

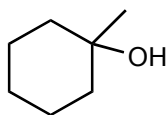
## HOMEWORK PROBLEMS: IR SPECTROSCOPY

1. You find a bottle on the shelf only labeled  $C_3H_6O$ . You take an IR spectrum of the compound and find major peaks at  $2950$ ,  $1720$ , and  $1400\text{ cm}^{-1}$ . Draw a molecule that might be the compound in the bottle.

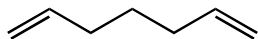
2. For each of the following compounds, draw an isomer that changes the functional groups in the molecule. Name all the functional groups. Indicate the major absorbances you would expect to find in the IR spectrum for each isomer, and highlight how you could use IR to tell them apart.

In each case I have shown just one possibility. Others will exist. Remember to check the molecular formulas to make sure you have created isomers.

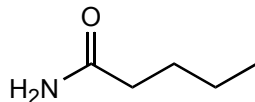
a.



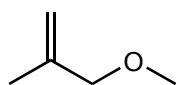
b.



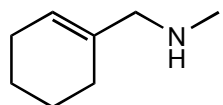
c.



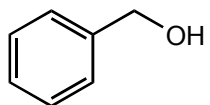
d.



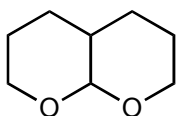
e.



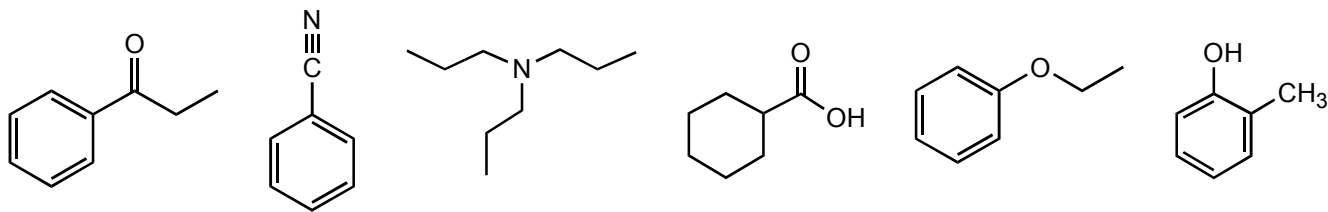
f.



g.



3. Given the following compounds and the data in the ensuing problems identify which compound corresponds with each scenario of given IR data.



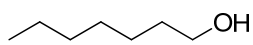
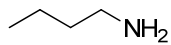
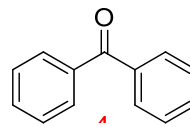
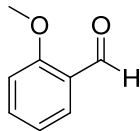
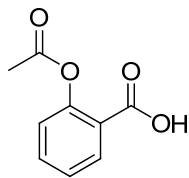
a. With O-H stretch at  $3414\text{ cm}^{-1}$ , aliphatic C-H, and aromatic/vinyl C-H (below and above  $3000\text{ cm}^{-1}$ ), must be:

b. With C=O peak at  $1687\text{ cm}^{-1}$  (C=O in conjugation), aliphatic C-H, and aromatic/vinyl C-H (below and above  $3000\text{ cm}^{-1}$ ), must be:

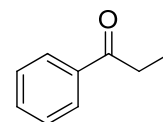
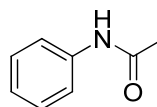
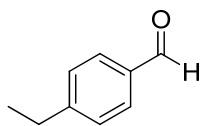
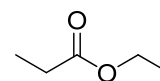
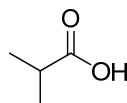
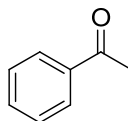
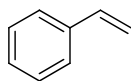
c. With only aliphatic C-H, must be:

4. For the infrared spectra below (numbers 1-6; and letters A-G), pick out the molecule from the list that would correspond to the spectrum for that compound.

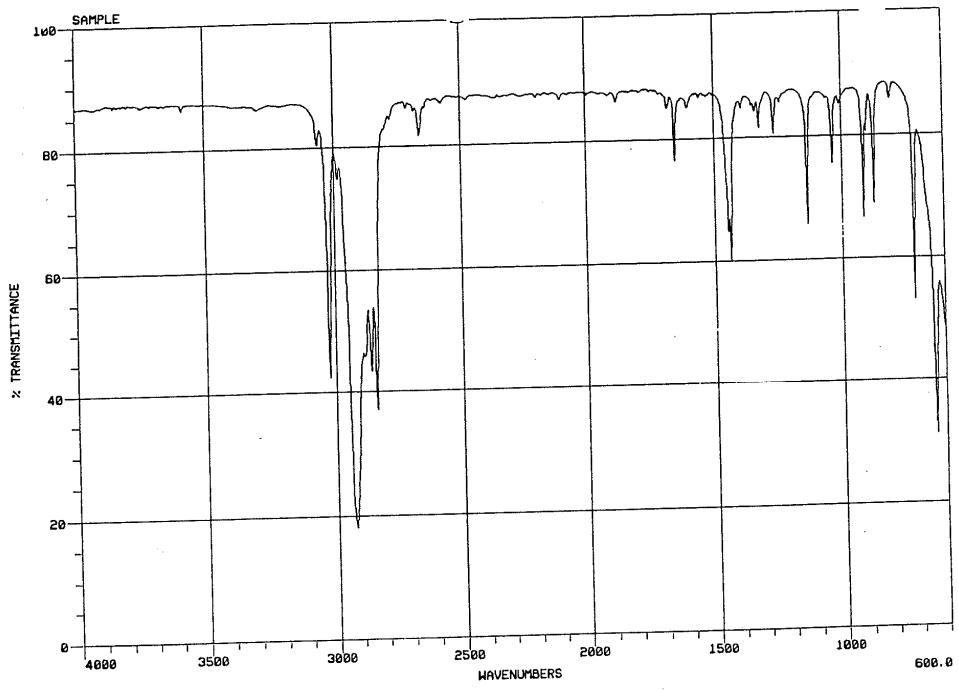
Spetra 1-6



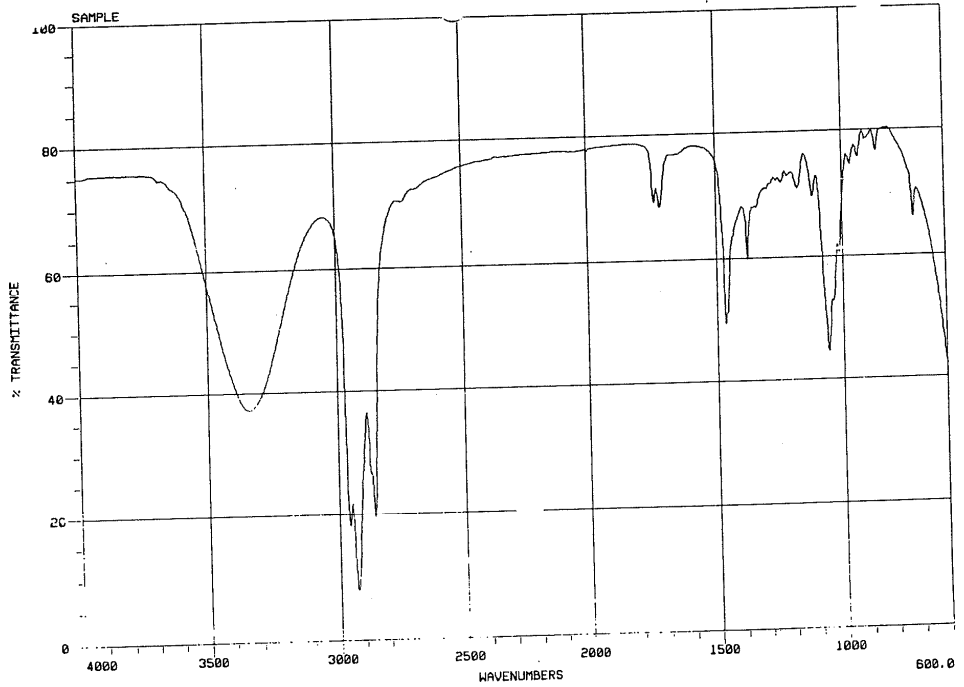
Spetra A-G



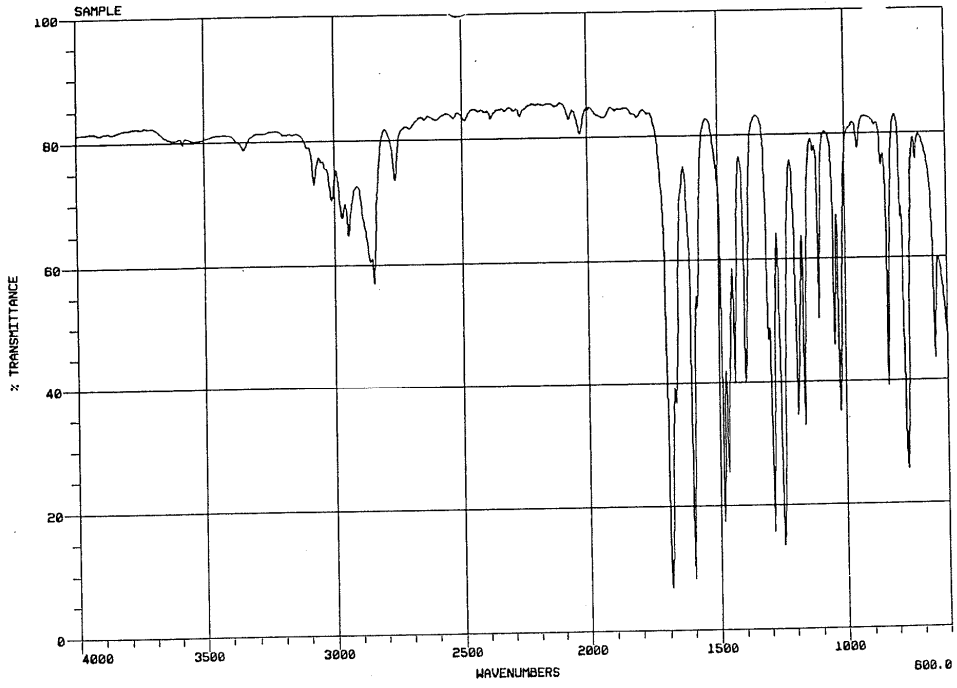
1.



