13A. Know the relationship between wavelength, frequency, wavenumber, and energy of light.

13A.1 Which has the higher energy?
a) light having a wavelength of 1×10^{-5}m and 1×10^{-8}m
b) light with frequency 1×10^{4} Hz or 1×10^{8} Hz
c) red light or blue light
d) ultraviolet light or infrared light

13A.2 Which has the highest frequency?
a) light with wavelength 650 nm or 253 nm
b) a photon with energy of 6×10^{-19} J or 9×10^{-19} J
c) visible light or radio waves

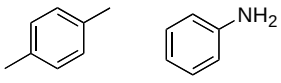
13A.3 The energy difference between two vibrational states is 25 kJ/mol, the energy difference between a set of π/ π * orbitals is 420 kJ/mol. Which will absorb longer wavelengths of light?

13A.4 The energy of a photon is
a) directly proportional to wavelength b) directly proportional to frequency c) neither

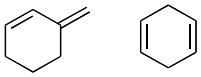
13A.5 Which region of the electromagnetic spectrum contains photons of the highest energy?
a) ultraviolet light b) radio waves c) infrared light d) X-rays E) visible light

13B. Know the relationship between extent of conjugation and peak wavelength absorbance, HOMO-LUMO energy difference and color of organic molecules.

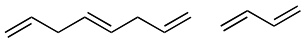
13B.1 Circle the molecule with the indicated property.



a) Has the largest peak wavelength absorbance.



b) Absorbs the highest energy photons.

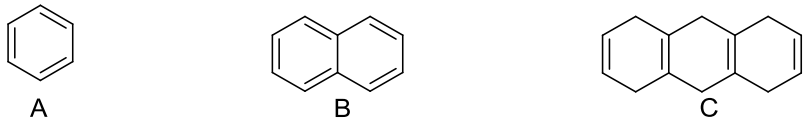


c) Has the smallest HOMO/LUMO gap.

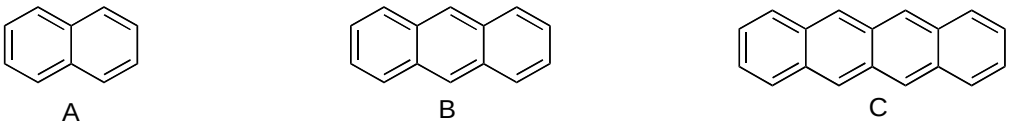
13B.2. Circle the appropriate word in each pair to complete the statement.

In UV spectroscopy, more conjugation leads to compounds absorbing (longer / shorter) wavelengths of (lower / higher) energy due to a (increased / decreased) gap between the HOMO and the LUMO.

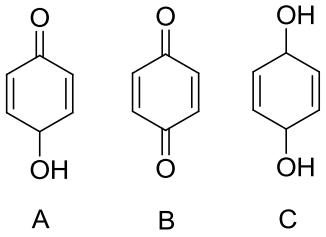
13B.3 Of the compounds below,
a) which has the largest energy difference between its HOMO and LUMO?
b) which has the longest peak wavelength absorbance?
c) which absorbs the highest energy photons?



13B.4 Of the compounds below,
a) which has the smallest gap between its HOMO and LUMO?
b) which has the longest peak wavelength absorption?
c) which absorbs the highest energy photons.?
d) is most likely to be colored?



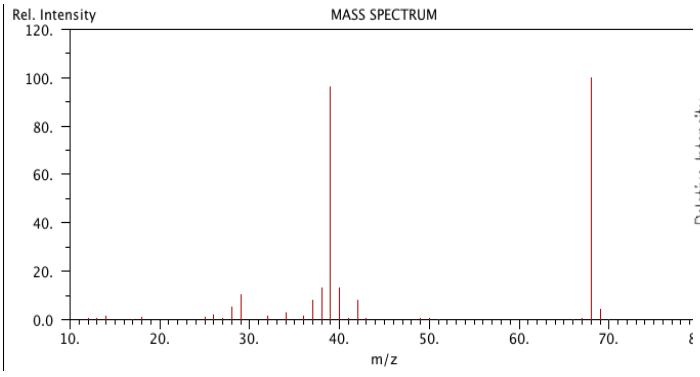
13B.5 Of the compounds below,
a) Which compound has the shortest peak wavelength absorbance?
b) Which compound has the smallest peak frequency absorbance?
c) Which compound has the largest gap between the HOMO and LUMO?



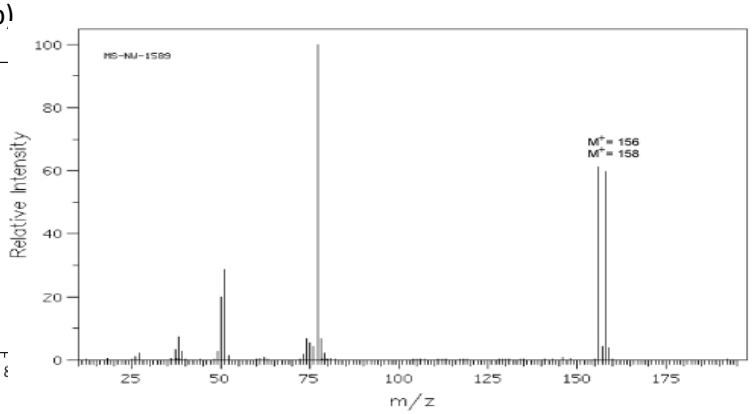
13C. Given a MS, identify and know the significance of the base peak, M+, and M+1 peak. Be able to distinguish between spectra containing chlorine, bromine or neither based on presence of and relative ratio of the M+2 peak

13C.1. For each mass spec below indicate if the compound contains bromine, chlorine or neither.

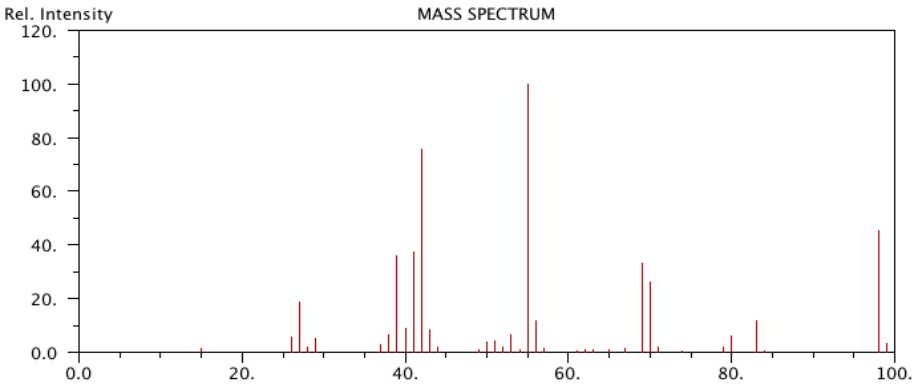
a)



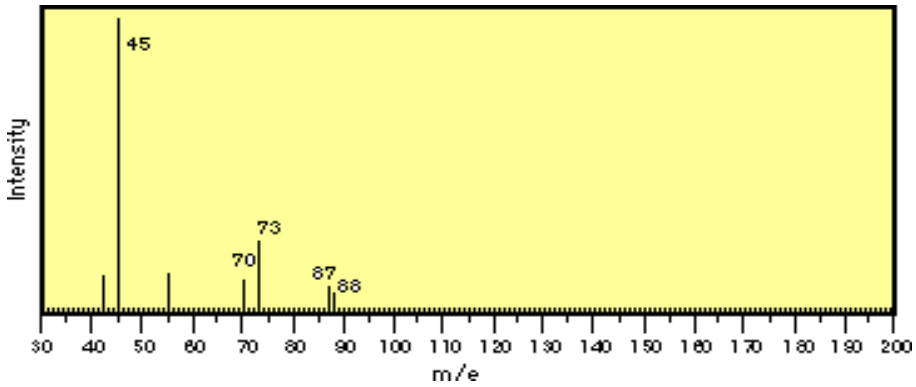
b)



13C.2. Based on the mass spec below, a) what is the molar mass of the compound? b) Does the substance contain chlorine?



