

REPRESENTATIVE CARBON COMPOUNDS

A STUDENT WHO HAS MASTERED THE MATERIAL IN THIS SECTION SHOULD BE ABLE TO:

1. 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
Compounds containing halogens (with C and H)
 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
Compounds containing nitrogen: amines (1°, 2°, 3°), amides, nitriles
2. Classify hydrogens attached to sp³ carbons as 1°, 2°, or 3°.
3. From a structural diagram of a molecule, predict whether or not it will have a dipole moment, and predict the direction of the dipole moment of the molecule if it exists.
4. Predict relative physical properties (including melting point, boiling point, and solubility) of compounds, based on the strength of the intermolecular forces and surface area of the compounds. Intermolecular forces include:
 ionic
 hydrogen bonding
 dipole-dipole
 London (Van der Waals attractive)
5. Define, recognize, and give examples of Bronsted-Lowry and Lewis acids and bases, including conjugate acids and bases. Also, predict the products of acid-base reactions. For some comments on how to do this see the next page.
6. Identify functional groups present in molecules from infrared (IR) spectroscopy data, and predict features of the IR spectra of molecules from their structures. Important IR absorption frequencies to know include:
 O—H (alcohols, hydrogen bonded): 3200-3550 cm⁻¹, strong and broad
 N-H: 3300-3500 cm⁻¹, medium intensity
 O—H (carboxylic acids): 2500-3000 cm⁻¹, broad peaks of variable intensity
 C=O: 1630-1780 cm⁻¹, strong absorption
If you need to use other frequencies to identify other functional groups (and sometimes you will), a table of IR frequencies will be provided.

General Comments on Acid-Base Reactions

Acid-Base reactions take place between a stronger acid and a stronger base to produce a weaker acid and a weaker base.

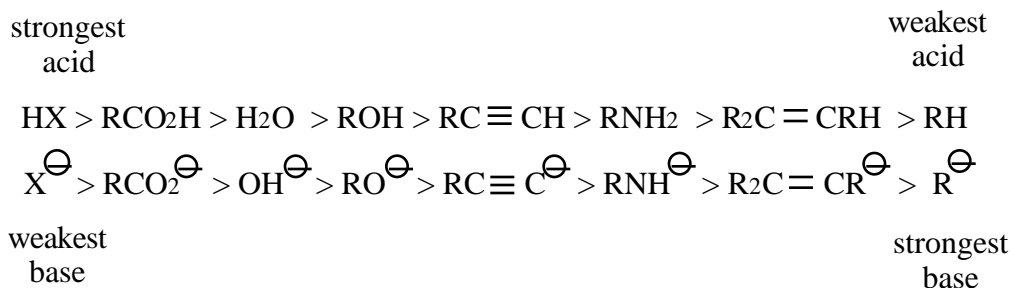
The newly formed acid is the conjugate acid of the starting base and the newly formed base is the conjugate base of the starting acid.

A conjugate acid is a stronger acid than the base it originated from and a conjugate base is a stronger base than the acid it originated from. For example, in the reaction



H_3O^+ is a conjugate acid of water, so it is a stronger acid than water, and Cl^- is a conjugate base of HCl , so it is a stronger base than HCl .

Stronger acids have weaker conjugate bases and stronger bases have weaker conjugate acids and vice versa. In this chart, HX indicates the strong mineral acids such as HCl , HBr , and HI .



Electron-withdrawing groups make acids stronger and electron-donating groups make bases stronger.

Acidity and basicity can be predicted from the periodic table.

For elements of the same group, the one that is further down in the periodic table forms stronger acids. This can be illustrated on the following example: H_2S is a stronger acid than H_2O (sulfur is in the third row and oxygen is in the second). PH_3 is a weaker base than NH_3 (phosphorus is in the third row and nitrogen is in the second).

