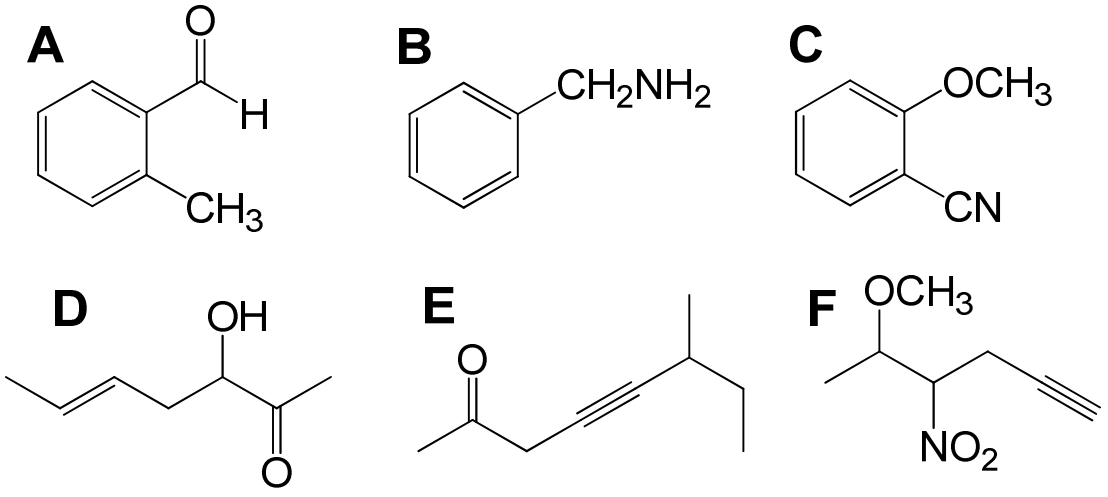
WORKSHEET I

1. Predict the positions of the major absorption bands in the IR spectra of the following compounds



2. Which compound would be expected to show intense IR absorption at 3300 cm^{-1}?

A) $CH_3C{\equiv}CCH_3$ **B)** butane **C)** but-1-ene **D)** $CH_3CH_2C{\equiv}CH$

3. Which compound would be expected to show intense IR absorption at 2820, 2710 and 1705 cm^{-1}?

A) $CH_3COCH_2CH_3$ **B)** $PhCOCH_3$ **C)** PhCHO **D)** $CH_2{=}CHCOCH_3$

4. Which compound would be expected to show intense IR absorption at 2250 cm^{-1}?

A) $CH_3CH_2CH_2CO_2H$ **B)** $(CH_3)_2CHCH_2OH$ **C)** $(CH_3)_2CHCN$ **D)** $CH_3CH_2CH_2CONH_2$

5. Deduce a possible structure for the following compounds from their IR absorptions below.

A C_3H_3Br: 3300, 2900, 2100 cm^{-1} **B** C_3H_5N: 2950, 2250 cm^{-1}

C C_5H_8O: 2950, 1750 cm^{-1} **D** C_4H_8O: 2950, 2820, 2715, 1715 cm^{-1}

E C_6H_{10}: 3040, 2980, 1660 cm^{-1}

6. How could IR spectroscopy be used to distinguish between the following pair of compounds? You should also list all the major absorption bands in the IR spectra of each of compound.

A $CH_3OCH_2CH_3$ and $CH_3CH_2CH_2OH$ **B** $HOCH_2CH_2CHO$ and $CH_3CH_2CO_2H$

C $CH_3COCH{=}CHCH_2CH_3$ and $CH_3COCH_2CH_2CH{=}CH_2$ **D** $CH_3CH_2C{\equiv}CH$ and $CH_3C{\equiv}CCH_3$