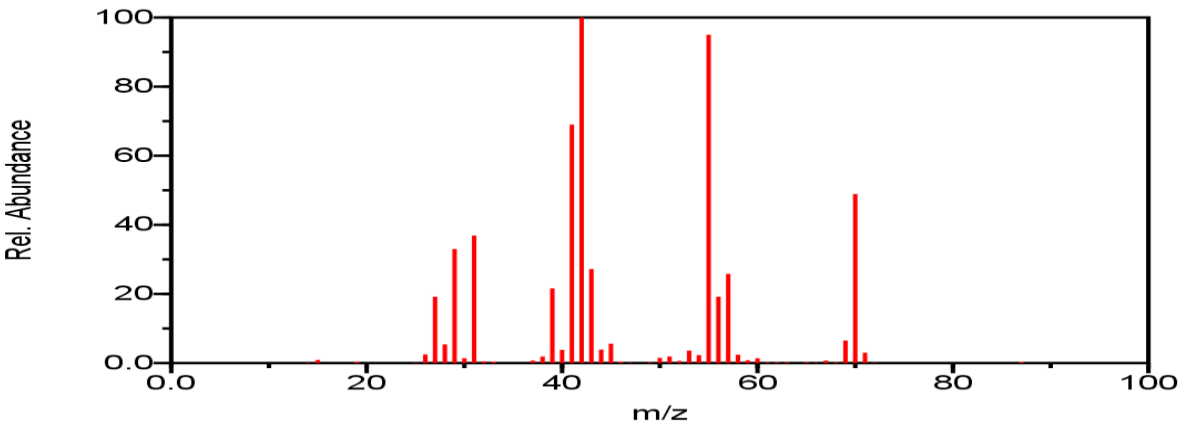
13C.3 Answer based on the mass spec below.



a) What is the molar mass of this compound?

b) What is the mass of the M+1 peak?.

13C.4



a) Based on the mass spec above, what is the molar mass of the compound?

b) Based on the mass spec above, what is the mass of the base peak?

13C.5 You observe a compound that exhibits a mass spectrum with peak at 160 and a peak at 162, both of equal intensity. This compound contains:

a) two chlorine atoms. b) one iodine atom. c) one bromine atom. d) two bromine atoms.

13C.6 The base peak in a mass spectrum is:

a) the highest mass peak
b) the lowest mass peak.
c) the peak corresponding to the molecular ion.
d) the peak with the greatest relative intensity.

13C.7 In the mass spectrum of CH_2Br_2, three peaks due to the molecular ion are observed at 172, 174, 176 in a 1:2:1 ratio. This is because:

a) bromine has three major isotopes
b) CH_2Br_2 readily loses two protons
c) bromine has two major isotopes
d) carbon has more than one isotope

13C.8 Can an exact mass obtained in a high-resolution mass spec distinguish between isomers such as CH_3OCH_3 and CH_3CH_2OH?

13C.9. a) What is the most important piece of information that can be derived from a mass spec? b) What is the name of the peak the gives this information?

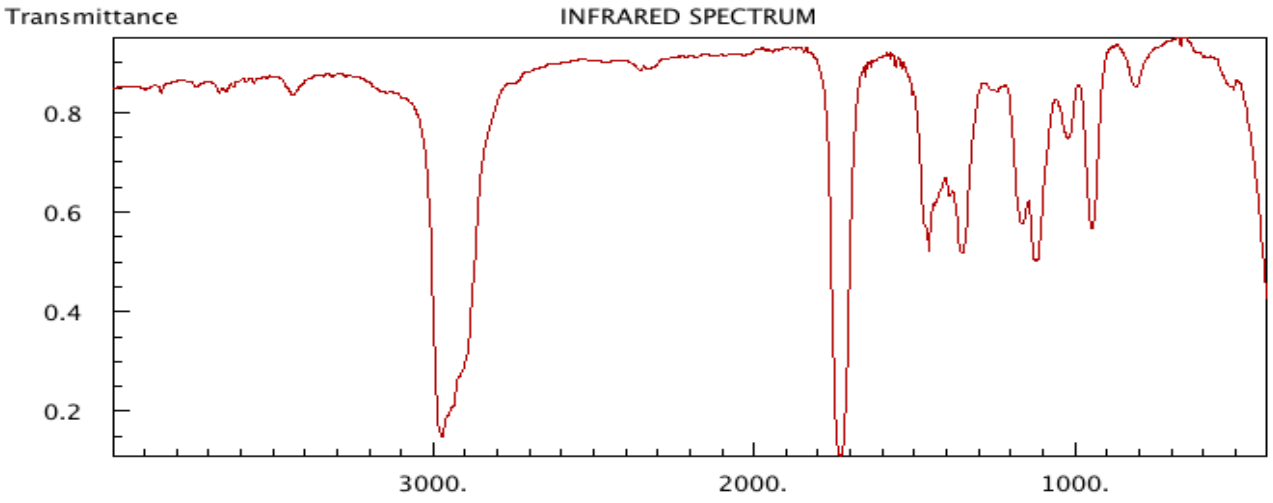
13C.10 Why do all organic mass spectra exhibit M+1 peaks?

13D. Given an IR spectrum and table of absorptions, identify the functional group of a molecule.

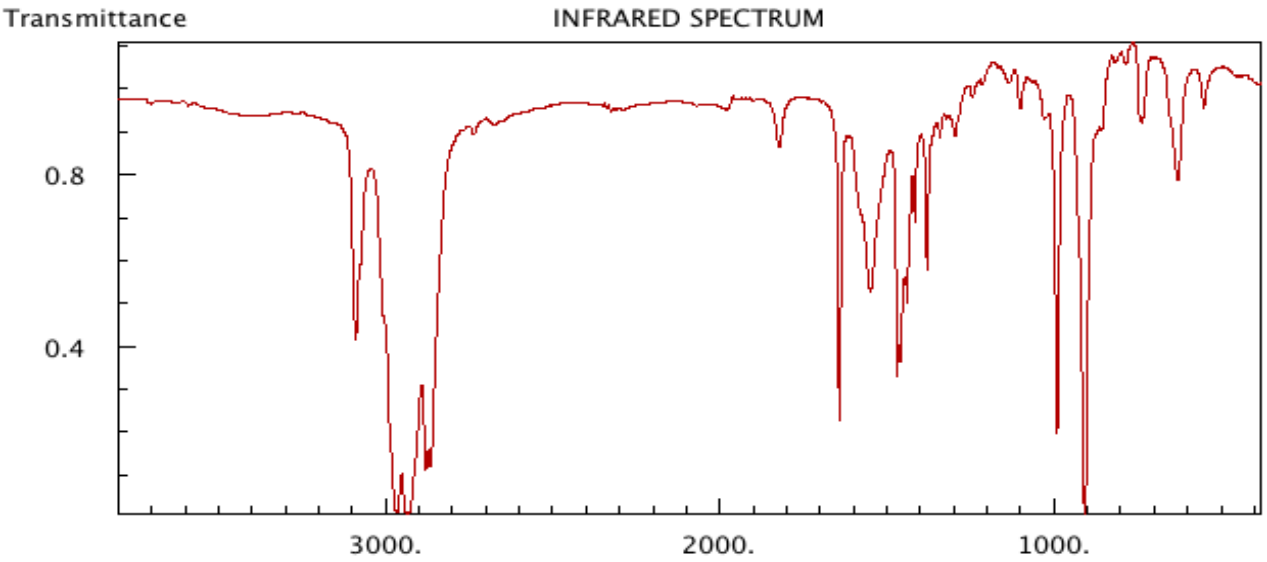
OCSL: 1.1 – 1.22

13D.1 Identify each of the spectra below as belonging to one of the following functional groups: alcohol, alkane, alkene, alkyne, amine, carboxylic acid, ketone. (8 points)

