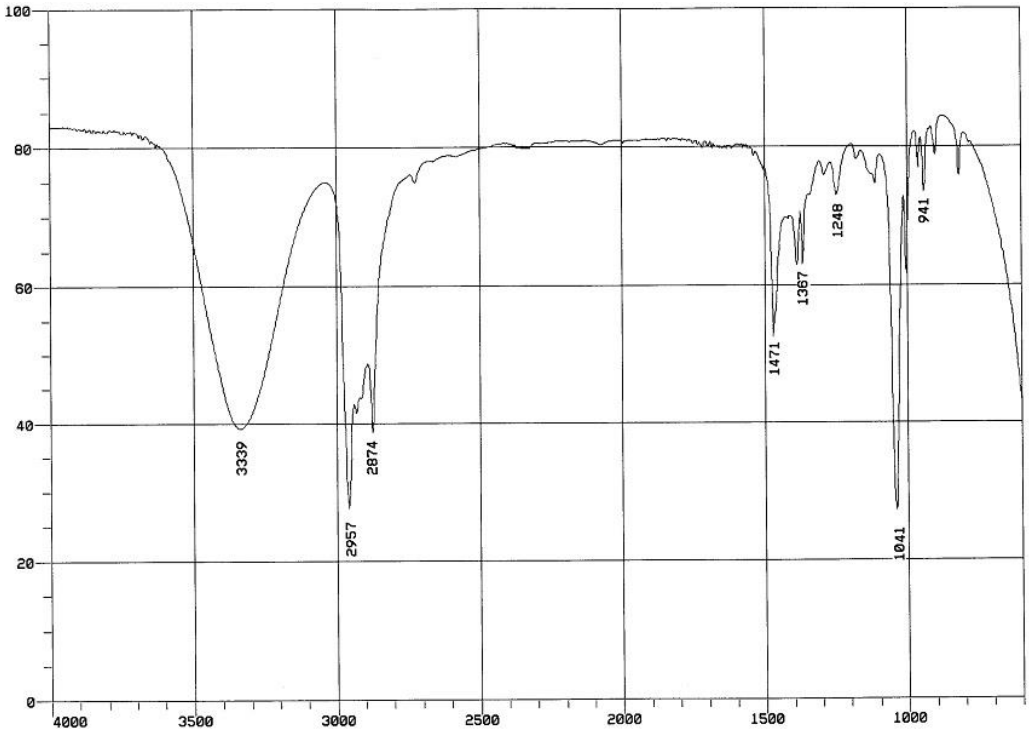
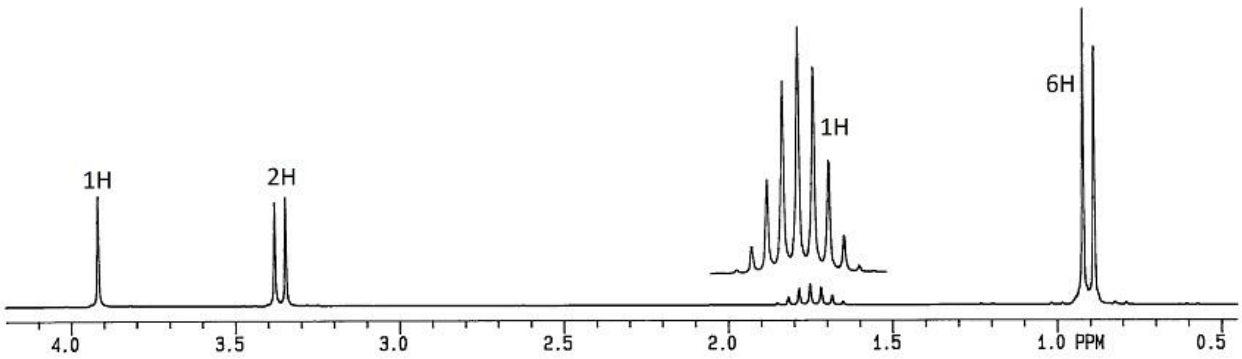
Midterm 2 – Review

