

MOLECULAR REPRESENTATIONS AND INFRARED SPECTROSCOPY

A STUDENT SHOULD BE ABLE TO:

1. Given a Lewis (dash or dot), condensed, bond-line, or wedge formula of a compound draw the other representations.
2. Give examples of, and recognize when given the structure, representatives of the following classes of compounds. Also, draw isomers of given compounds.

Hydrocarbons (compounds containing C and H only)

Saturated - alkanes

Unsaturated - alkenes (olefins), alkynes, aromatics

Organic compounds containing halogens

Alkyl halides (1° , 2° , 3°)

Compounds containing oxygen:

C-O single bonds only: alcohols (1° , 2° , 3°), ethers

C=O compounds: aldehydes, ketones, carboxylic acids, esters, acyl halides, anhydrides

Compounds containing nitrogen: amines (1° , 2° , 3°), amides, nitriles

Compounds containing sulfur: thiols, sulfides

3. Identify functional groups present in molecules from infrared (IR) spectroscopy data, and predict features of the IR spectrum of molecules from their structures. Important IR absorption frequencies to know include:
 - O—H (alcohols, hydrogen bonded): $3200-3550\text{ cm}^{-1}$, strong and broad
 - N-H: $3300-3500\text{ cm}^{-1}$, medium intensity
 - O—H (carboxylic acids): $2500-3000\text{ cm}^{-1}$, broad peaks of variable intensity
 - C=O: $1630-1780\text{ cm}^{-1}$, strong absorptionIf you need to use other frequencies to identify other functional groups (and sometimes you will), a table of IR frequencies will be provided.
4. Apply concepts learned in Module 1.

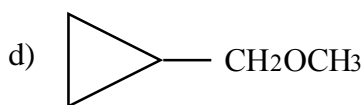
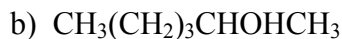
Simplified Table of Main IR Frequencies

Wave number, cm^{-1}	Functional Group	Peak Description
3300 – 3600	O-H (alcohol)	Strong and broad
2500 – 3000	O-H (carboxylic acids)	Very broad (over $\sim 500 \text{ cm}^{-1}$), often looks like distorted baseline, can reach above 3000 cm^{-1} .
3200 – 3500	N-H	Doublet in case of NH_2 group of a primary amine or amide
3300	$\text{C}\equiv\text{C}-\text{H}$ terminal alkyne	Usually sharp and strong
3000 - 3100	$\text{C}=\text{C}-\text{H}$ alkene or arene	Often weak, overlaps with CH alkane absorption
2800 – 3000	C-H (sp^3 carbon)	Strong, broad and multi-banded
2250 - 2220	$\text{C}\equiv\text{N}$	Medium intensity
2100 - 2260	$\text{C}\equiv\text{C}$ alkyne	Medium intensity for terminal alkynes, very weak for internal
1680 – 1820	C=O (amides, ketones, aldehydes, carboxylic acid, esters)	Very strong; lower frequency for amides and when C=O is conjugated
1600 – 1650	C=C alkene, aromatic ring	Check to see if you have C-H unsaturated $>3000 \text{ cm}^{-1}$ (if not, it's completely substituted)
~ 1600	$-\text{NH}_2$ (bending) 1° amines and amides	Only if you have corresponding N-H peak at $3200\text{-}3500 \text{ cm}^{-1}$ (this peak may be mistaken for C=C otherwise)
1200	Ar-O	Strong (look for $\text{C}-\text{H}$ & $\text{C}=\text{C}$ first)
1050-1150	C-O	
690 and 750	phenyl group	Strong (look for $\text{C}-\text{H}$ & $\text{C}=\text{C}$ first)

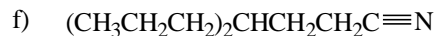
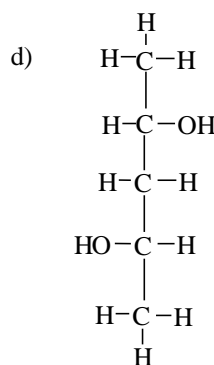
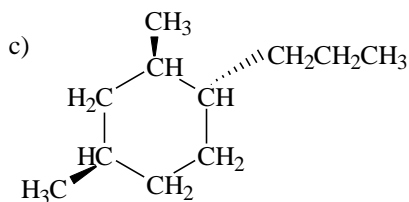
To best prepare for this module, please work Chapter 2 Skill Builder problems and Chapter 15 Skill Builder problems (IR problems only) in the textbook.