E $CH_2{=}CHCH_2CH(CH_3)_2$ and $CH_3CH_2CH_2CH(CH_3)_2$

7. Ethyne (HC≡CH) does not show IR absorption in the region 2000-2500 cm^{-1} because:

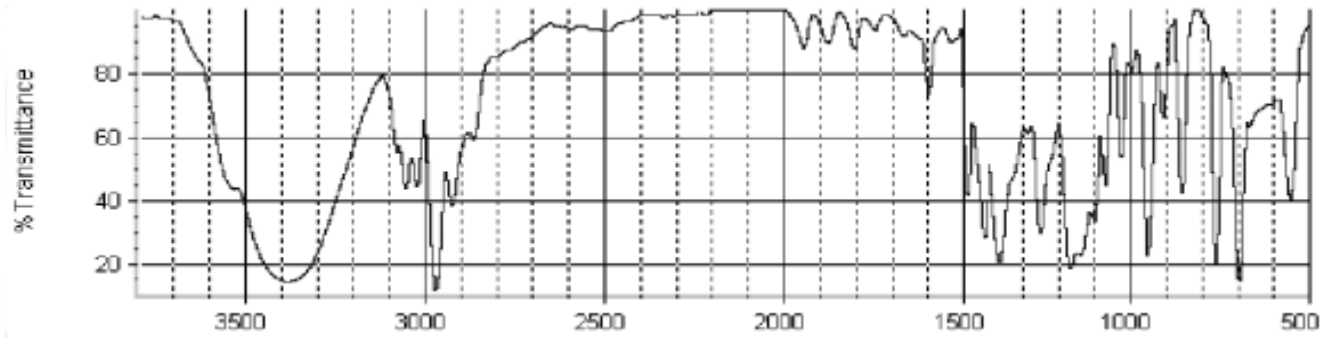
A) C–H stretches occur at lower energies.

B) C≡C stretches occur at about 1640 cm^{-1}.

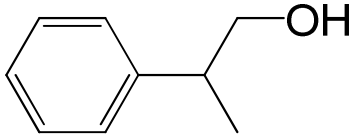
C) there is no change in the dipole moment when the C≡C bond in ethyne stretches.

D) there is a change in the dipole moment when the C≡C bond in ethyne stretches.

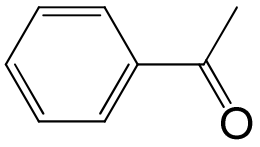
8. Which of the following structures is consistent with the IR spectra shown below?