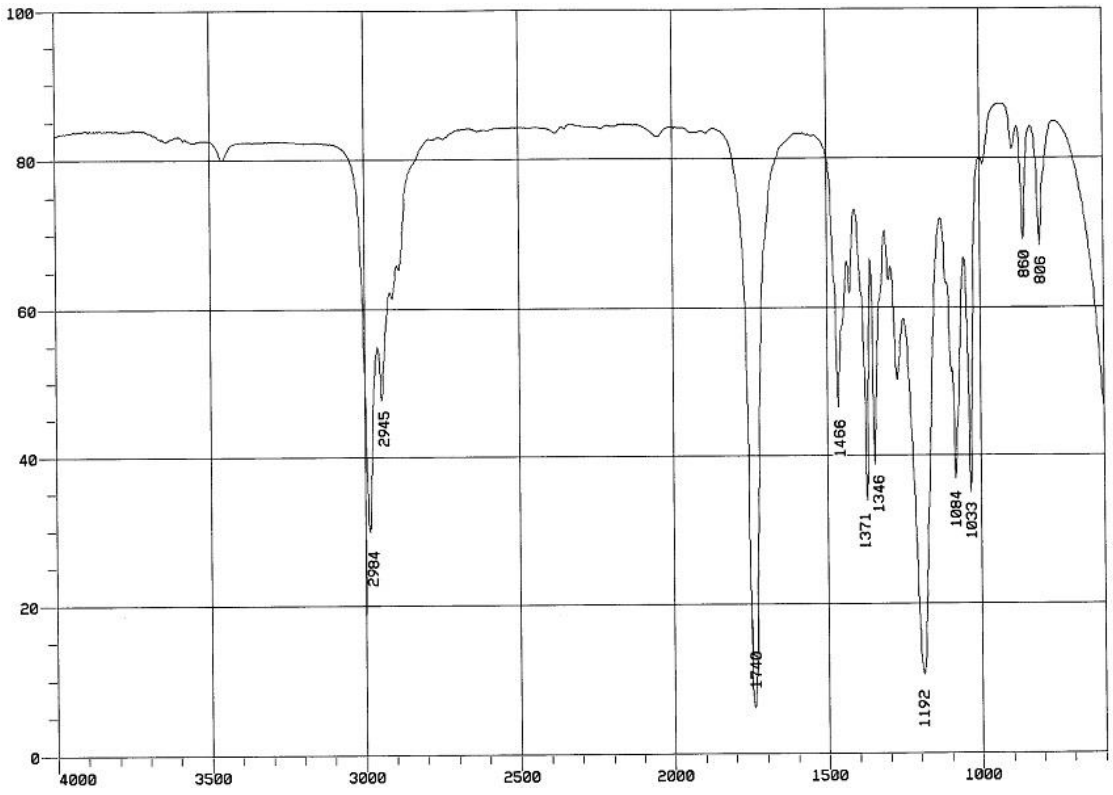
Chapters 17 – 19

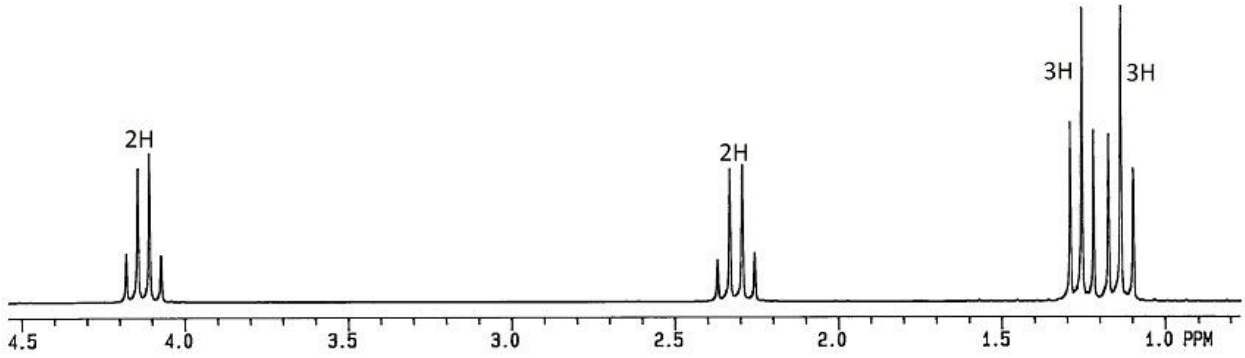
1. A. Identify the compounds using IR and NMR data given for each:
   $C_4H_{10}O$