A STUDENT WHO HAS MASTERED THE OBJECTIVES FOR THIS UNIT SHOULD BE ABLE TO SOLVE THE FOLLOWING PROBLEMS AND RELATED ONES:

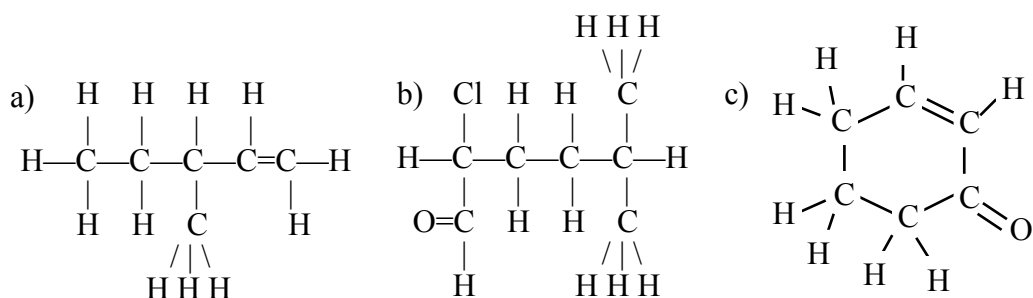
1.1 Draw complete structures (showing all atoms, bonds as lines, and non-bonding valence electrons as dots) for the following compounds:



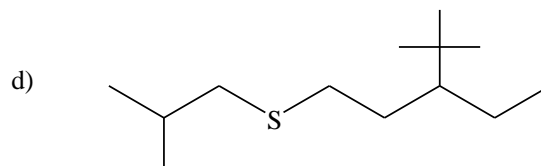
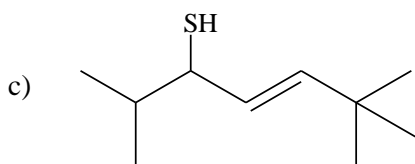
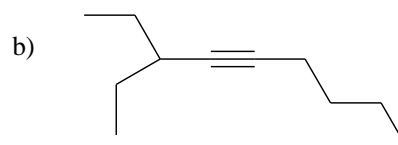
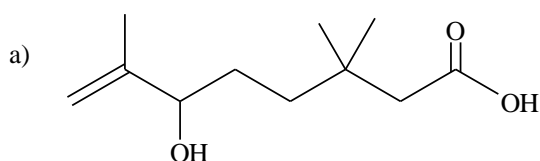
1.2 Draw a bond-line structure for each of the following compounds. Use dashes and wedges to indicate three-dimensional geometry where appropriate.



1.3 Draw both condensed and bond-line structures for (a) and (b); draw a bond-line formula for (c).



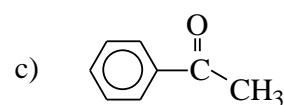
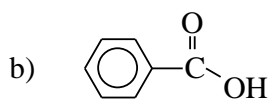
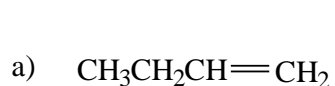
1.4 Draw condensed formulas for each of the following.



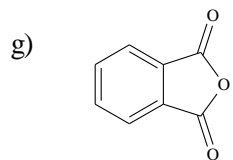
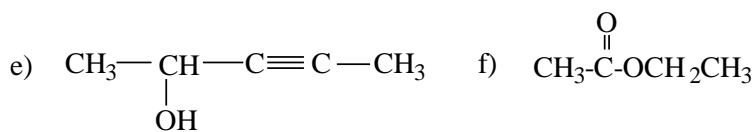
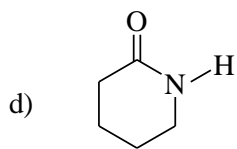
2.1 Draw the structure of an example of each of the following classes of compounds. **Do not use the symbol "R."**

- | | | |
|---------------|-------------|--------------------|
| a) alkane | b) ether | c) 2° amine |
| d) 3° alcohol | e) aldehyde | f) 1° alkyl halide |
| g) thiol | h) alkyne | i) acyl chloride |