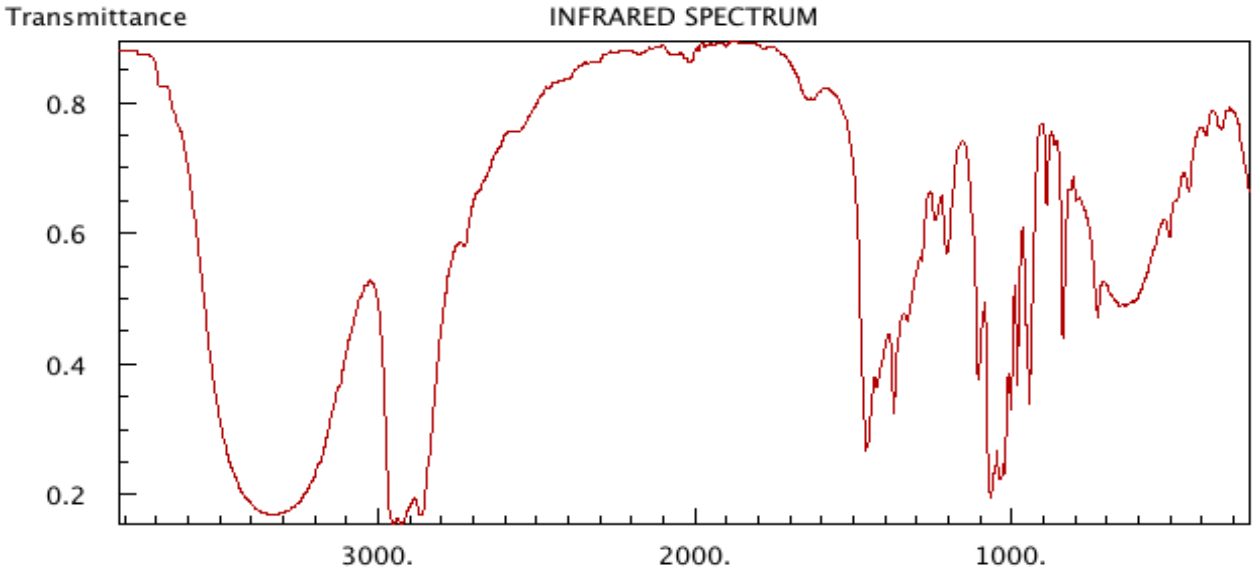
a)



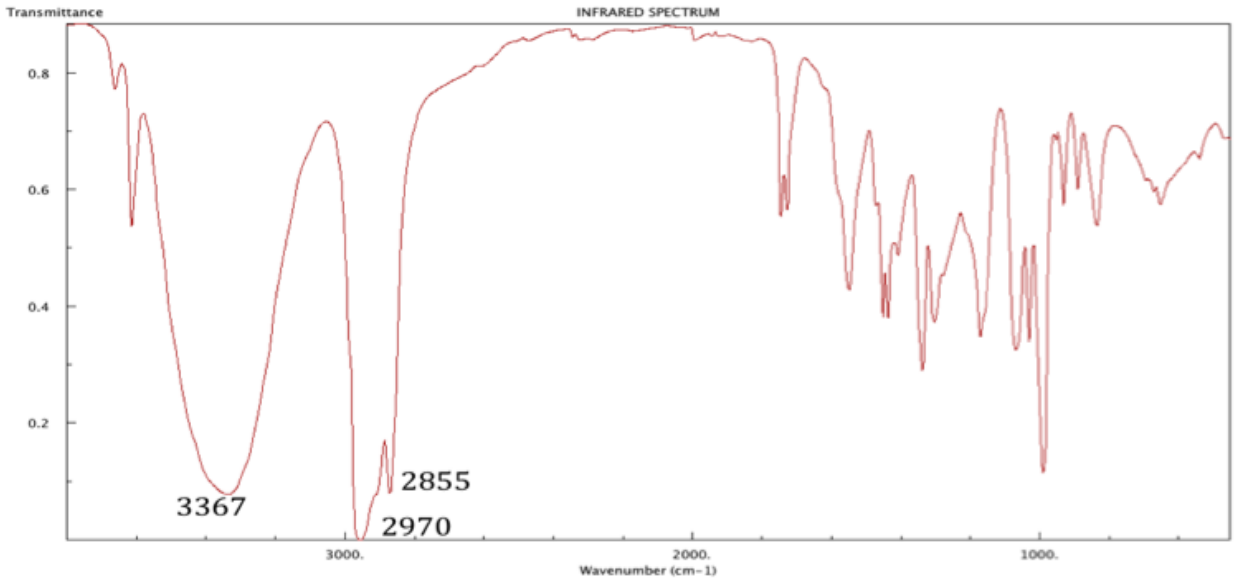
b)


Transmittance
INFRARED SPECTRUM
0.8
0.4
3000.
2000.
1000.

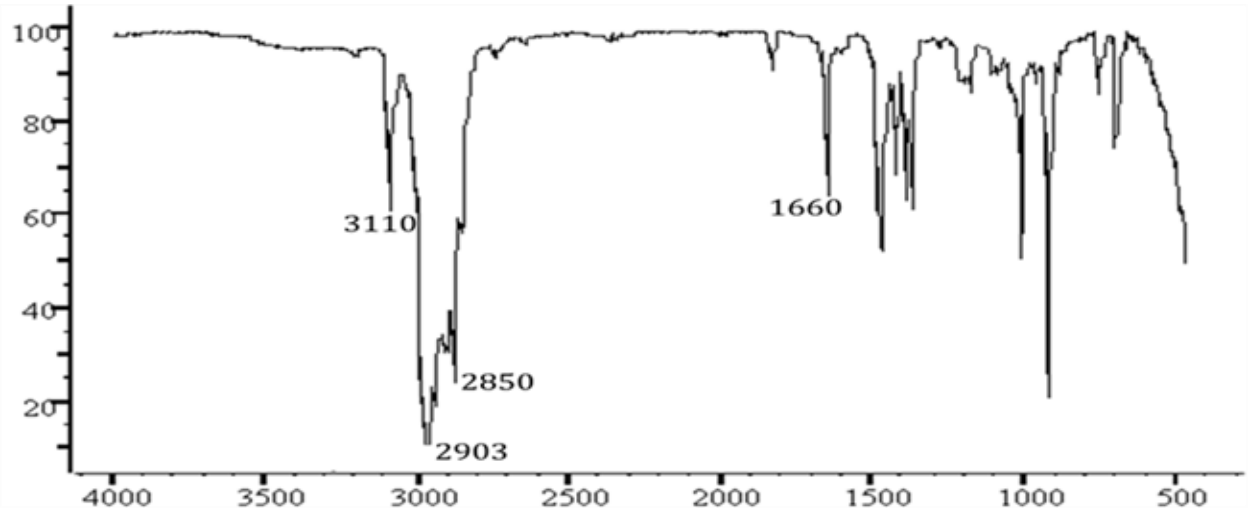
c)


Transmittance
INFRARED SPECTRUM
0.8
0.6
0.4
0.2
3000.
2000.
1000.

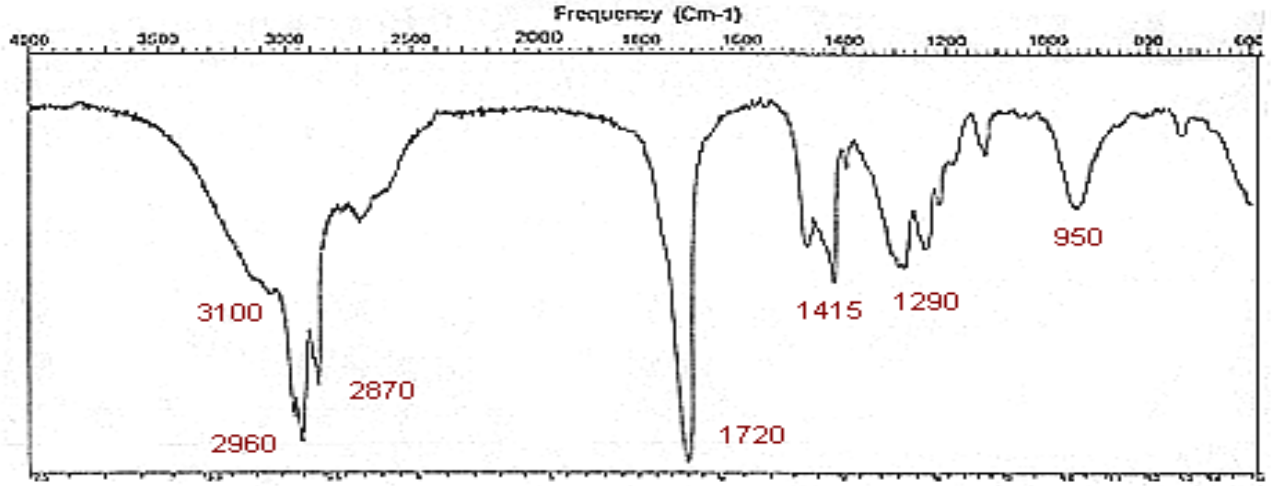
d)


Transmittance
INFRARED SPECTRUM
0.8
0.6
0.4
0.2
3367
2855
2970
3000.
2000.
1000.
Wavenumber (cm-1)