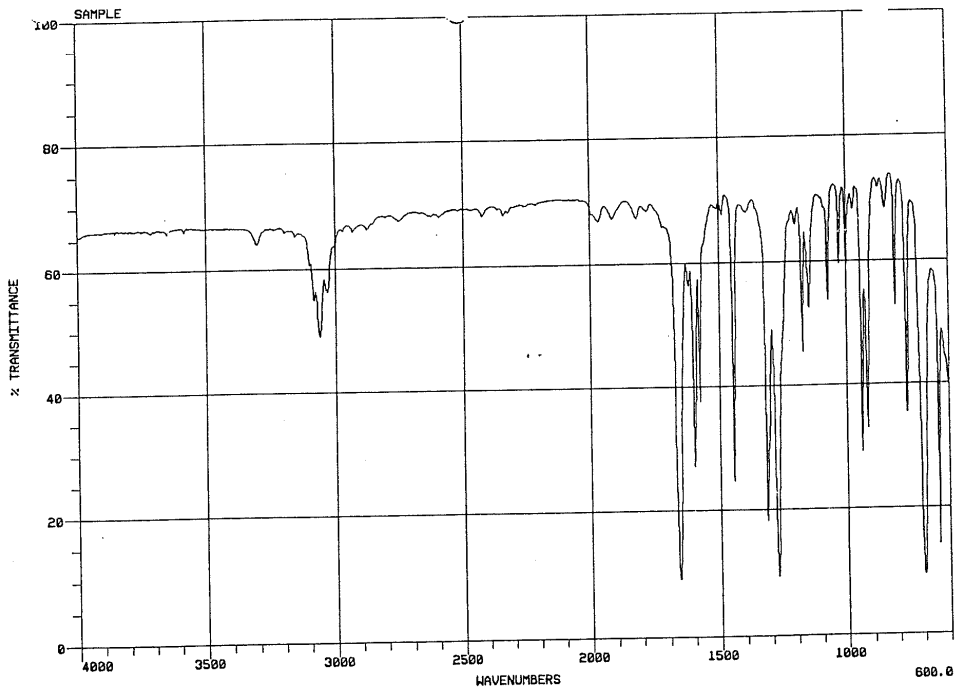
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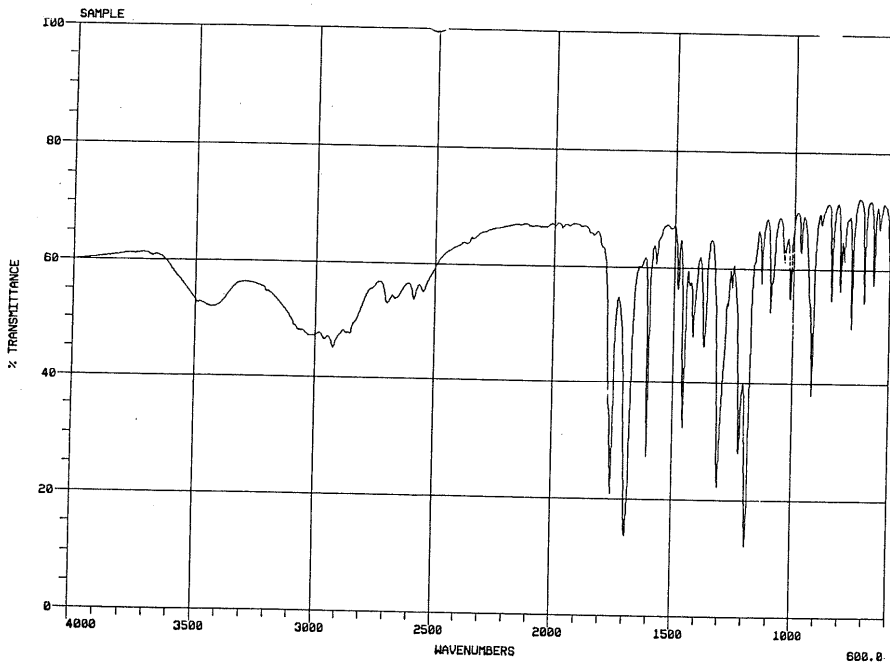
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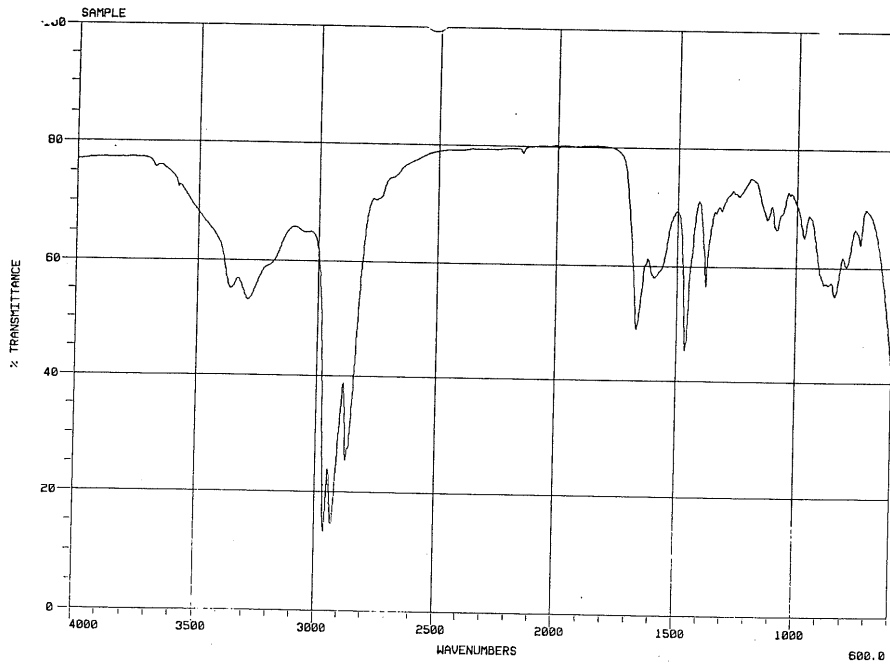
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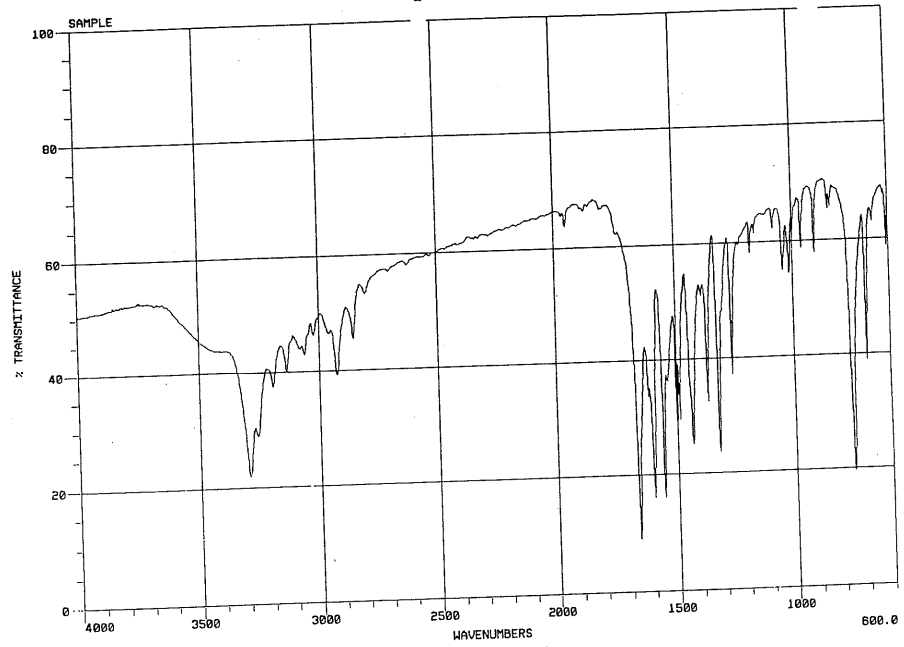
5.



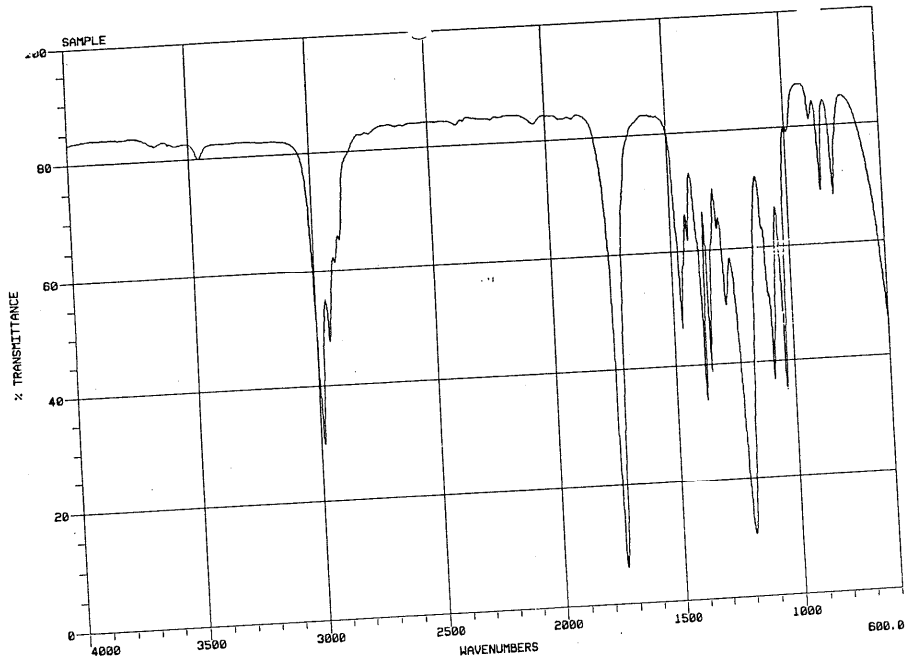
6.