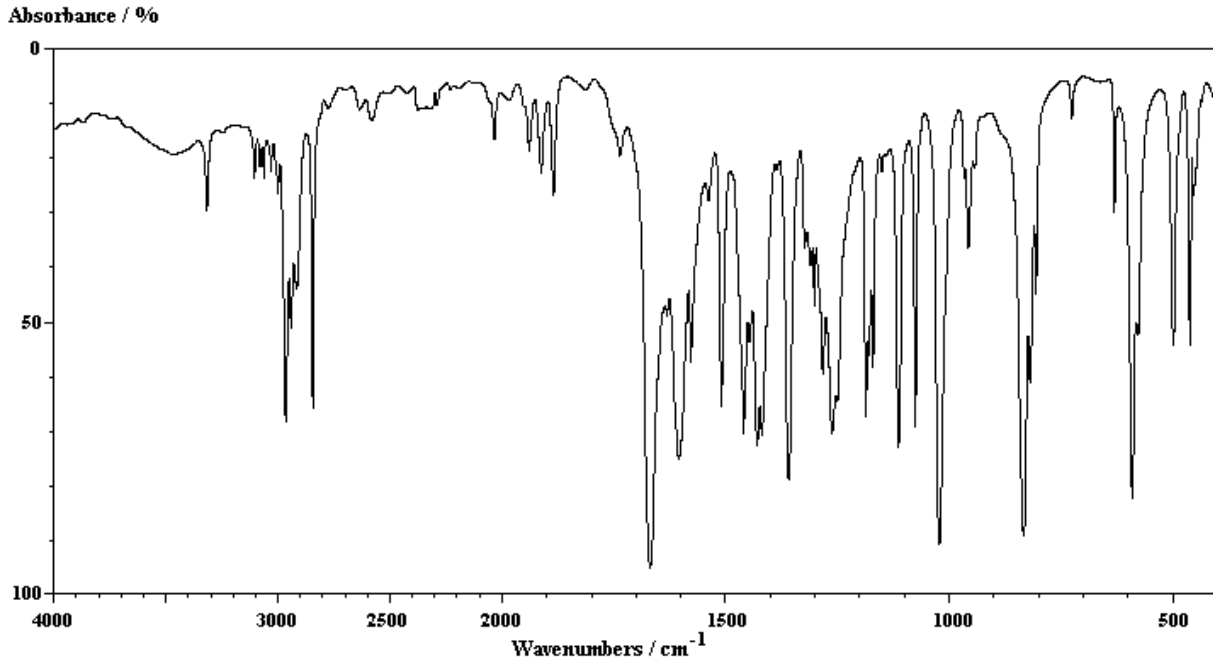


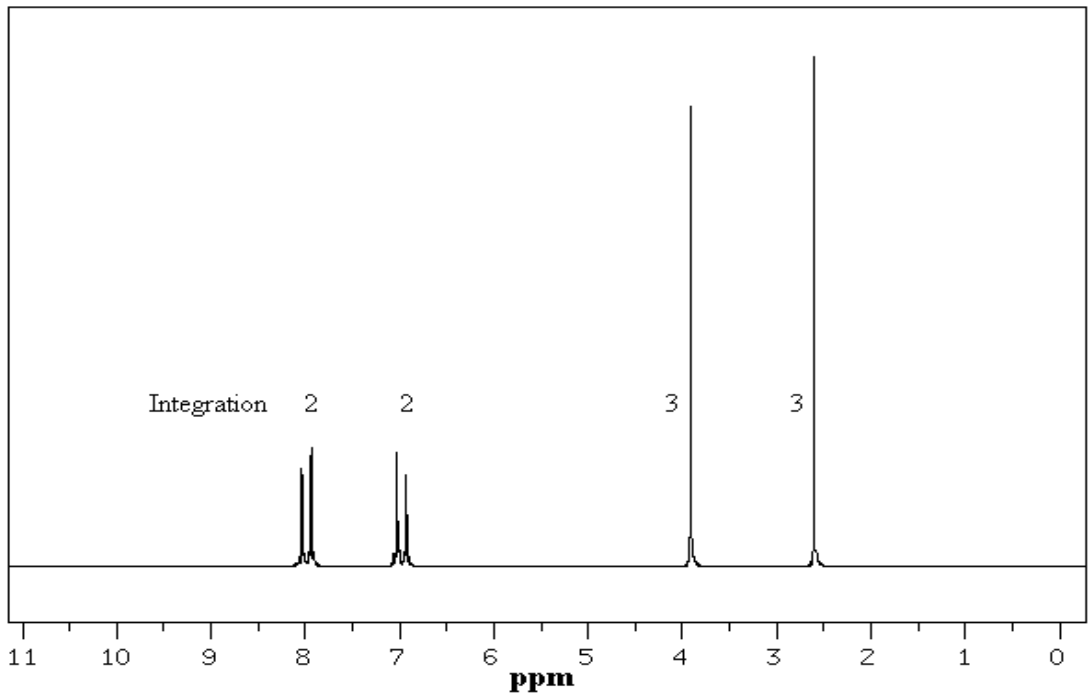
B. $C_5H_{10}O_2$


100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
2984
2945
1740
1466
1371
1346
1192
1084
1033
860
806


2H
2H
3H
3H
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0 PPM

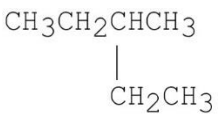
C. $C_9H_{10}O_2$


Absorbance / %
0
50
100
4000
3000
2500
2000
1500
1000
500
Wavenumbers / cm-1

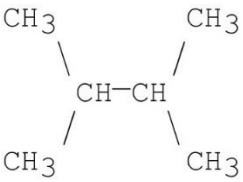

Integration 2 2 3 3
11 10 9 8 7 6 5 4 3 2 1 0
ppm

2. Which of the following structures will give a base peak of 43 in mass spectrometry?

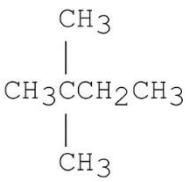
A)



B)

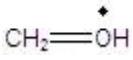


