Chem 31 Class Packet

Periodic Table of Elements

1 H 1.00794																	2 He 4.00260
3 Li 6.941	4 Be 9.01218											5 B 10.811	6 C 12.011	7 N 14.0067	8 O 15.9994	9 F 18.99840	10 Ne 20.1797
11 Na 22.98977	12 Mg 24.305											13 Al 26.98154	14 Si 28.0855	15 P 30.97376	16 S 32.066	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	21 Sc 44.9559	22 Ti 47.88	23 V 50.9415	24 Cr 51.9961	25 Mn 54.9380	26 Fe 55.847	27 Co 58.9332	28 Ni 58.6934	29 Cu 63.546	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.9216	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.4678	38 Sr 87.62	39 Y 88.9059	40 Zr 91.224	41 Nb 92.9064	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.9055	46 Pd 106.42	47 Ag 107.8682	48 Cd 112.411	49 In 114.82	50 Sn 118.710	51 Sb 121.757	52 Te 127.60	53 I 126.9045	54 Xe 131.29
55 Cs 132.9054	56 Ba 137.327	57 La* 138.9055	72 Hf 178.49	73 Ta 180.9479	74 W 183.85	75 Re 186.207	76 Os 190.2	77 Ir 192.22	78 Pt 195.08	79 Au 196.9665	80 Hg 200.59	81 Tl 204.3833	82 Pb 207.2	83 Bi 208.9804	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra 226.0254	89 Ac† 227.0278	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (268)	110 (269)	111 (272)	112 (277)		114 (285)		116 (289)		118 (293)

*Lanthanide Series	58 Ce 140.115	59 Pr 140.9077	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.965	64 Gd 157.25	65 Tb 158.9254	66 Dy 162.5	67 Ho 164.9303	68 Er 167.26	69 Tm 168.9342	70 Yb 173.04	71 Lu 174.967
†Actinide Series	90 Th 232.0381	91 Pa 231.0359	92 U 238.0289	93 Np 237.048	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)

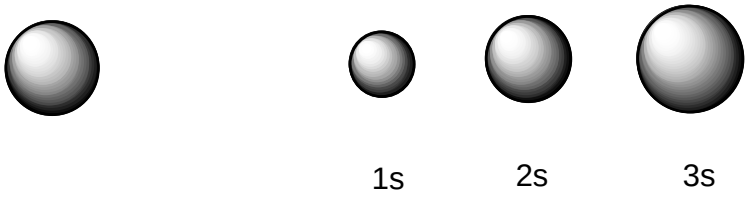
Organic Chemist's View of the Periodic Table of Elements

1 H 1.00794																6 C 12.011
3 Li 6.941	6 C 12.011											5 B 10.811	6 C 12.011	7 N 14.0067	8 O 15.9994	9 F 18.99840	6 C 12.011
11 Na 22.98977	12 Mg 24.305											13 Al 26.98154	14 Si 28.0855	15 P 30.97376	16 S 32.066	17 Cl 35.4527	6 C 12.011
19 K 39.0983	20 Ca 40.078	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	35 Br 79.904	6 C 12.011
6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	53 I 126.9045	6 C 12.011
6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011
6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	110 (269)	111 (272)	112 (277)		114 (285)		116 (289)		118 (293)

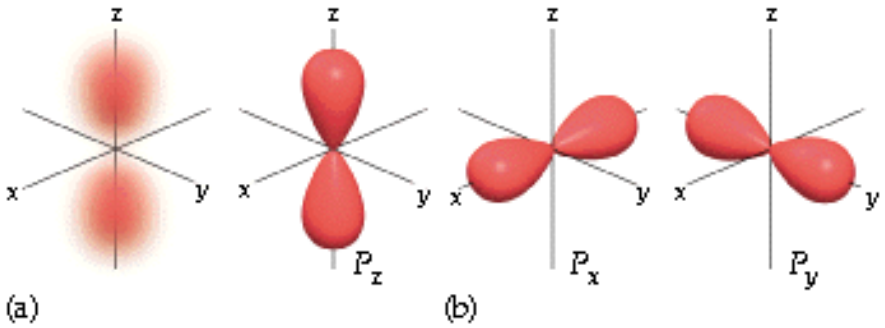
*Lanthanide Series	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011
†Actinide Series	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011	6 C 12.011

Orbital Shapes and Size

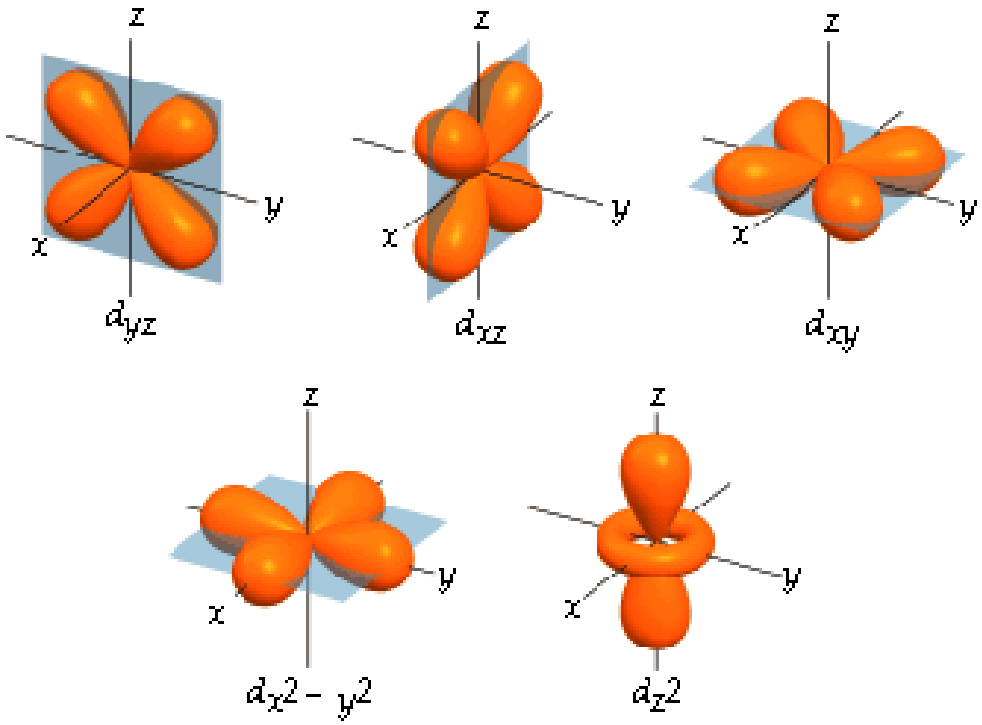
s orbitals



p orbitals



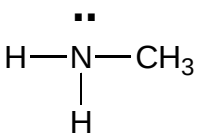
d orbitals



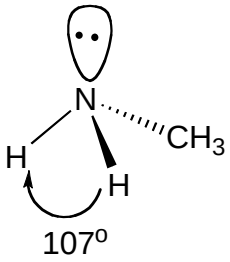
Hybridization:

Nitrogen:

H_2NCH_3



Tetrahedron
Pyramidal
(or Trigonal Pyramidal)



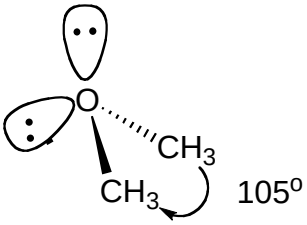
Methyl Amine

3 atoms bonded to nitrogen
plus lone pair: Need 4 orbitals $\xrightarrow{H}$ **sp^3**

Oxygen:

H_3COCH_3

Tetrahedron
Angular or
Bent



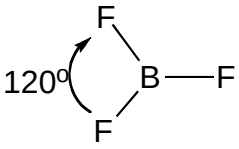
Dimethyl Ether

2 atoms bound to oxygen
plus 2 lone pairs. Need 4 orbitals $\xrightarrow{H}$ **sp^3**

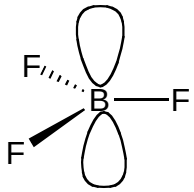
Boron:

Trigonal Planar

BF_3



Boron Trifluoride

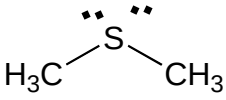


side view

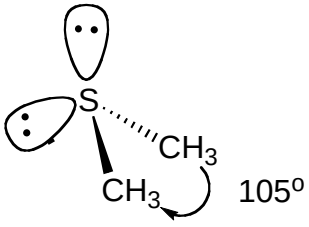
3 valence electrons
Can only form 3 bonds.
Need 3 orbitals $\xrightarrow{H}$ **sp^2**

Sulfur:

H_3CSCH_3



Tetrahedron
Angular

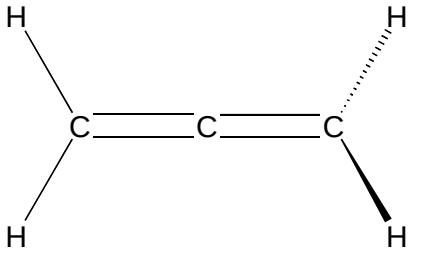


Dimethyl Sulfide

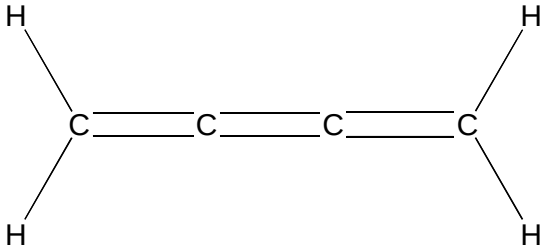
6 valence electrons- 2 lone pairs
Can only form 2 bonds, plus 2 lone pairs
Need 4 orbitals $\xrightarrow{H}$ **sp^3**

Orbital Picture Drawing Practice

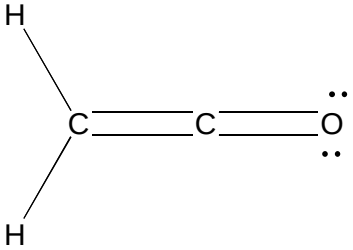
For the following compounds, draw an orbital picture showing the s-bonds and lines and the p-bonds as overlapping p-orbitals. Are the H's in allene and cumulene coplanar? Are the H's and the nonbonding electrons on oxygen in ketene coplanar?



Allene

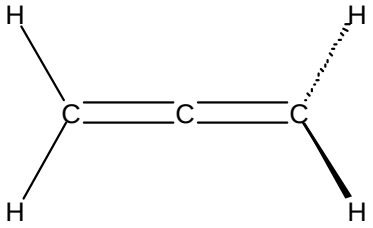


Cumulene



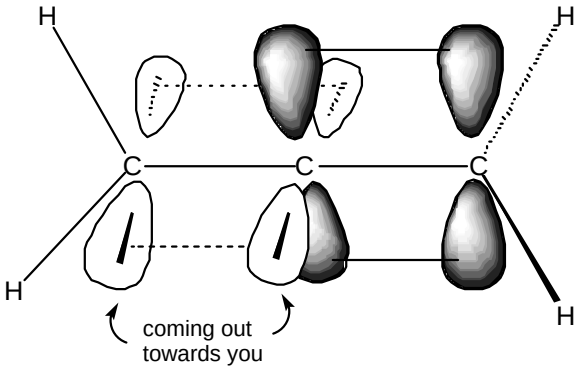
Ketene

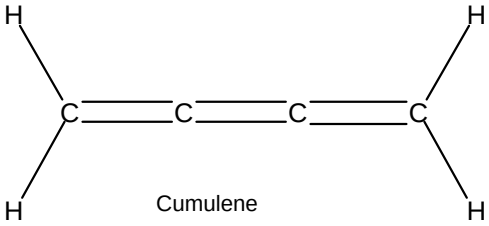
Orbital Picture Answers:



Allene

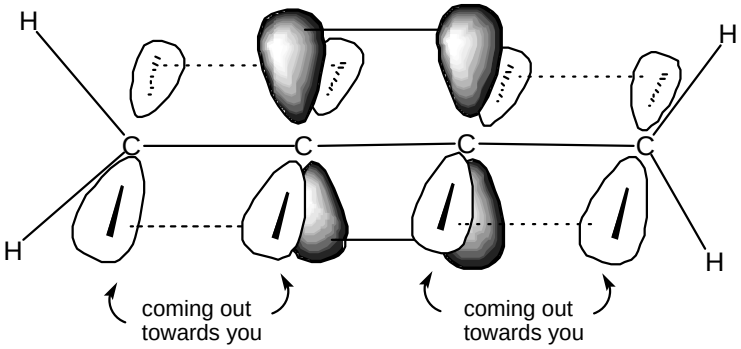
H's are not coplanar

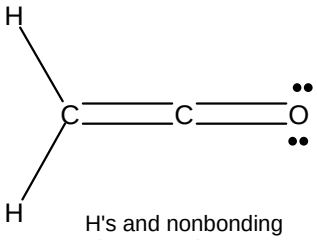




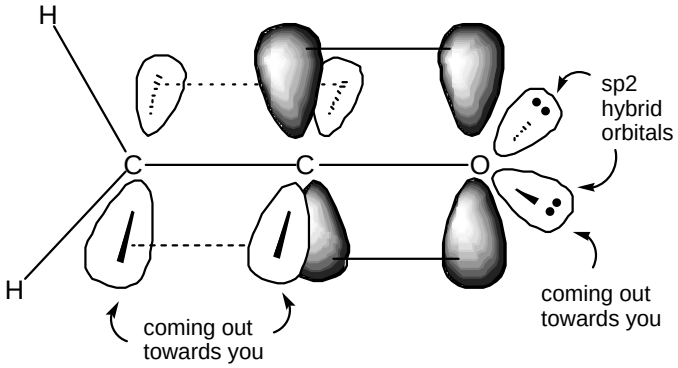
Cumulene

H's coplanar





H's and nonbonding electron pair are not coplanar



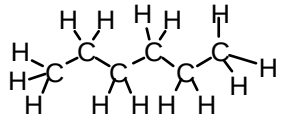
Skeletal Drawings in Organic Chemistry

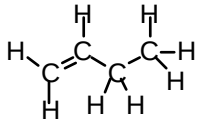
Rules:

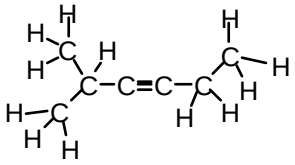
1. Carbon atoms are represented by the ends of lines or the junctions between lines without using the chemical symbol, C. The lines represent the bonds between carbon atoms.
2. Hydrogen atoms attached to carbon atoms are not shown explicitly. Sufficient hydrogen atoms are assumed to be attached to the carbons so that each carbon has four bonds. Be sure to count the correct number of bonds - double bonds count as two bonds and triple bonds count as three bonds.
3. All other types of atoms (e.g. O, S, N, Cl) are shown explicitly.
4. Hydrogens attached to atoms other than carbon are always shown explicitly.
5. Nonbonding electron pairs on atoms are not typically shown. Sufficient nonbonding pairs are assumed so that each atom has a full outer shell of 8 electrons.

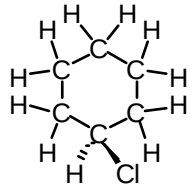
Note- at times carbon atoms, assumed hydrogens and nonbonding electron pairs will be shown for emphasis.

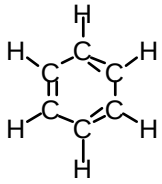
Examples and Practice – Convert the following Lewis structures to skeletal drawings and convert the following skeletal drawings to complete Lewis structures.

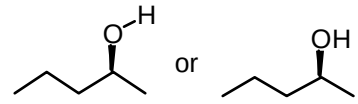


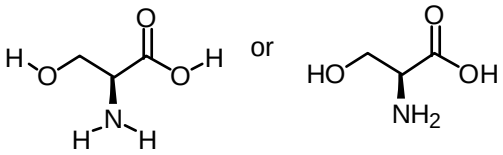









O
H
or
OH


O
H
O
O
H
N
H
H
or
O
HO
OH
NH2

Skeletal Drawings in Organic Chemistry

Rules:

1. Carbon atoms are represented by the ends of lines or the junctions between lines without using the chemical symbol, C. The lines represent the bonds between carbon atoms.
2. Hydrogen atoms attached to carbon atoms are not shown explicitly. Sufficient hydrogen atoms are assumed to be attached to the carbons so that each carbon has four bonds. Be sure to count the correct number of bonds - double bonds count as two bonds and triple bonds count as three bonds.
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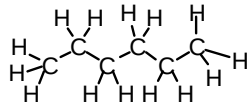
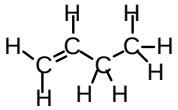
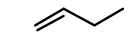
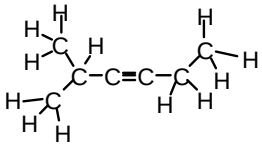
Note- at times carbon atoms, assumed hydrogens and nonbonding electron pairs will be shown for emphasis.