For elements in the same row, the strongest acid is to the right and the strongest base is to the left. HF is a stronger acid than H_2O ; $^{\ominus}\text{CH}_3$ is a stronger base than $^{\ominus}\text{NH}_2$. Be careful, however; CH_4 is a weaker base than NH_3 because CH_4 has no pair of valence electrons.

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 =C-H & C=C first)
1050-1150	C-O	
690 and 750	phenyl group	Strong (look for =C-H & C=C first)

A STUDENT WHO HAS MASTERED THE OBJECTIVES ON THE PREVIOUS PAGE SHOULD BE ABLE TO SOLVE THE FOLLOWING PROBLEMS AND RELATED ONES:

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

a) alkane

b) ether

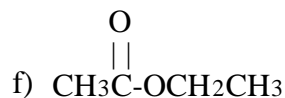
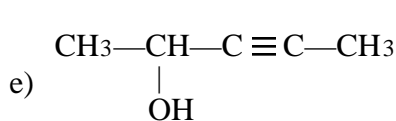
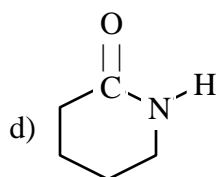
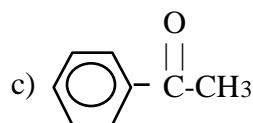
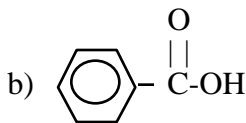
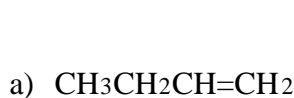
c) 2° amine

d) 3° alcohol

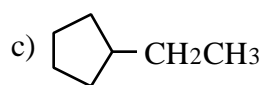
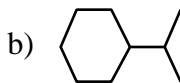
e) aldehyde

f) 1° alkyl halide

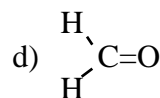
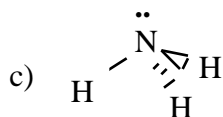
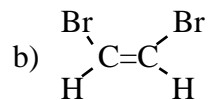
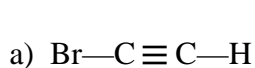
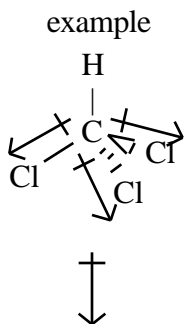
1.2 Name the functional group or groups present in each of the following molecules. Indicate 1°, 2°, or 3° when appropriate.



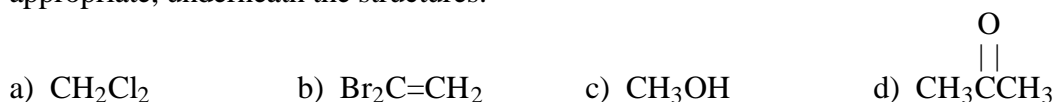
2.1 How many 1°, 2°, and 3° hydrogens are present in each of the following molecules?



3.1 Indicate directions of individual bond dipoles of the following compounds. Also indicate the directions of the overall dipoles, if appropriate, underneath the structures.



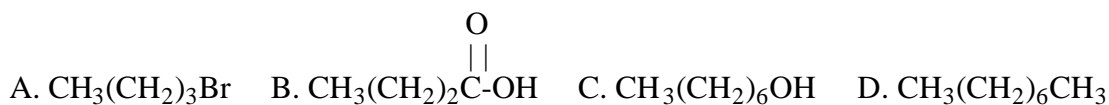
3.2 Draw the molecules in their approximate shapes, and indicate the overall dipoles, if appropriate, underneath the structures.



4.1 Which of these compounds has the highest boiling point? Which has the lowest?



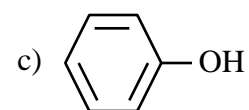
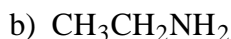
4.2 Which of the following compounds is most soluble in water? Which is the least soluble?



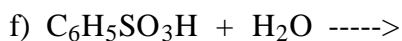
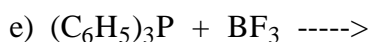
5.1 Give the conjugate acid and conjugate base of each of the following substances.

