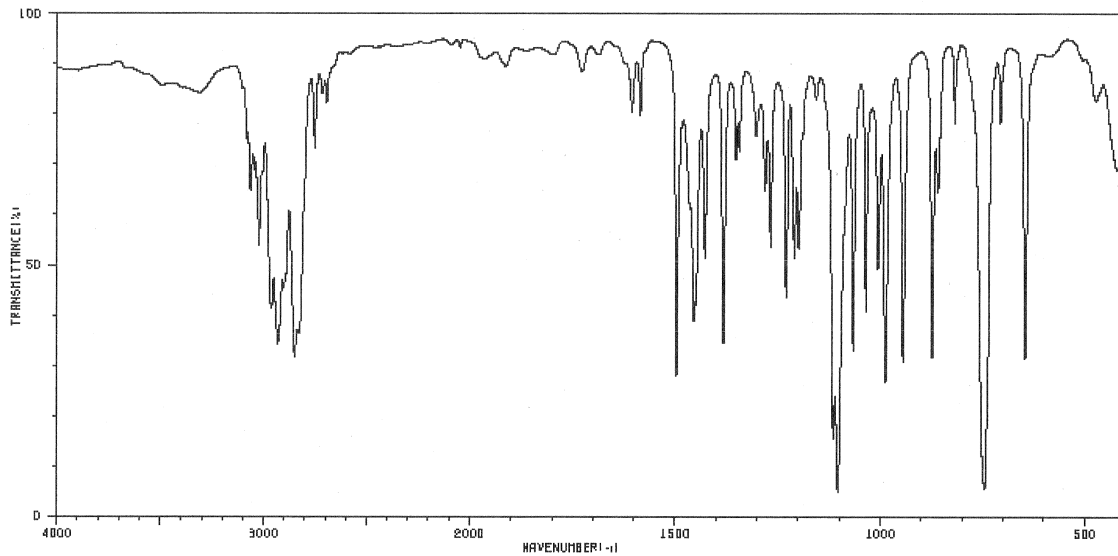
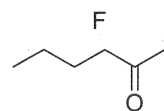
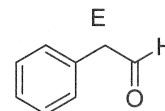
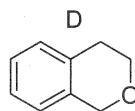
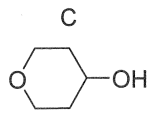
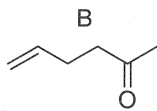
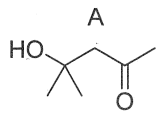
Letter here