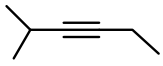
Example and Practice – Convert the following Lewis structures to skeletal drawings and convert the following skeletal drawings to complete Lewis structures.

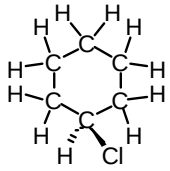


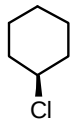


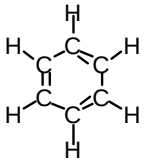


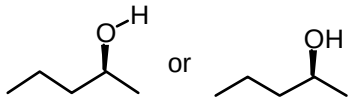


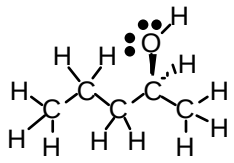


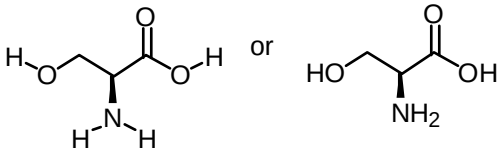


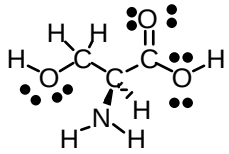





O
H
or
OH


H
O
H
H
H
C
C
C
C
H
H
H
H
H
H
H
H
H


O
H
O
O
H
N
H
H
or
O
HO
OH
NH2


O
H
H
H
O
C
C
O
H
C
H
N
H
H

Drawing Lewis Structures

1. Sum the valence electrons from all atoms.

(Use the periodic table as necessary to help you determine the number of valence electrons each atom.) For an anion, add an electron for each negative charge. For a cation, subtract an electron for each positive charge. Don't worry about keeping track of which electrons come from which atoms. Only the total number is important.

2. Write the symbols for the atoms to show which atoms are attached to which, and connect them with a single bond (a dash, representing two electrons). Chemical formulas are often written in the order in which the atoms are connected in the molecule or ion, as in HCN. When a central atom has a group of other atoms bonded to it, the central atom is usually written first, as in CO_3^{2-} and SF_4. In other cases, you may need more information before you can draw the Lewis structure.

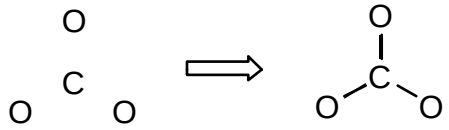
3. Complete the octets of the atoms bonded to the central atom. (Remember, however, that hydrogen can have only two electrons.)

4. Place any leftover electrons on the central atom, even if doing so results in more than an octet.

5. If there are not enough electrons to give the central atom an octet, try multiple bonds. Use one or more of the unshared pairs of electrons on the atoms bonded of the central atom to form double or triple bonds.

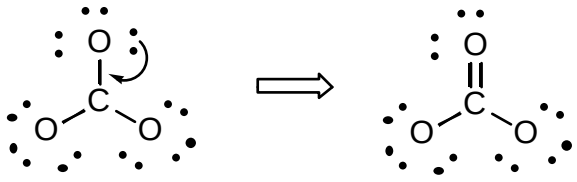
Example: CO_3^{-2}

1. Total valence electrons = 4 + 3 x 6 + 2 = 24 electrons
   (H) (O) (Charge)
2. Place the atoms in order of attachment, and
3. Place a bond (using a line) between attached atoms. Each bond accounts for two electrons.



4. Fill in remaining electrons on the peripheral atoms first to achieve and octet for those atoms. Do not put electrons on hydrogen atoms. Any leftover electrons go on the central atom.

   24 – 6 bonding electrons = 18 electrons on perpheral atoms.



5. Check for octets on all atoms. If central atom does not have an octet, "move" electrons from peripheral atoms "in" creating multiple bonds to the central atom. Do this until octet on central atom is achieved.

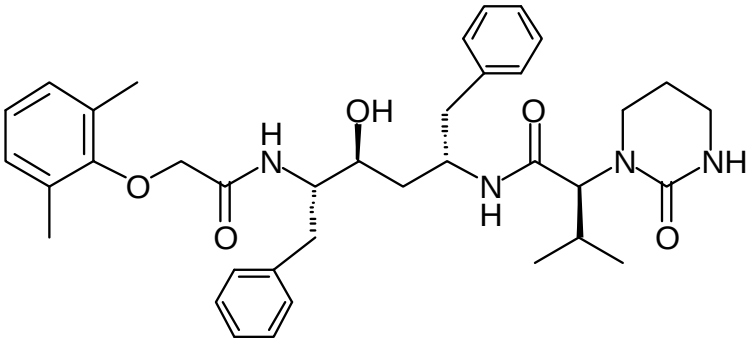
   Oxygens have octet, carbon has only 6 electrons. Move one pair in, gives carbon octet See picture above.

Electronegativity of the Elements

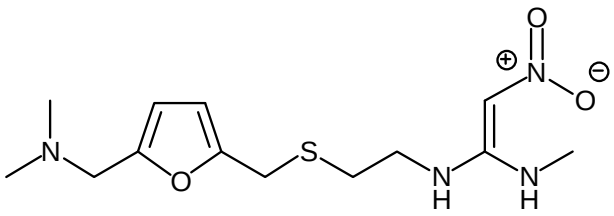
1 H 1.00794																	2 He 4.00260
3 Li 6.941	4 Be 9.01218											5 B 10.811	6 C 12.011	7 N 14.0067	8 O 15.9994	9 F 18.99840	10 Ne 20.1797
11 Na 22.98977	12 Mg 24.305											13 Al 26.98154	14 Si 28.0855	15 P 30.97376	16 S 32.066	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	21 Sc 44.9559	22 Ti 47.88	23 V 50.9415	24 Cr 51.9961	25 Mn 54.9380	26 Fe 55.847	27 Co 58.9332	28 Ni 58.6934	29 Cu 63.546	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.9216	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.4678	38 Sr 87.62	39 Y 88.9059	40 Zr 91.224	41 Nb 92.9064	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.9055	46 Pd 106.42	47 Ag 107.8682	48 Cd 112.411	49 In 114.82	50 Sn 118.710	51 Sb 121.757	52 Te 127.60	53 I 126.9045	54 Xe 131.29
55 Cs 132.9054	56 Ba 137.327	57 La* 138.9055	72 Hf 178.49	73 Ta 180.9479	74 W 183.85	75 Re 186.207	76 Os 190.2	77 Ir 192.22	78 Pt 195.08	79 Au 196.9665	80 Hg 200.59	81 Tl 204.3833	82 Pb 207.2	83 Bi 208.9804	84 Po (209)	85 At (210)	86 Rn (222)

Structures of Some Common Pharmaceuticals

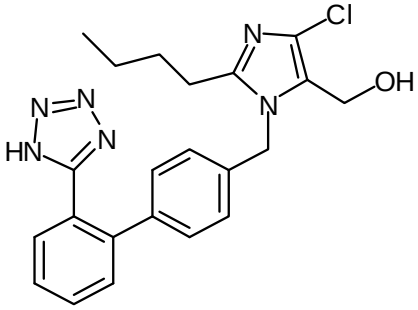
Fill in the correct number of H's and nonbonding electrons for each structure below. Assume zero charge unless a charge is given.



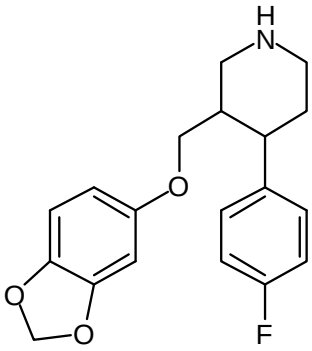
Lopinavir
HIV Protease Inhibitor



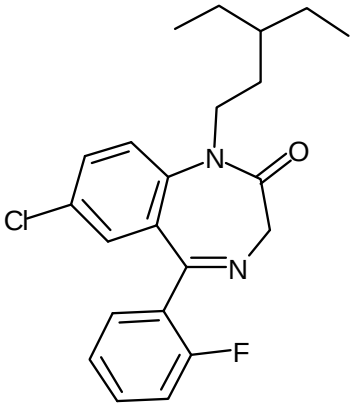
Zantac -Ulcer medication



Losartan
Angiotensin II Antagonist



Paxil
Antidepresant



Flurazepam
Treatment for Sleep Disorders

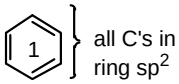
Key:

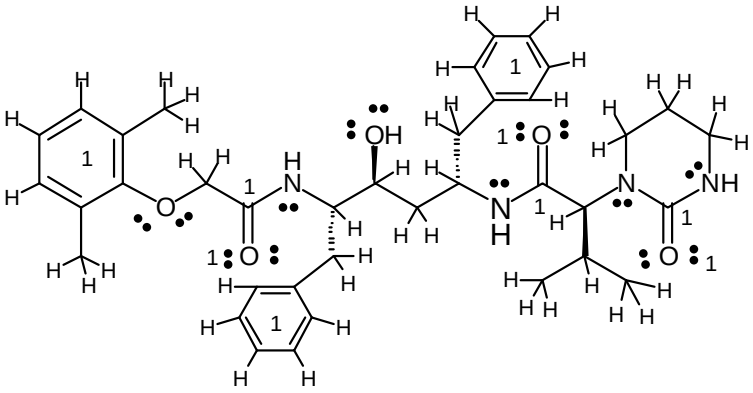
Structures of Some Common Pharmaceuticals

Fill in the correct number of H's and nonbonding electrons for each structure below. Assume zero charge unless a charge is given.

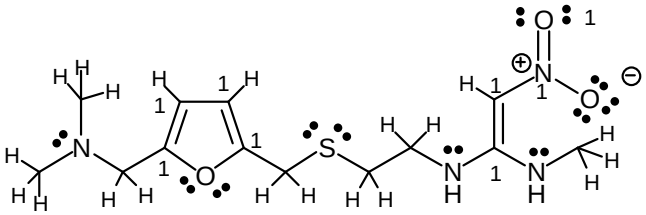
Hybridization:
1 - sp^2
all other sp^3

there are no sp C's

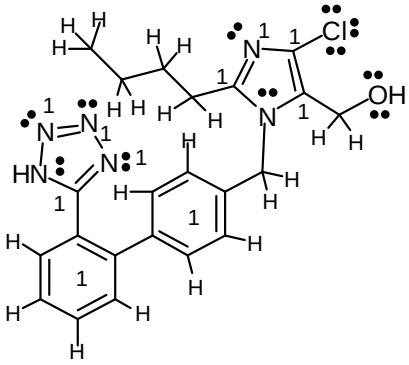




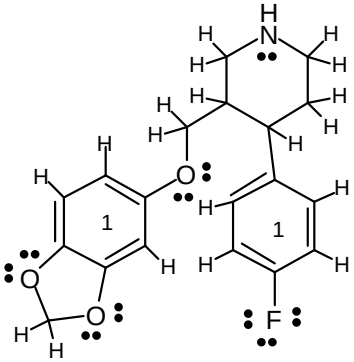
Lopinavir
HIV Protease Inhibitor



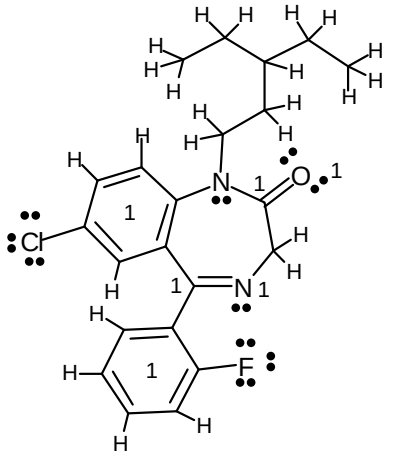
Zantac -Ulcer medication



Losartan
Angiotensin II Antagonist



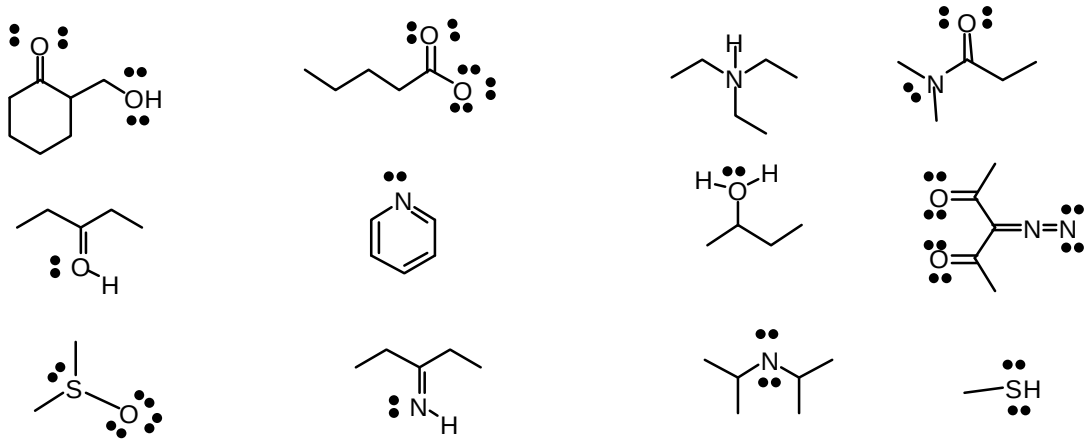
Paxil
Antidepresant



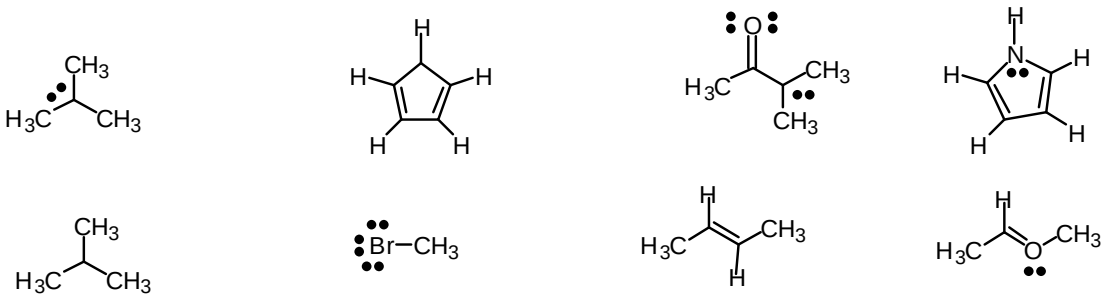
Flurazepam
Treatment for Sleep Disorders

Formal Charge Practice:

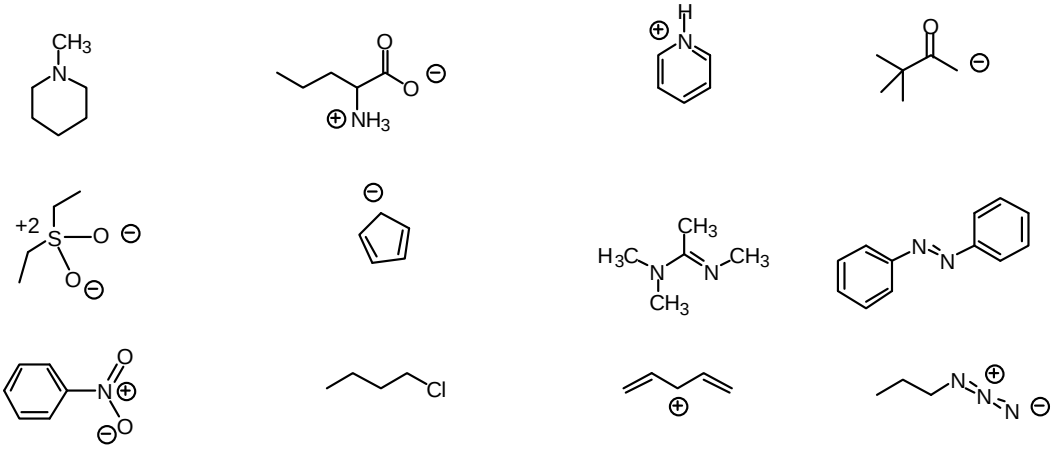
1. For the following compounds, determine the formal charge for all the heteroatoms (O, N and S). All nonbonding electrons are shown. For carbon atoms, assume zero charge and fill in the correct number of assumed hydrogens. Note: there are no assumed electrons on carbon, they have to be explicitly shown with nonbonding electrons and/or with a charge notation.



2. For the following compounds, determine the charge for all the atoms. All assumed hydrogens and nonbonding electrons are shown.