A.

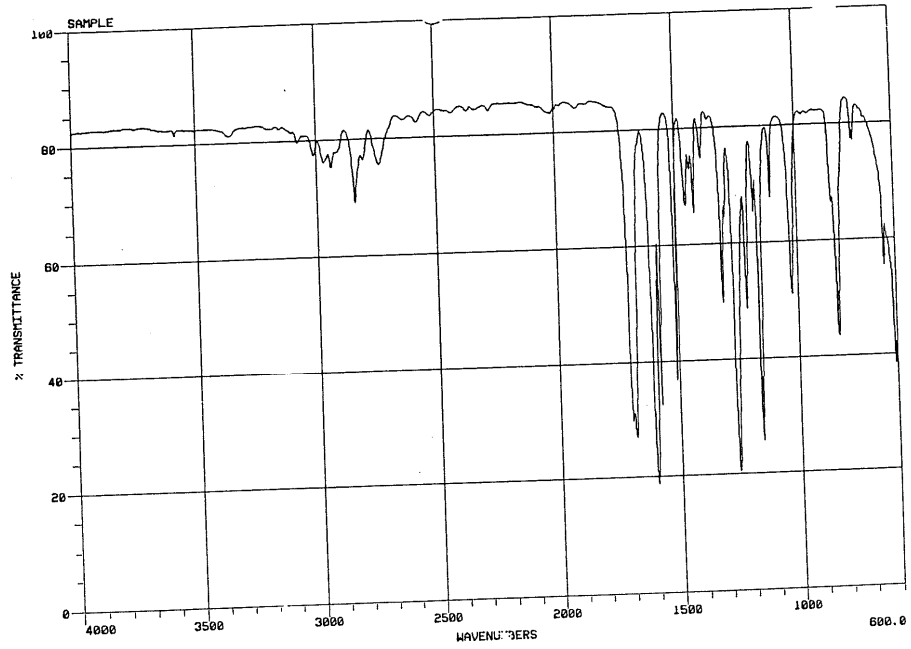


B.

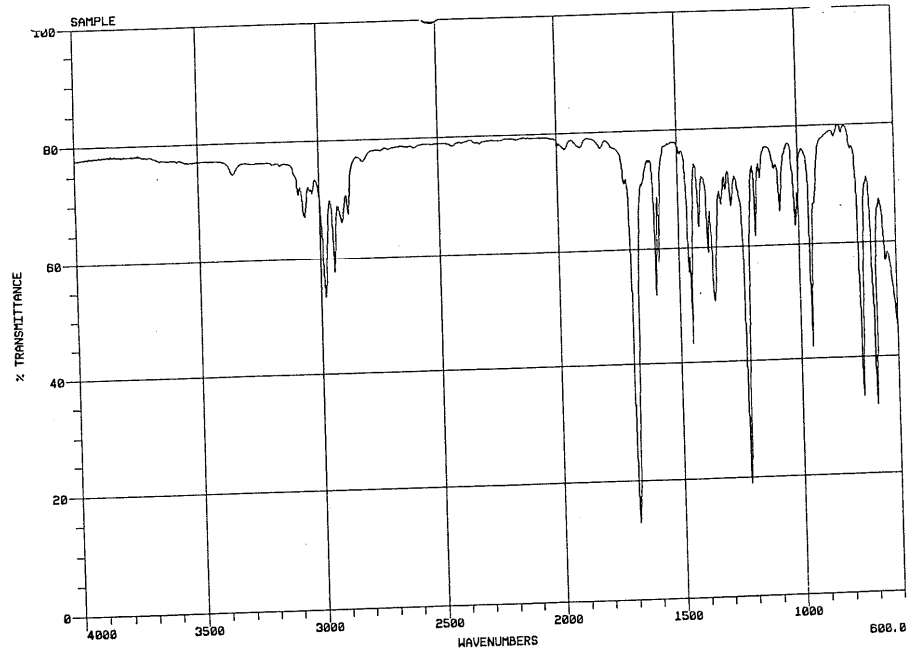




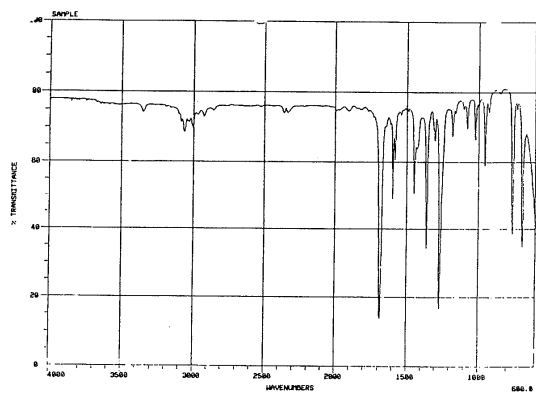
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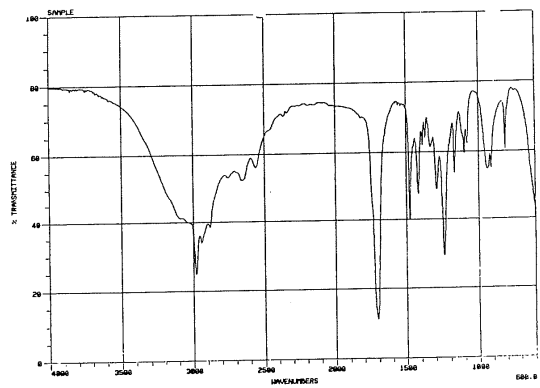
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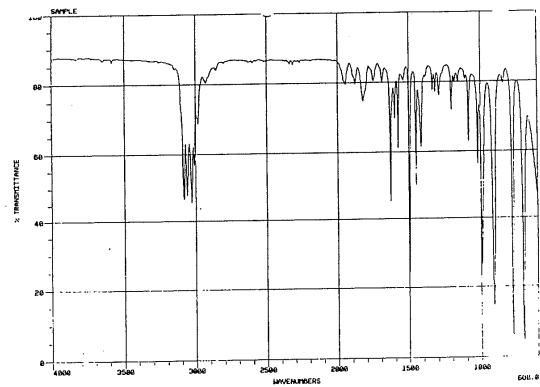
E.



F.

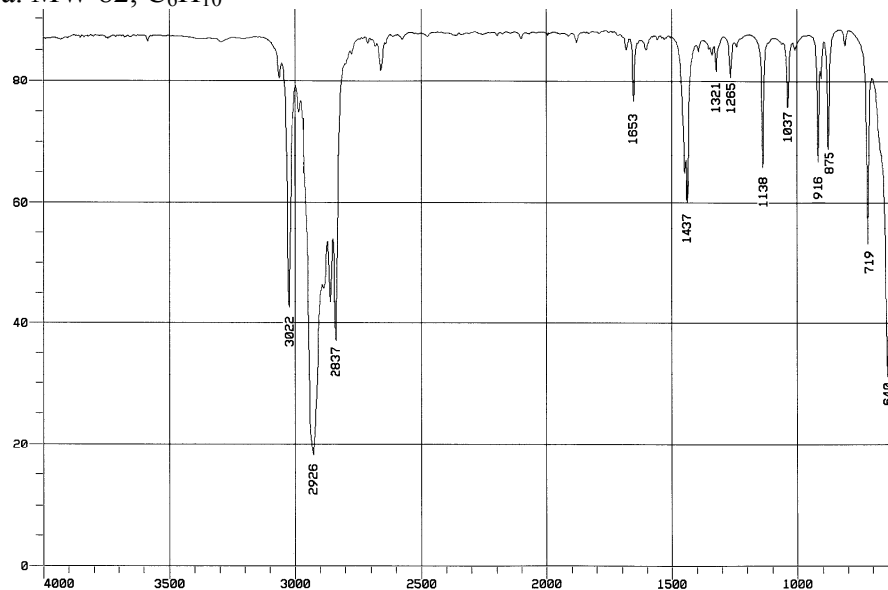


G.

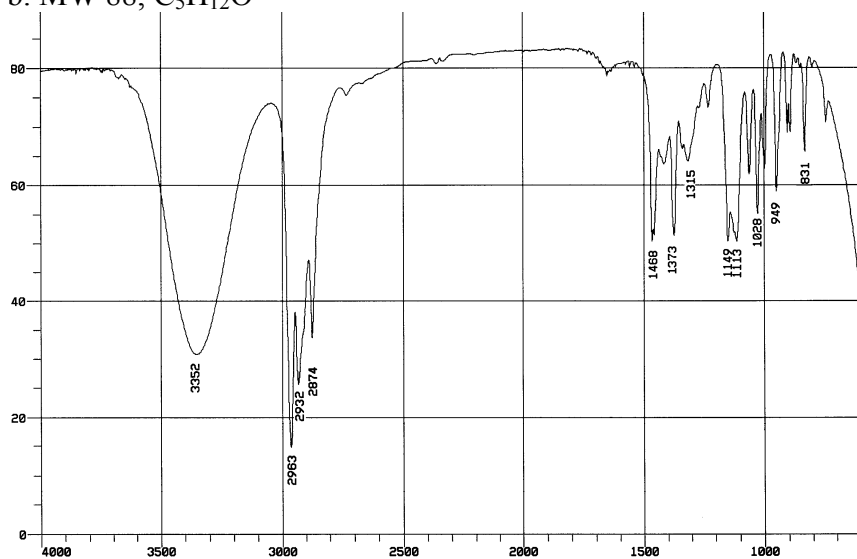


5. For each case, draw at least one possible isomer that is consistent with the molecular formula and the IR spectrum. MULTIPLE CORRECT ANSWERS, I PROVIDED ACTUAL COMPOUND IN THE ANSWER KEY.