2.2 Name the functional group or groups in each of the following molecules. Indicate 1°, 2°, or 3° where appropriate.



2.2 (Continued)



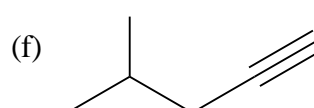
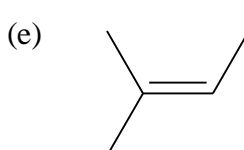
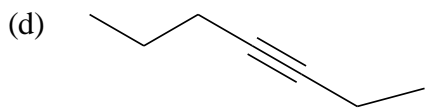
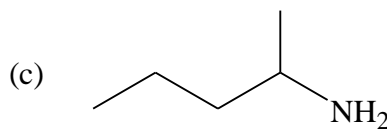
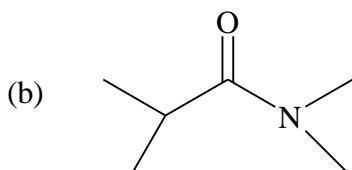
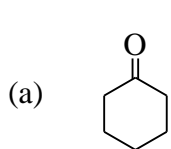
3.1 Based on the IR data given, what functional group(s) can be present in these compounds?

- a) A strong absorption at 1710 cm^{-1} , no N in the molecular formula, no O-H peaks present.
- b) A strong absorption at 1720 cm^{-1} and a broad absorption between $2500\text{-}3000\text{ cm}^{-1}$.
- c) An oxygen-containing compound with a strong absorption at $3200\text{-}3400\text{ cm}^{-1}$, no N in the molecular formula, no peak at $1680\text{-}1820\text{ cm}^{-1}$.

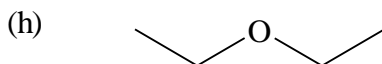
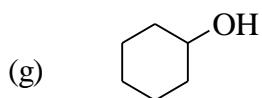
3.2 An oxygen-containing compound does not have IR peaks in either the $3200\text{-}3600\text{ cm}^{-1}$ region or the $1630\text{-}1780\text{ cm}^{-1}$ region. Which of the following general formulas fits this IR spectrum?

- A. ROH B. RCOOH C. RCOR D. ROR

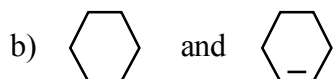
3.3 For each of the following compounds, determine whether or not you would expect its IR spectrum to exhibit a signal to the left of 3000 cm^{-1} .



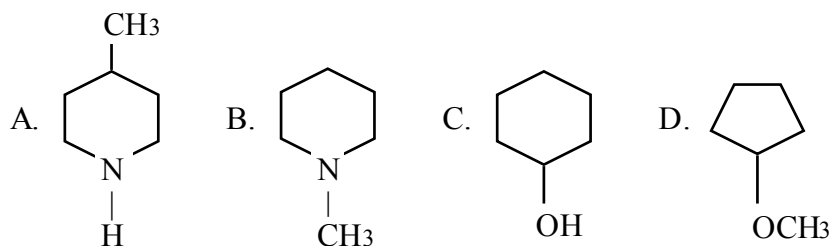
3.3 Continued.



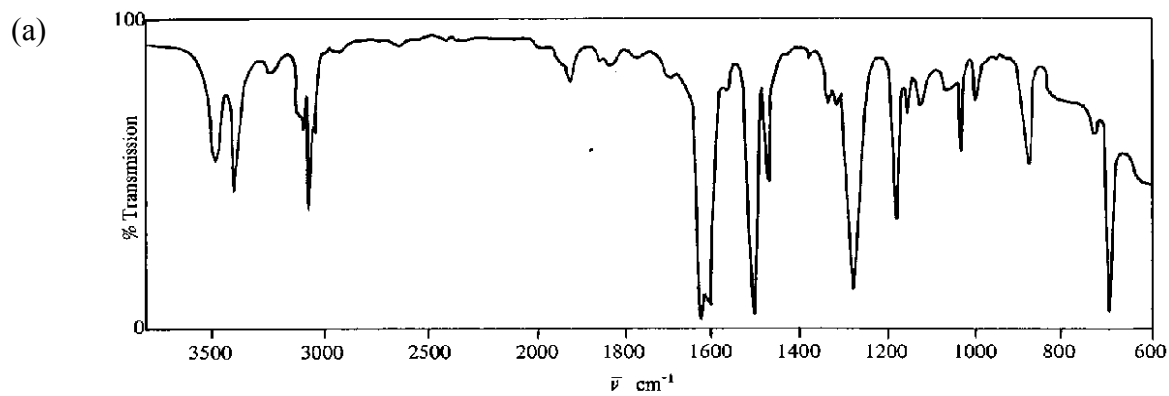
3.4 What IR frequencies would enable a chemist to distinguish between these?