3. For the following compounds, all charges are shown as they might typically be in texts or the chemical literature. Add to these structures the correct number of assumed nonbonding electrons and hydrogens *consistent with the formal charges as shown*. Recall from the drawing conventions, hydrogens are always shown on heteroatoms (O, N and S) so only hydrogens on carbons are assumed and need to be added to the structure below. As always, assume zero charge unless a charge is shown.



Formal Charge Practice: Key

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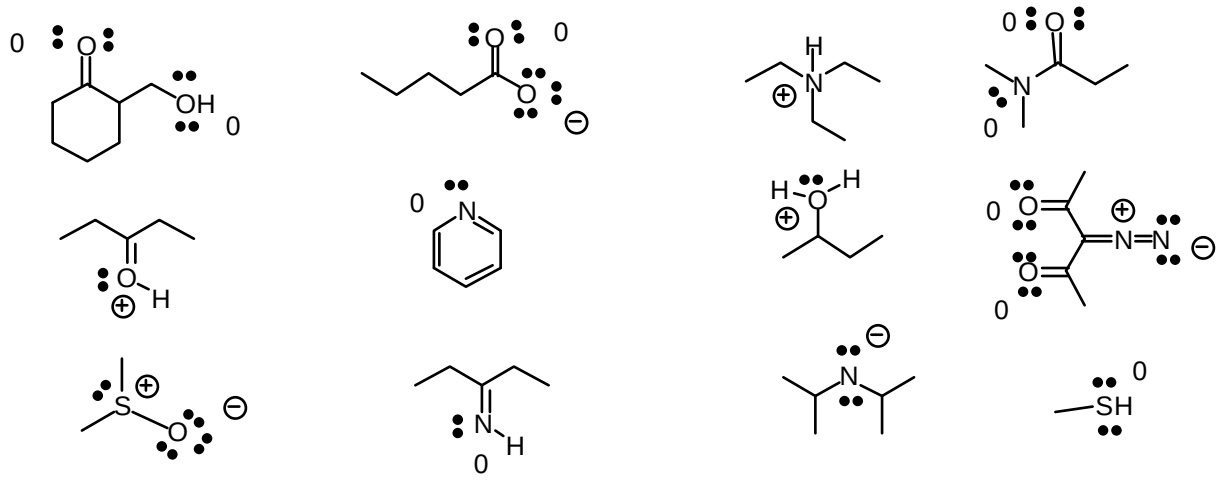
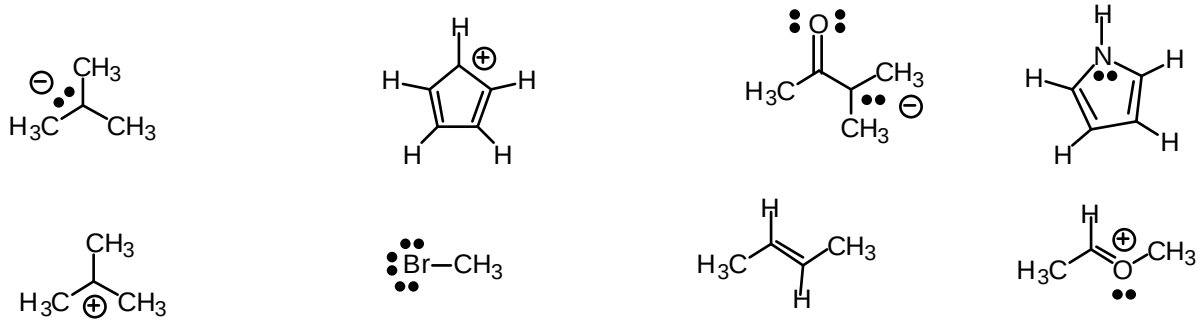


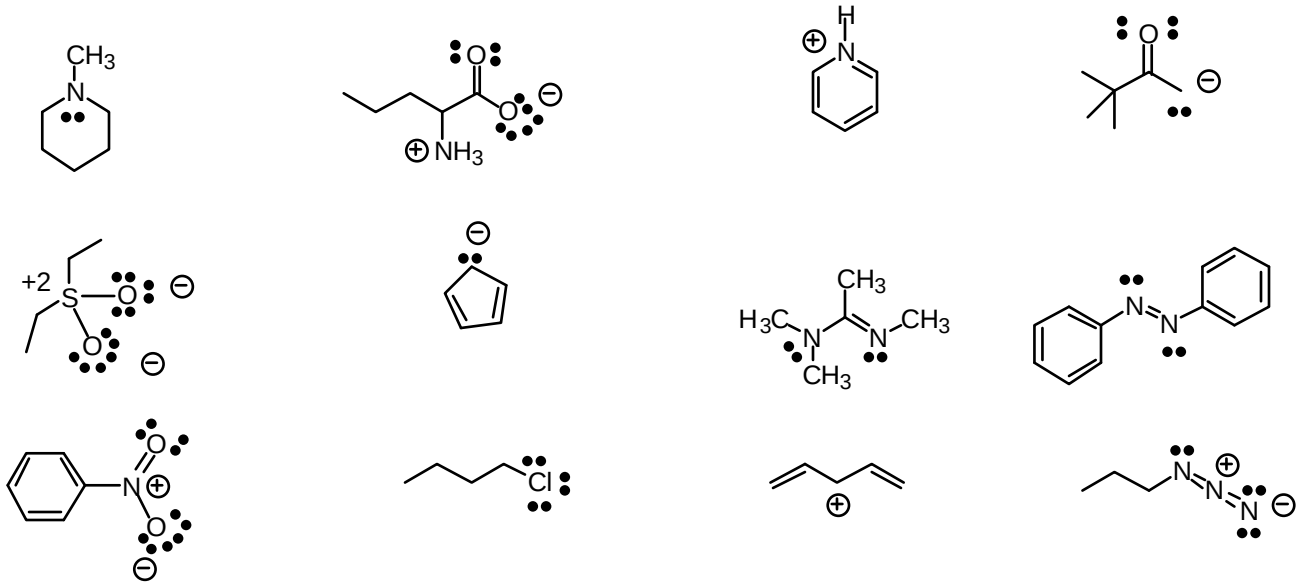
all carbons zero charge-i did not fill in H's since it would be too much in this graphic
if you have questions concerning number of Hs, email me or come see me in office hours

2. For the following compounds, determine the charge for all the atoms. All assumed hydrogens and nonbonding electrons are shown.



all other atoms that no charge is shown- zero charge

3. For the following compounds, all charges are shown as they might typically be in texts or the chemical literature. Add to these structures the correct number of assumed nonbonding electrons and hydrogens *consistent with the formal charges as shown*. Recall from the drawing conventions, hydrogens are always shown on heteroatoms (O, N and S) so only hydrogens on carbons are assumed and need to be added to the structure below. As always, assume zero charge unless a charge is shown.



electrons are filled in to meet the charge given. cation on carbon has three bonds no e-pairs; anion on carbon has three bond 1 e-pair. again all other atoms that no charge is shown- zero charge, go back and confirm that for each atom and recognize the assumed Hs and e-pairs

Resonance Form Rules:

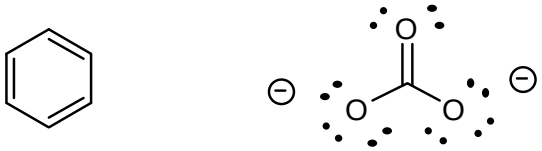
1. Resonance forms differ only in the location of pi bonding electrons and non-bonding electrons. No atoms change position.

A common error in drawing resonance structures is to disregard hydrogen atoms- Draw in H's so you do not move any atoms in the process of drawing resonance structures.

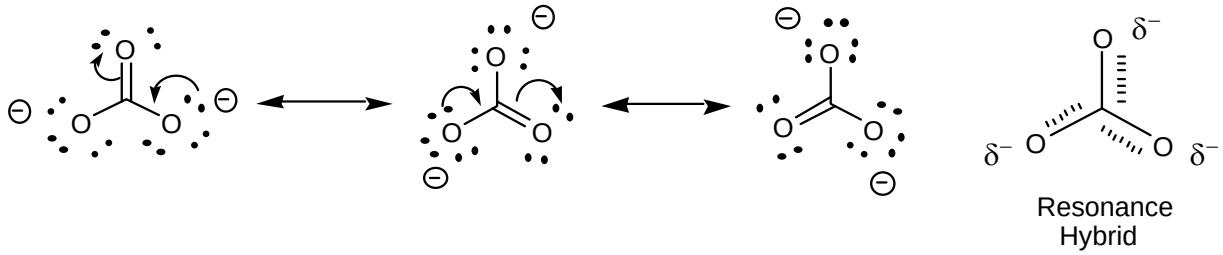
2. Resonance forms are localized "versions" of the major contributing structures to the "actual" structure. You can think of the actual structure as an average between the two or more resonance structures. A resonance hybrid is a useful way of depicting a molecule with many resonance forms.
3. Resonance forms do not have to be equivalent. The more stable resonance form will be the larger contributor to the resonance hybrid.
4. Rules of valency must be followed - do not exceed normal valency to draw extra resonance structures. Never more than 8 electrons around an atom, although you can have less than 8.
5. Resonance and the opportunity for resonance results in overall stabilization for the molecule - "Resonance Stabilization". This information is extremely useful in predicting a molecules reactivity.

<u>Resonance Forms</u>: Drawing and Interpreting

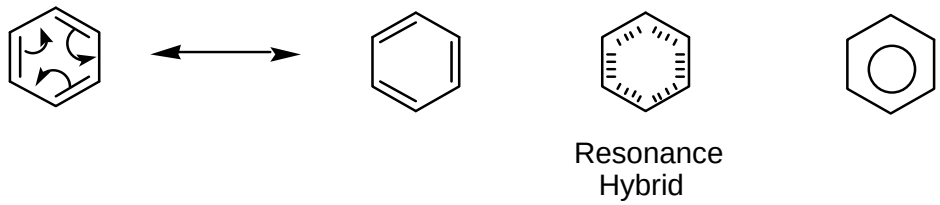
Resonance is a valuable tool to explain and predict a molecules behavior and the results of chemical reactions. For example: How might one explain that for benzene and carbonate the interatomic distances are all the same?



There are three possible resonance forms of carbonate - no one resonance form is more stable than any others; all the oxygens share the negative charge equally, as demonstrated by the resonance hybrid.

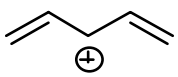


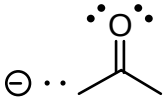
The benzene ring has two contributing resonance structures, which contribute equally to the resonance hybrid. In fact, you will often see the benzene ring depicted as a resonance hybrid using the shorthand notation of a circle in the center of the ring. (Although we will not use this notation!)

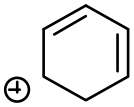


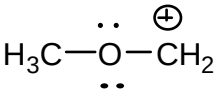
Resonance Practice Problems

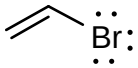
1. Draw the important resonance structures for each of the following molecules.

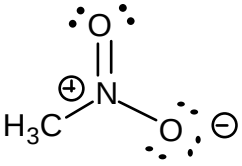


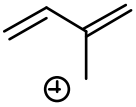


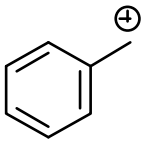


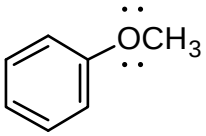


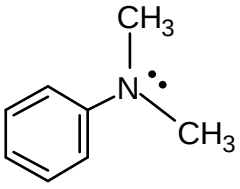


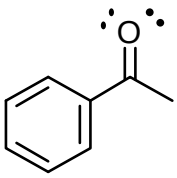


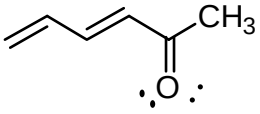






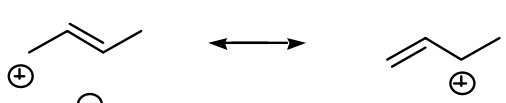




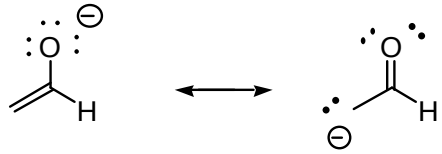


2. Draw the Resonance Hybrid (using dashed bond as partial bonds and partial charges) for the following resonance structures.

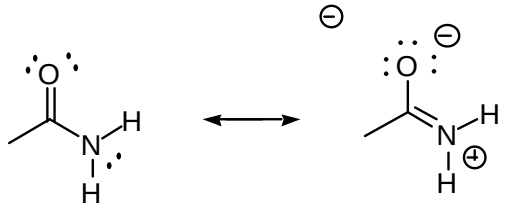
a.



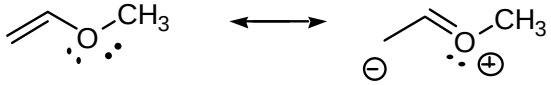
b.



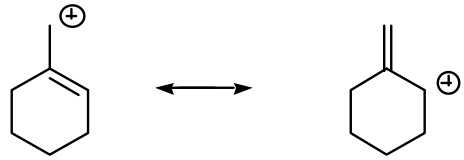
c.



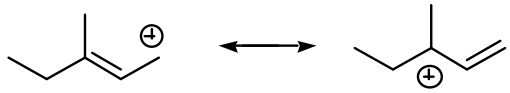
d.



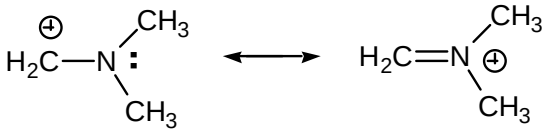
e.



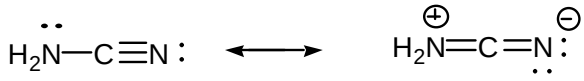
f.



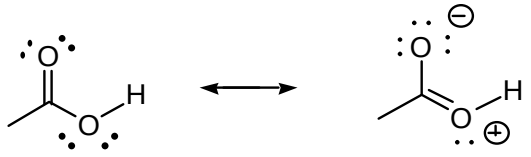
g.



h.

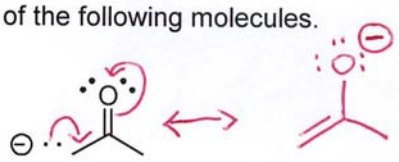


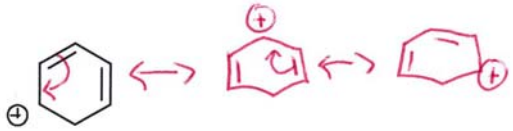
i.

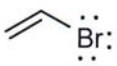


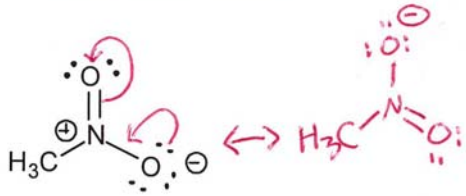
Resonance Practice Problems

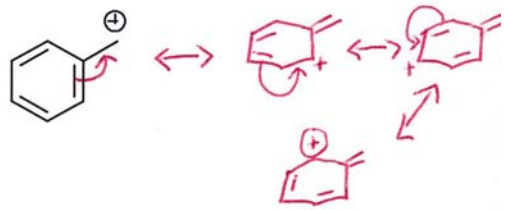
1. Draw the important resonance structures for each of the following molecules.

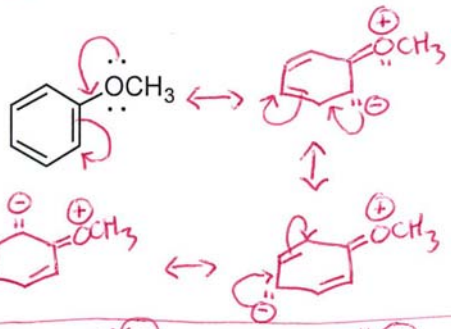


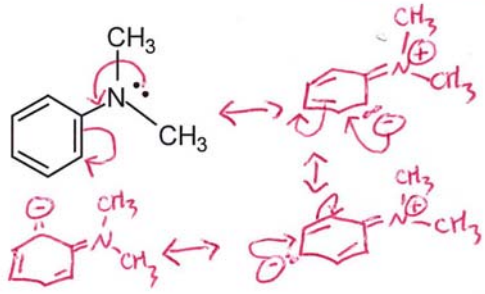


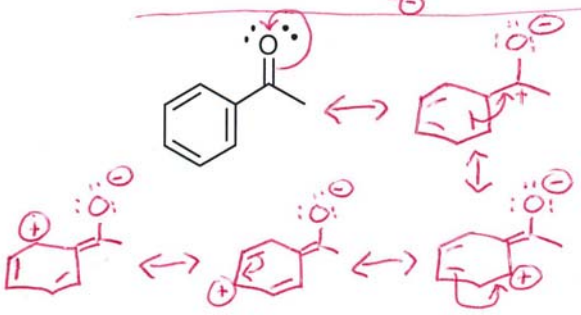






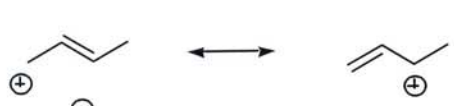




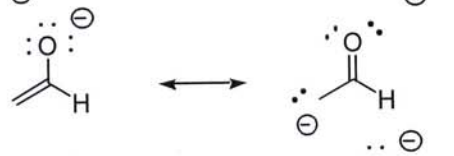


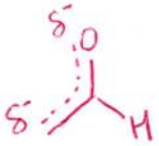
2. Draw the Resonance Hybrid (using dashed bond as partial bonds and partial charges) for the following resonance structures.

a.