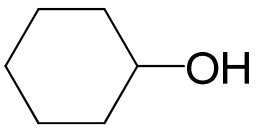
A



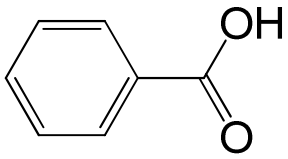
B



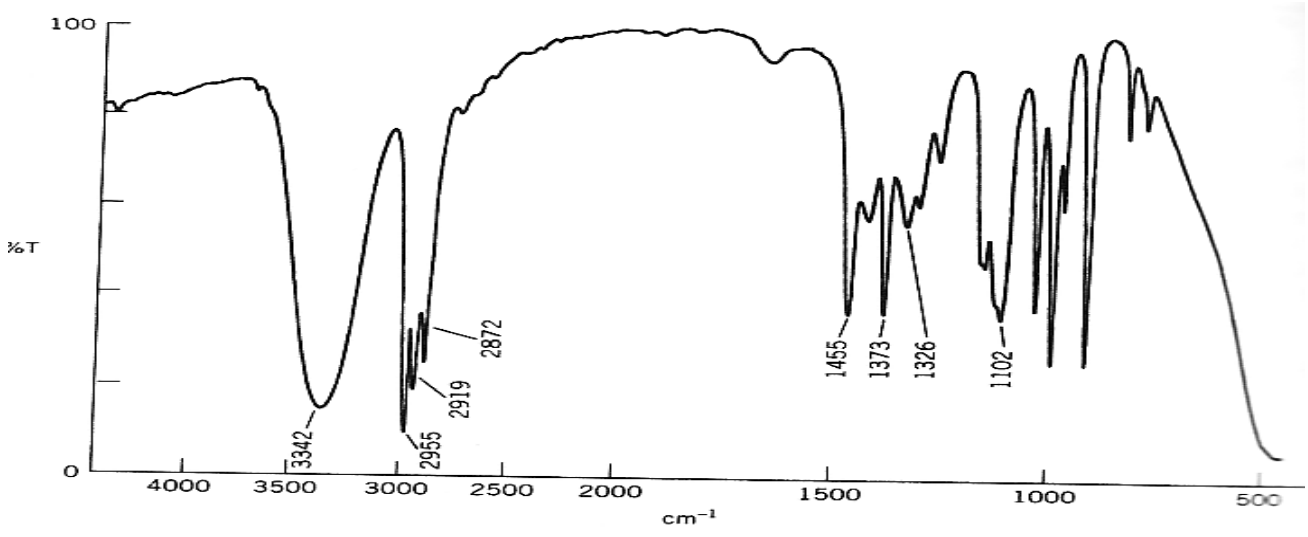
C



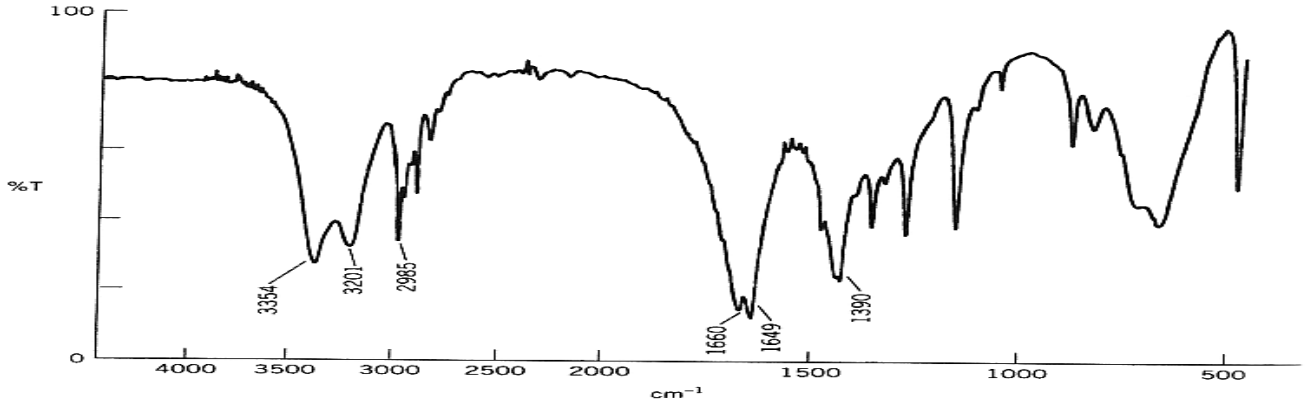
D



9. Explain which functional group(s) is present in the compound that has the following IR spectra
The molecular formula is $C_4H_{10}O$



10. Explain which functional group(s) is present in the compound that has the following IR spectra The molecular formula is C_4H_9NO



11. Which compound would be expected to show intense IR absorption at 1715 cm^{-1}?

A) $(CH_3)_2CHNH_2$ **B)** hex-1-yne **C)** 2-methylhexane **D)** $(CH_3)_2CHCO_2H$

12. Which compound would be expected to show intense IR absorption at 3363, 3185, 1660 cm^{-1}?

A) $CH_3CH_2CH_2OH$ **B)** $(CH_3)_2CHNH_2$ **C)** $CH_3CH_2CONH_2$ **D)** but-1-ene

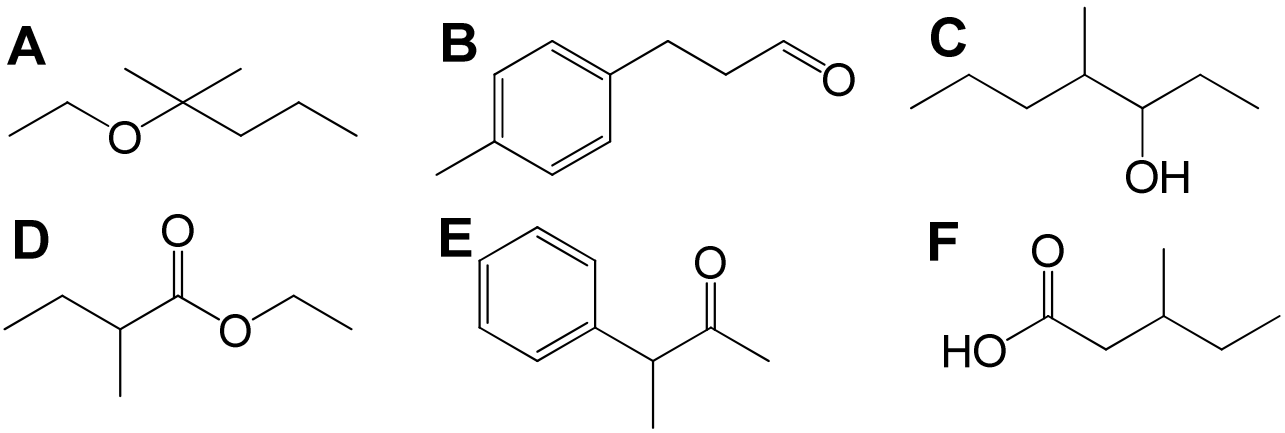
13. 2-Methylhexane shows an intense peak in the mass spectrum at *m/z* = 43. Propose a likely structure for this fragment.