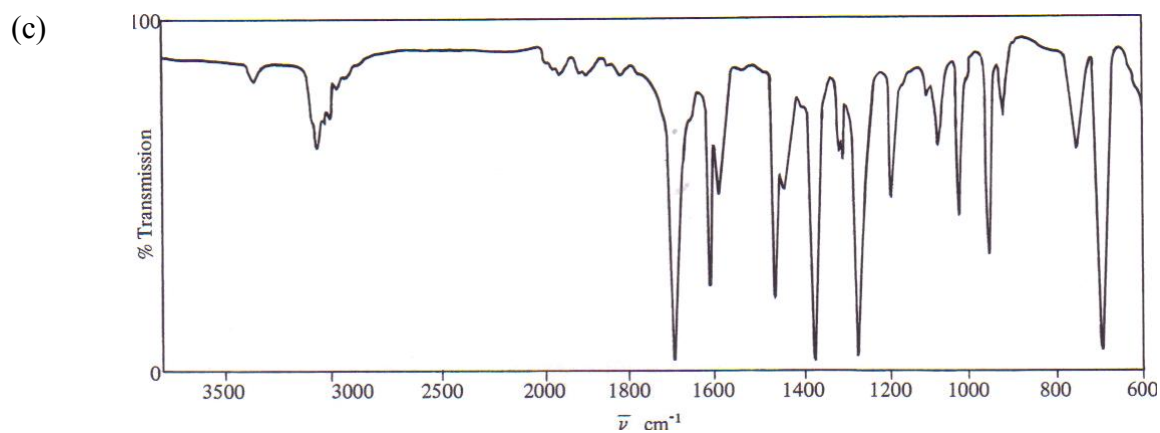
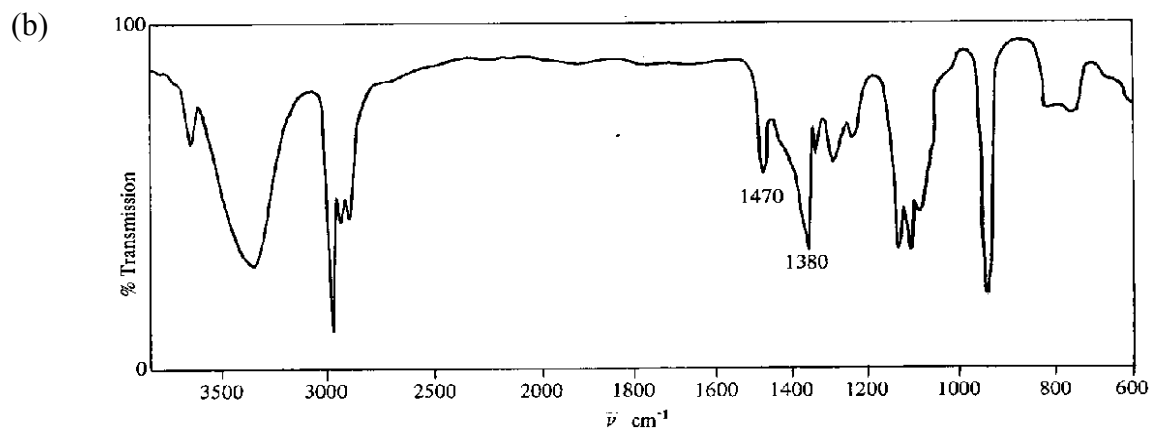
3.5 An unknown compound having the formula $\text{C}_6\text{H}_{13}\text{N}$ had a peak in its IR spectrum at 3350cm^{-1} . Which of the following compounds is consistent with this?