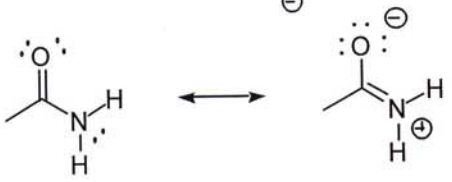


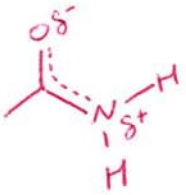
b.





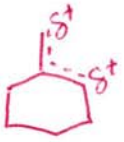
c.





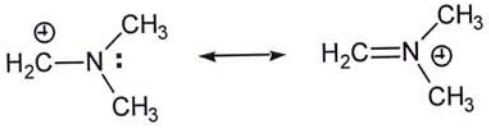
d.

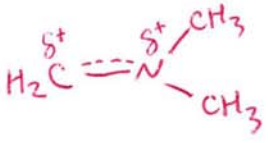
e.



f.

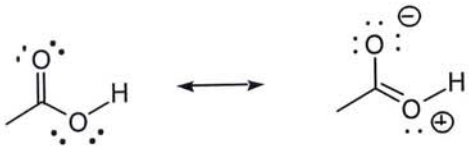
g.

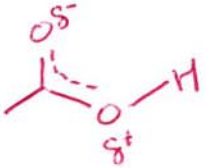




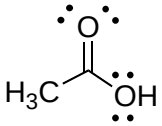
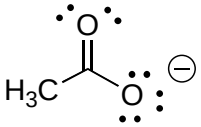
h.

i.





pKa Table: Acidity and Basicity

	Acid	pKa	Conjugate Base	
Weak Acid	CH_4	49	$\ominus :CH_3$	**Strong Base**
	NH_3	36	$\ominus :NH_2$	
	$H-C\equiv C-H$	25	$H-C\equiv C:^{\ominus}$	
	H_3C-OH	16	$H_3C-O:^{\ominus}$	
	$H_2O:$	15.7	$\ominus :OH$	
	$^{\oplus}NH_4$	9.2	NH_3	
		4.8		
	H-F:	3.2	:F: $^{\ominus}$	
	$H_3O^{\oplus}$	-1.7	H_2O	
Strong Acid	H-Cl:	-7.0	:Cl: $^{\ominus}$	**Weak Base**

pKa Table: Acidity and Basicity

	Acid	pKa	Conjugate Base	
Weak Acid	CH_4	49	$^{\ominus}:CH_3$	Strong Base
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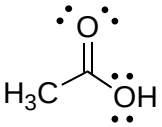
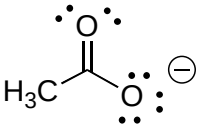
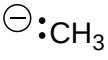
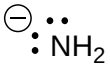
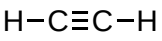
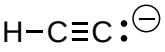
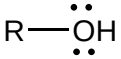
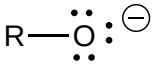
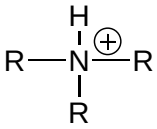
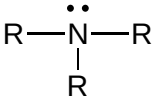
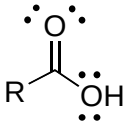
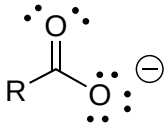
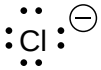
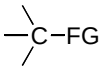
	H_2O	15.7	$^{\ominus}:OH$	
	$^{\oplus}NH_4$	9.2	NH_3	
		4.8		
	H-F:	3.2	:F:$^{\ominus}$	
	$H_3O^{\oplus}$	-1.7	H_2O	
	H-Cl:	-7.0	:Cl:$^{\ominus}$	
	H-Br:	-9.0	:Br:$^{\ominus}$	
Strong Acid	H-I:	-10.0	:I:$^{\ominus}$	Weak Base

pKa Table: Acidity and Basicity

	Acid	pKa	Conjugate Base	
Weak Acid		49		**Strong Base**
		36		
		25		
		~16-18		
		15.7		
		~10		
		9.2		
		~5		
		3.2		
		-1.7		
Strong Acid		-7.0		**Weak Base**

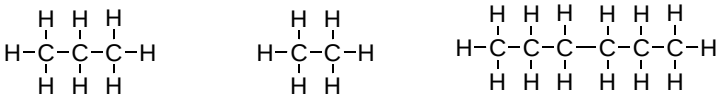
FUNCTIONAL GROUPS: Organized by class or similar structural feature

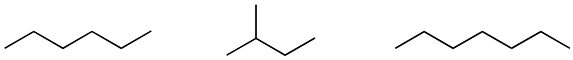
-Functional groups are show with the minimum structural components to define the functional group

- The functional groups are often shown as:  This implies that the a carbon is required to define the functional group, but any other atom can be attached at the end of the three lines attached to the carbon.

-Example molecules are shown using the standard drawing conventions, circle and label each functional group

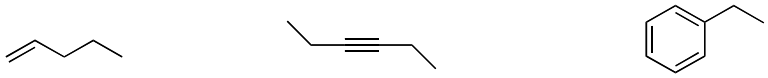
Hydrocarbon Chain - Alkane



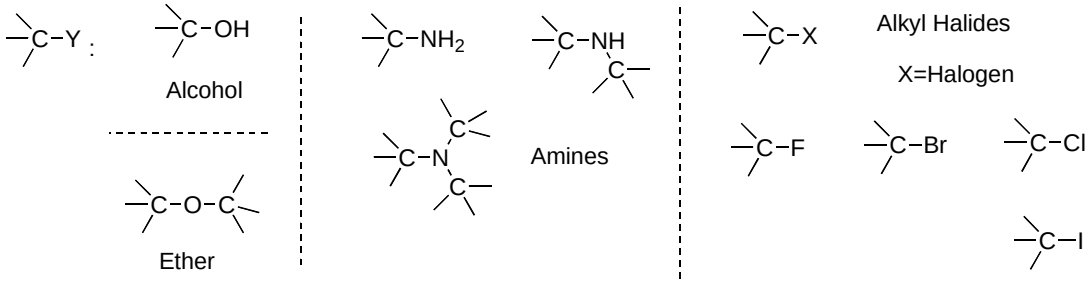
Examples: 

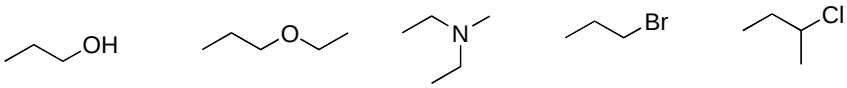
Compounds Containing C-C Multiple Bonds

Alkene Alkyne Aromatic Ring or Arene Ring

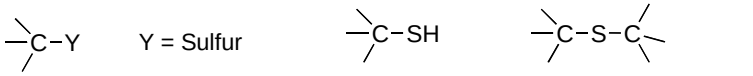
Examples: 

C-Y Containing Funtional Groups: Y is some electronegative atom (N, O, F, Cl, Br, I, S etc.)



Examples: 

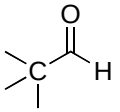
Less Important C-Y Containing Functional Groups:

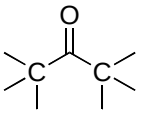


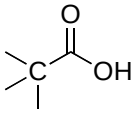
Examples: 

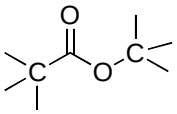
FUNCTIONAL GROUPS, continued

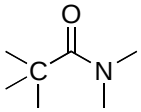
Carbonyl Compounds: General class of compounds all containing a carbonyl or 

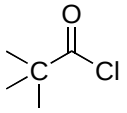
 Aldehyde

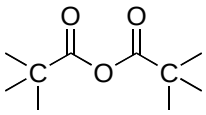
 Ketone

 Carboxylic Acid

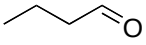
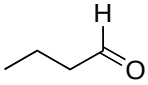
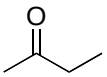
 Ester

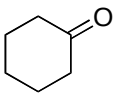
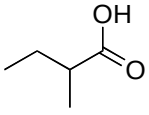
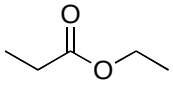
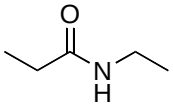
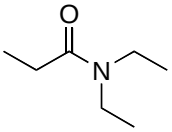
 Amide

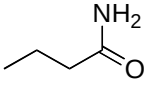
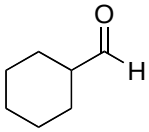
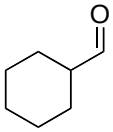
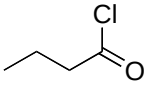
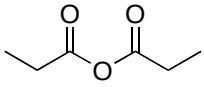
 Acid Chloride

 Anhydride

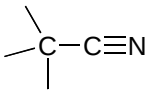
Examples:

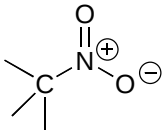
 or  

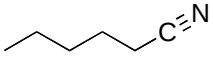
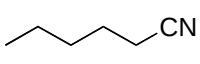
  or   

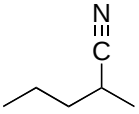
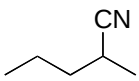
Other Functional Groups to Know:

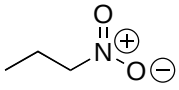
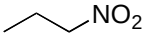
 Nitrile

 Nitro

Examples:

 or 

 or 

 or 

Infrared Spectroscopy: Simplified Correlation Table

	Frequency	Intensity
O-H	3400 cm^{-1}	Large, Broad
Carboxylic Acids	3200-2500 cm^{-1}	Large, Broad
C-H		
Aliphatic	Below 3000 cm^{-1}	Large
Aromatic & Vinyl	Above 3000 cm^{-1}	Medium
Aldehyde	2850, 2750 cm^{-1}	Medium (Two Peaks)
C=O	1690 cm^{-1} - 1715 cm^{-1}	Large, Sharp
Ester	1735 cm^{-1}	Large, Sharp
Conjugation	1690 cm^{-1}	Large, Sharp
C≡C	2250-2100 cm-1	Small
C≡N	2250 cm-1	Medium
-NO_2	1600, 1500 cm^{-1}	Large (Two peaks)

EXAMPLE SPECTRA - IR FALL - Chem 35

1.

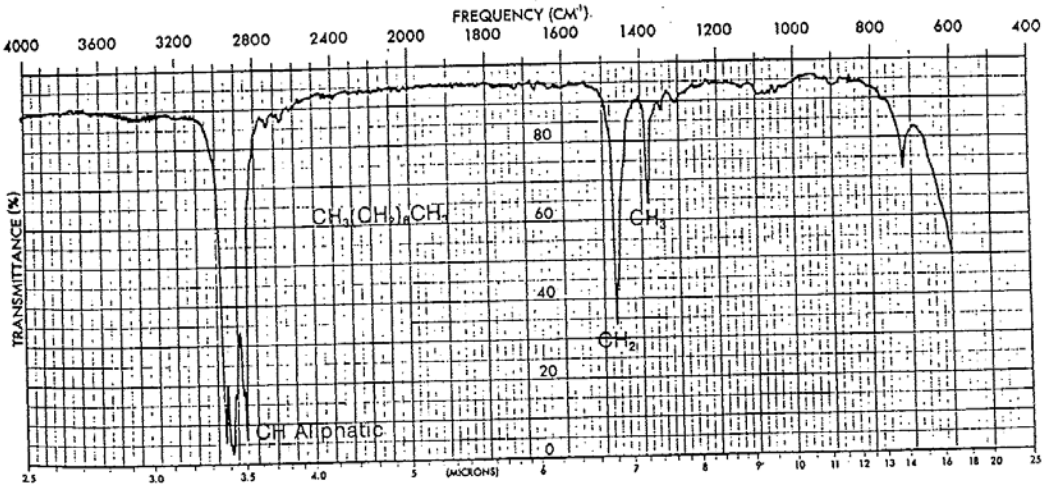


FIGURE 2-7 The Infrared Spectrum of Decane (Neat Liquid, Salt Plates)

2.

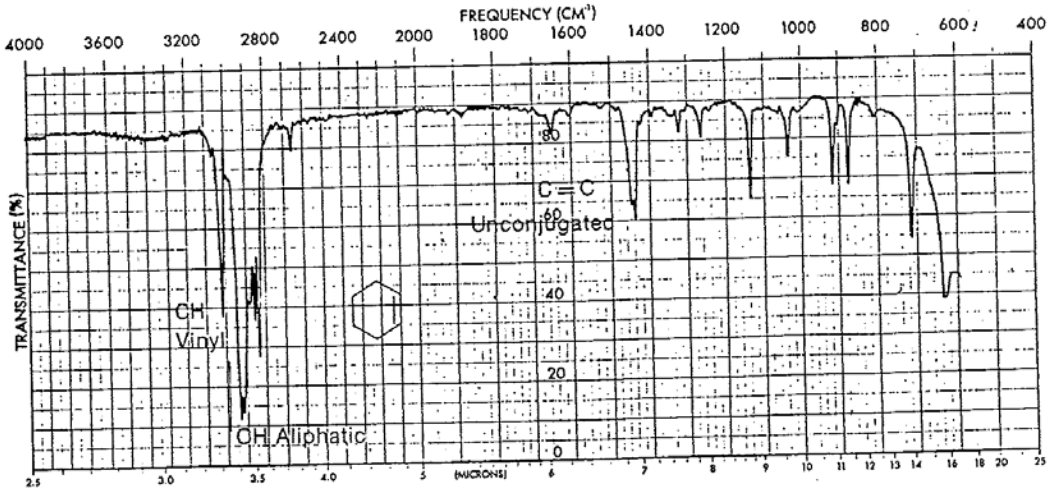


FIGURE 2-9 The Infrared Spectrum of Cyclohexene (Neat Liquid, Salt Plates)

3.

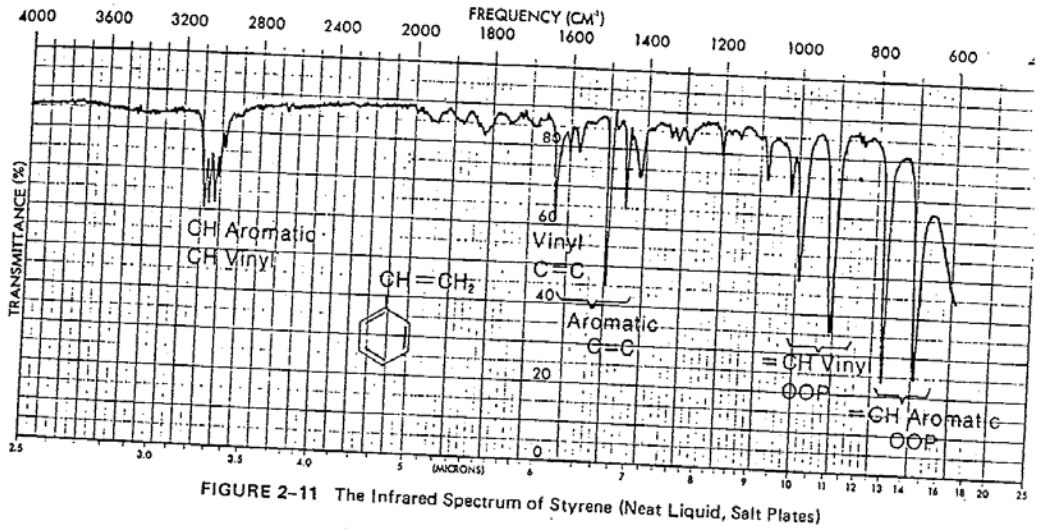


FIGURE 2-11 The Infrared Spectrum of Styrene (Neat Liquid, Salt Plates)

4.