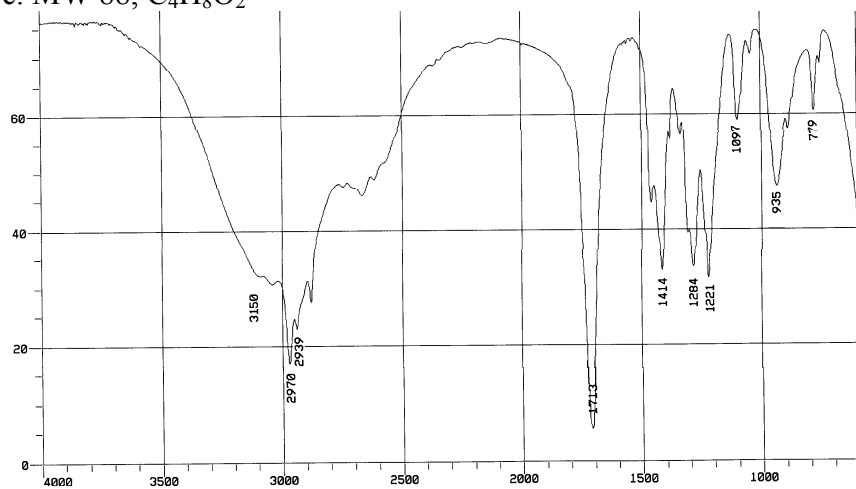
a. MW 82,  $C_6H_{10}$



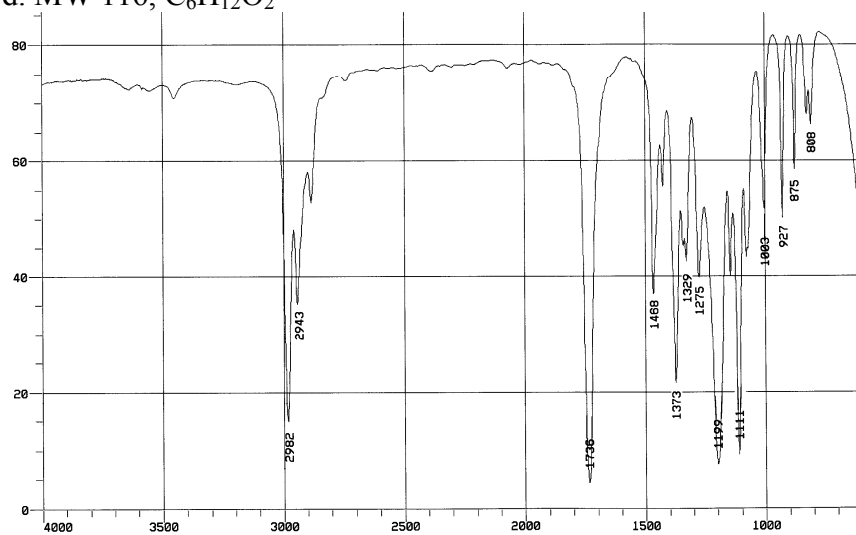
b. MW 88,  $C_5H_{12}O$



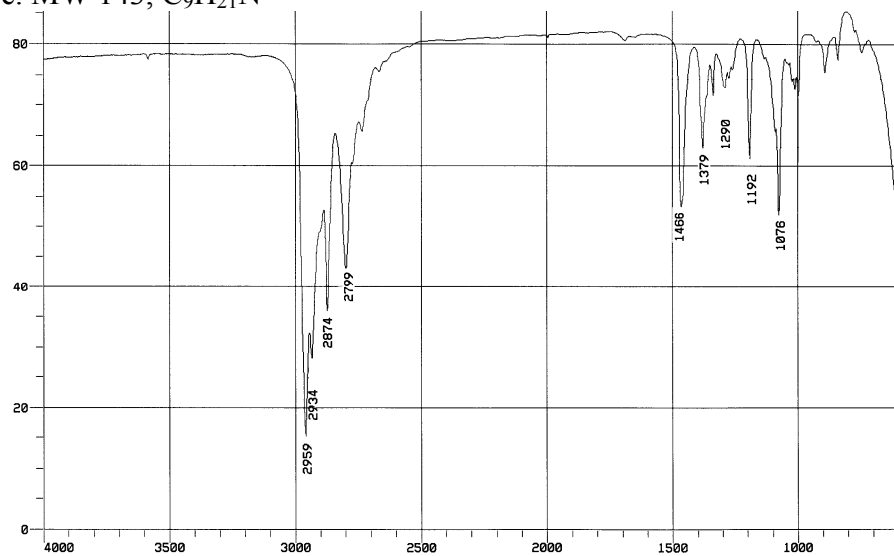
c. MW 88, C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>



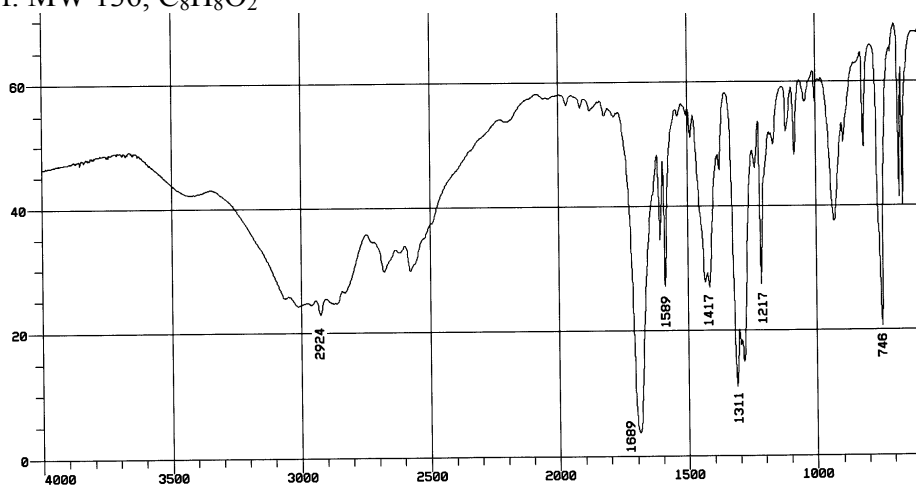
d. MW 116, C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>



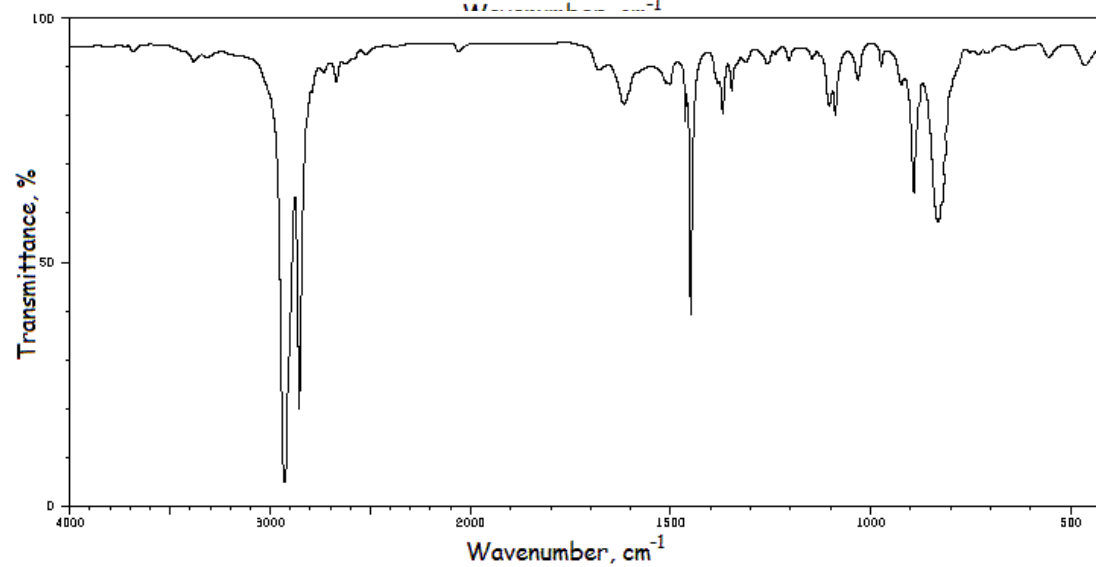
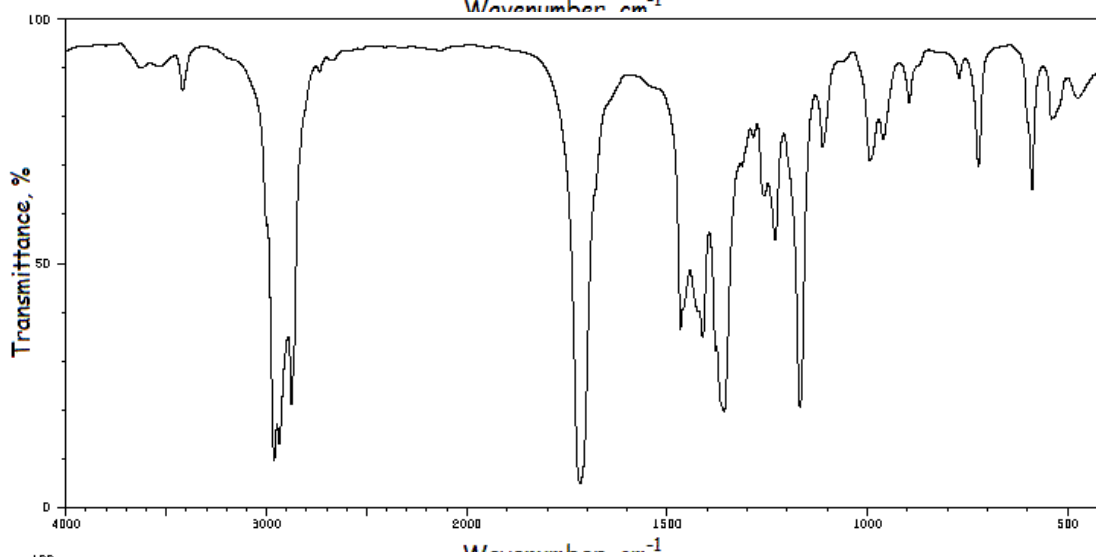
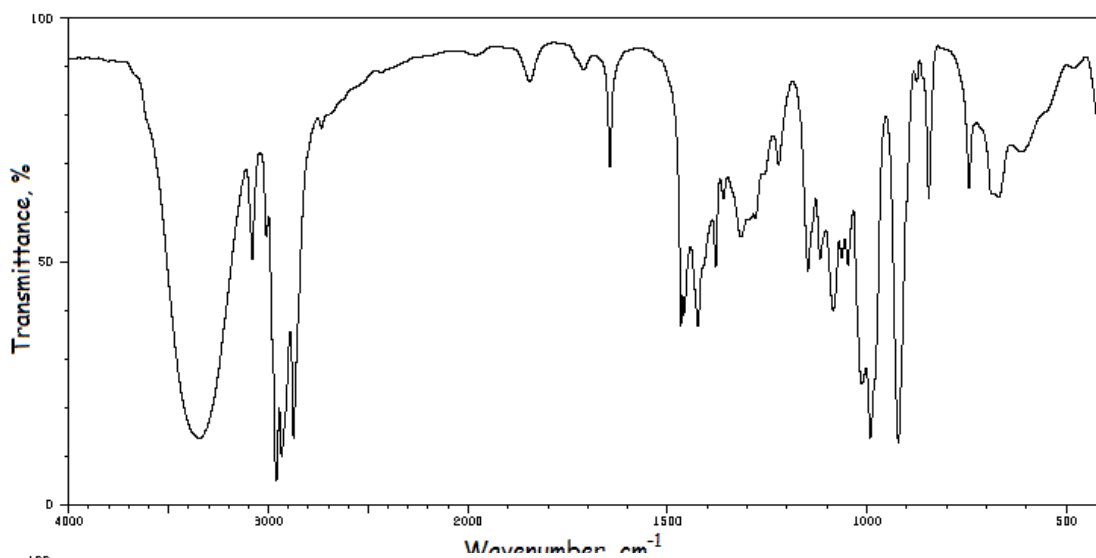
e. MW 143, C<sub>9</sub>H<sub>21</sub>N