3.6 For each of the following IR spectra, identify whether it is consistent with the structure of a ketone, an alcohol, a carboxylic acid, a primary amine, or a secondary amine. Explain your answer.



3.6 (Continued)

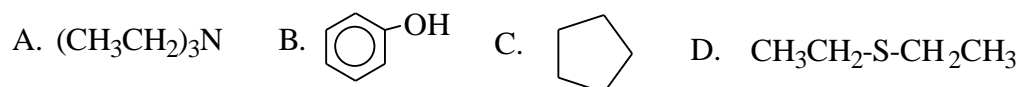


4.1 Draw all constitutional isomers of C_3H_9N and identify the functional group present in each one. Indicate 1° , 2° , and 3° if appropriate.

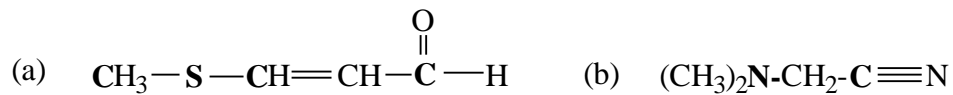
4.2 Which of the following compounds is most soluble in water? Which is most soluble in hexanes?

- (a) $CH_3CH_2NH_2$ (b) $CH_3(CH_2)_2\overset{O}{\parallel}C-OH$
- (c) $CH_3(CH_2)_3CH_3$ (d) $(C_2H_5)_2CHCH_2Br$

4.3 Which compound has the highest boiling point? Which has the lowest?



4.4 Provide hybridizations and approximate bond angles around the atoms that are in bold. You may need to add lone pairs to complete the octet.

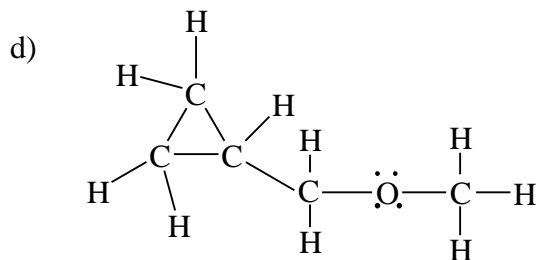
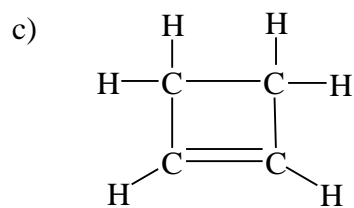
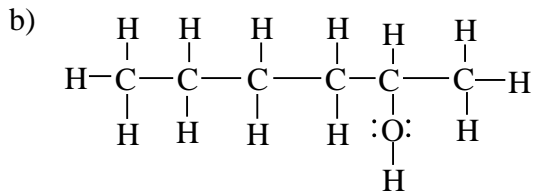
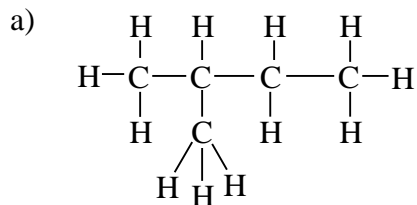


hybridization _____ _____ _____ _____ _____ _____

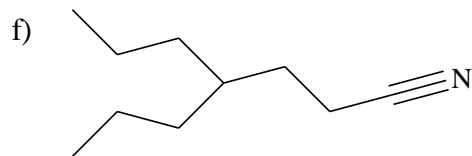
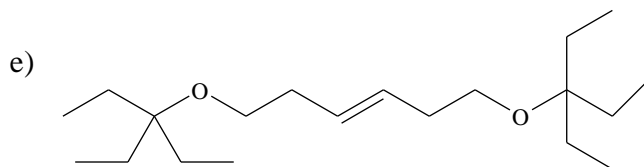
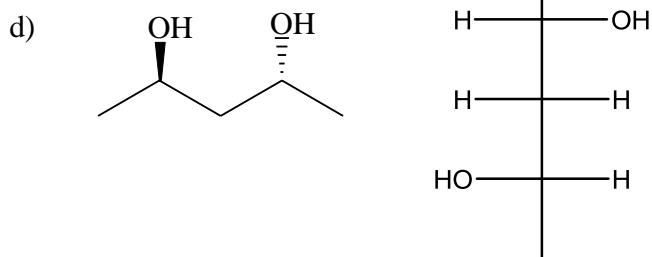
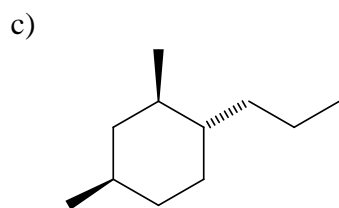
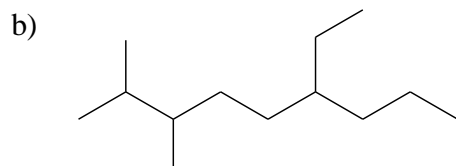
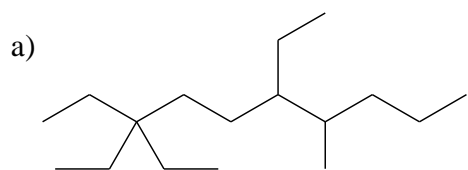
bond angle _____ _____ _____ _____ _____ _____