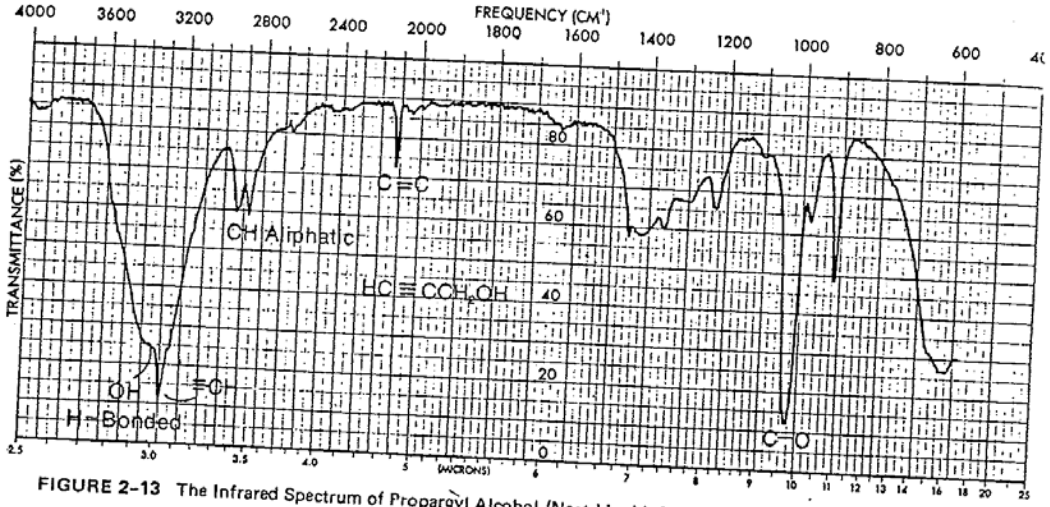


FIGURE 2-13 The Infrared Spectrum of Propargyl Alcohol (Neat Liquid, Salt Plates)

5.

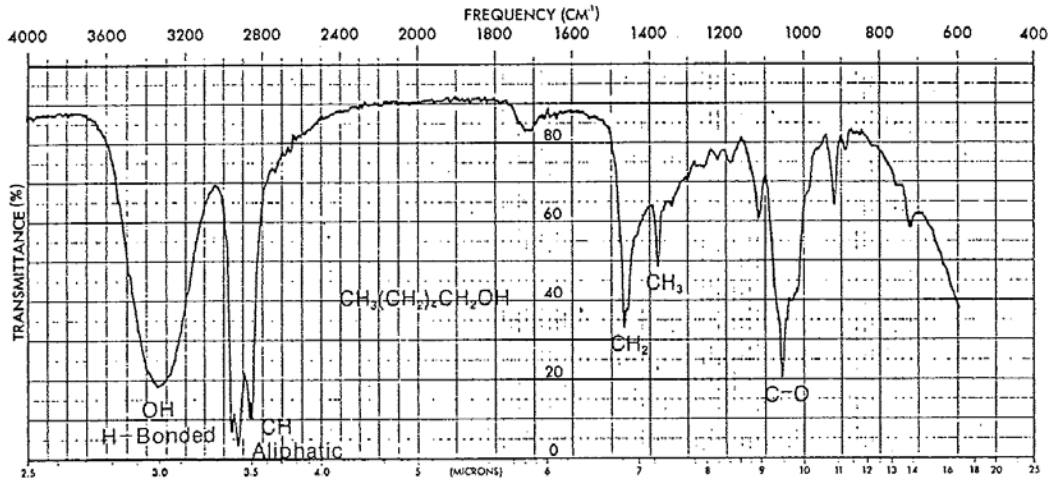


FIGURE 2–26 The Infrared Spectrum of 1–Hexanol (Neat Liquid, Salt Plates)

6.

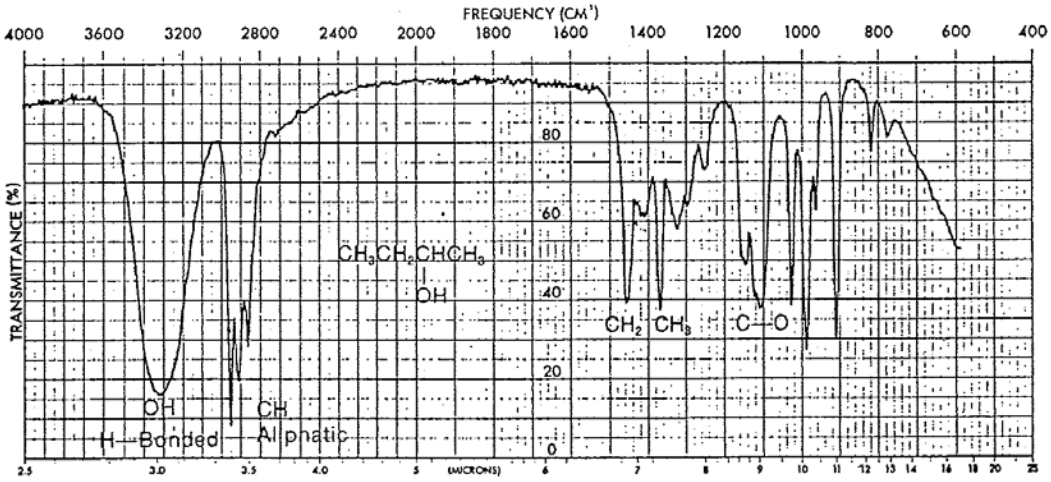


FIGURE 2–27 The Infrared Spectrum of 2-Butanol (Neat Liquid, Salt Plates)

7.

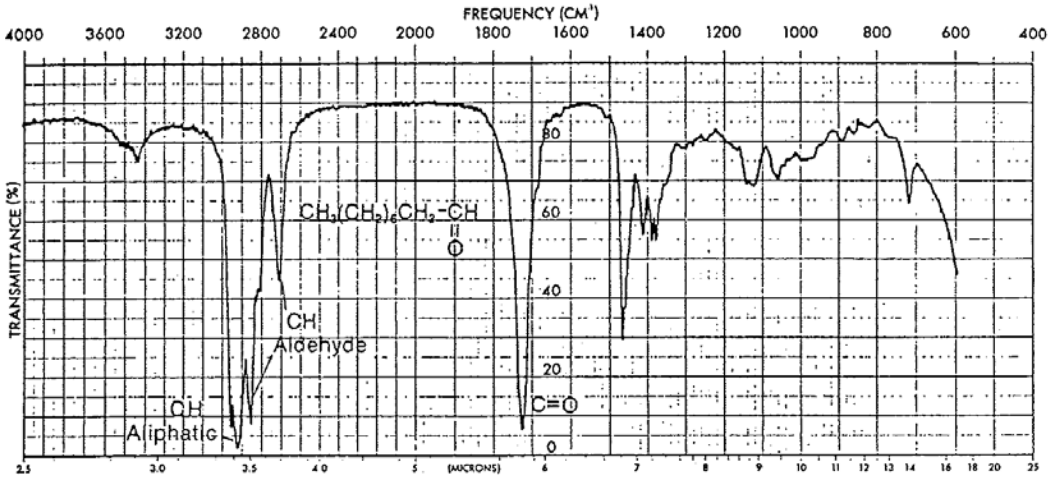


FIGURE 2–33 The Infrared Spectrum of Nonanal (Neat Liquid, Salt Plates)

8.

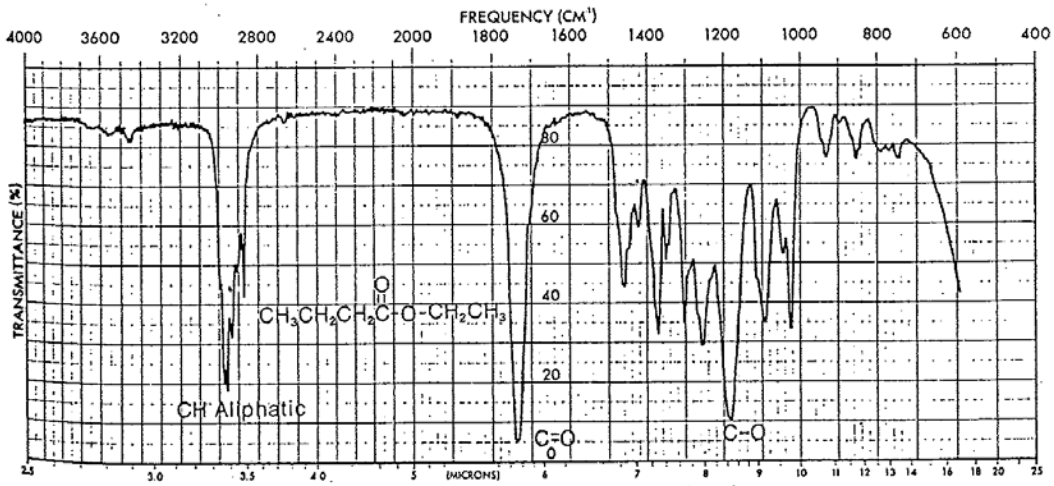


FIGURE 2–43 The Infrared Spectrum of Ethyl Butyrate (Neat Liquid, Salt Plates)

9.

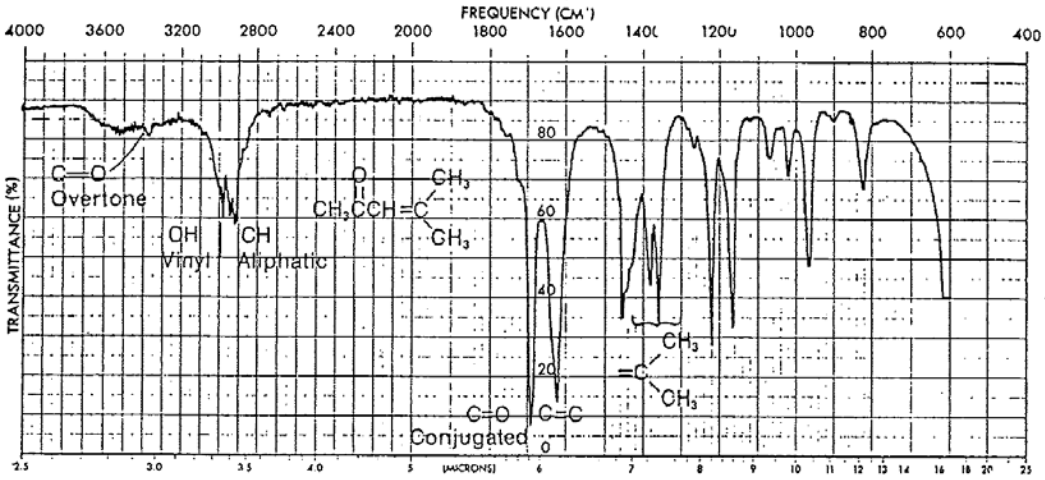


FIGURE 2–36 The Infrared Spectrum of Mesityl Oxide (Neat Liquid, Salt Plates)

10.

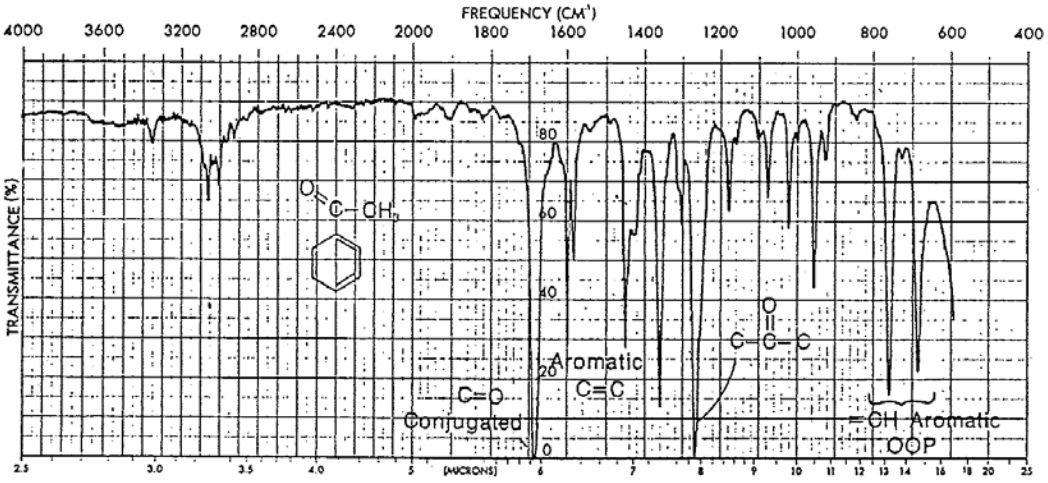


FIGURE 2–37 The Infrared Spectrum of Acetophenone (Neat Liquid, Salt Plates)

11.

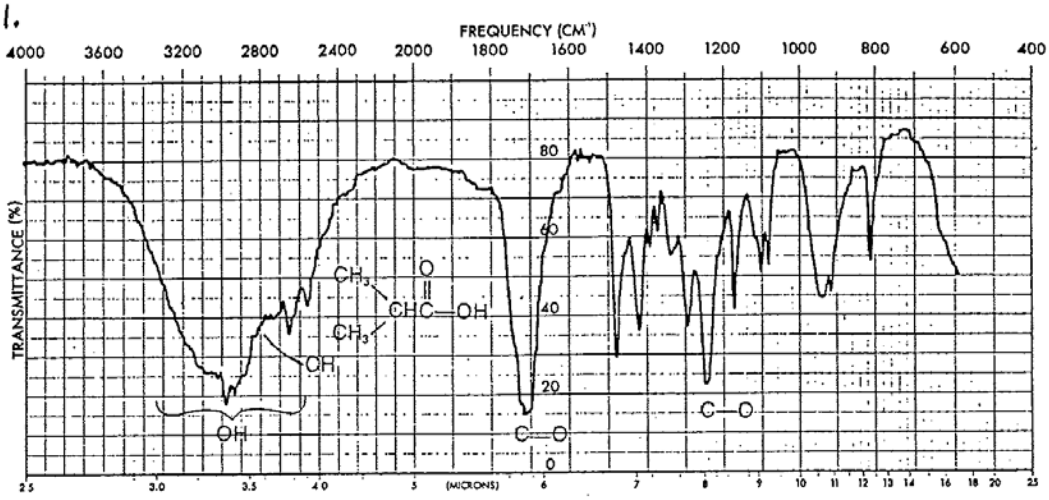


FIGURE 2–41 The Infrared Spectrum of Isobutyric Acid (Neat Liquid, Salt Plates)

12.

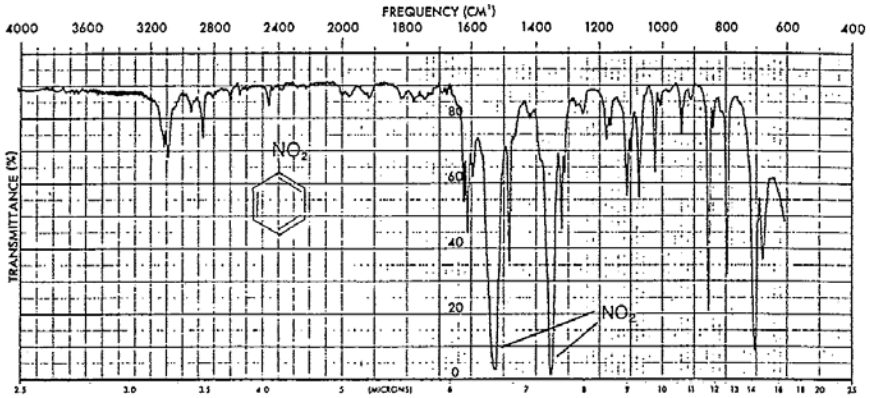


FIGURE IR–12. Infrared spectrum of nitrobenzene, neat

13.