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





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



D

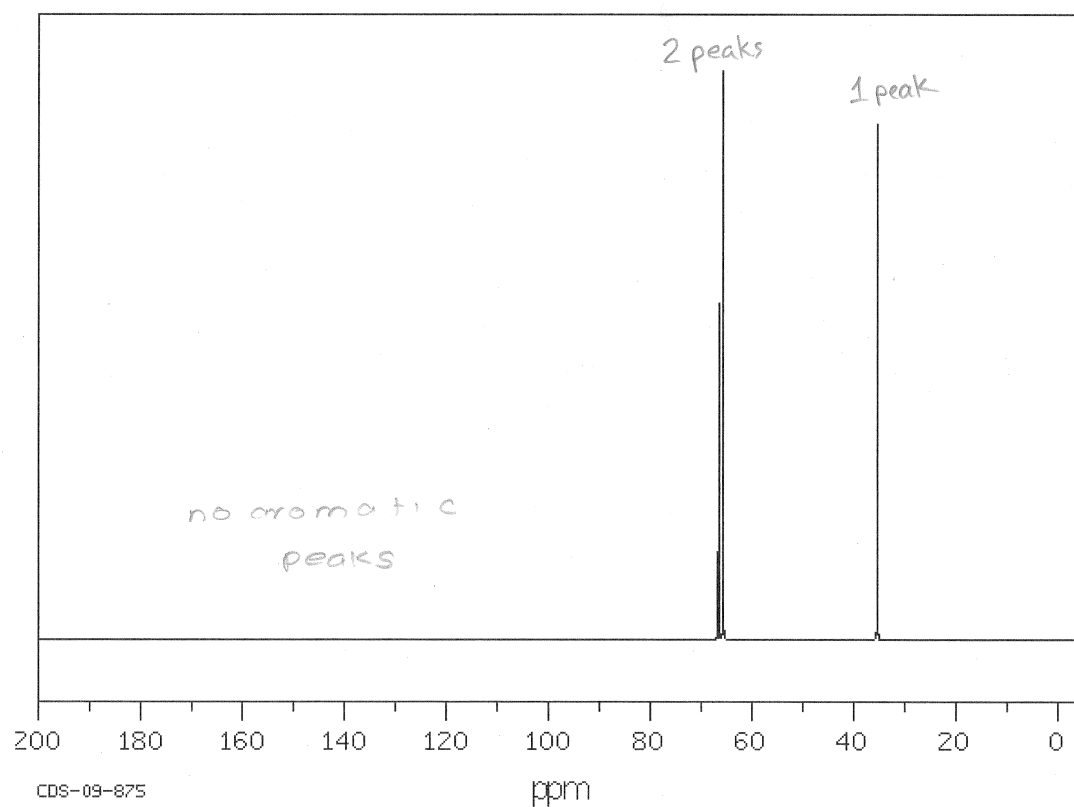
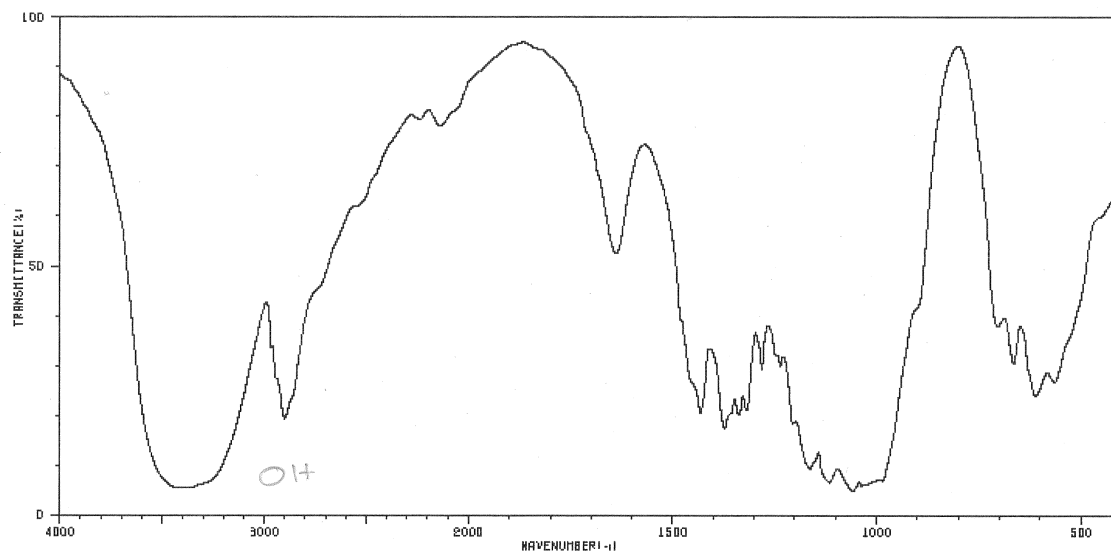
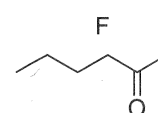
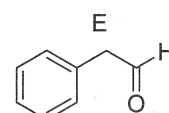
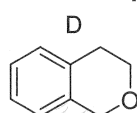
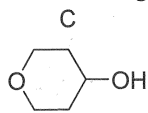
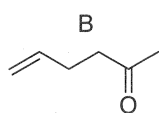
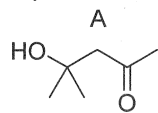
Letter here

can't be A, B, C, F (no aromatic ring)

alkyl region has 6 H

only answer is D.