C)

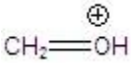


3. Give the ion that corresponds a m/z ratio of 31 in a mass spectrum of 1-butanol.

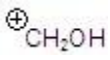
A)



B)

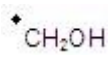


C)



D)

E)



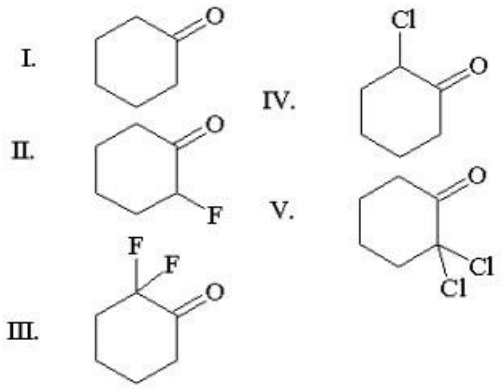
4. Know how frequency, wavelength, wavenumber and energy are related.

5. Know the two factors that IR frequencies depend on

6. Know the common bond frequency regions for IR and how they could slightly vary depending on the overall functional group.

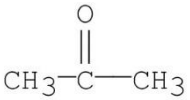
7. Compare the IR frequencies of an acid chloride, ester, aldehyde, ketone, carboxylic acid with reasoning.