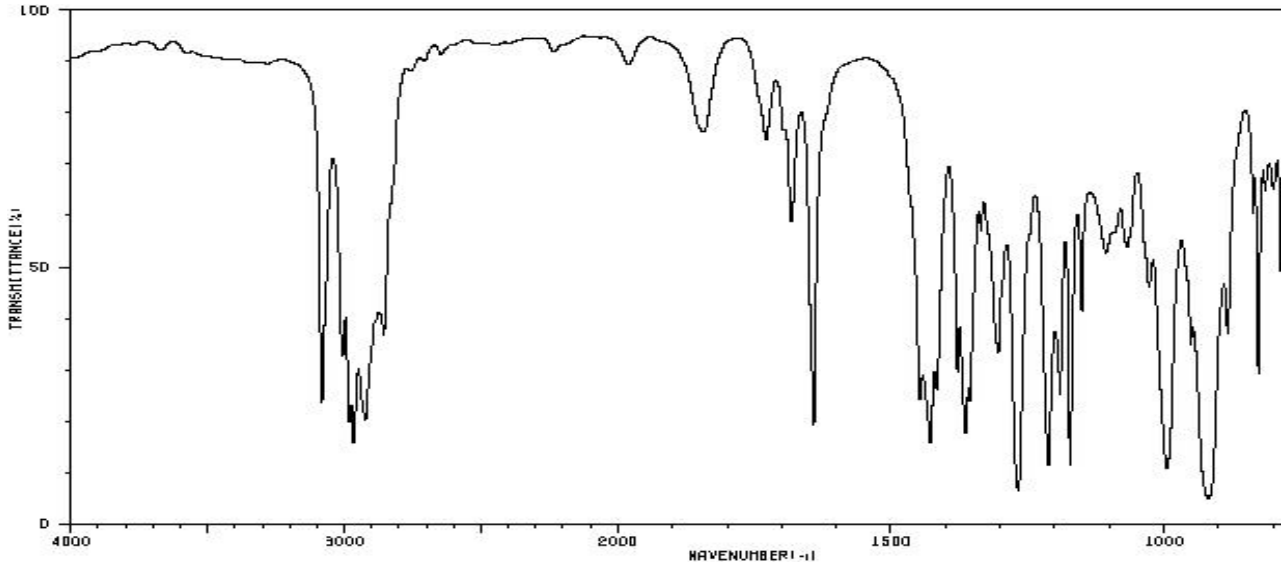
e)


100
80
60
40
20
3110
2850
2903
1660
4000
3500
3000
2500
2000
1500
1000
500

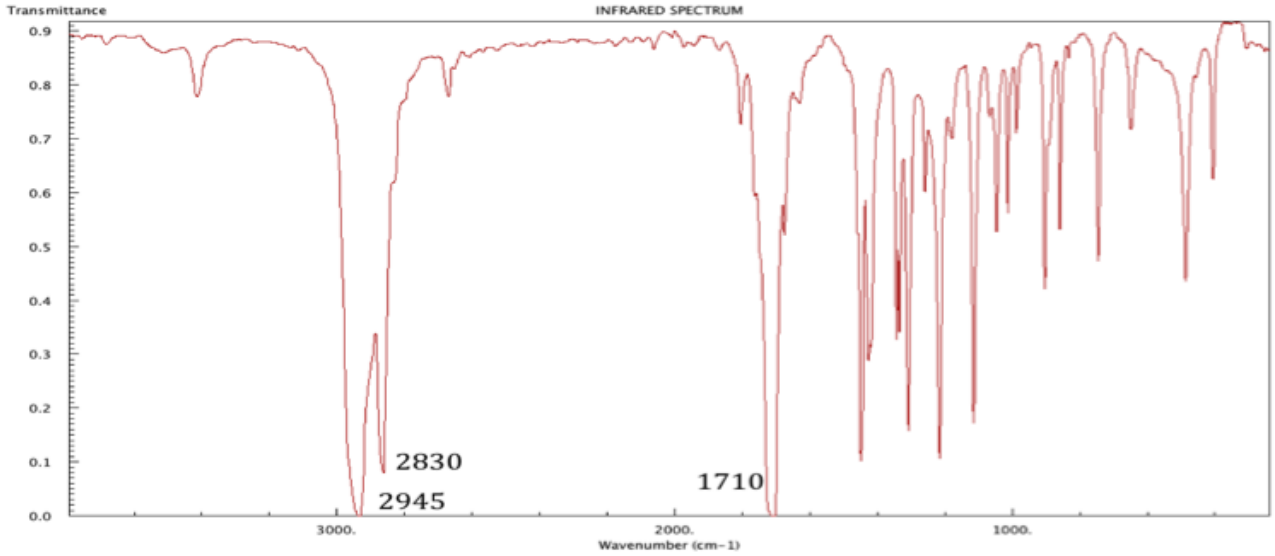
f)


Frequency (Cm-1)
3100
2870
2960
1720
1415
1290
950

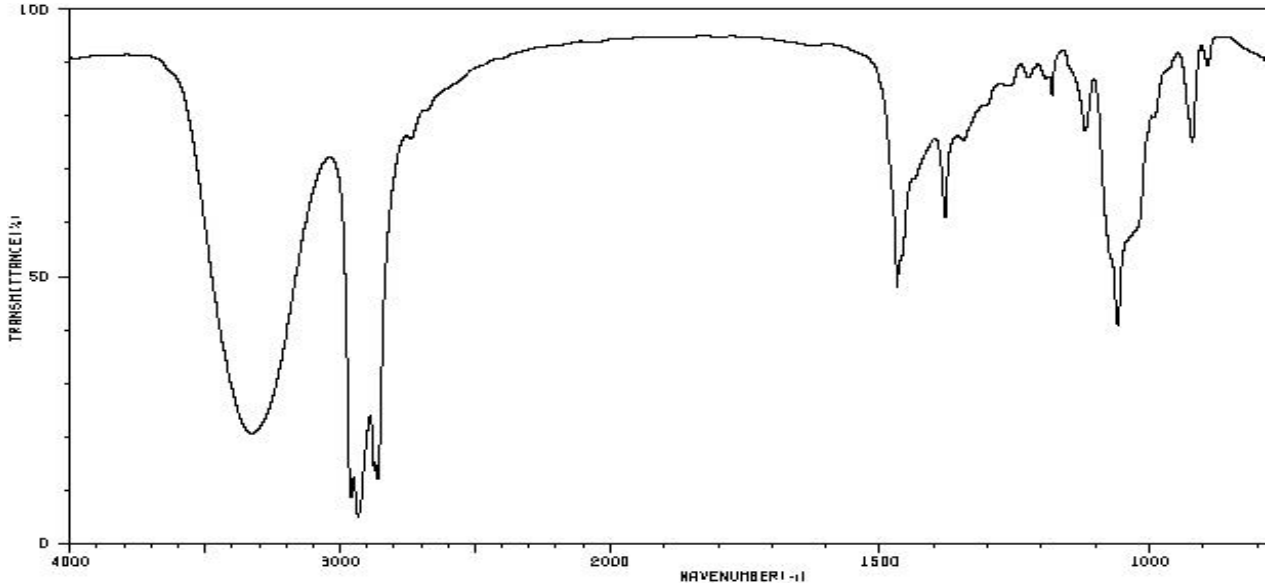
g)


100
50
0
TRANSMITTANCE(%)
4000
3000
2000
1500
1000
WAVENUMBER(-1)