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



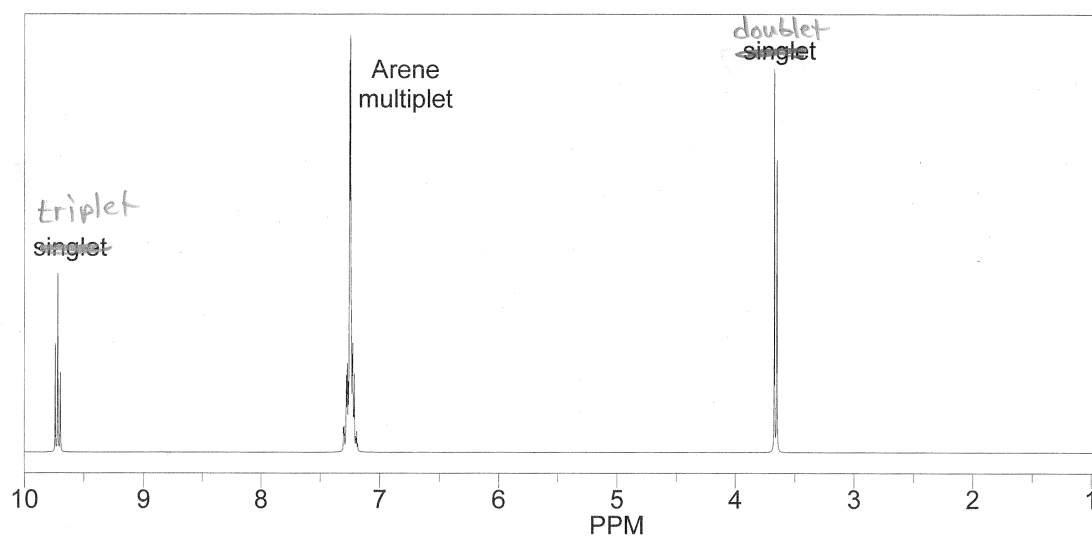
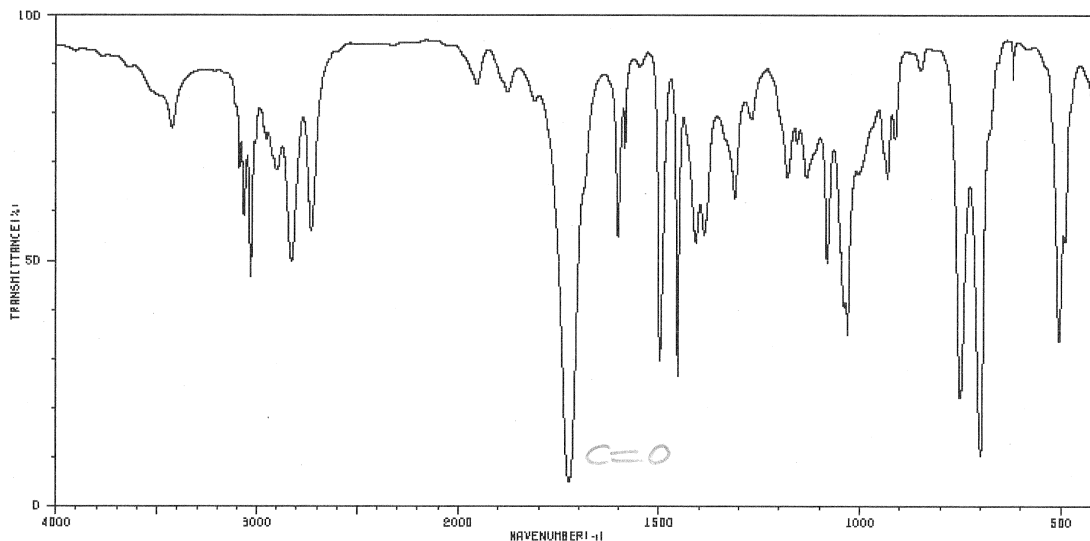
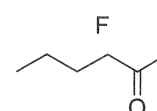
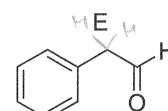
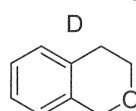
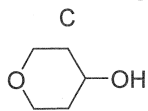
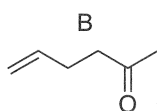
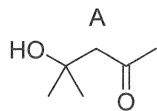
CDS-09-875

can't be D, E, B, F

C

Letter  
here

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



E

Letter here

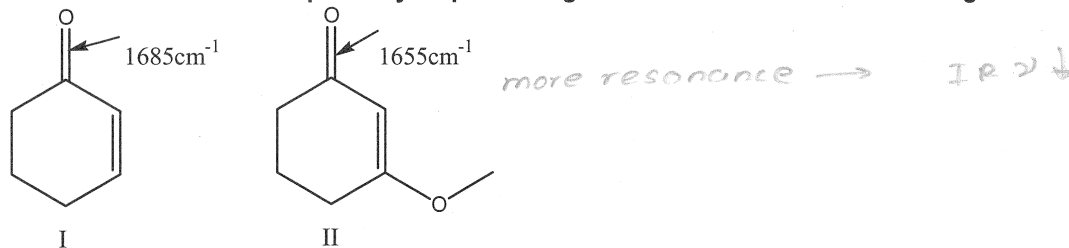
can't be A, B, C, F (no aromatic)