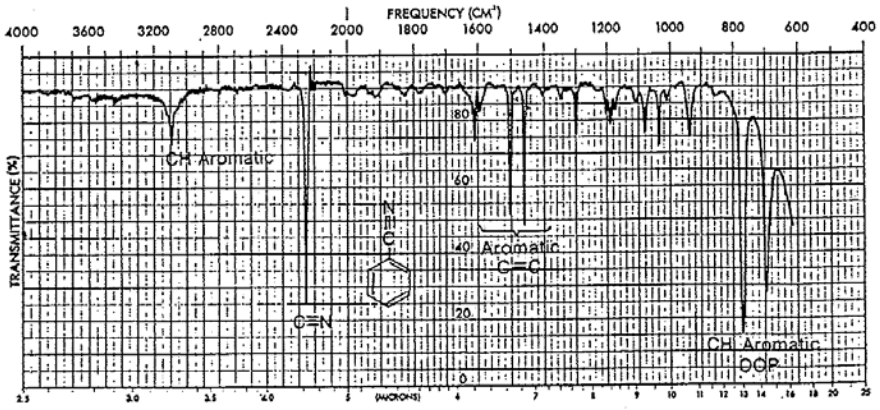
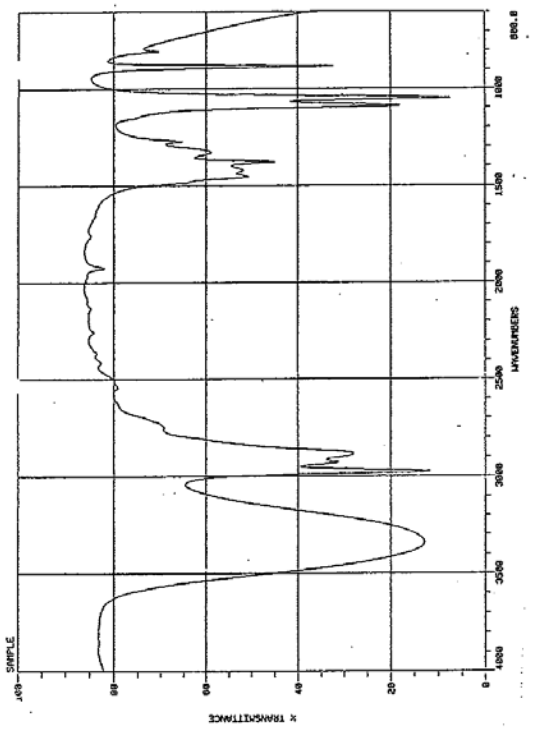
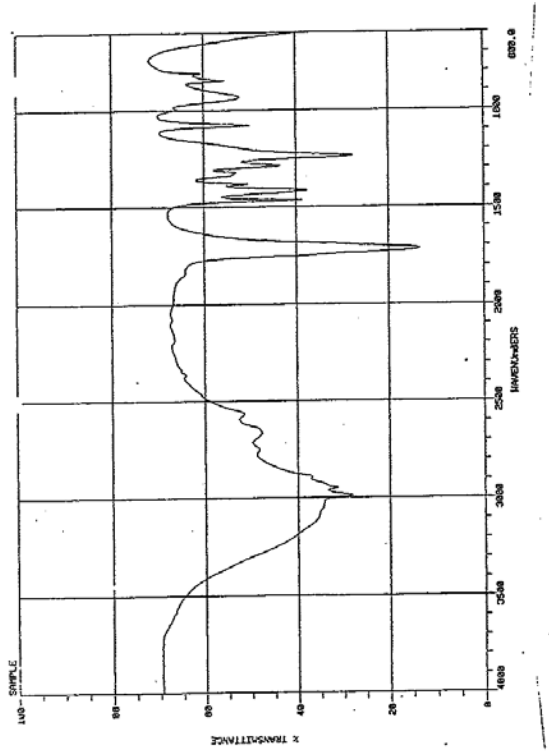
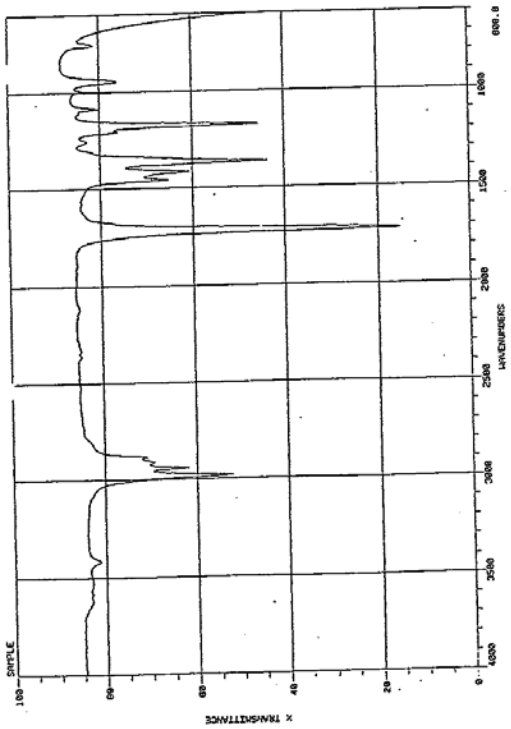


FIGURE IR–13. Infrared spectrum of benzonitrile (neat liquid, salt plates)

For the following IR spectra, determine the main functional group.

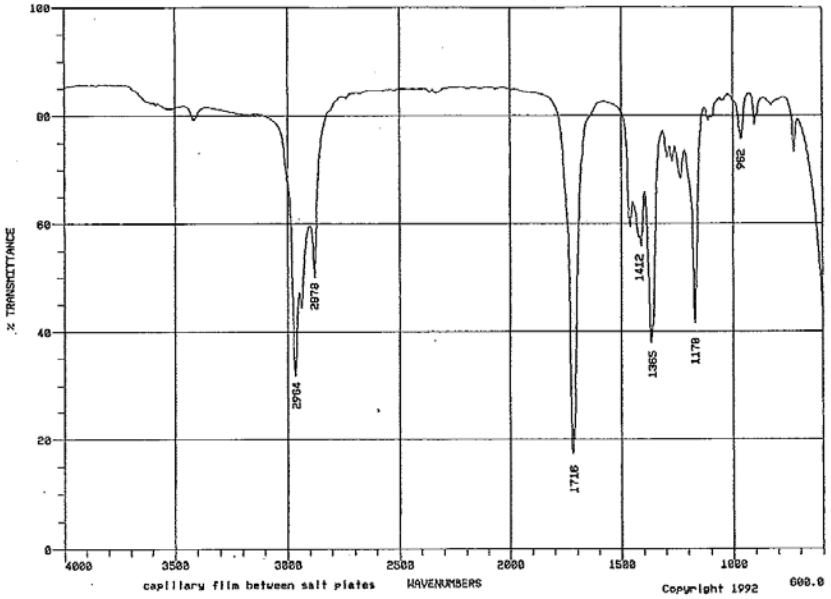




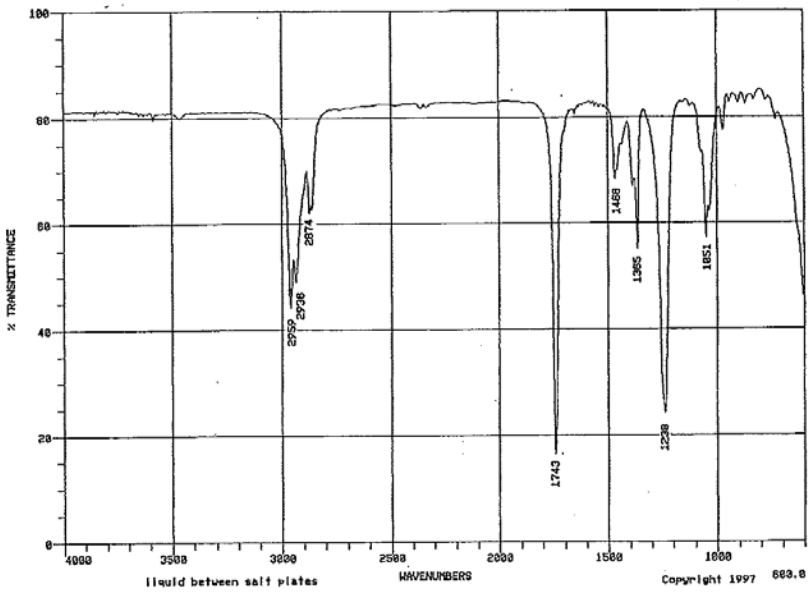


IR Practice:

1.

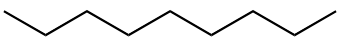


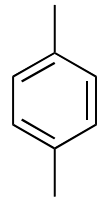
2.

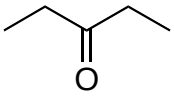


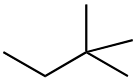
^{13}C NMR Problem Set:

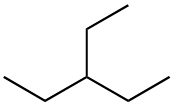
1. Determine the numbers of peaks observed in the ^{13}C NMR spectrum for the following compounds.

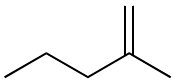


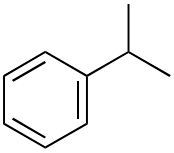


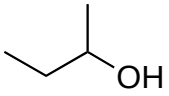




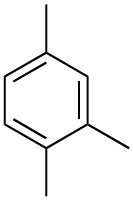


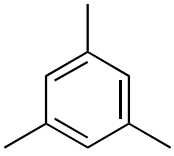






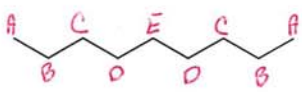
2. You have been given a sample that contains one of the two following compounds. How would determine which compound you have?





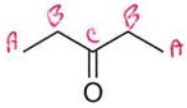
^{13}C NMR Problem Set:

1. Determine the numbers of peaks observed in the ^{13}C NMR spectrum for the following compounds.

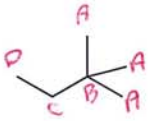


5

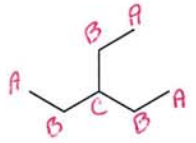
3



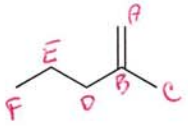
3



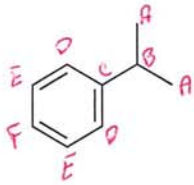
4



3



6



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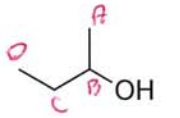
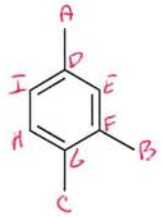
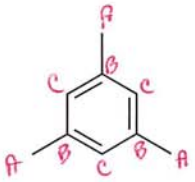


4

2. You have been given a sample that contains one of the two following compounds. How would determine which compound you have?

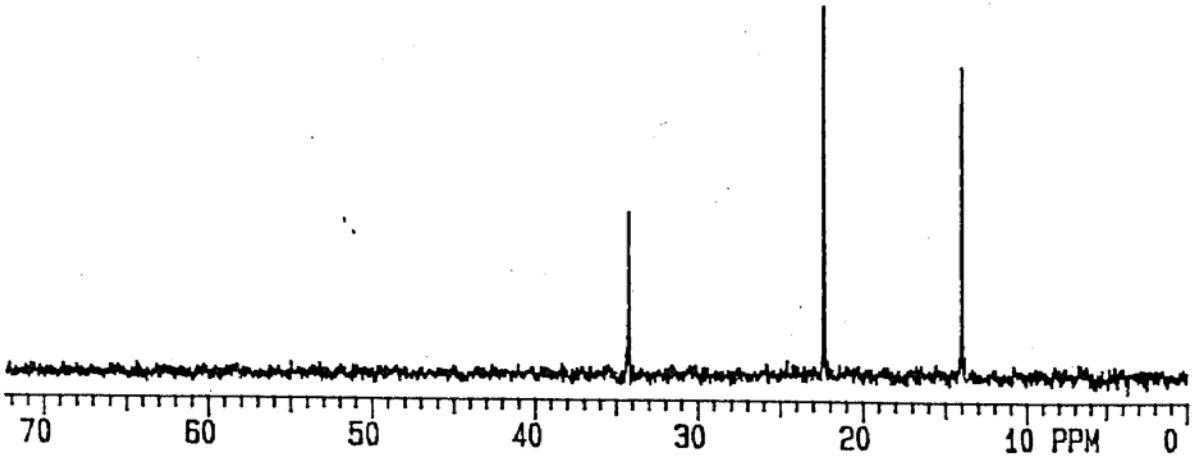


9 signals in ^{13}C (no symmetry)



only 3 signals in ^{13}C due to symmetry

C-13 NMR



Nomenclature Rules : IUPAC System

Prefix-Parent-Suffix

A. Define the Parent Chain:

1. Pick out the longest continuous carbon chain.
2. With two chains the same length: chose the one with largest number of branches.
3. Number the carbon chain from the end nearest to the first branching on the chain.

B. Assemble the Prefix:

1. Name the substituents *****(see below for special cases- **F*** and **G***)
2. Give a location number on the parent chain for each substituent
3. For more than one of the same substituent use prefixes (di, tri, tetra, penta etc.) and the location numbers separated by a comma. i.e. 2, 6-dimethyl

C. Suffix: Family Designation

1. For the family of Alkanes: -ane.
2. Other family suffixes will be learned in due course.

D. Writing the Name:

1. Written as a single word, hyphens separating the numbers and words. (i.e. no spaces in a chemical name)
2. Write the substituents in alphabetical order.
   a. Use the main name of the substituent for order placement.
   b. Any number prefixes (di, tri, tetra) and hyphenated prefixes (*sec*-, *tert*- or *t*-) **are not** used for alphabetizing purposes.
   c. Non hyphenated prefixes such as iso **are** used in alphabetizing (i.e. isopropyl and isobutyl).

F*. Complex Substituents:

1. Begin numbering at the point of attachment to the main chain of the molecule.
2. Number the longest chain and name it as an alkyl substituent (i.e. propyl, butyl, pentyl etc.)
3. Create a prefix using the rules above for naming the substituents and giving location numbers on the chain.
4. This name is set off in parenthesis with a location number on the main chain in front.

G. Common Names for Substituents:

1. Nonsystematic common names to know: isopropyl, tert-butyl or t-butyl isobutyl.
You might encounter but will not be expected to know: sec-butyl, isobutyl. (see below for structures).
2. Others are less common and can be named by complex substituent rules.

Names of Straight Chain Alkanes:

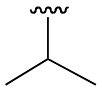
C1- methane	C6- hexane	C11- undecane
C2- ethane	C7- heptane	C12- dodecane
C3- propane	C8- octane	C13- tridecane
C4- butane	C9- nonane	
C5- pentane	C10- decane	

Most Common Alkyl Groups:

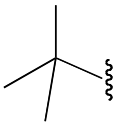
Methyl: $-CH_3$ Ethyl: $-CH_2CH_3$ Propyl: $-CH_2CH_2CH_3$
Butyl: $-CH_2CH_2CH_2CH_3$ Pentyl: $-CH_2CH_2CH_2CH_2CH_3$

Common Groups Structures:

Need to know:

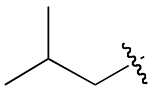


isopropyl

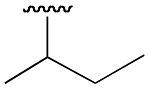


tert -butyl or *t*-butyl

Other common groups:

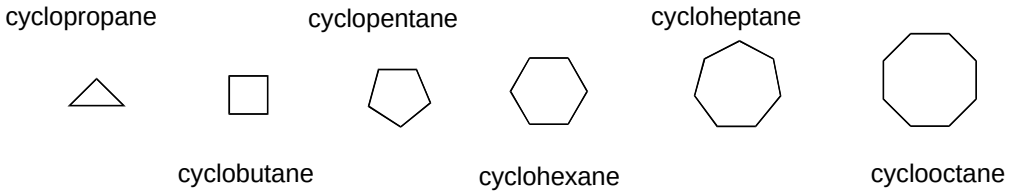


isobutyl



sec-butyl

Cycloalkanes:



Naming Cycloalkanes:

A. Parent Cyclic is usually the main name

1. Unless side branch has more carbons than cyclic then named as a substituent on the chain
2. Cycloalkanes as substituents are named as alkyl group (i.e. cyclopropyl, cyclobutyl, cyclopentyl, etc).

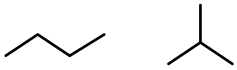
B. Number from point of attachment of the substituent

1. If more than one substituent, number on the ring to achieve the lowest location numbers.
2. If location numbers are the same for two numbering schemes:
   a. Give number priority to the groups by alphabetical priority (i.e. number ethyl before methyl).
   b. Halogens are named exactly like alkyl groups. Use fluoro, chloro, bromo, iodo in naming prefix with location number before name.

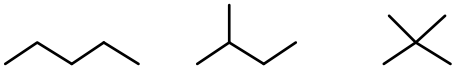
Isomers[1]

Different compounds having the same molecular formula are called isomers. Simply stated, for a specific molecular formula, how many unique structures exist? When these structures have completely different atom-atom attachments (or the atoms in the molecule are bonded together in fundamentally different ways), we refer to such compounds as constitutional or structural isomers. Since this is the most simple form of isomerism, we can just say "isomers" and the structural/constitutional term is implied. There are two structural or constitutional isomers of C_4H_{10} and three for C_5H_{10}. The structural formulas for these molecular formulas are drawn below. These structures represent all the possible C_4H_{10} and C_5H_{10} compounds that can exist for these specfic molecular formulas. Note that there are no double or triple bonds and no rings in any of these structures. We will discuss these structural features below when we consider the Degree of Unsaturation.