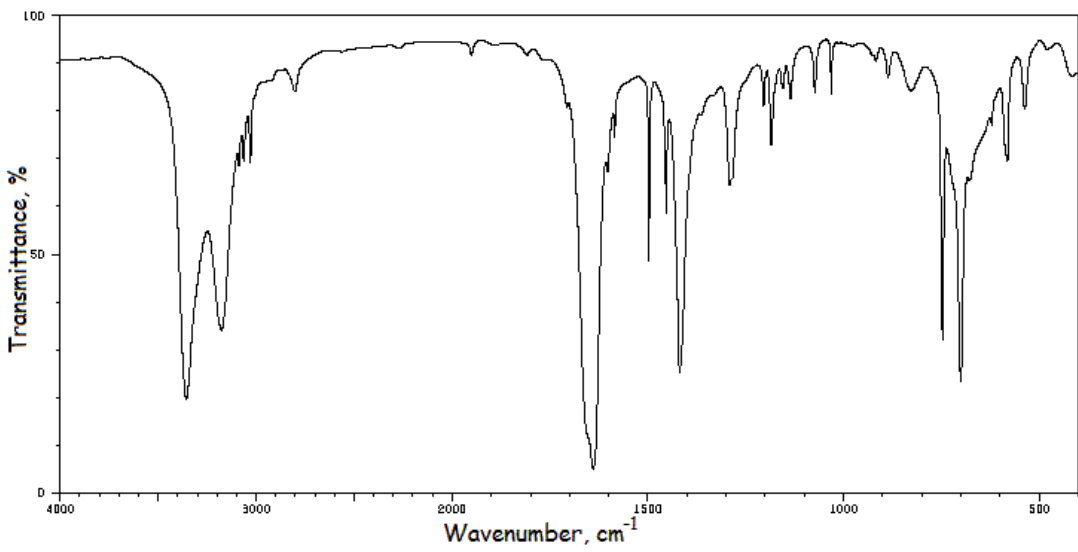
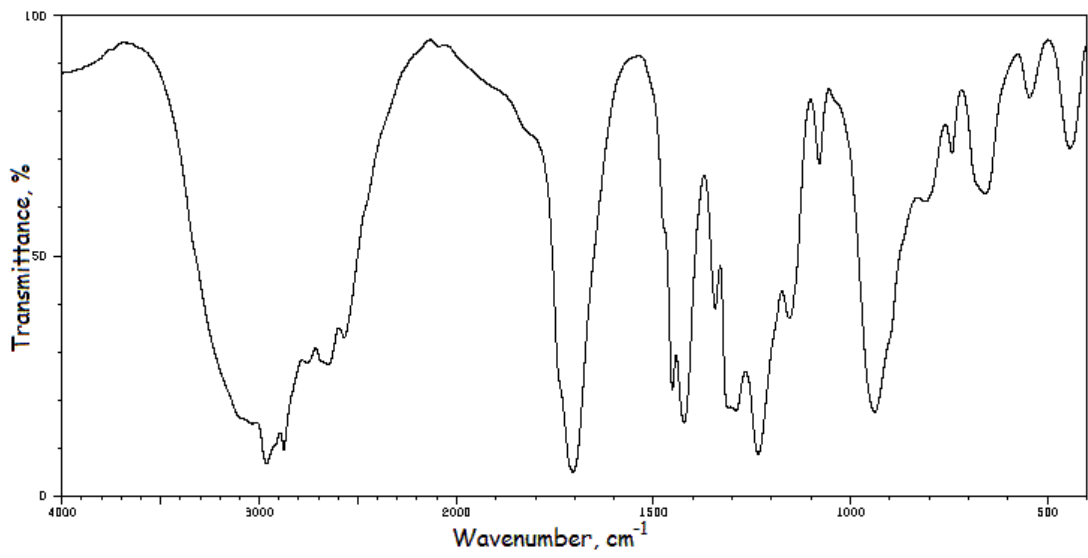
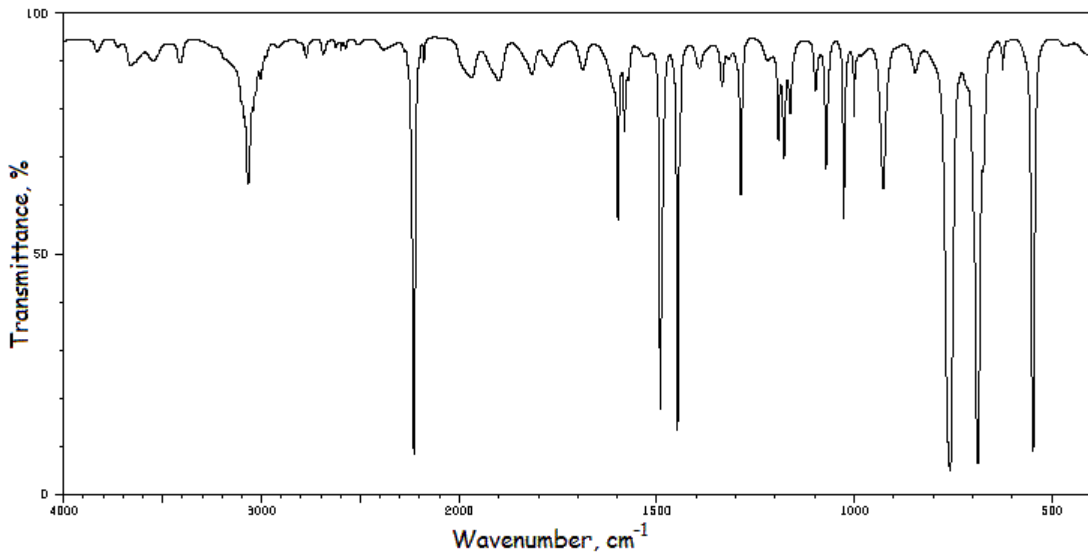