contains  $\text{C}=\text{O}$

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

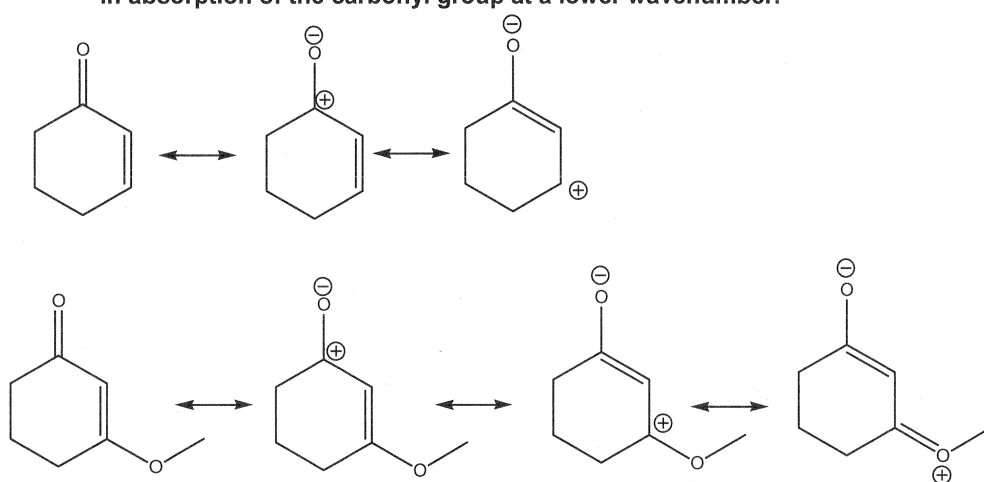
Example: (this will not be provided on the exams)

For the following pair of compounds the expected stretching absorption of the C=O bond is  $1685\text{cm}^{-1}$  &  $1655\text{cm}^{-1}$  respectively. Explain using both words and structural drawings.

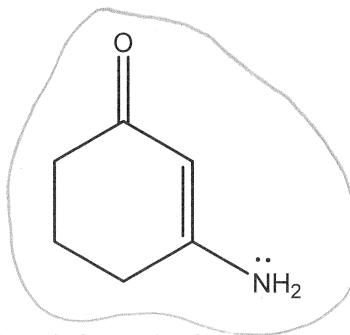
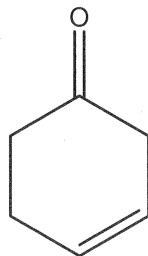
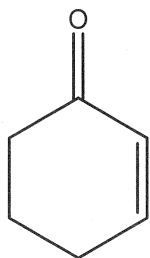
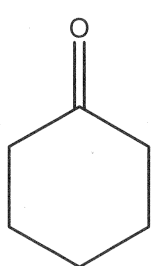


Both compounds I and II have conjugated double bond that allows for single bond character to the carbonyl group.

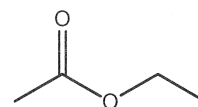
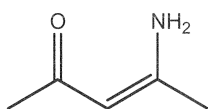
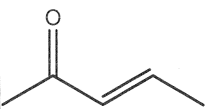
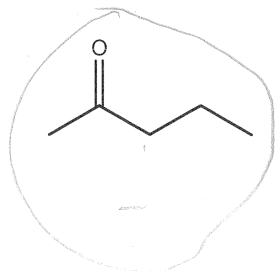
- For compound II the oxygen atom allows for additional resonance structures, which results in more single bond character for the carbonyl group. This results in absorption of the carbonyl group at a lower wavenumber.



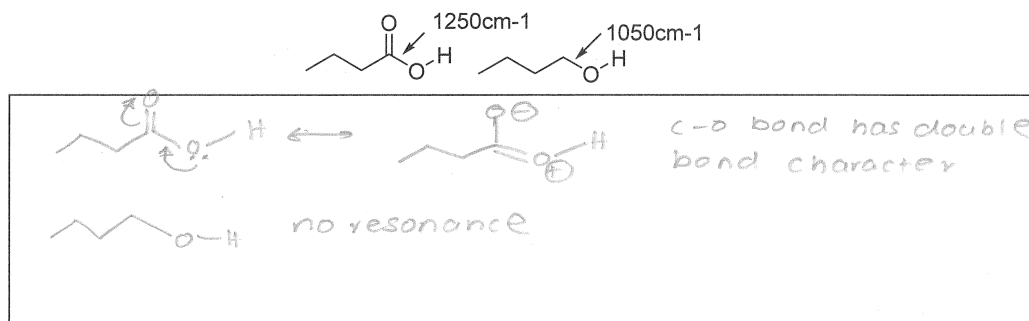
36) CIRCLE the compound that has the LOWEST wavenumber for carbonyl absorption?