Conjugate Acid

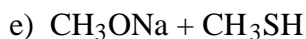
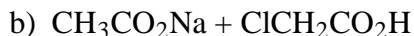
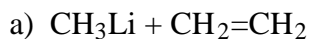
Conjugate Base



5.2 For each of the following reactions, identify which reactant is the acid and which is the base. Then give the product(s) of the reaction. It is useful to show unshared electron pairs.



5.3 For each of the following reactions, write the acid/base reaction product or indicate no reaction.



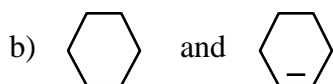
6.1 Based on the IR data given, what functional group(s) can be present in these compounds?

a) A strong absorption at 1710 cm^{-1} , no N in the molecular formula, no O-H peaks present

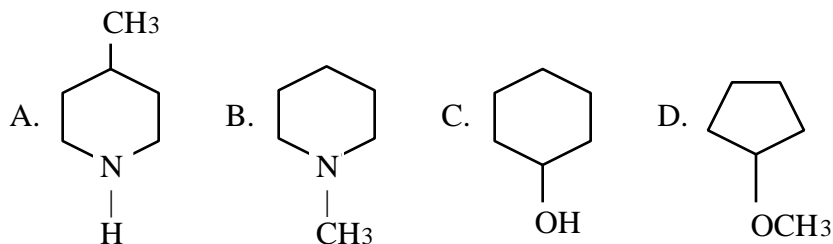
b) A strong absorption at 1720 cm^{-1} and a broad absorption between $2500\text{--}3000\text{ cm}^{-1}$.

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

a) $\text{CH}_3\text{CH}_2\text{OH}$ and $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$



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



6.4 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

ANSWERS TO THE SAMPLE PROBLEMS:

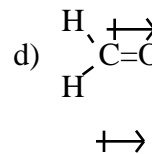
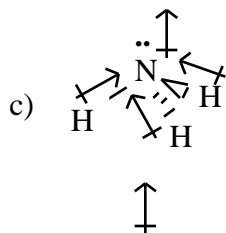
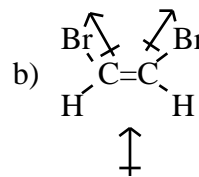
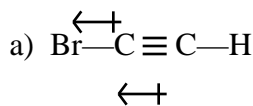
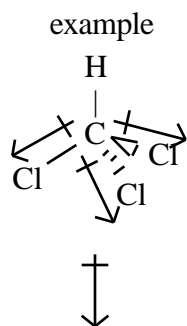
- 1.1 a) alkane $\text{CH}_3\text{CH}_2\text{CH}_3$
 b) ether $\text{CH}_3\text{-O-CH}_2\text{CH}_3$
 c) 2° amine $\text{CH}_3\text{-NH-CH}_2\text{CH}_3$
 d) 3° alcohol $\begin{array}{c} \text{OH} \\ | \\ \text{CH}_3\text{-C-CH}_2\text{CH}_3 \\ | \\ \text{CH}_3 \end{array}$
 e) aldehyde $\begin{array}{c} \text{O} \\ || \\ \text{CH}_3\text{CH}_2\text{CH}_2\text{C-H} \end{array}$
 f) 1° alkyl halide $\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$

Note: There are many compounds that are correct answers to Question 1.1. Their structures may be drawn as complete Lewis structures, as condensed structures (as above), or as bond-line formulas.