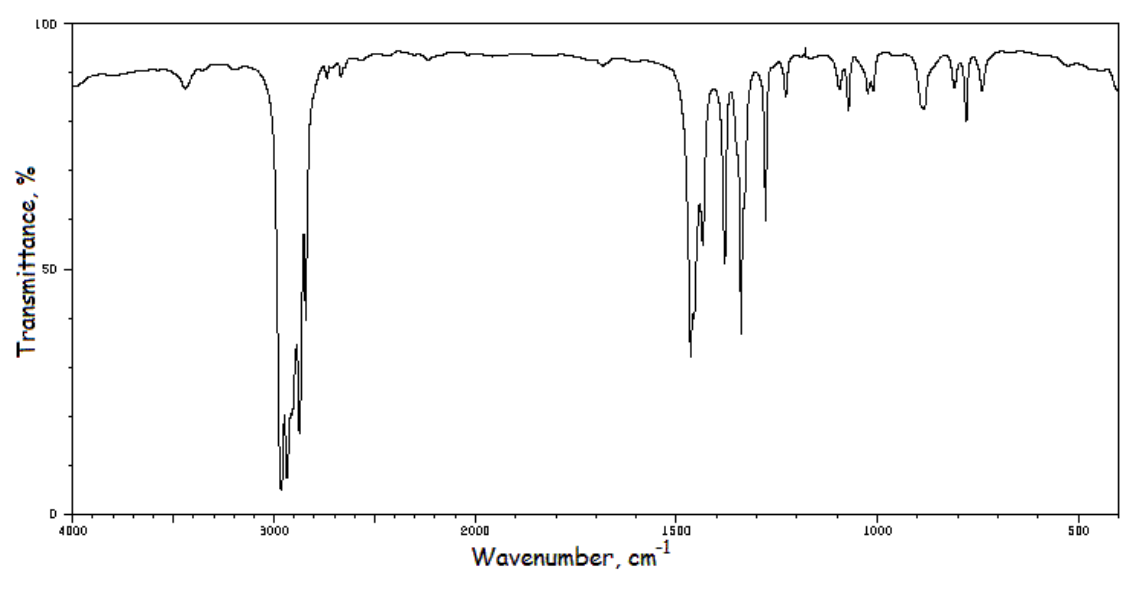
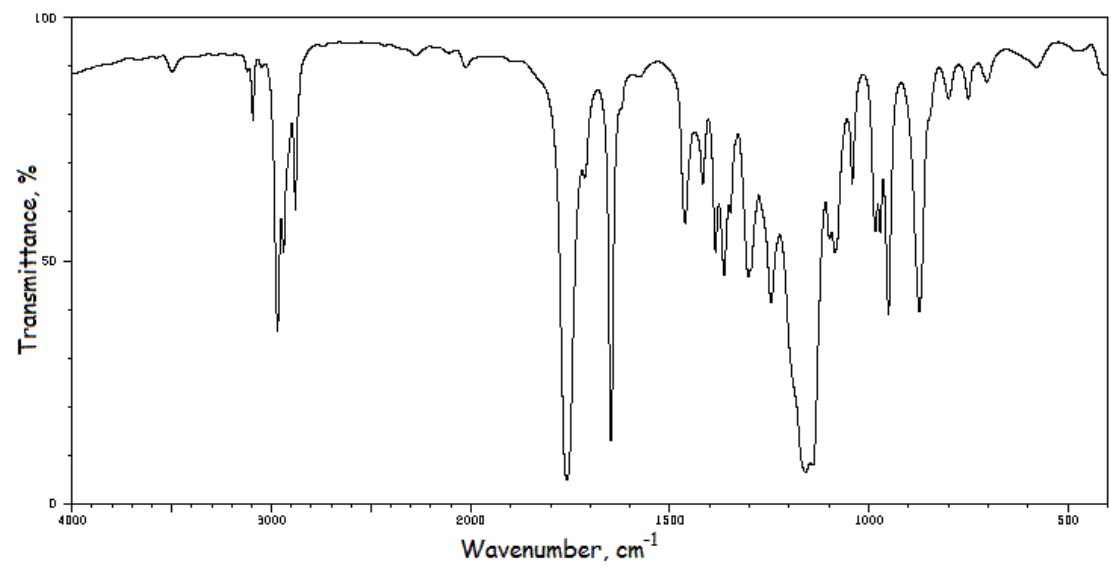
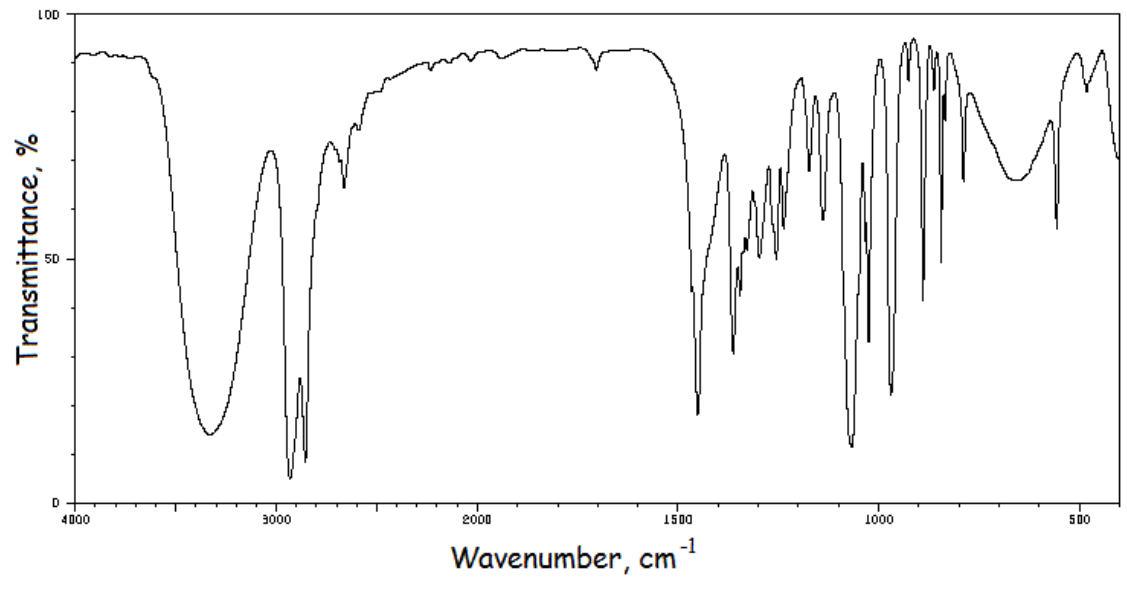
f. MW 136, C<sub>8</sub>H<sub>8</sub>O<sub>2</sub>



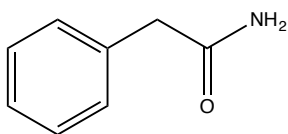
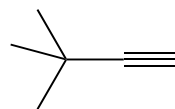
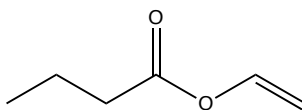
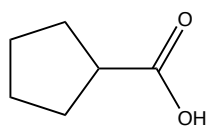
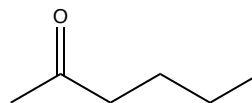
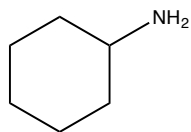
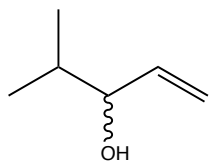
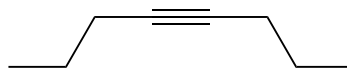
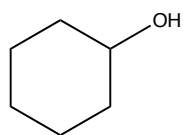
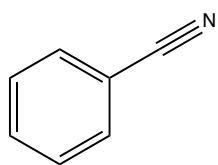
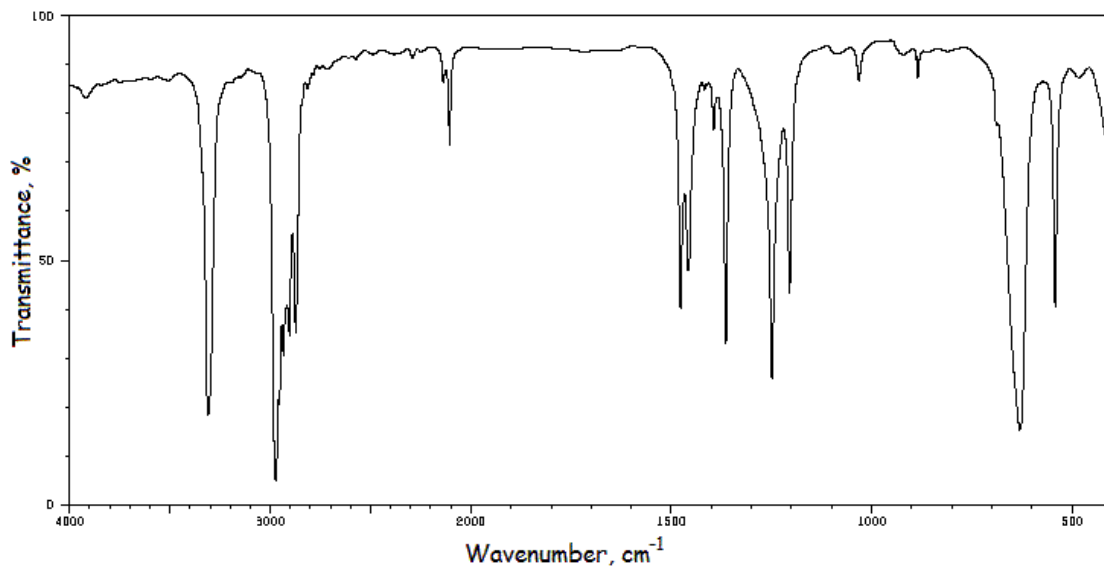
Each one of the following IR spectra (shown below) corresponds to one of the ten compounds at the bottom of the list. Match each spectrum to the correct structure. Look for important functional groups.









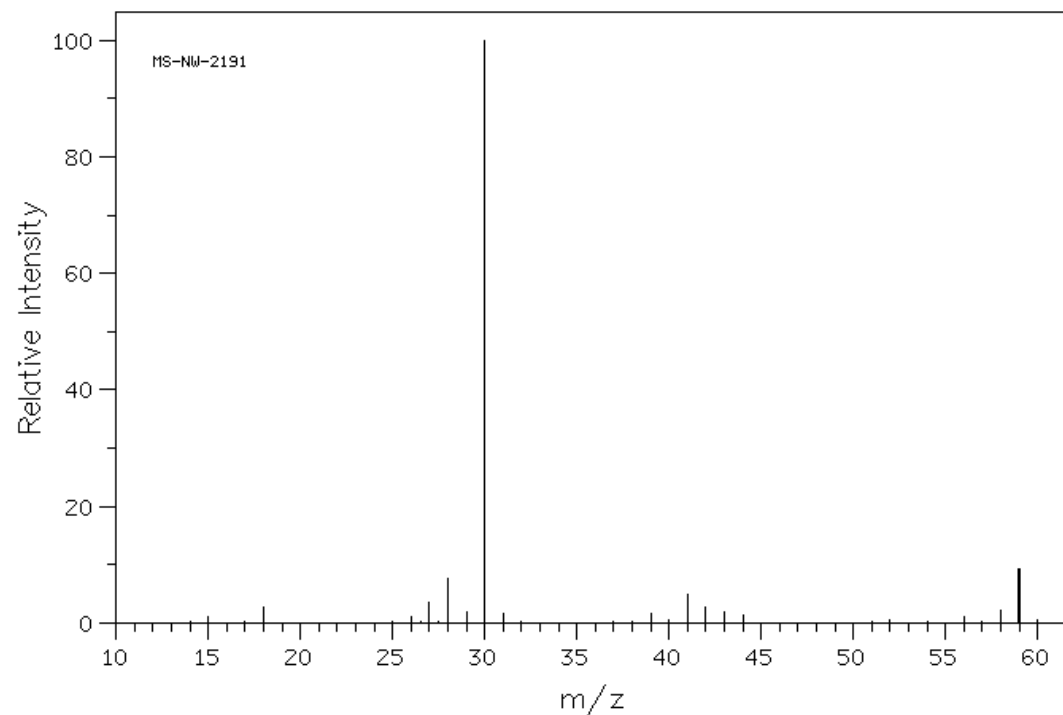
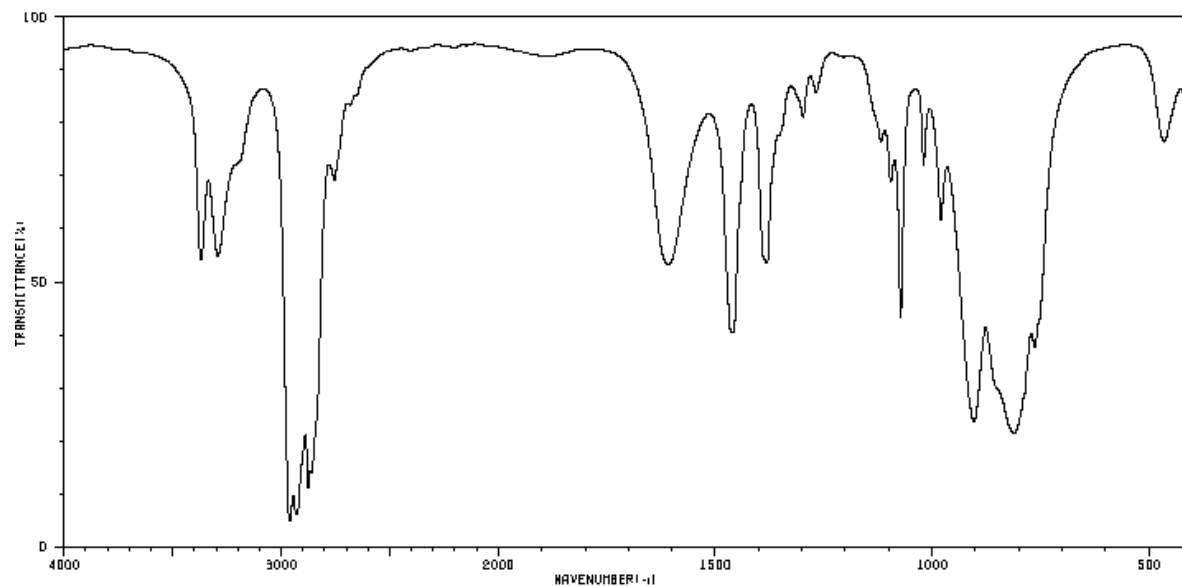