37) CIRCLE the compound that has the HIGHEST wavenumber for carbonyl absorption?



38) The C—O absorption in carboxylic acids appears around  $1250\text{cm}^{-1}$ , where as the C—O absorption in alcohol appears around  $1050\text{cm}^{-1}$ . Explain why.



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

- A) C=C
- B) O—H
- C) C=O
- D)  $\text{sp}^3\text{C—H}$
- E) A and D

Ans:

A

40) Diluted alcohols show a \_\_\_\_\_ absorption distinctly  $\sim 3600\text{cm}^{-1}$ , due to \_\_\_\_\_.

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

Ans:

C

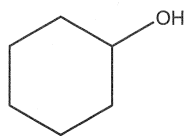
41) Concentrated alcohols show a \_\_\_\_\_ absorption in the region between  $3200\text{--}3600\text{cm}^{-1}$ , due to \_\_\_\_\_.

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

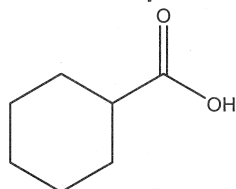
Ans:

B

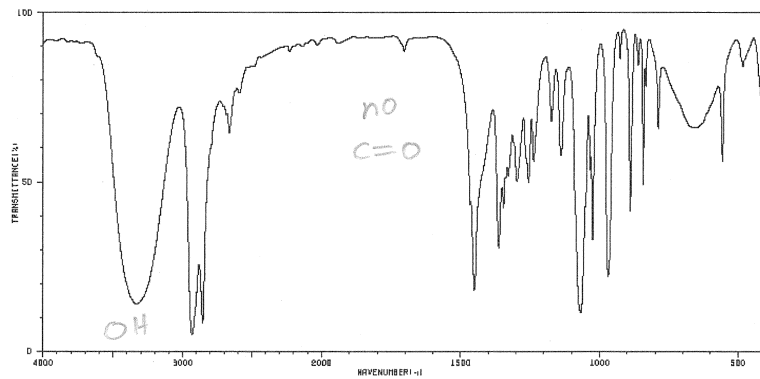
42) Match each compound to its IR spectrum below