SOLUTIONS TO SAMPLE PROBLEMS:

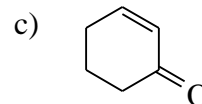
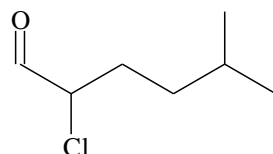
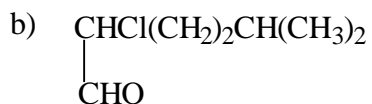
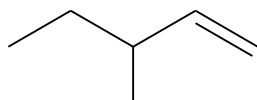
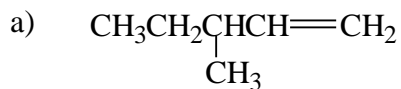
1.1 Draw complete structures:



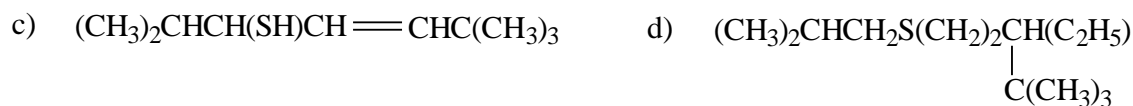
1.2 Draw a bond-line structure:



1.3



1.4 Condensed formula:

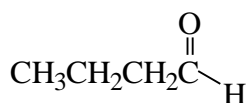
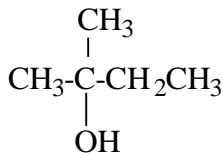


2.1 There are numerous other correct answers. These are just examples.

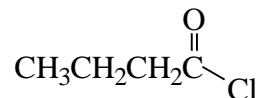
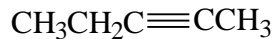
a) alkane b) ether c) 2° amine



d) 3° alcohol e) aldehyde f) 1° alkyl halide



g) thiol h) alkyne i) acyl chloride



2.2 a) alkene b) aromatic, carboxylic acid c) aromatic ring, ketone

d) amide e) 2° alcohol, alkyne f) ester

g) aromatic ring, anhydride h) thiol i) sulfide

3.1 a) Aldehyde, ketone, ester, anhydride b) Carboxylic acid c) alcohol

3.2 D

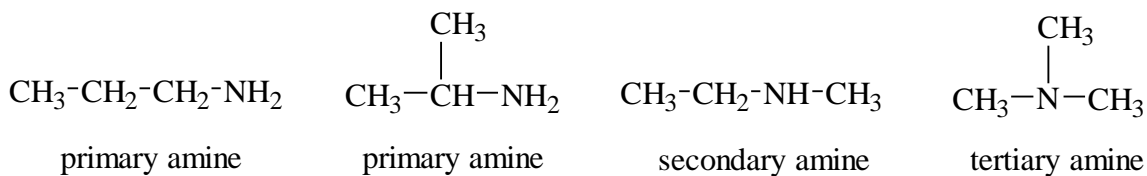
3.3 (a) no (b) no (c) yes (d) no (e) yes (f) yes (g) yes (h) no

3.4 (a) 3300-3600 cm^{-1} (OH) (b) 1600-1650 (C=C) (c) 3000-3100 (=C-H)

3.5 A

3.6 (a) primary amine (3500 cm^{-1}) (b) alcohol (broad band 3350 cm^{-1})
(c) ketone (C=O, near 1700 cm^{-1})