## Combined IR Spectroscopy and Mass Spectrometry Problems

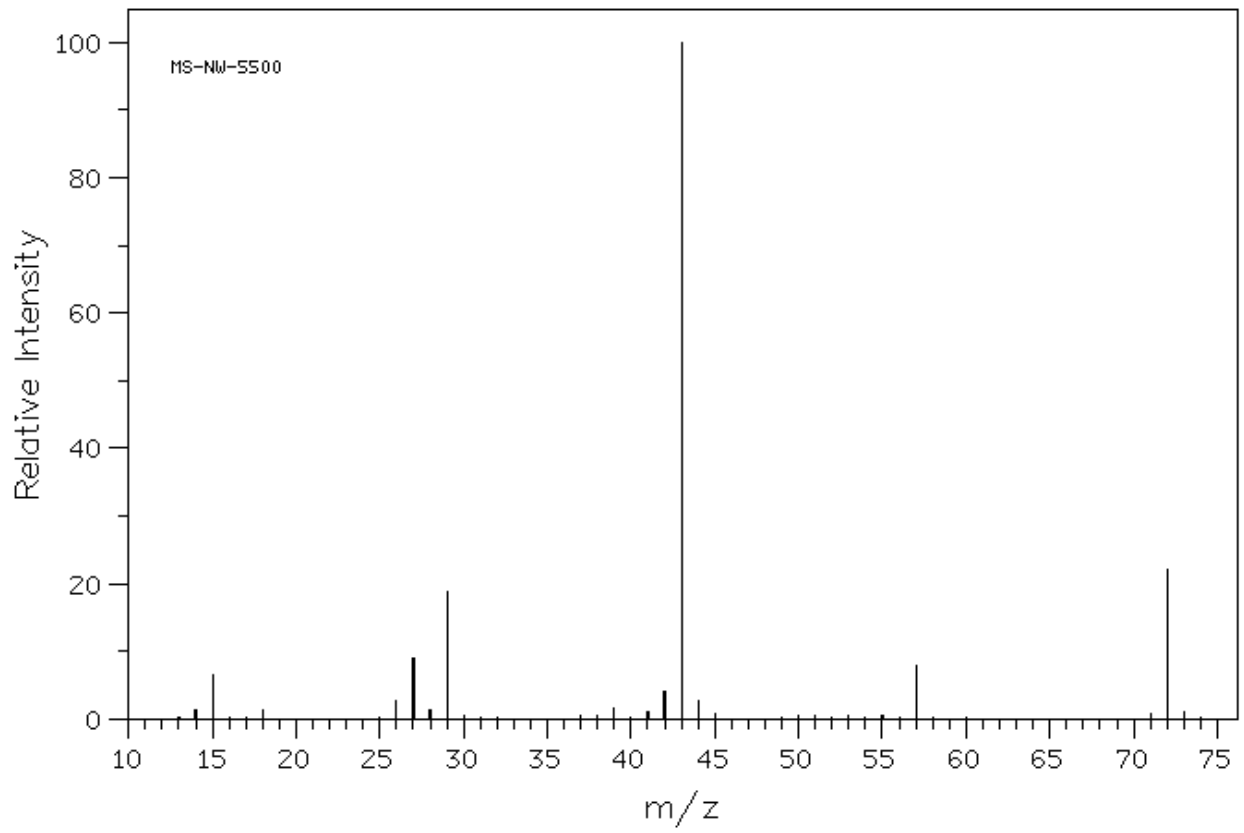
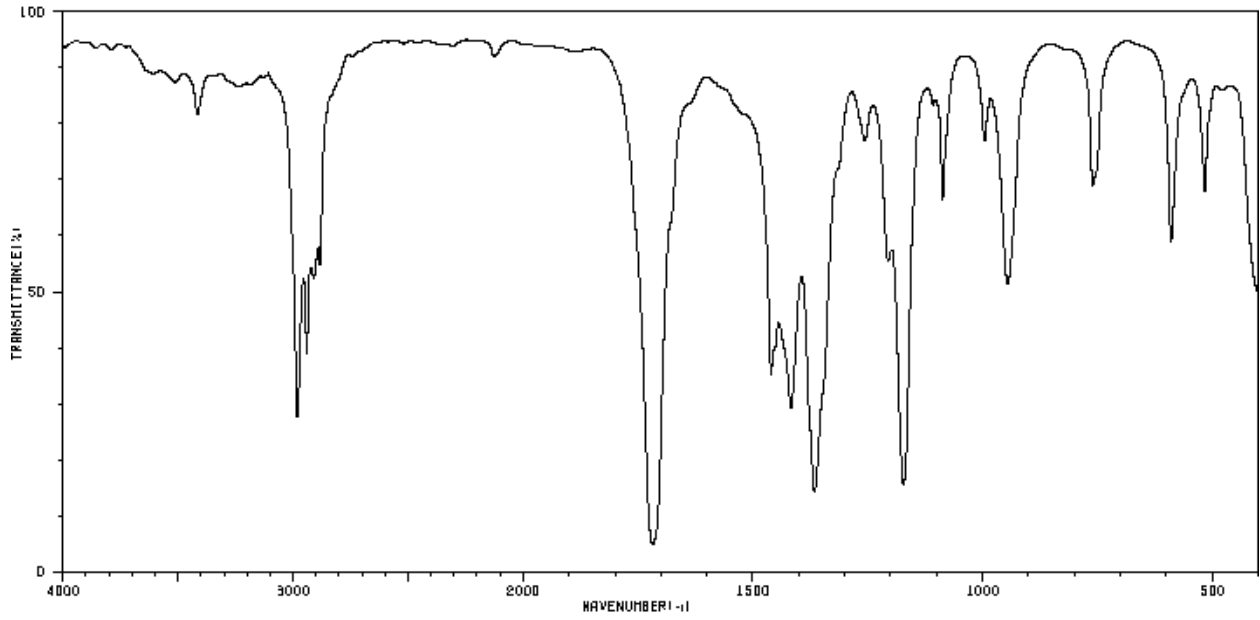
Determine the molecular formula and possible structures for each unknown based on the given spectra. Use the IR Correlation Table. Note:  $\text{DOU} = \#C_s + 1 - 0.5(\#H_s - \#N_s + \#\text{halogens})$ .

SHOW YOUR WORK!