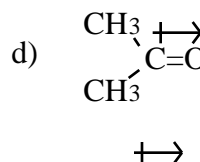
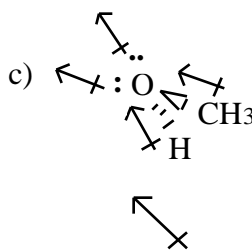
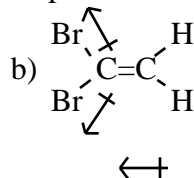
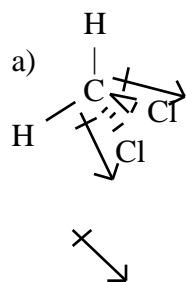
- 1.2 a) alkene b) carboxylic acid, aromatic ring c) ketone, aromatic ring d) amide
 e) 2° alcohol, alkyne f) ester

- 2.1 a) nine 1° H's, 2 2°, and 1 3°; b) 6 1°, 10 2°, and 2 3° H's; c) 3 1°, 10 2°, and 1 3° H

- 3.1 Bond dipoles and overall dipoles:

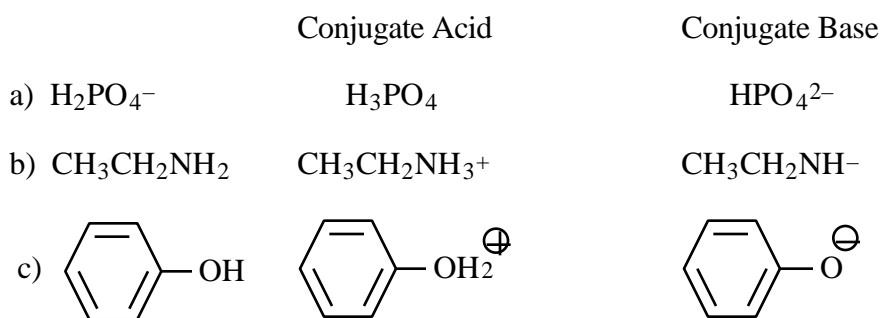


- 3.2 Shapes and overall dipoles:

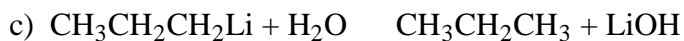
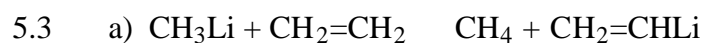
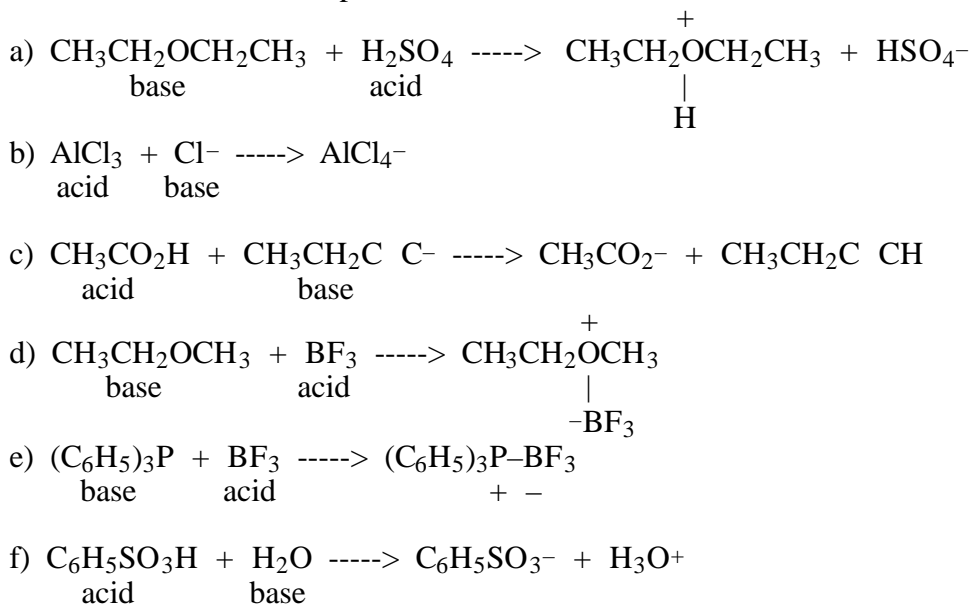


- 4.1 B has the highest boiling point, and A has the lowest.
 4.2 B is the most soluble in water, and D is the least soluble.