8. Which of the following carbonyl groups exhibits the highest wavenumber in infrared spectroscopy and why?



9. Look the spectra we worked on in class and some extra ones posted on class notes and practice.

10. Which of the following compounds has a vibration that is infrared inactive?

A) $CH_3—C{\equiv}C—H$ B) H_2O C)  D) CO_2

11. Which of the following species has a characteristic broad absorption at 3200-3500 cm^{-1} in its IR spectrum?

A) $PhCH_2CH_3$

B) $PhCH_2N(CH_3)_2$

C) $PhCH_2CO_2CH_3$

D) $PhCH_2CH_2OH$

12. How could IR spectroscopy be used to distinguish between the following pair of compounds?

a. Alcohol and ether

b. Ether and carboxylic acid

c. Alkane and alkene

d. Different amines

e. Acid chloride and aldehyde

f. Ketone and aldehyde

g. Sp3 carbon carbon bond, sp2 carbon carbon bond, sp carbon carbon bond

h. Sp3 carbon hydrogen bond, sp2 carbon hydrogen bond, sp carbon hydrogen bond

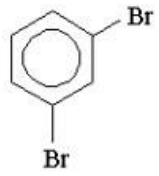
13. Practice mass spec problems of determining molecular formula using M, M+1 and M+2 values and relative abundances.

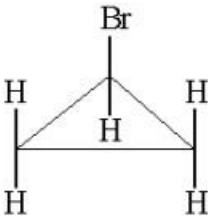
14. What are shielded and deshielded protons. Where do they show up on the NMR spectrum?

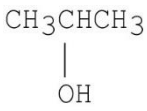
15. What do NMR intensities tell you and how to use them to determine number of chemically equivalent hydrogens?

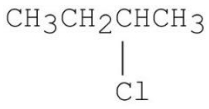
16. Practice determining peak positions and splitting patterns from structures or spectra.

17. How many signals would you expect to see in the ^{1}H NMR spectrum of the following compounds?

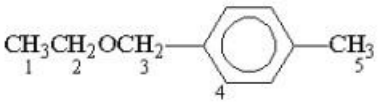
a. 

b. 

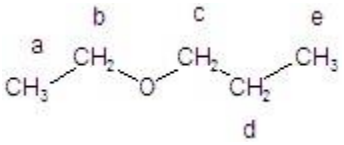
c. 

d. 

18. Which of the following protons gives an NMR signal with the lowest chemical shift value (farthest upfield)?



19. Give the splitting pattern for each proton in the ^{1}H NMR spectrum.

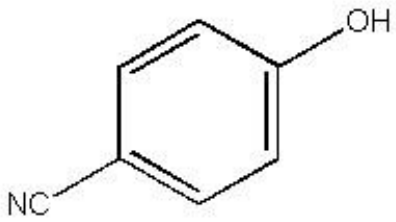


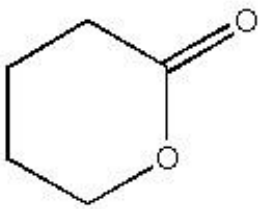
20. Deduce the identity of the following compound from the spectral data given.

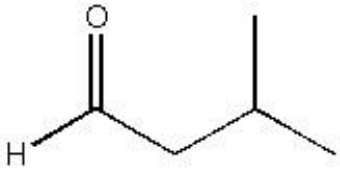
a. $C_4H_8O_2$: ^{1}H NMR, δ 1.23 (3H, triplet), 2.00 (3H, singlet), 4.02 (2H, quartet); IR, 2980, 1740 cm-1

b. C_4H_7BrO: δ 2.2 (3H, singlet), 3.5 (2H, triplet), 4.5 (2H, triplet)

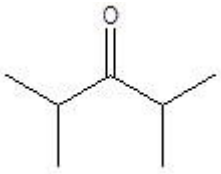
21. Which of the following compounds has a triplet at 9.8 in its ^1H NMR spectrum?