A

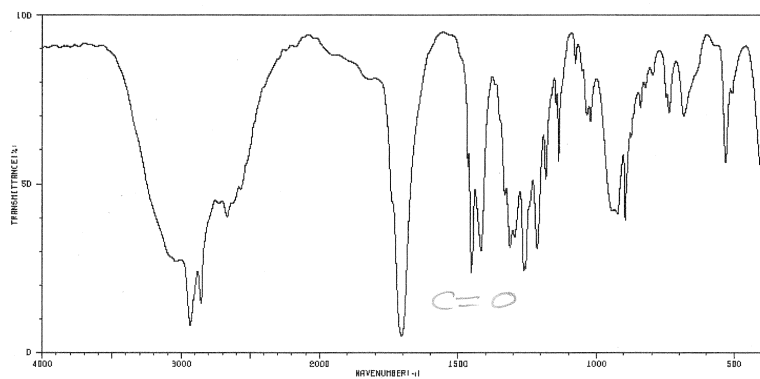


B



A

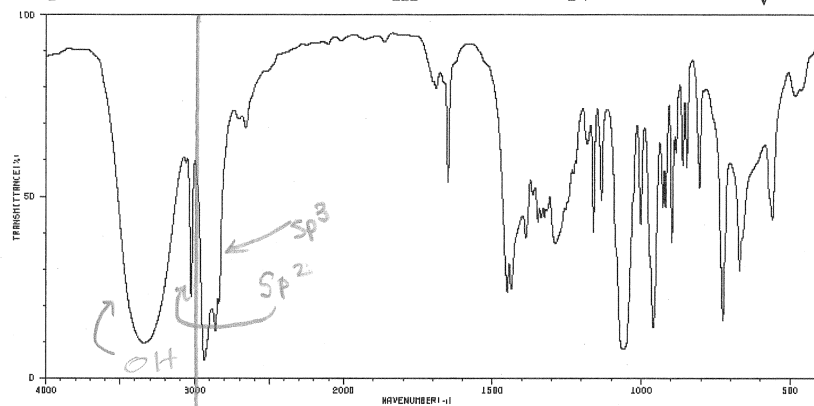
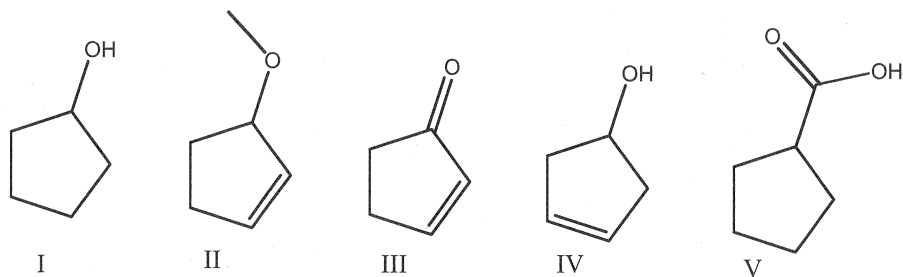
Letter here



B

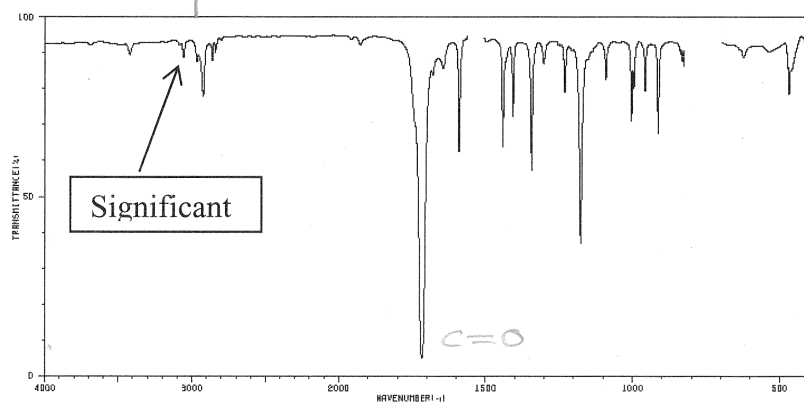
Letter here

43) Match each IR spectrum below to a compound.



IV

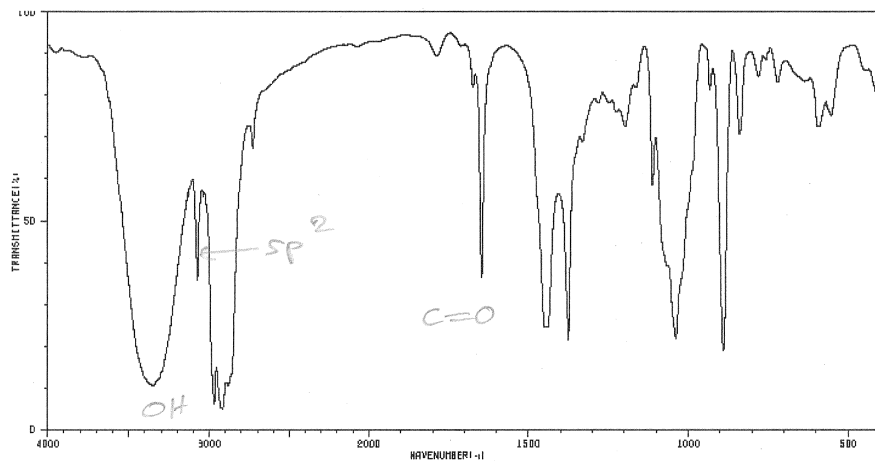
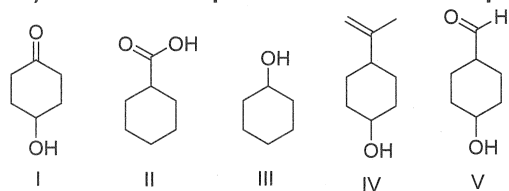
Letter here