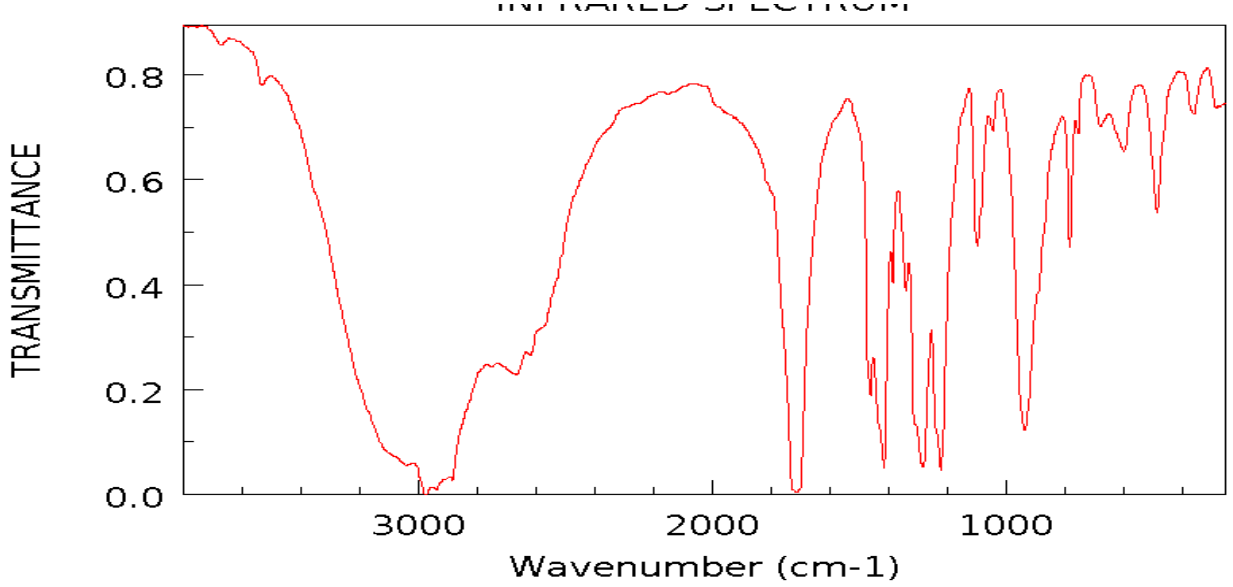
h)


Transmittance
INFRARED SPECTRUM
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
2830
2945
1710
3000.
2000.
1000.
Wavenumber (cm-1)

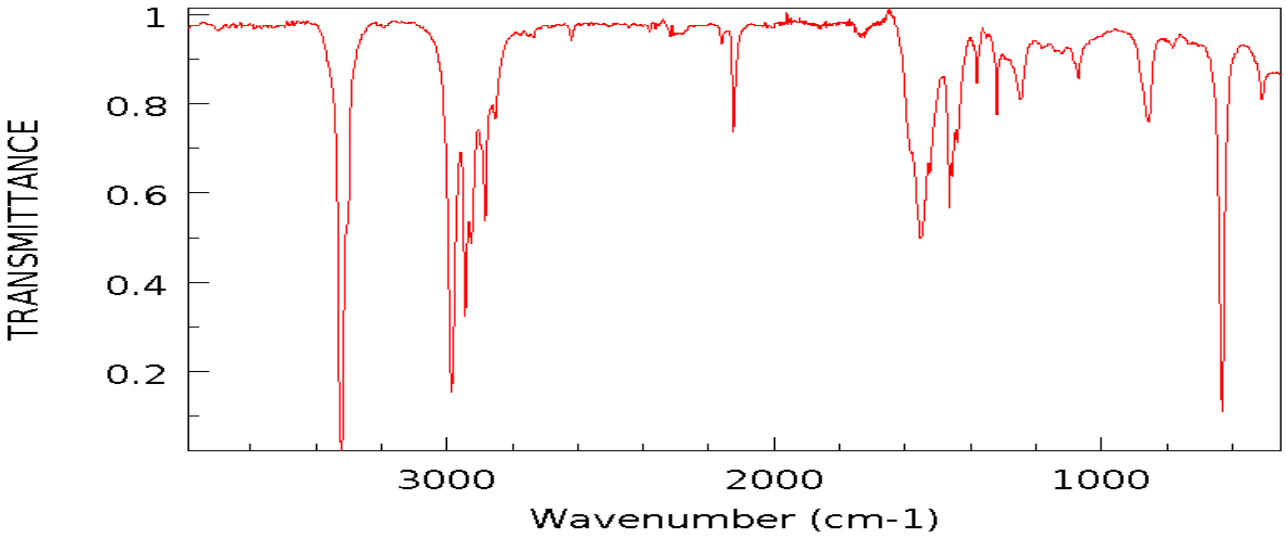
i)


100
50
0
4000
3000
2000
1500
1000

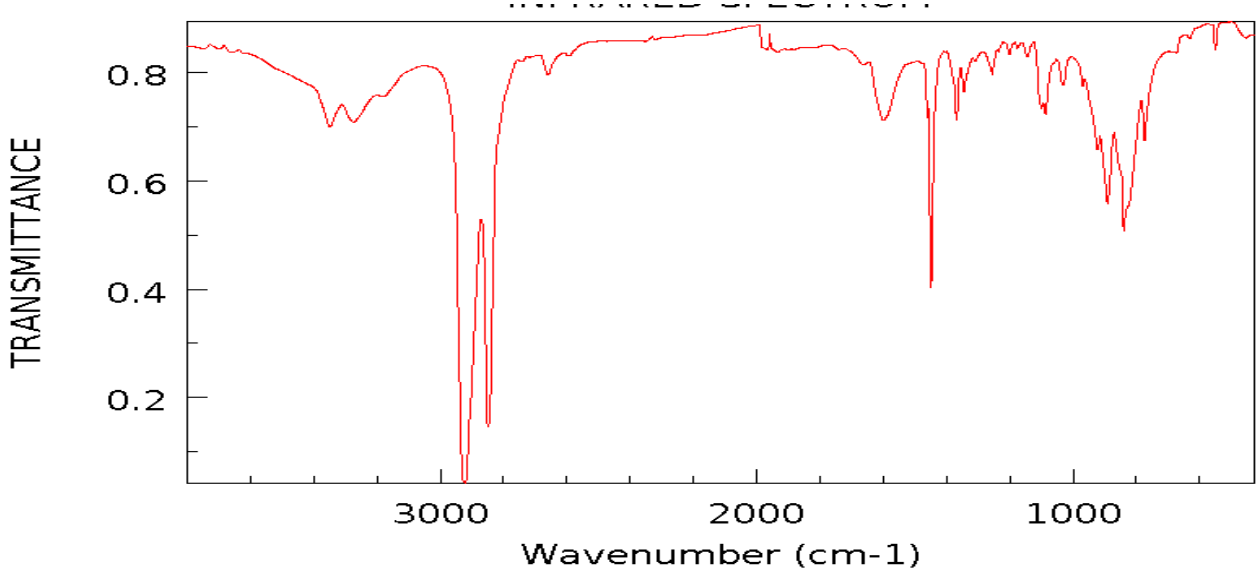
j)


TRANSMITTANCE
0.8
0.6
0.4
0.2
0.0
3000
2000
1000
Wavenumber (cm-1)

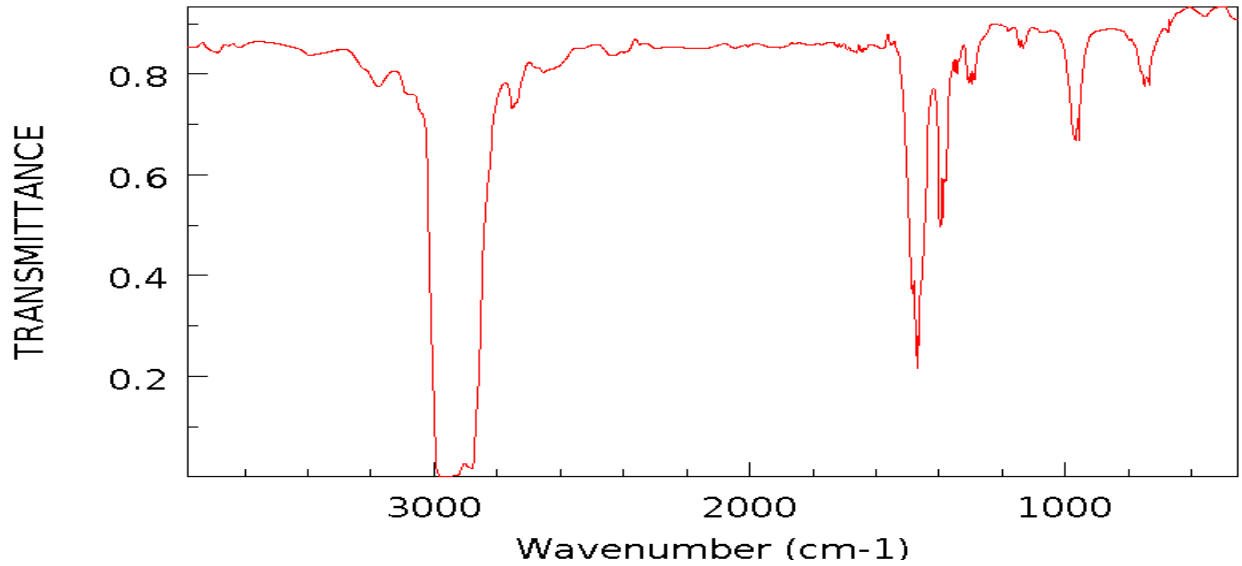
k)