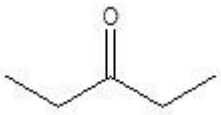


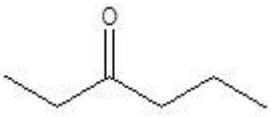




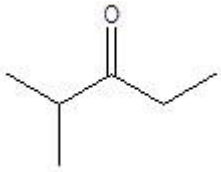
22. Give the structure of a compound that has a formula of $C_6H_{12}O$ and has a triplet (3H, 1.1 ppm), doublet (6H, 1.2 ppm), quartet (2H, 2.4 ppm), and septet (1H, 2.7 ppm) in the ^1H NMR spectrum.

A) 

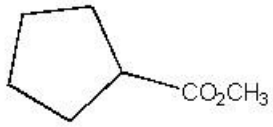
B) 

C) 

D) 

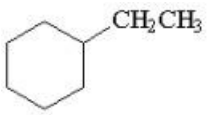
E) 

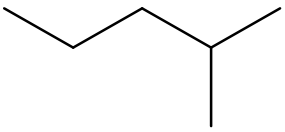
23. How many distinct carbon signals are expected in the proton-decoupled ^{13}C NMR spectrum of the compound below?

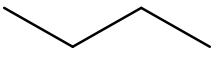


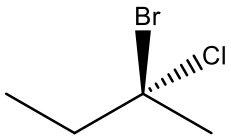
24. Write down all steps involved in the monobromination of cyclohexane:

25. How many products are formed from the monochlorination of the following? Ignore stereoisomers.

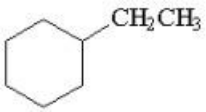
a. 

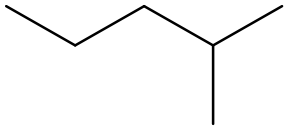
b. 

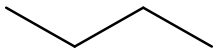
c. 

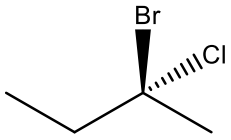
d. 

26. Write down the major products formed from the bromination of the following?

a. 

b. 

c. 

d. 

27. During the free radical chlorination of methane, which of the following reactions has the lowest collision frequency?

A) $Cl\cdot + \cdot CH_3 \rightarrow CH_3Cl$

B) $Cl\cdot + Cl_2 \rightarrow Cl_2 + Cl\cdot$

C) $\cdot CH_3 + CH_4 \rightarrow CH_4 + \cdot CH_3$

D) $\cdot CH_3 + Cl_2 \rightarrow CH_3Cl + Cl\cdot$

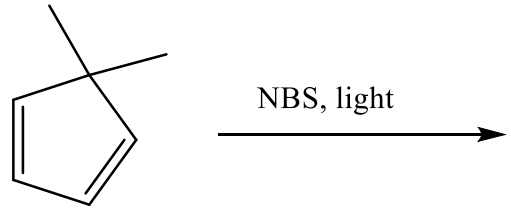
28. How many monochlorinated products would be obtained from 2-methylbutane? Show the structures and give their IUPAC names.

29. Know how to identify initiation, propagation, or termination steps.

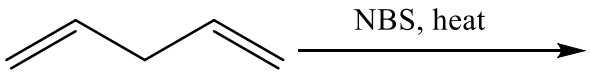
30. Know the energy diagrams from chlorination and bromination.

31. Determine the products of the following reactions:

a.

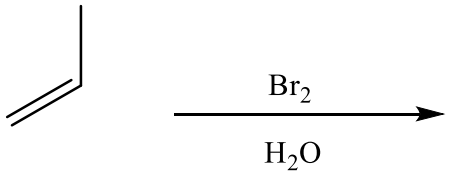


b.

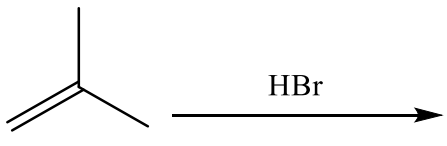


a.

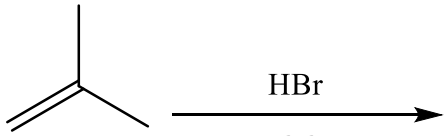
b.



c.



d.



e.