II

Letter here

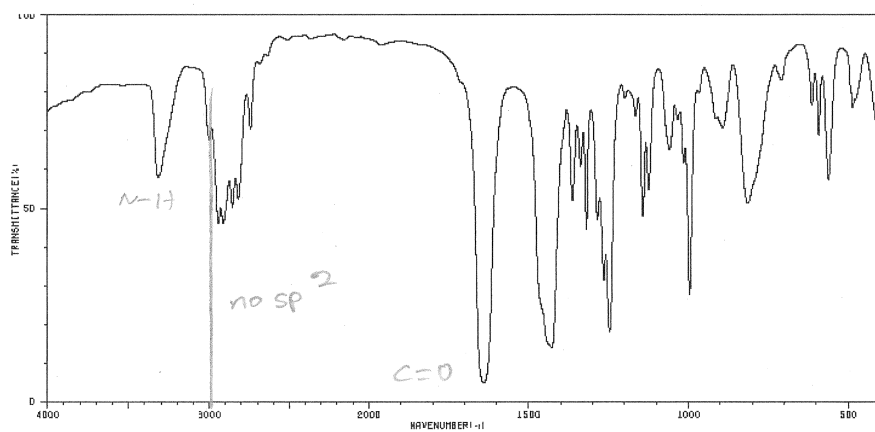
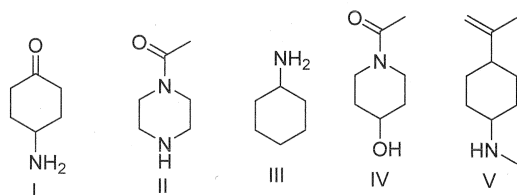
44) Match the IR spectrum below to a compound.



IV

Letter here

45) Match the IR spectrum below to a compound.

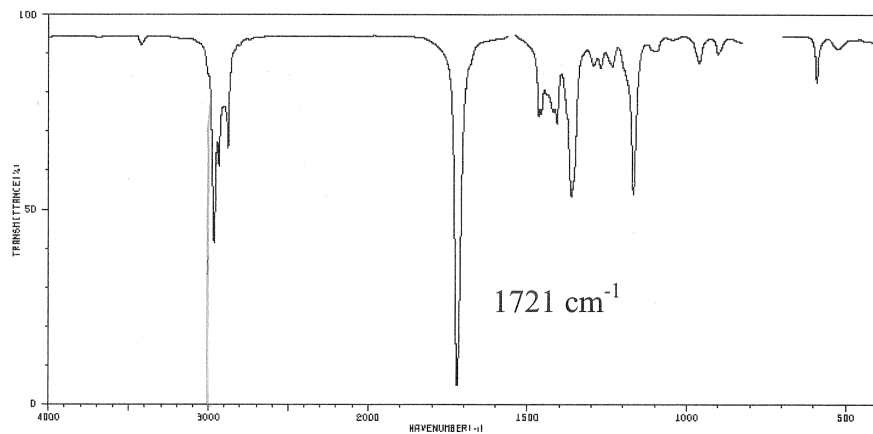
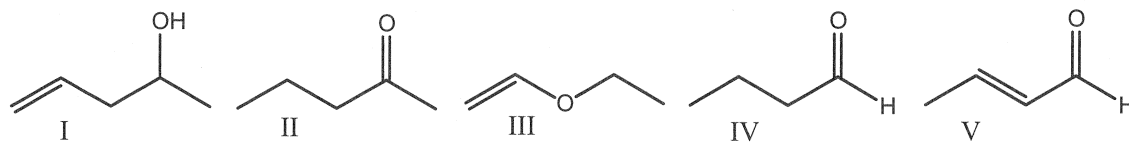