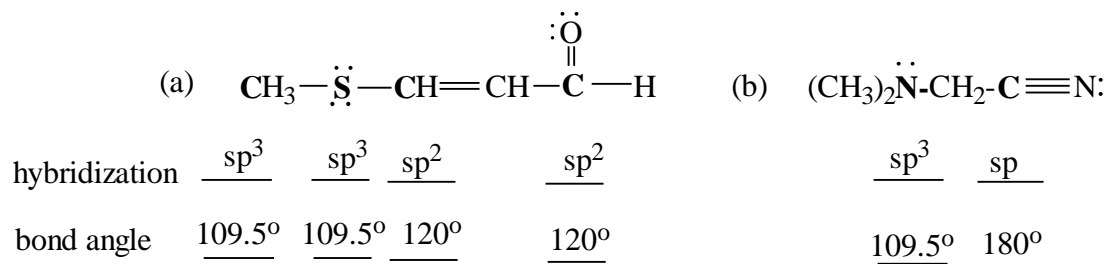
4.1



4.2 A is most soluble in water; C is most soluble in hexanes

4.3 B has the highest bp; C has the lowest bp

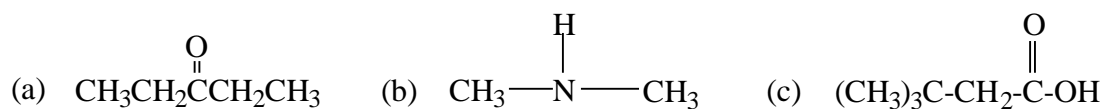
4.4



Name _____
Organic Chemistry 2210 DR

Second Drill Test (Sample A)
Answer All Questions

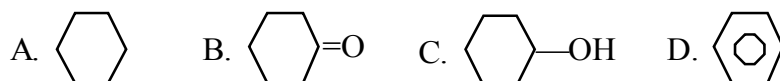
1. Name the functional group in each of the following compounds, indicating 1°, 2°, or 3° if appropriate.



2. Give specific examples (**do not use R**) for each of the following types of compounds.

a) 3° alcohol b) ester c) aldehyde d) sulfide

3. Which of these compounds has a peak in its IR spectrum nearest 3030 cm^{-1} ?



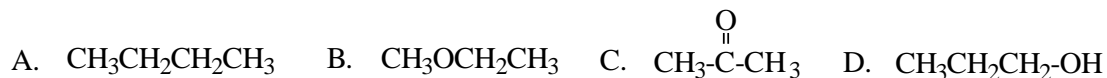
4. Which of the following functional groups does not show any absorption bands in the $3300\text{-}3500\text{ cm}^{-1}$ region of the infrared spectrum?

A. alcohols B. primary amines C. secondary amines D. tertiary amines

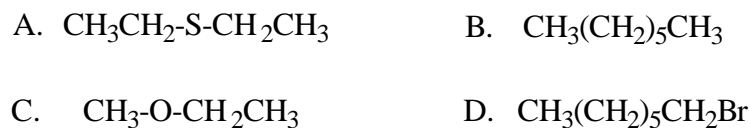
5. What IR frequencies would enable a chemist to distinguish between these?



6. Which of the following compounds has the highest boiling point?

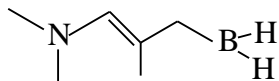


7. Which of the following compounds is most soluble in water? Which is most soluble in hexanes?

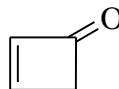


1. Draw structures as indicated.

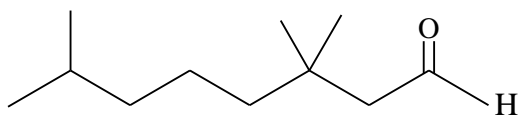
(a) Lewis structure of



(b) an isomer of



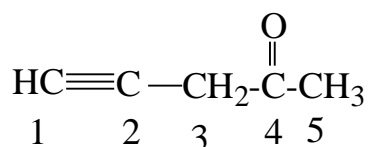
(c) condensed formula for



(d) a bond-line formula for



2. Consider the molecule below. Give:



(a) the hybridization of C2 _____

(b) the hybridization of C4 _____

(c) the O-C4-C5 bond angle _____

3. Draw the structure of an example (**do not use R**) of each of the following classes of compounds.

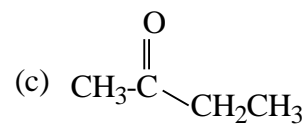
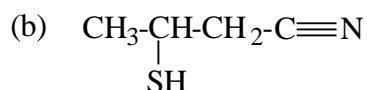
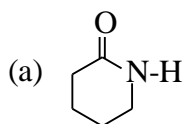
(a) 1° amine