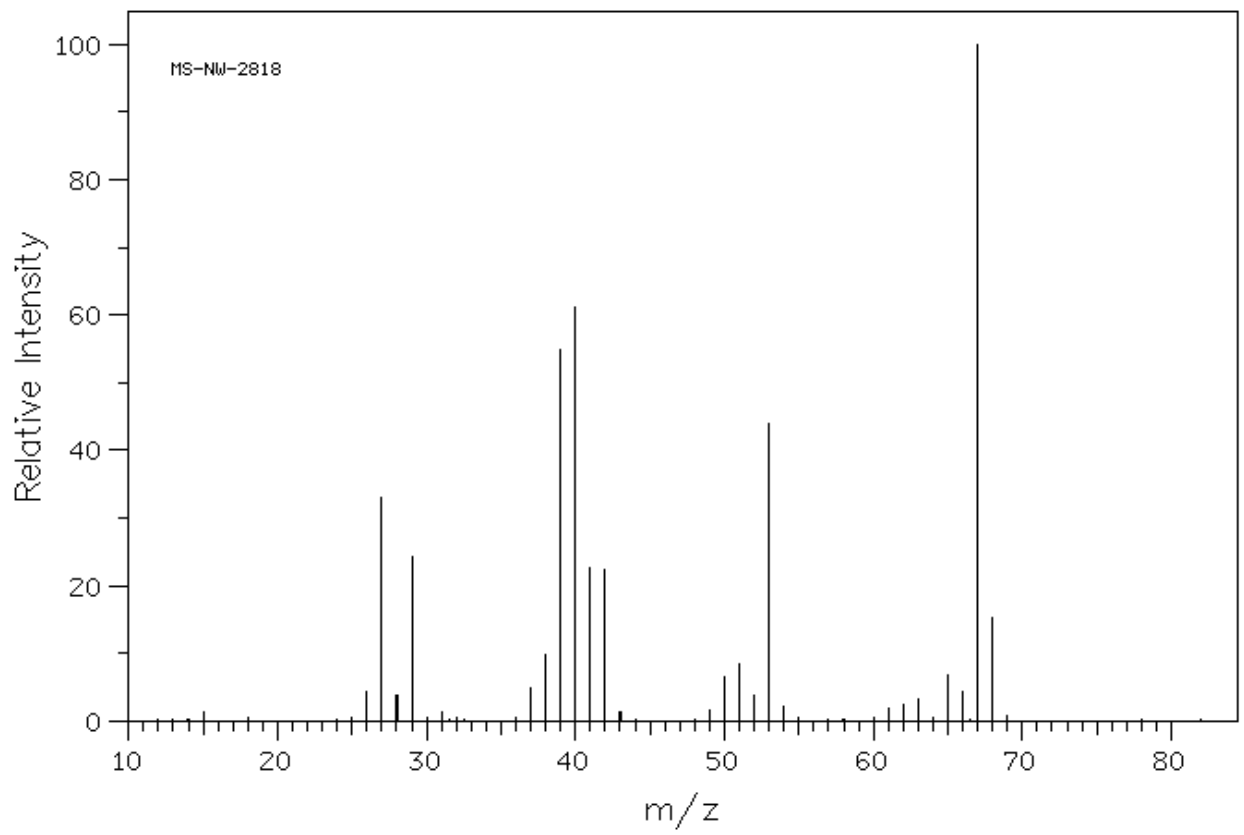
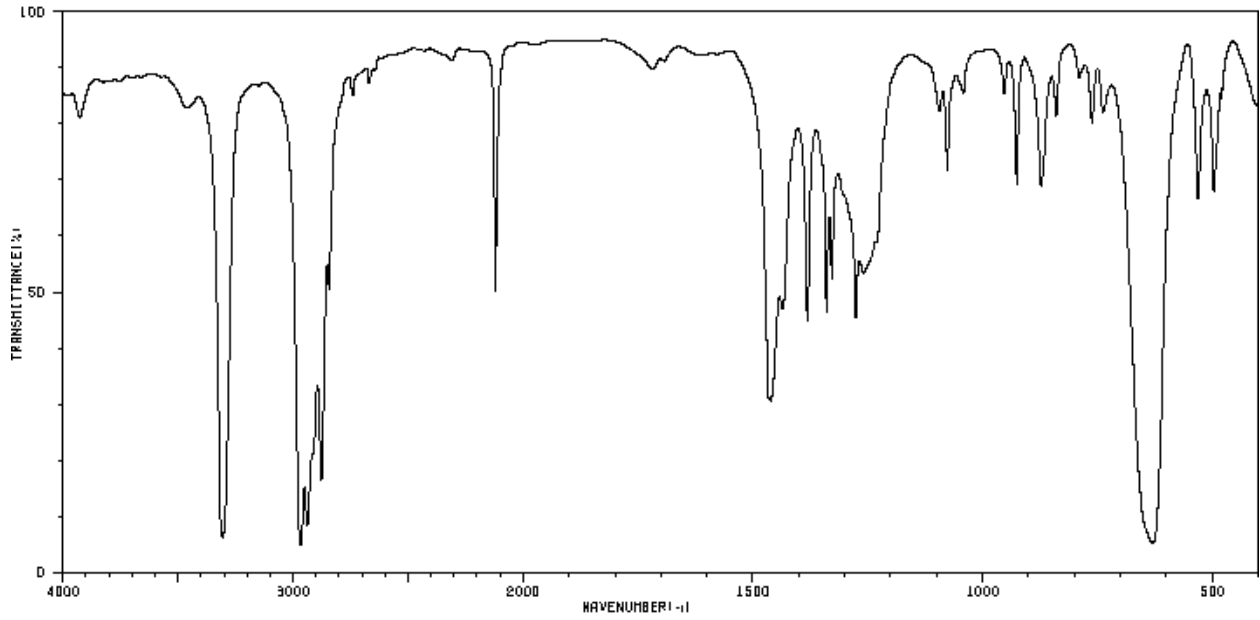
1.



2.

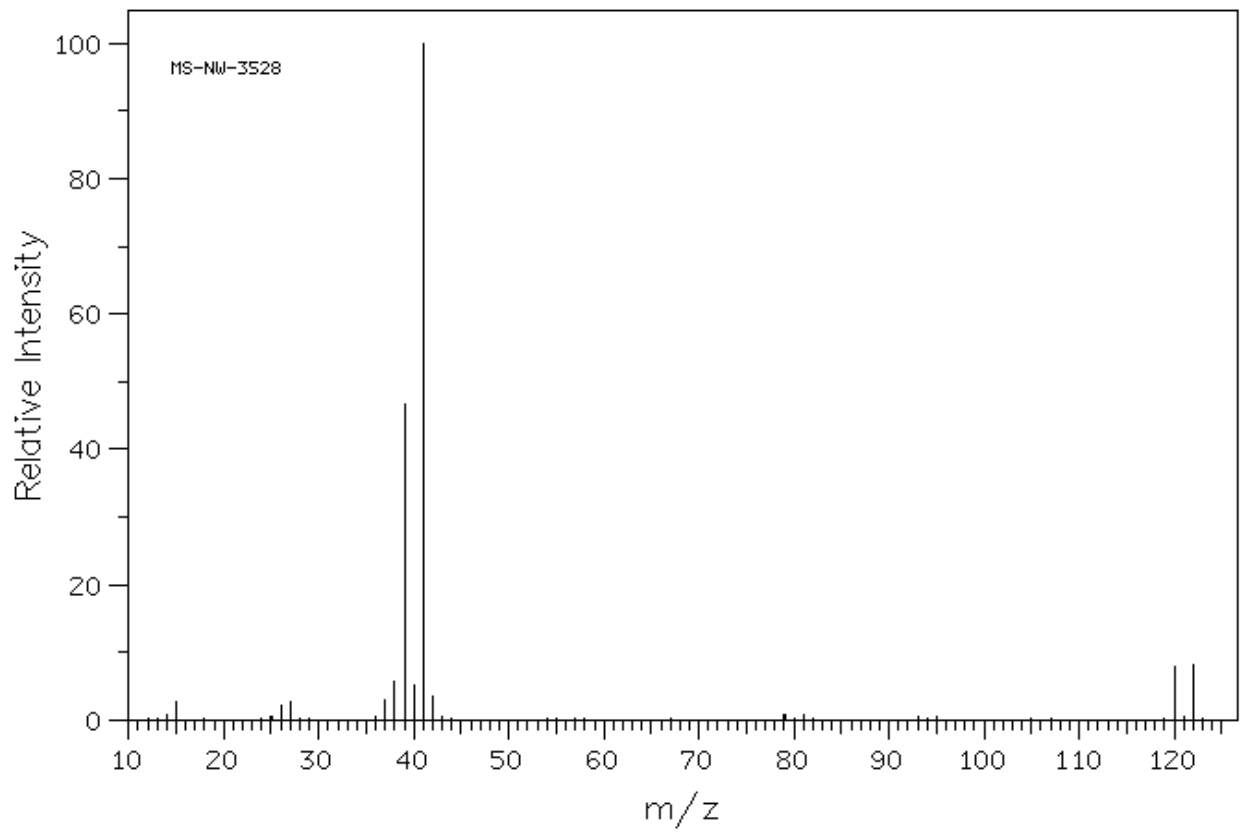
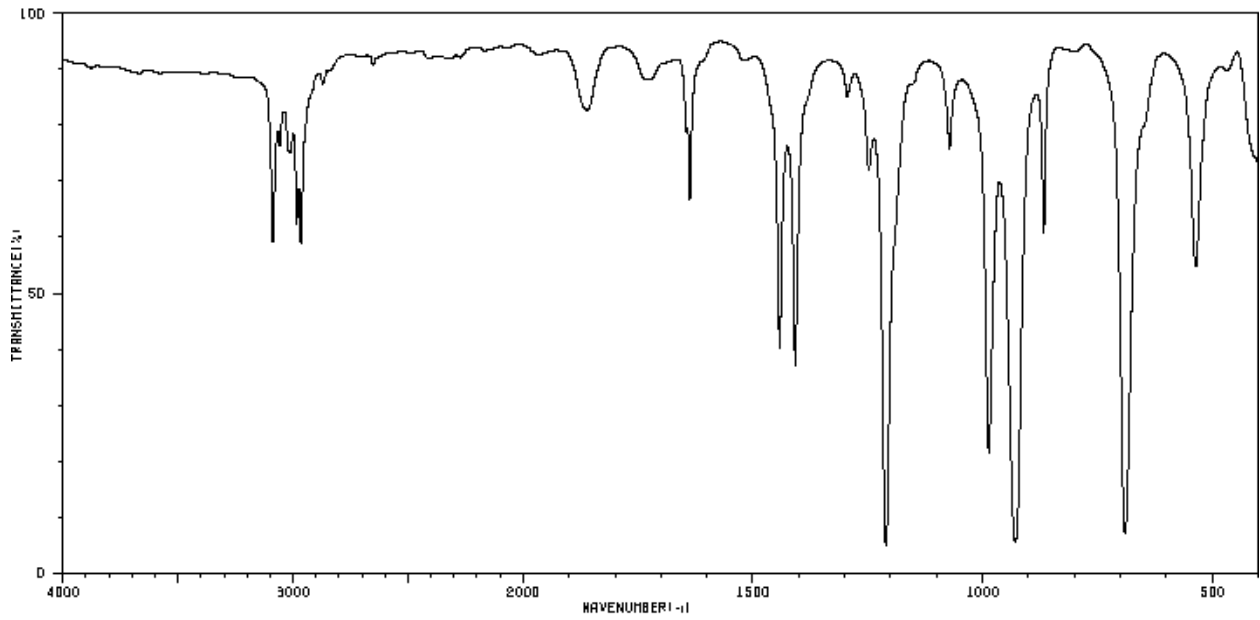


3.



$M^+ = 68$

4.



5.