14. Which compound would show a larger than usual M+2 peak in the mass spectrum?

A) $CH_3CH_2SCH_3$ **B)** $(CH_3)_2CHNH_2$ **C)** $CH_3CH_2CO_2H$ **D)** $CH_3(CH_2)_2CH_3$

15. Sodium borohydride can be used to reduce cyclohexanone to cyclohexanol. How could one use IR to determine if all starting material had been consumed?

16. Predict the major fragments and their *m/z* that would appear in the mass spectra of these compounds:



17. **a)** Both $C_6H_{10}O$ and C_7H_{14} have the same nominal mass, namely 98. Show how these compounds can be distinguished by the *m/z* ratio of their molecular ions in high-resolution mass spectrometry.

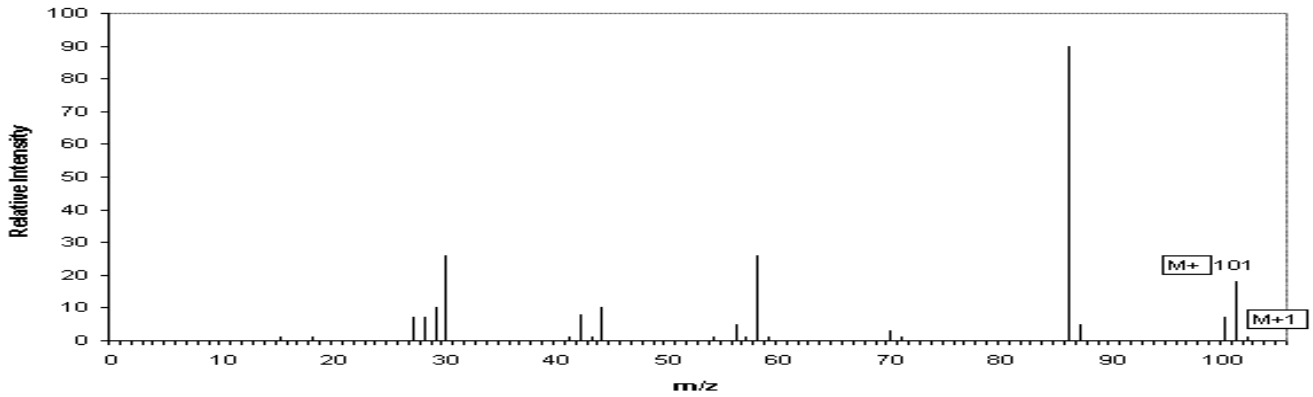
b) same question for C_6H_9N and C_5H_5NO.

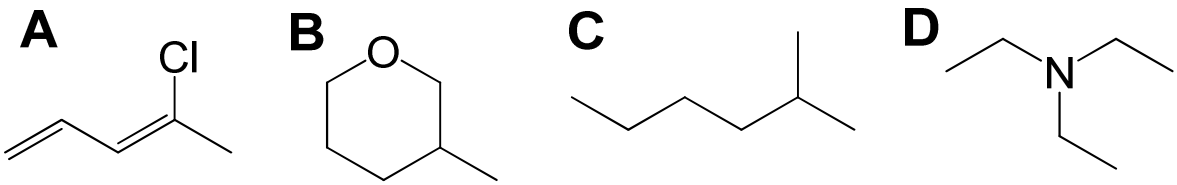
18. Carboxylic acids often give a strong fragment ion at *m/z* (M-17). What is the likely structure of this cation? Show by drawing contributing structures that it stabilized by resonance.

19. The base peak in the mass spectrum of propanone (acetone) occurs at *m/z* 43. What cation does this peak represents?

20. A characteristic peak in the mass spectrum of most aldehydes occurs at *m/z* 29. What cation does this peak represent? (This fragment is not ethyl cation, $CH_3CH_2^+$, if you don't remember the functional group in aldehydes, check your list of functional groups for help).