II

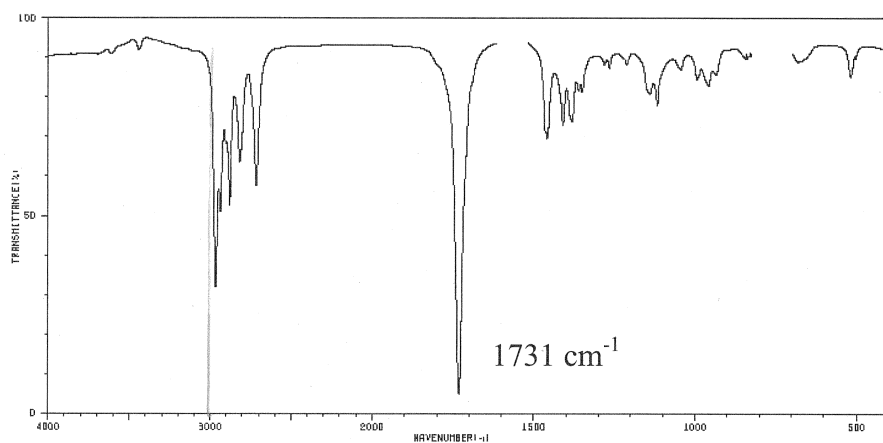
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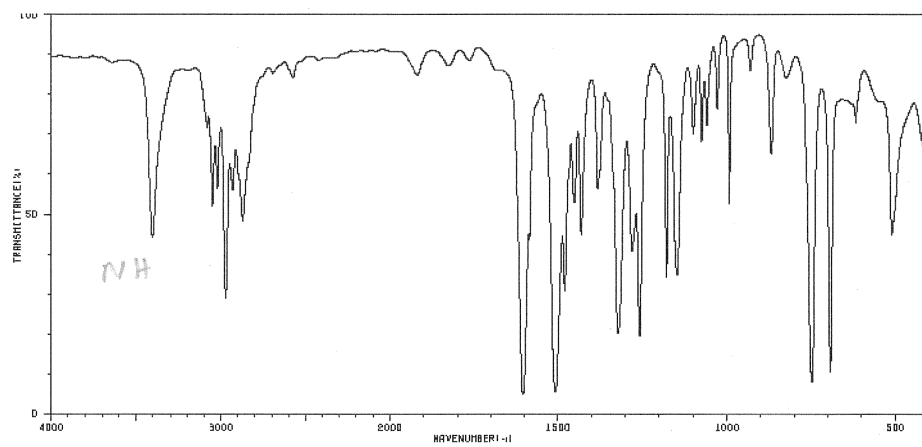
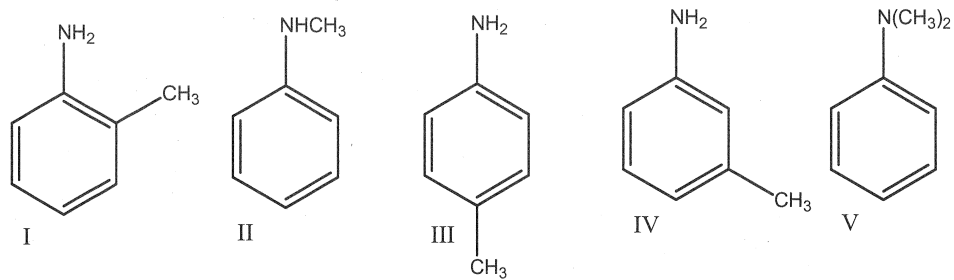
46) Match the IR spectrum below to a compound.



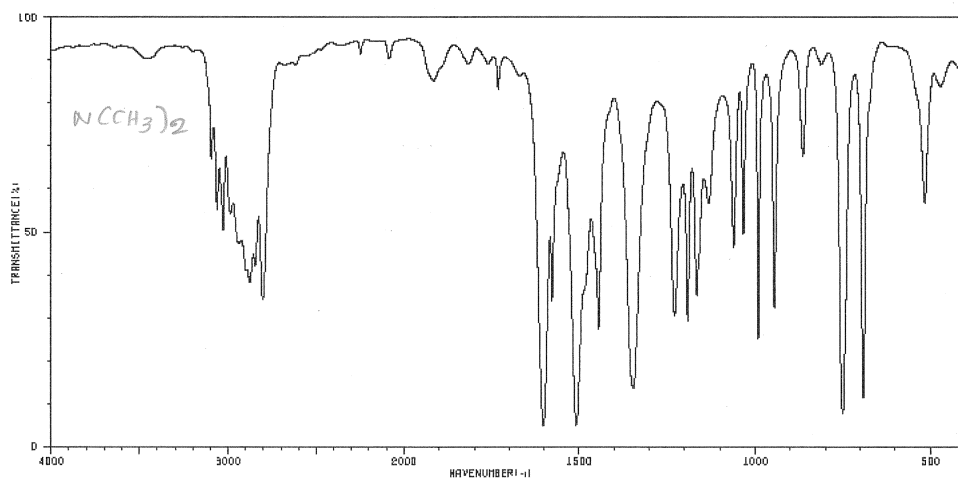
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Letter here



Letter here



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