TRANSMITTANCE
1
0.8
0.6
0.4
0.2
3000
2000
1000
Wavenumber (cm-1)

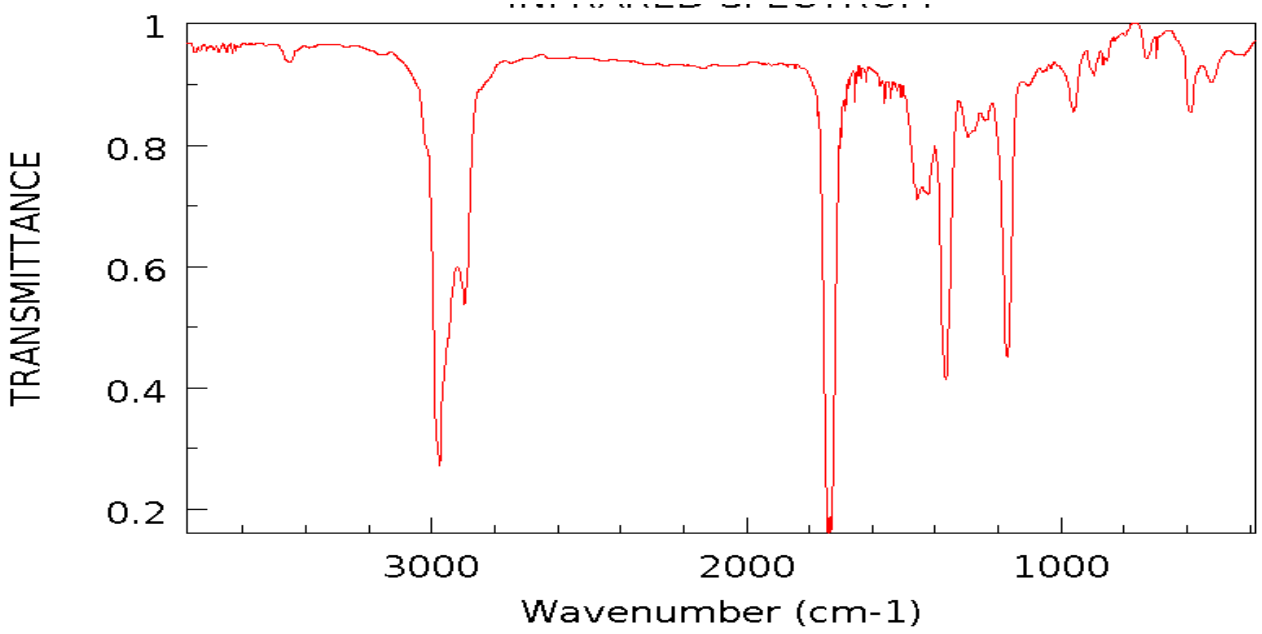
l)


TRANSMITTANCE
0.8
0.6
0.4
0.2
3000
2000
1000
Wavenumber (cm-1)

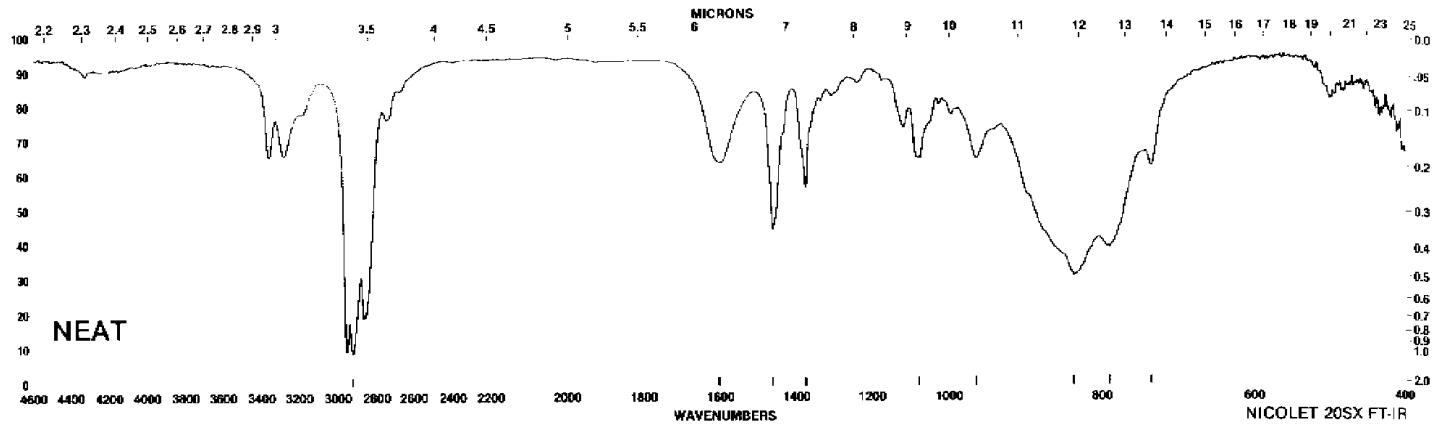
m)


TRANSMITTANCE
0.8
0.6
0.4
0.2
3000
2000
1000
Wavenumber (cm-1)

n)

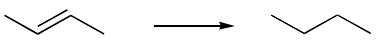


o)

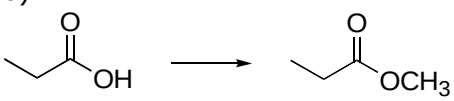


13D.2 What peaks would you expect to appear or disappear in the IR spectrum after the following transformations?

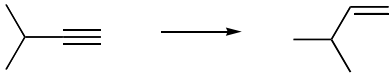
a)



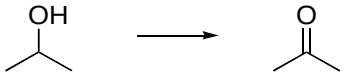
b)



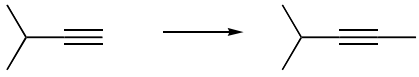
c)



d)



e)

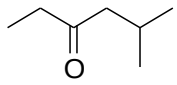


13E. Given a structure predict the number of ^{1}H and ^{13}C peaks in its NMR spectrum.

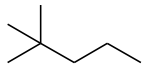
OCSL: 2.1 – 2.11

13E.1 Indicate the number of ^{13}C and ^{1}H NMR peaks that would be observed for the following compounds. (10 points)

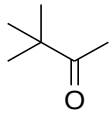
a)



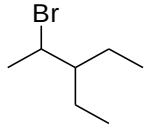
b)



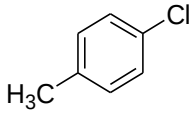
c)



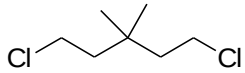
d)



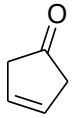
e)



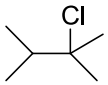
f)



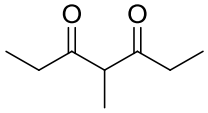
g)



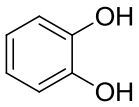
h)



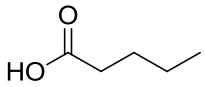
i)



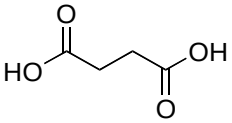
j)



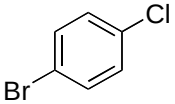
k)



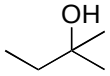
l)



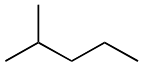
m)



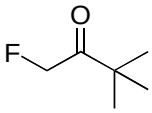
n)



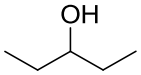
o)



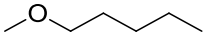
p)



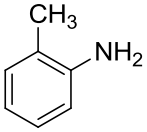
q)



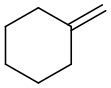
r)



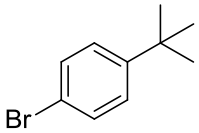
s)



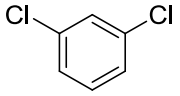
t)



u)



v)

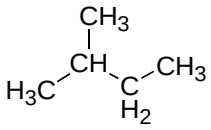


13F. Given a table predict the approximate chemical shift of different ^{1}H and ^{13}C peaks.