21. Which of the following structures is consistent with the mass spectrum shown below?





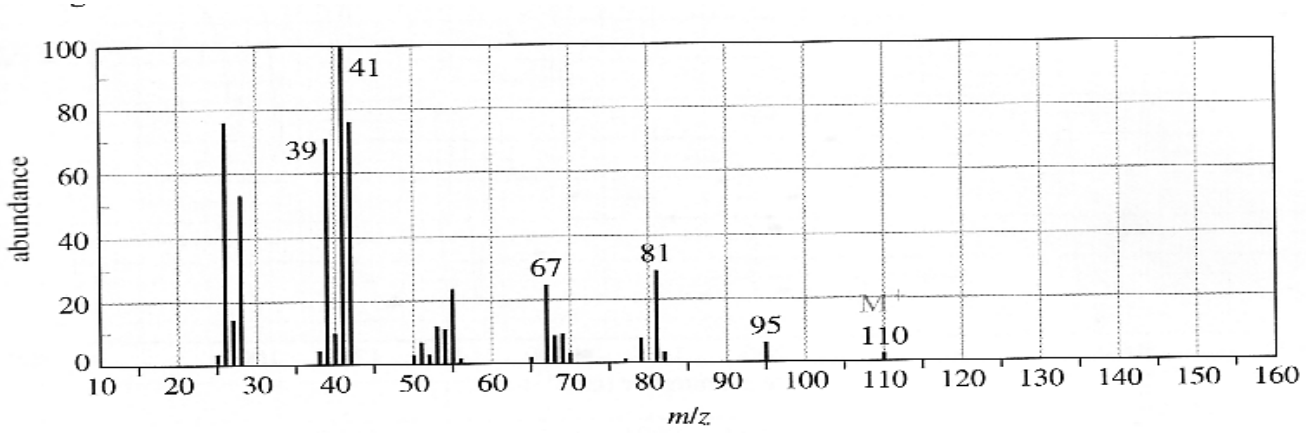
23. An unknown, foul-smelling hydrocarbon gives the mass spectrum and infrared spectrum shown.

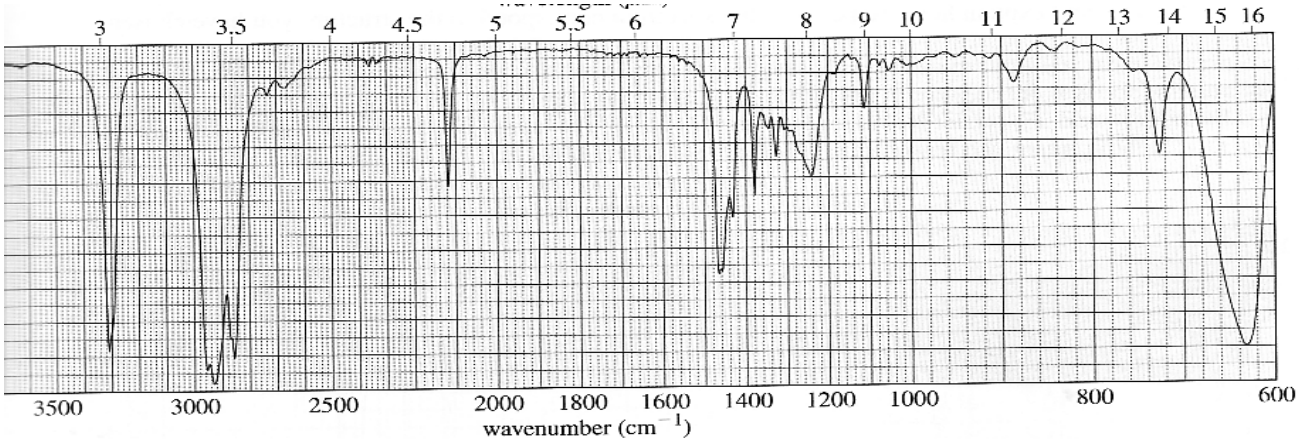
a) Use the mass spectrum to propose a molecular formula. How many elements of unsaturation are there?

b) Use the IR spectrum to determine the functional group(s), if any.

c) Propose one or more structures for this compound. What parts of the structure are uncertain? If you knew that hydrogenation of the compound gives n-octane, would the structure still be uncertain?

d) Propose structures for the major fragments at 39, 67, 81 and 95 in the mass spectrum. Explain why the base peak is so strong.


100
80
60
40
20
0
abundance
41
39
67
81
95
M+
110
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160
m/z


3 3.5 4 4.5 5 5.5 6 7 8 9 10 11 12 13 14 15 16
3500 3000 2500 2000 1800 1600 1400 1200 1000 800 600
wavenumber (cm⁻¹)