(b) acyl chloride

(c) ether

(d) 2° alkyl bromide

4. Name the functional group or groups present in each of the following molecules. Indicate 1°, 2°, or 3° when appropriate.

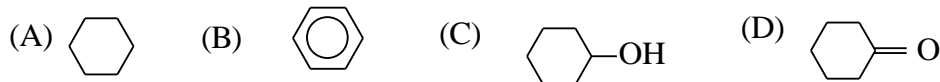


5. **Multiple Choice**

(1) An oxygen-containing compound which shows no IR absorption at $1630\text{-}1780\text{ cm}^{-1}$ or $3200\text{-}3500\text{ cm}^{-1}$ is likely to be what type of compound?

- (A) an amide (B) an alcohol (C) a ketone (D) an ether

(2) Which of these compounds has a peak in its IR spectrum at $1630\text{-}1780\text{ cm}^{-1}$?



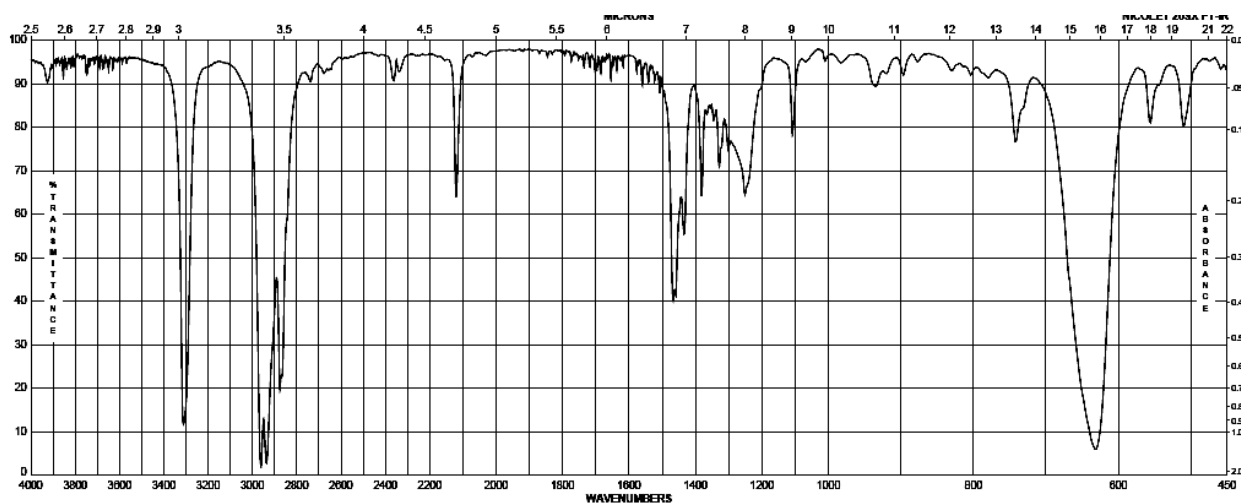
(3) Which of the following compounds has the highest boiling point?

- (A) $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (B) $\text{CH}_3\text{-}\overset{\text{O}}{\parallel}\text{C}\text{-CH}_3$
 (C) $\text{CH}_3\text{OCH}_2\text{CH}_3$ (D) $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$

(4) Which of the following compounds is **least soluble** in water?

- (A) $\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$ (C) $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{OH}$
 (B) $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$ (D) $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{Br}$

6. Indicate which of the four compounds below is responsible for the IR spectrum shown below. **Explain your answer.**



- (A) $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}\equiv\text{CCH}_3$ (B) $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$
 (C) $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH}$ (D) $\text{CH}_3\text{CH}_2\text{CH}_2\overset{\text{O}}{\parallel}\text{COH}$