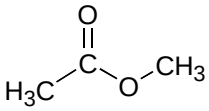
OCSL: 2.12 – 2.19, 2.49 – 2.55

13F.1 Determine the ^{1}H and ^{13}C chemical shift range for each group of protons in the following molecules.

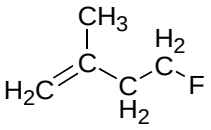
a)



b)

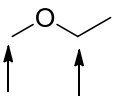


c)

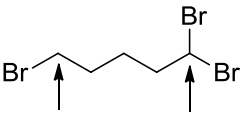


13F.2 Which of the indicated protons in each pair absorbs further downfield? Circle the arrow for each.

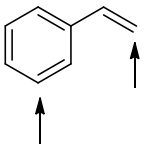
a)



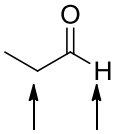
b)



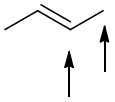
c)



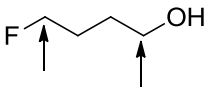
d)



e)

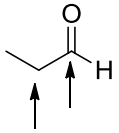


f)

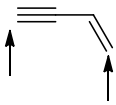


13F.3 Which of the indicated carbons in each pair absorbs further downfield? Circle the arrow for each.

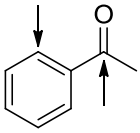
a)



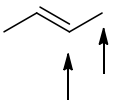
b)



c)

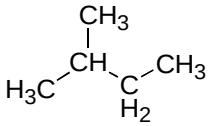


d)

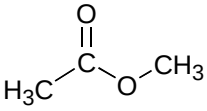


13F.4 For each of the following molecules, circle the proton(s) which would give the highest ppm peak.

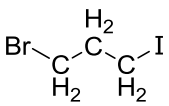
a)



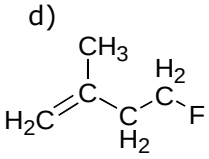
b)



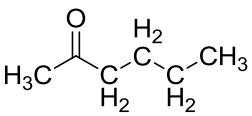
c)



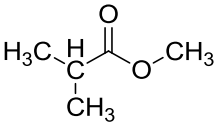
d)



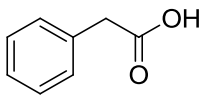
e)



f)



g)



13G. Predict integration values of ^{1}H spectra.

OCSL: 2.20 – 2.23

13G.1 Predict the integration ratios of peaks in the following molecules.

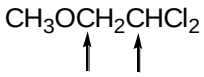
a) b) c) d)

13H. Predict splitting patterns of protons in a structure.

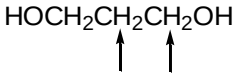
OCSL: 2.24 – 2.34

13H.1 Predict the splitting pattern at the indicated groups of Hs.

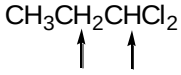
a)



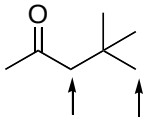
b)



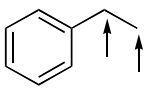
c)



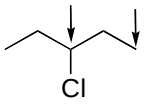
d)



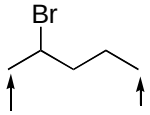
e)



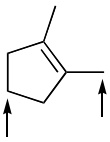
f)



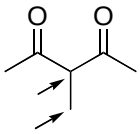
g)



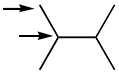
h)



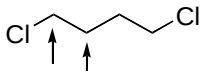
i)



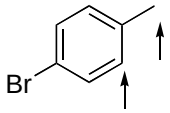
j)



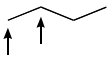
k)



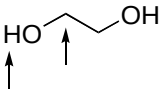
l)



m)



n)



13I. Use number of peaks, chemical shift, integration and splitting data to match a structure to its NMR spectrum.

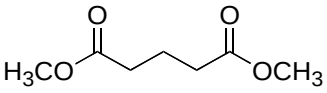
OCSL: 2.42 – 2.48

13I.1 For the molecules below, give each type of hydrogen a number, then predict the chemical shift, integration and splitting of each peak.

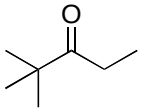
For each:

Peak number	Approx. ppm	integration	splitting

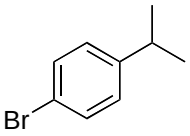
a)



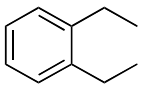
b)



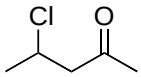
c)



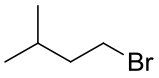
d)



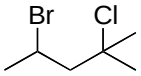
e)



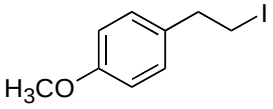
f)



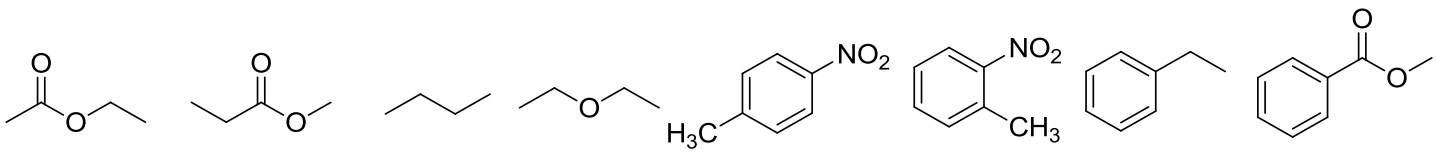
g)



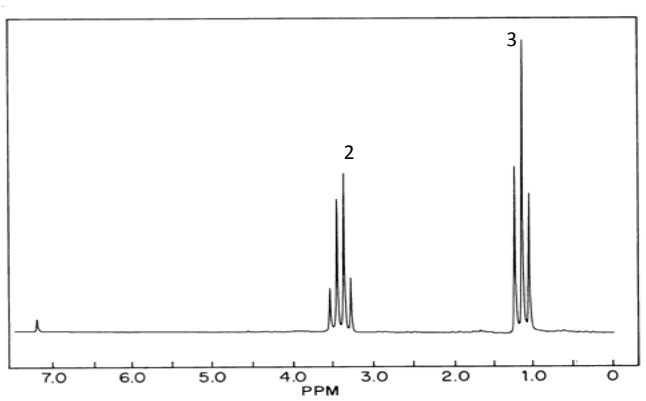
h)



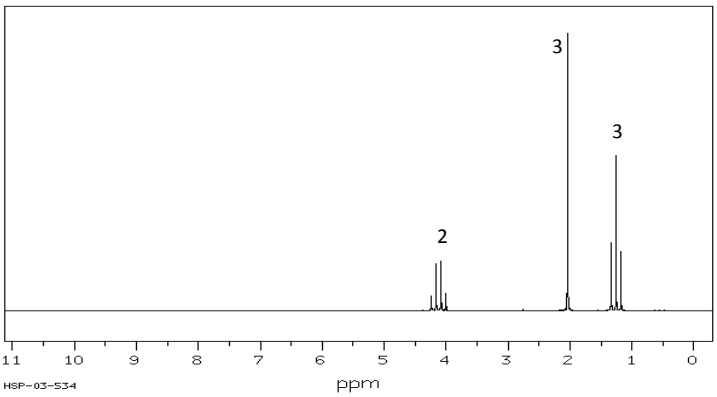
13I.2 Match each of the spectra below to one of the following compounds.