5.1 Conjugate acids and conjugate bases:

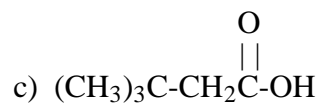
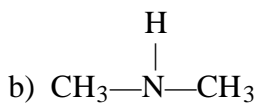
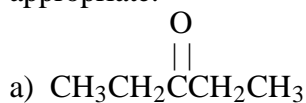


5.2 Acids, bases, and reaction products.



- | | | |
|-----|-------------------------------|--------------------|
| 6.1 | a) Ketone, aldehyde, or ester | b) Carboxylic acid |
| 6.2 | a) OH absorption | b) C=C absorption |
| 6.3 | A | |
| 6.4 | D | |

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



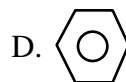
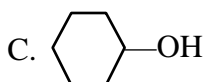
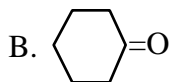
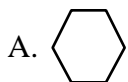
2. Give specific examples (don't use R) for each of the following types of compounds.

a) 3° alcohol

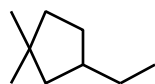
b) ester

c) aldehyde

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



4. Consider the following structure, and fill in the blanks.

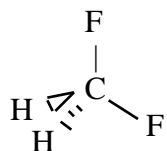


This compound contains: _____ 1° hydrogens

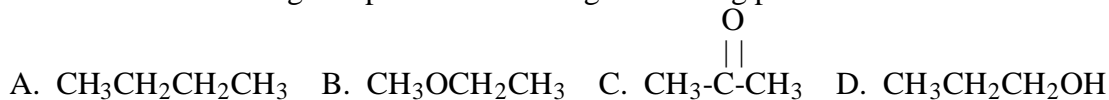
_____ 2° hydrogens

_____ 3° hydrogens

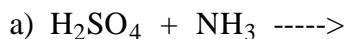
5. Indicate the direction of the dipole moment of the molecule shown.



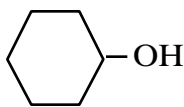
6. Which of the following compounds has the highest boiling point?


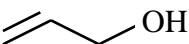
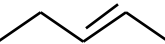
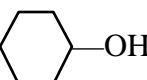


7. Predict the product of each of the following reactions. Hint: Show unshared electron pairs as needed.

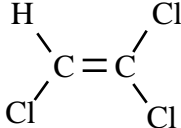


- Draw the structure of an example (do not use R) of each of the following classes of compounds.
 - ether
 - amide
 - 2° alkyl bromide

- What family does each of the compounds shown belong to? Be specific; indicate 1°, 2°, or 3° if appropriate.
 - 
 - $\text{CH}_3\text{CH}_2\overset{\text{O}}{\parallel}\text{C}-\text{OH}$
 - CH_3NHCH_3

- Which of the following compounds has absorptions in the 3400-3650 cm^{-1} and 1640-1680 cm^{-1} regions of the IR spectrum?
 - 
 - 
 - 
 - 

- Which of the compounds shown is the LEAST soluble in water?
 - NaCl
 - CH_3OH
 - $\text{CH}_3\overset{\text{O}}{\parallel}\text{CCH}_3$
 - $\text{CH}_3\text{CH}_2\text{CH}_3$

- Indicate the direction of the dipole moment of the molecule shown.
 

- Which of the following compounds has the highest boiling point?
 - $\text{CH}_3\overset{\text{O}}{\parallel}\text{C}-\text{OLi}$
 - $\text{CH}_3\overset{\text{O}}{\parallel}\text{CCH}_3$
 - $\text{CH}_3\overset{\text{O}}{\parallel}\text{C}-\text{OH}$
 - $\text{CH}_3\overset{\text{O-H}}{\mid}\text{CHCH}_3$

- Which of these molecules has the largest dipole moment?
 - H-C C-H
 - Br-C C-Br
 - H-C C-Br

- What is the strongest type of intermolecular force present in a pure sample of $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$?