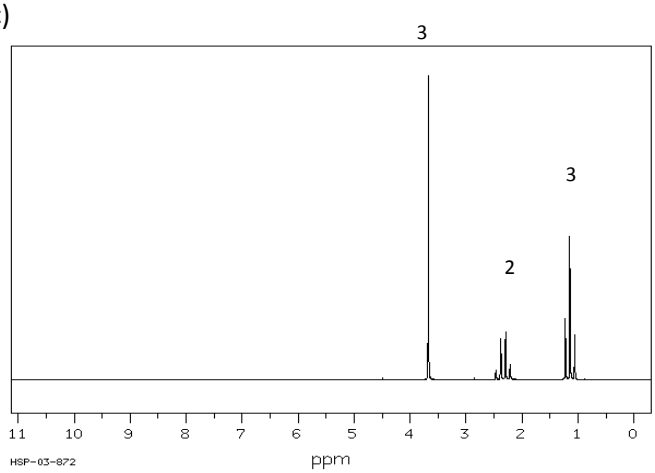
a)



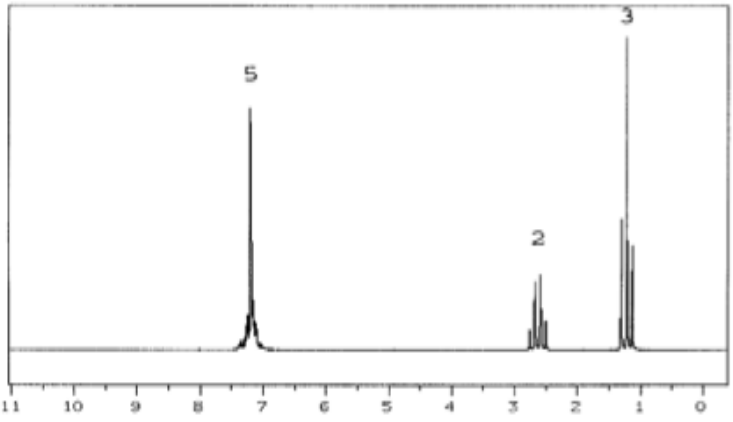
b)



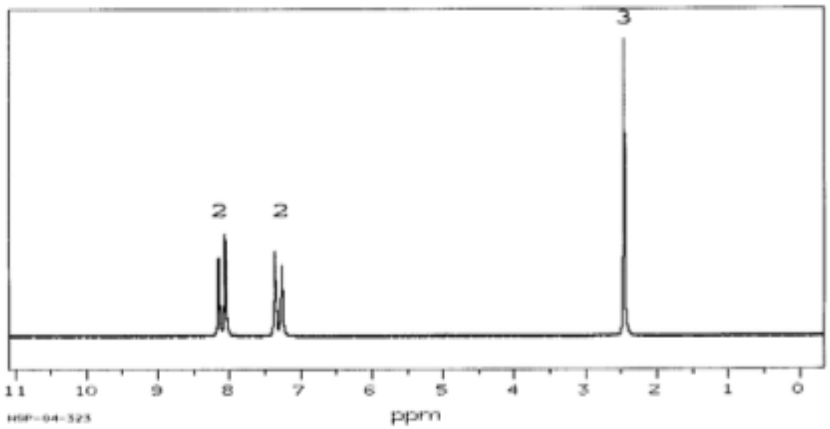
c)



d)

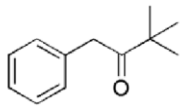


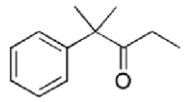
e)

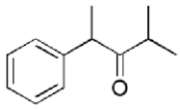


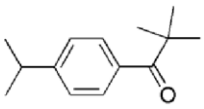
13I.3 Circle the compound that best matches the NMR data below.

absorption	ppm	ratio of absorbing H's
singlet	1.0	6
triplet	1.2	3
quartet	2.2	2
broad singlet	7.0	5

A. 

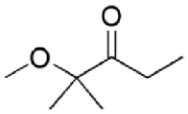
B. 

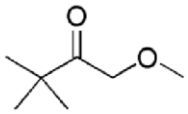
C. 

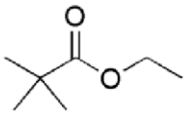
D. 

13I.4. Circle the compound that best matches the NMR data below.

absorption	ppm	ratio of absorbing H's
singlet	1.0	9
triplet	1.2	3
quartet	3.5	2

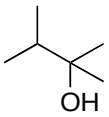
A. 

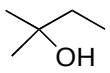
B. 

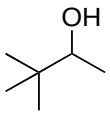
C. 

13I.5 Circle the compound that best matches the NMR data below.

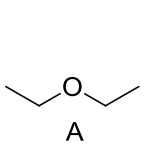
absorption	**d**	**H ratio**
singlet	1.0	9
doublet	1.2	3
singlet	3.0	1
quartet	3.5	1

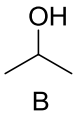


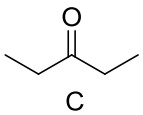


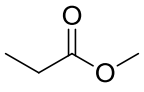


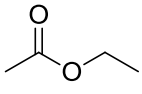
13I.6. Match the ^{1}H NMR signals below to one of the following compounds:

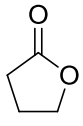

A


B


C


D


E

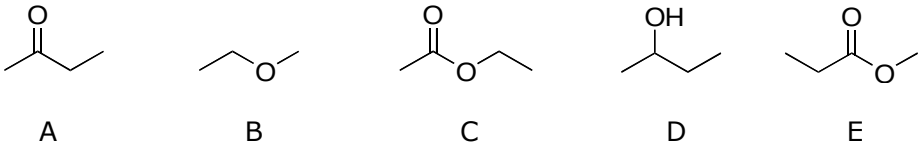

F

a) 4.2 ppm (quartet), 2.0 ppm (singlet), 1.3 ppm (triplet) 2:3:3 ratio

b) 3.7 ppm (singlet), 2.3 ppm (quartet), 1.2 ppm (triplet) 3:2:3 ratio

c) 3.7 ppm (quartet), 1.0 ppm (triplet) 2:3 ratio

13I.7. Match the ^{1}H NMR signals below to one of the following compounds:



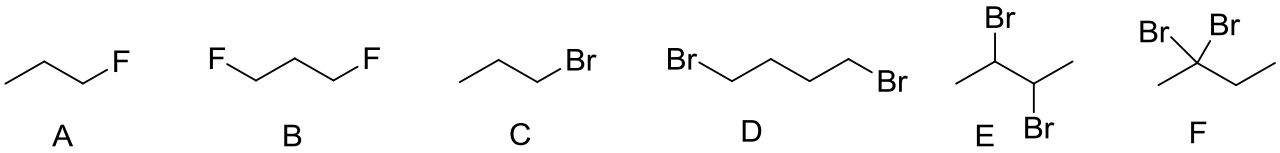
A B C D E

a) 3.4 (singlet, 3H); 2.3 (quartet 2H); 1.1 (triplet, 3H)

b) 4.1 (quartet 2H); 1.9 (singlet, 3H); 1.2 (triplet, 3H)

c) 2.5 (quartet 2H); 2.1 (singlet, 3H); 0.9 (triplet, 3H)

13I.8 . Match the ^{1}H NMR signals below to one of the following compounds:



A B C D E F

a) 3.6 ppm (quartet), 1.4 ppm (doublet) 1:3 ratio

b) 3.5 ppm (triplet), 1.4 ppm (triplet) 2:2 ratio

c) 3.4 ppm (triplet), 1.3 ppm (sextet), 1.0 ppm (triplet) 2:2:3 ratio

d) 4.4 ppm (triplet), 1.4 ppm (sextet), 1.1 ppm (triplet) 2:2:3 ratio

13J. Know the basic workings of UV-VIS, mass spec, HRMS, GCMS, IR, and NMR and what information can be gained from them.

13J.1 Which technique is most typically used to identify substances in a mixture?

a) GC MS b) High Resolution Mass Spec c) IR d) ^{1}H NMr e)^{13}C NMR

13J.2 Absorption of what type of electromagnetic radiation results in transitions among nuclear magnetic spin states?

a) ultraviolet light b) radio waves c) infrared light d) X-rays E) visible light

13J.3. Which one of the following pieces of information cannot be obtained from an infra-red spectrum?

a) the molar mass c) the presence of C=O bonds

b) the presence of O-H bonds d) the identity of a compound through comparison with other spectra

13J.4. In infrared spectroscopy, absorption of electromagnetic radiation results in transitions between _____ energy levels.

a) vibrational b) electronic c) rotational d) nuclear

13J.5. What type(s) of molecular motion is (are) observed using infrared spectroscopy?

a) Stretching and bending b) Rotation and excitation c) Spin flipping d) Fragmentation

13J.6 Which analytical technique involves an electron moving from a higher to a lower energy level?

a) Mass Spec b) UV-Vis c) IR d) ^{1}H NMr e)^{13}C NMR

13J.7 Infrared spectroscopy can be used to identify which of the following?

a) molecular weight. b) melting point. c) conjugation. d) functional groups.

13J.8 Which technique requires magnets to create a difference in energy levels?

a) Mass Spec b) UV-Vis c) IR d) NMR

13J.9 In Mass Spec, the path of ions after deflection depends on

a) only the mass of the ion

b) only the charge on the ion

c) both the charge and the mass of the ion

d) neither the charge nor the mass of the ion