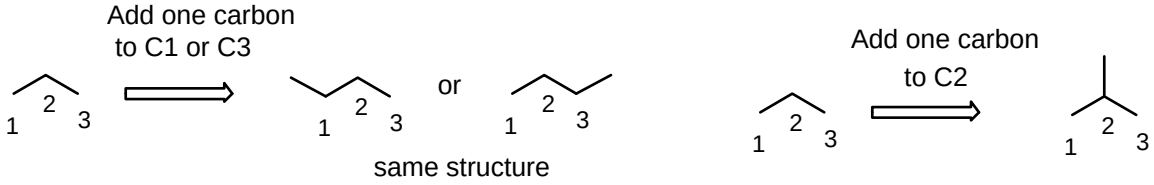
Two Structural Formulas for C_4H_{10} Isomers



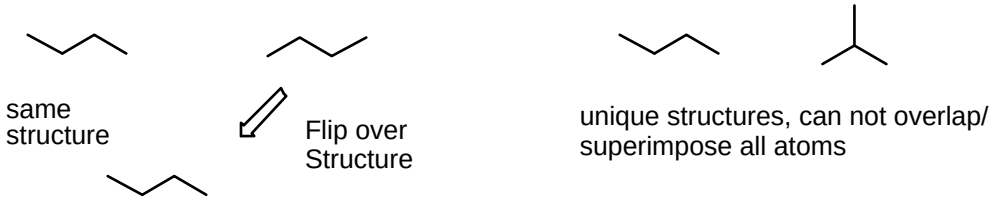
Three Structural Formulas for C_5H_{12} Isomers



A simple method for drawing isomers is to begin with a three carbon chain and draw all the possible permutations for adding the number of carbons to complete the molecular formula. For example, we can work through drawing the different isomers for C_4H_{10} in the following systematic manner:



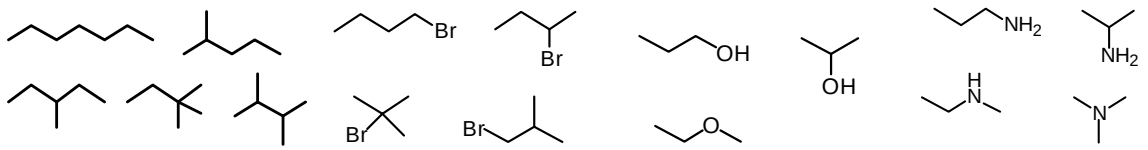
We also need to develop the ability to "see" if a structure is unique or not. Although this seems very obvious with simple structures, for more complicated structures we determine if the compounds are *superimposable*. We envision picking up one of the structures and placing the molecule on top of the other and if all the atoms match up (are superimposable), then the structures are equivalent. This is especially easy if you make models of each molecule you are comparing with your molecular model kits. Eventually, you will not need models as often because you will develop 3D-imaging capability so you can do the “mental gymnastics” in your head.



When drawing isomers that correspond to a molecular formula containing noncarbon atoms (O, N, S, Halogens etc.), we have to be careful to follow the bonding rules to draw valid structures. This is very good practice and a good test whether you have the bonding rules firmly in your understanding of organic structures. Try drawing the isomers for the following molecular formulas--the answers are on the following page:

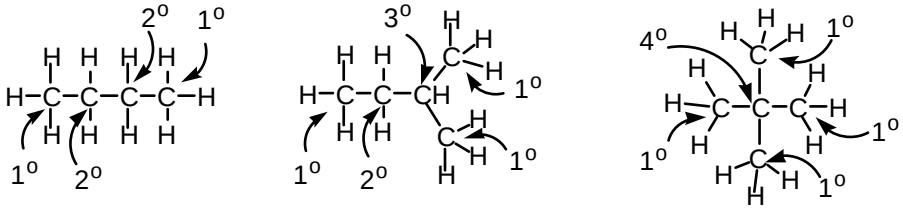
C_6H_{14} C_4H_9Br C_3H_8O C_3H_9N

C_6H_{14} C_4H_9Br C_3H_8O C_3H_9N

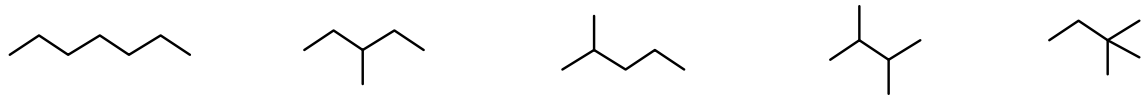


Degree of Substitution

When discussing a compounds structure, it is often useful to distinguish different groups of carbon atoms by their structural features. One such description is to look at how many carbon chains are attached to any specific carbon atom. We refer to this as *degree of substitution*. A primary carbon (1º) is one that is bonded to no more than one other carbon atom. A secondary carbon (2º) is bonded to two other carbon atoms, tertiary (3º) is bonded to three other carbon atoms and quaternary (4º) carbon atoms are bonded four other carbons. It is important to recognize that when considering the degree of substitution for any atom, we only count the number of ***carbon*** atoms directly attached to the carbon atom being examined. The three C_5H_{12} isomers shown below illustrate the use of this terminology:



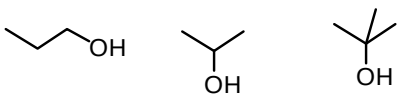
To practice with the C_6H_{14} isomers, determine the number of each type substituted carbon for each compound:



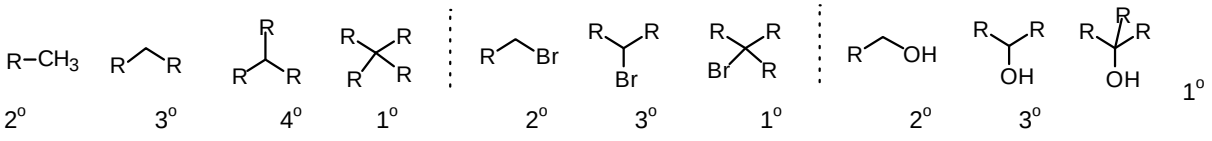
1º:__2º:__3º:__4º:__ 1º:__2º:__3º:__4º:__ 1º:__2º:__3º:__4º:__ 1º:__2º:__3º:__4º:__ 1º:__2º:__3º:__4º:__

We will use these terms often to refer to a carbon atom and its substitution. The degree of substitution can be important to the stability of a charged carbon, like a carbocation, or the reactivity of an alkyl halide. For example, we will refer to alkyl halides as 1º, 2º and 3º, which tells us the number of carbon-chain substituents attached to the carbon that bears the halogen. Below are examples of 1º, 2º and 3º bromides. Note, that you can not have a 4º alkyl halide, there would no place to put the halogen, or you would have too many bonds to carbon!!

We can use this terminology to refer to other compounds as well. For example, determine the degree of substitution of the following alcohols:



Finally, there is another term that is used when discussing the number of substituents in a more general way. To refer to a carbon chain without specifying its structure, we use the term R-group. An R-group can be a hydrocarbon chain with any structure, number atoms, number of branches etc. Below are some general examples of degree of substitution for alkanes, alkyl halides and alcohols using the R-group designation for the carbon chains attached:



Degree of Unsaturation- Molecular Formula Analysis

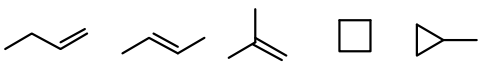
Although skeletal or Lewis structures are essential to describe a unique organic compound, it is often useful to evaluate the structural information that may be obtained directly from a molecular formula. As we saw from our discussion of isomers above, many structures can be drawn with the same molecular formula. By examining the molecular formula, we can determine some of the structural features of the isomer compounds we could draw for a given molecular formula. Two useful rules for the examination of alkane (C and H only) molecular formulas are below:

1. The number of hydrogen atoms that can be bonded to a given number of carbon atoms is limited by the maximum number of bonds to a carbon atom - four. For compounds of carbon and hydrogen (hydrocarbons) the maximum number of hydrogen atoms that can be bonded to n carbons is 2n + 2 (n is an integer). Consider CH_4, n=1, therefore 2n + 2 = 4. In a chain of carbon atoms, the middle carbons will have two hydrogens each and the two end carbons have three hydrogens each. For a six-carbon chain (n = 6) we have $CH_3CH_2CH_2CH_2CH_2CH_3$, and the total number of hydrogen atoms using the 2n+2 formula is (2 x 6) + 2 = 14. Below are some possible and impossible molecular formulas. Note that the molecular formula can have less than a 2n+2 number but not more than 2n+2.

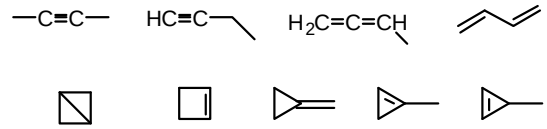
Some Plausible Molecular Formulas:	Some Impossible Molecular Formulas:
C_7H_{16}, C_9H_{18}, $C_{15}H_{28}$, C_6H_{10}	C_8H_{20}, $C_{23}H_{50}$, C_5H_{16}, C_4H_{12}

2. The number of hydrogen atoms in stable compounds of carbon and hydrogen reflects the number of double bonds and rings in their structural formulas. Consider a hydrocarbon with a molecular structure consisting of a simple chain of four carbon atoms, $CH_3CH_2CH_2CH_3$. The molecular formula is C_4H_{10} (maximum number of hydrogens = 2n+2, where n=4, number of H's is 10). If a molecular formula has this maximum number we refer to that molecule as "saturated", meaning the molecule has as many hydrogens as it can "hold" (like a saturated solution has as much solute as can dissolve). If the four carbon atoms form a ring, two hydrogens must be “removed” from the structure to adhere to the bonding rules for carbon. Similarly, the introduction of a double bond requires the loss of two hydrogens, and a triple bond the loss of four hydrogens. For each two hydrogens that are "missing" from the saturated molecular formula (C_nH_{2n+2}), we refer to that as one *degree of unsaturation*. Again, for each degree of unsaturation, there must be either a π bond or a ring in the possible isomeric structures that are drawn.

C_4H_8: 1^o of unsaturation, 1 π-bond or 1 ring



C_4H_6: 2^o of unsaturation, 2 π-bonds or 2 rings or 1 π-bond and 1 ring

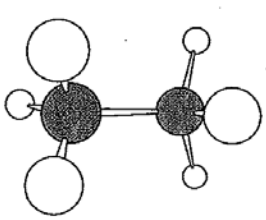


From the above discussion and examples, the molecular formula of a hydrocarbon can give some structural information, which helps us in drawing isomers. In comparing C_4H_{10} and C_4H_8, there are two hydrogens missing (1^o of unsaturation) so we know a π-bond or ring must be included in the structures we draw. All the possible structures have to have either one of these structural features. As you can see for C_4H_6 isomers above, the process of drawing isomers can become complicated rather quickly and it is often challenging to draw all the possible structural permutations, especially for molecular formulas with more carbons. We will not expect that you can draw the 20 isomers for specific molecular formula, but for small molecules, drawing isomers is good practice and reinforces much of the structural basics we have been learning.

1. Adapted from Virtual Text in Organic Chemistry, William Reusch, Michigan State University.

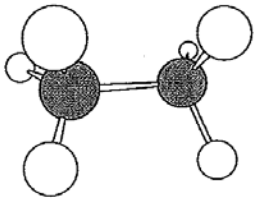
Introduction to Molecular Models

Ethane:



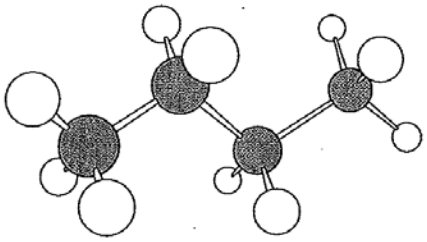
Staggered

OR



Eclipsed

Butane:



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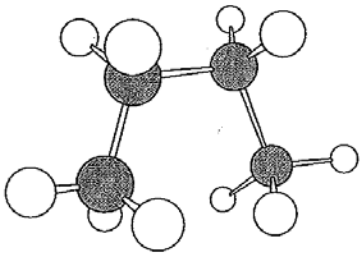

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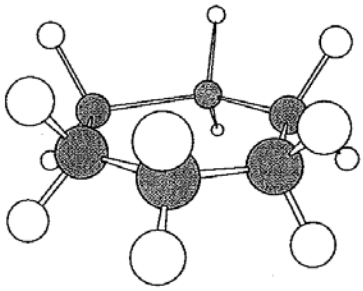
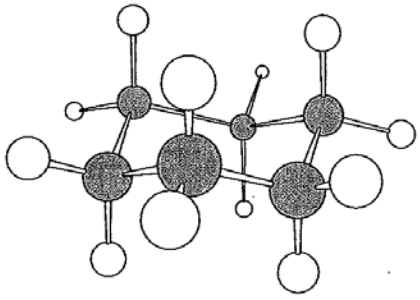
Cyclohexane:



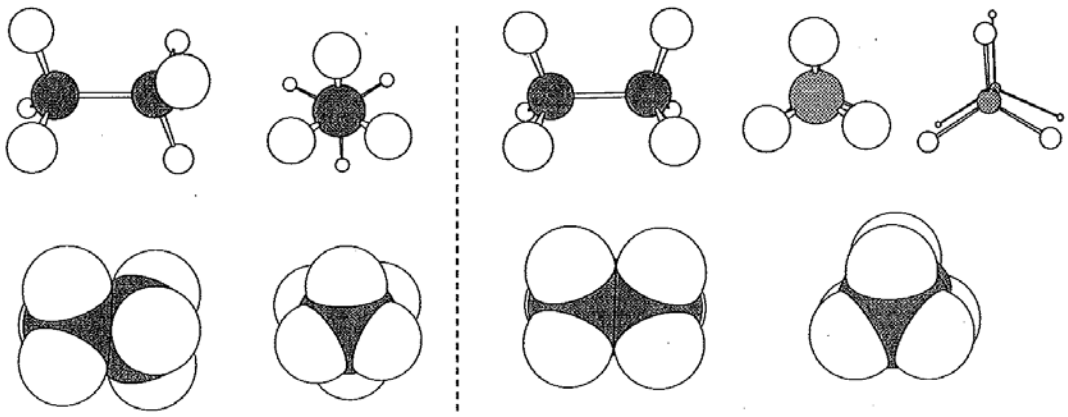
Planar

OR

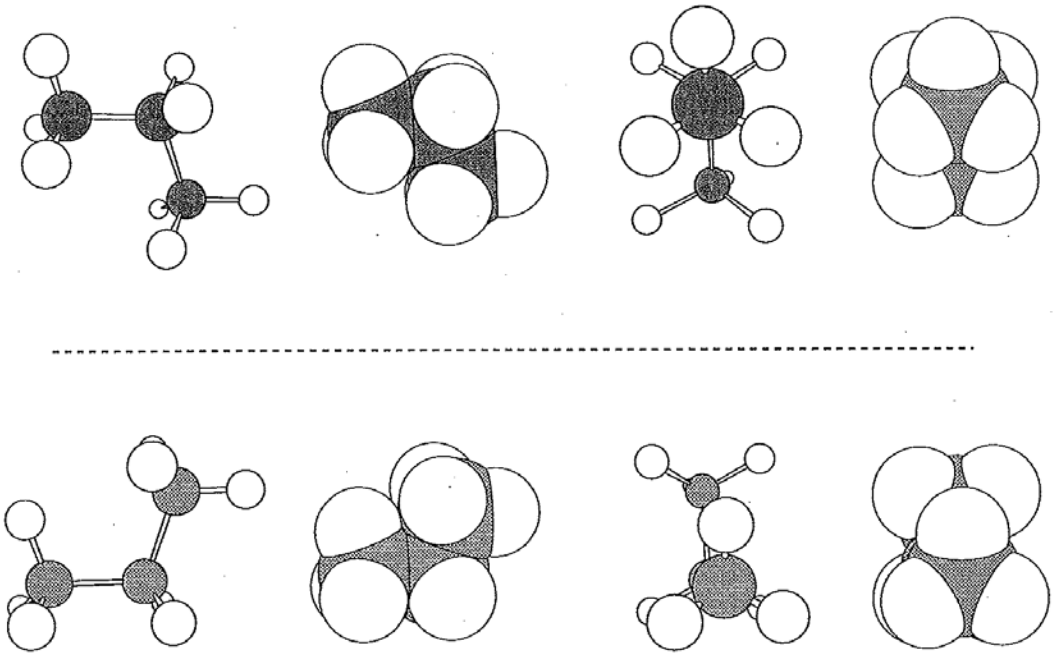


Chair

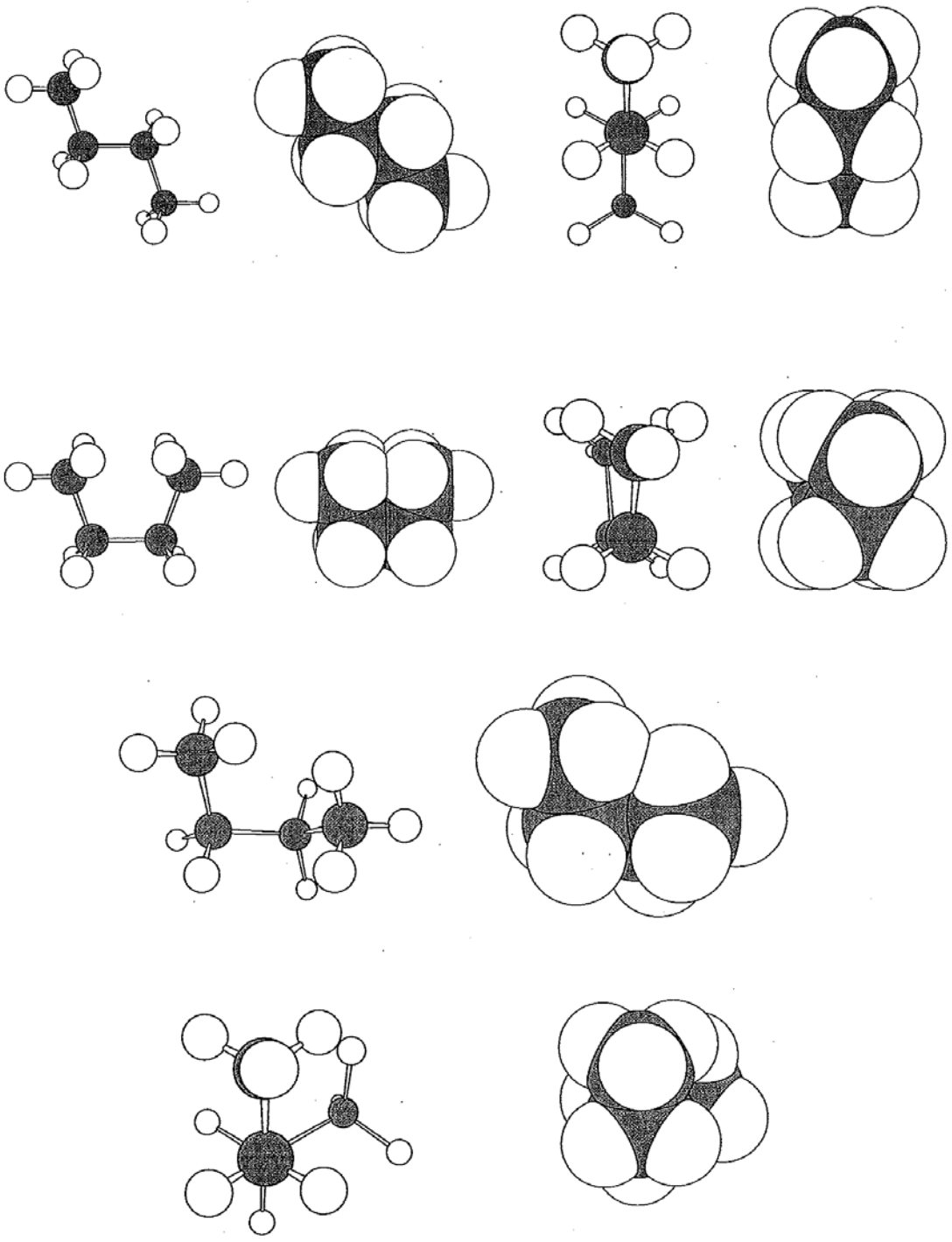
Ethane Conformations



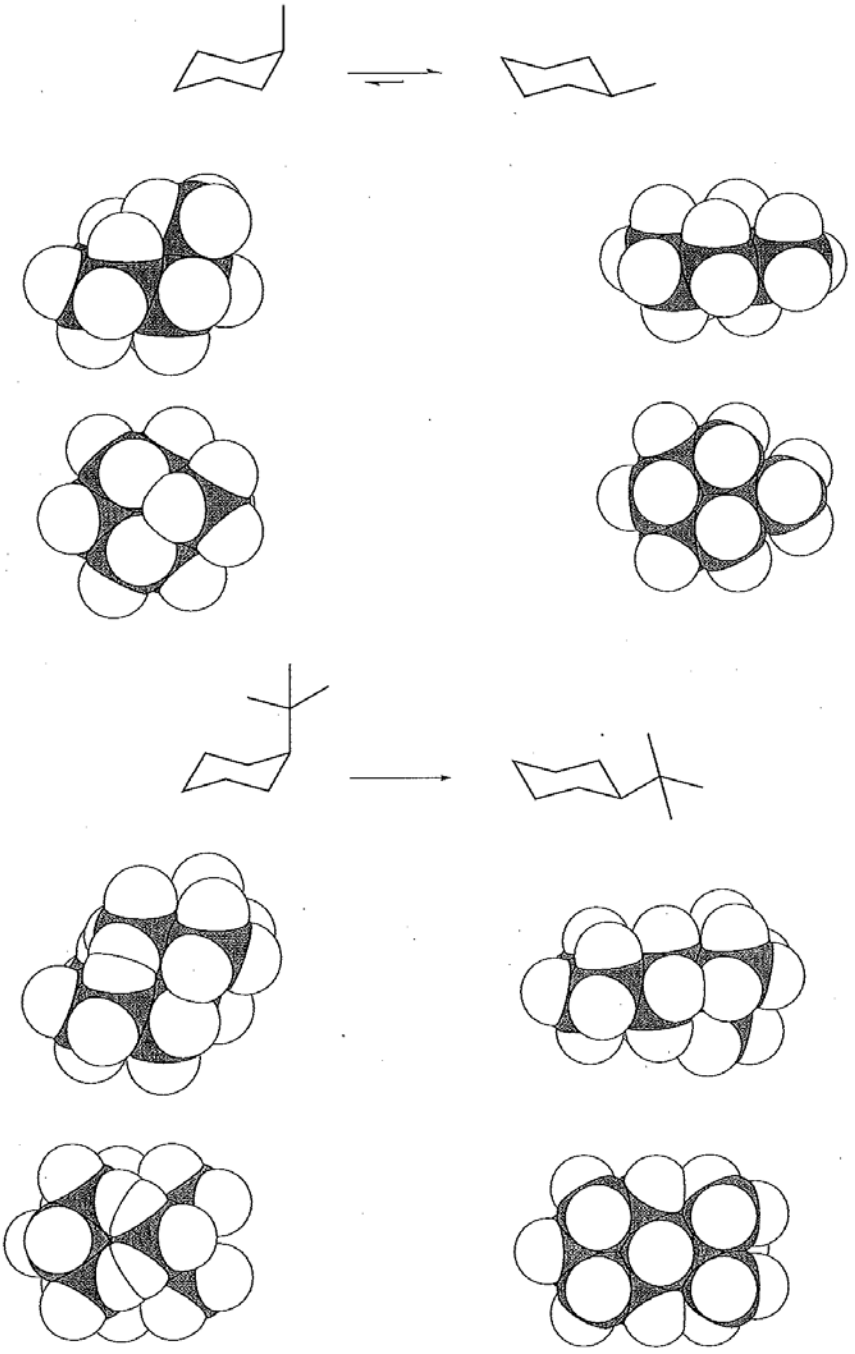
Propane Conformations



Butane Conformations

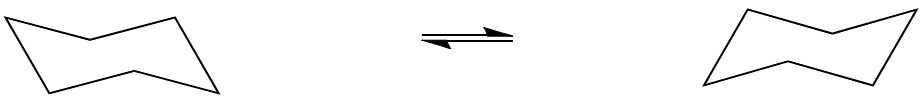


Substituted Cyclohexanes-Space Filling Pictures
Methyl versus t-Butyl



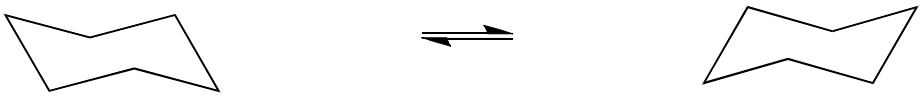
Cyclohexane Practice:

Fill in Axial and Equatorial H's



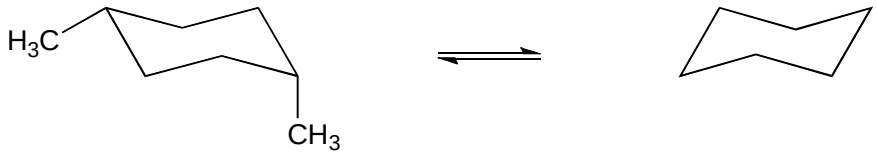
Redraw the scheme above in your best chair rendering:

Draw the two ring-flip isomers of Methylcyclohexane, include all H's on the ring

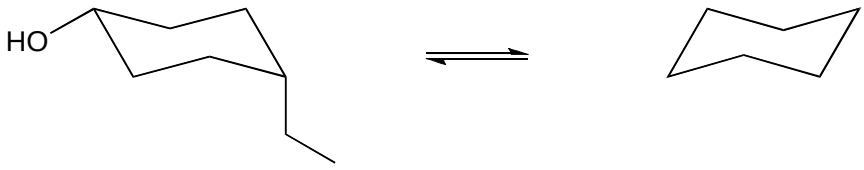


Conformational Analysis Practice

1.

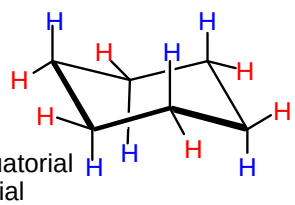


2.

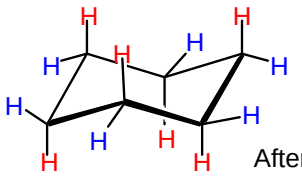


Cyclohexane Practice:

Fill in Axial and Equatorial H's



red H's equatorial
blue H's axial

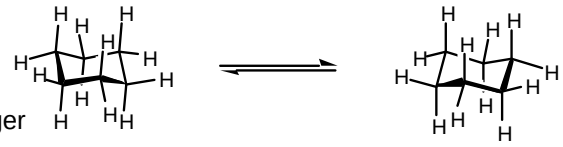


After ring flip:

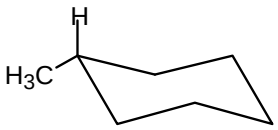
red H's axial
blue H's equatorial

Redraw the scheme above in your best chair rendering:

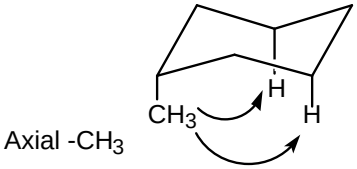
easy if you have a chemical drawing program! Try to make it look like these only bigger



Draw the two ring-flip isomers of Methylcyclohexane, include all H's on the ring



equatorial -CH_3
no steric interactions



Axial -CH_3

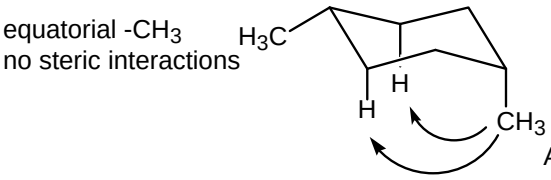
2 x 1, 3 CH_3-H Diaxial interactions
2 x 0.9=1.8 kcal/mol

Conformational Analysis Practice

1.

Ratio 50:50 since the same energy

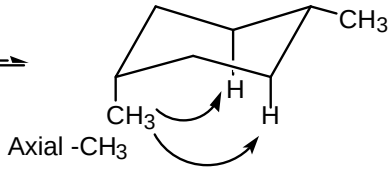
equatorial -CH_3
no steric interactions



Axial -CH_3

2 x 1, 3 CH_3-H Diaxial interactions
2 x 0.9=1.8 kcal/mol

equatorial -CH_3
no steric interactions



Axial -CH_3

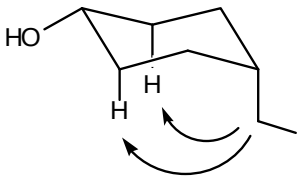
2 x 1, 3 CH_3-H Diaxial interactions
2 x 0.9=1.8 kcal/mol

2.

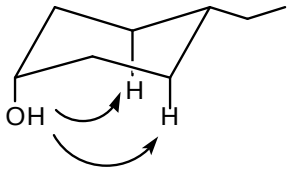
Ratio about 17:83 since 0.9 kcal/mol energy difference

equatorial -CH_2CH_3
no steric interactions

equatorial -OH
no steric interactions

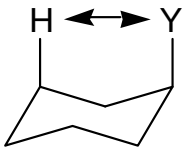


2 x 1, 3 -CH_2CH_3-H Diaxial interactions
2 x 0.95=1.9 kcal/mol



2 x 1, 3 OH-H interactions
2 x 0.5= 1.0 kcal/mol

Steric Strain Due to 1,3-Diaxial Interactions



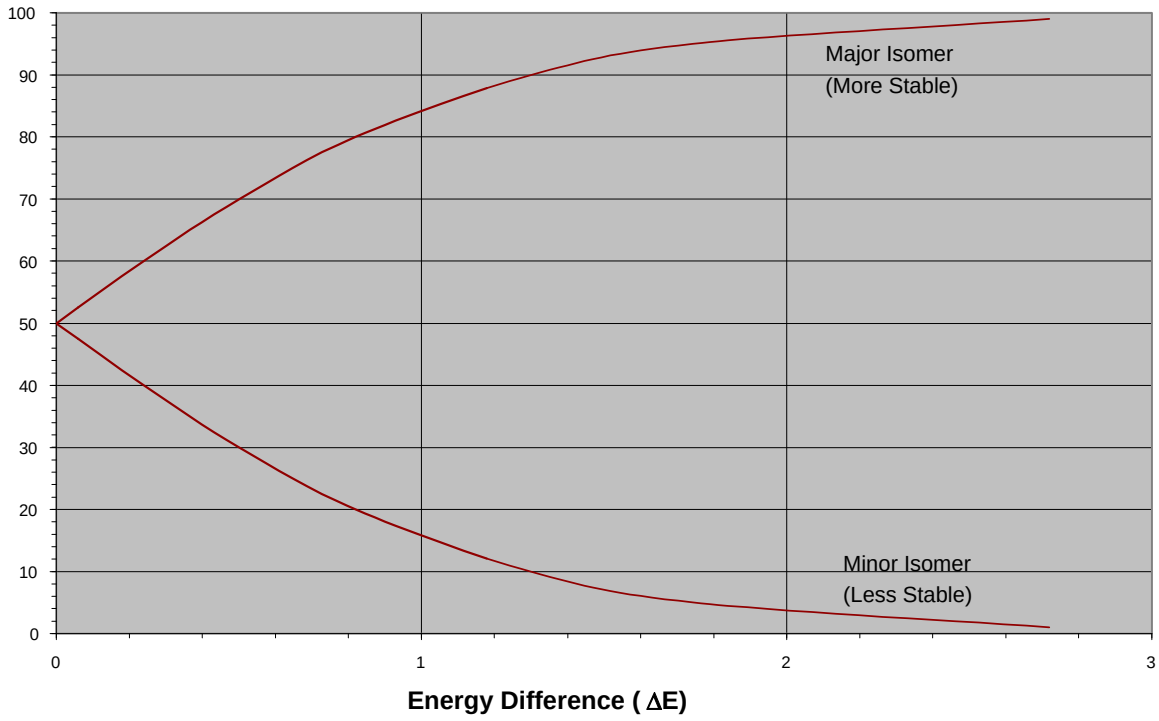
Strain of one H-Y 1,3-diaxial interaction		
Y	(kcal/mol)	(kJ/mol)
-F	0.12	0.5
-Cl	0.25	1.4
-Br	0.25	1.4
-OH	0.5	2.1
$-CH_3$	0.9	3.8
$-CH_2CH_3$	0.95	4.0
$-CH(CH_3)_2$	1.1	4.6
$-C(CH_3)_3$	2.7	11.3
$-C_6H_5$	1.5	6.3
-COOH	0.7	2.9
-CN	0.1	0.4

Relationship Between Stability and Isomer Percentages at Equilibrium**

More stable isomer (%)	Less stable isomer (%)	Energy difference at 25˚C (kcal/mol)	(kJ/mol)
50	50	0	0
75	25	0.651	2.72
90	10	1.302	5.45
95	5	1.744	7.29
99	1	2.722	11.38
99.9	0.1	4.092	17.11

**The values in this table are calculated from the equation $K = e^{-(\Delta E/RT)}$, where K is the equilibrium constant between isomers; e ≈ 2.718 (the base of natural logarithms); ΔE = energy difference between isomers; T = absolute temperature (in kelvins); and R = 1.986 cal/mol •K (the gas constant).

Energy Difference and Isomer Ratio



Energy Difference (ΔE)

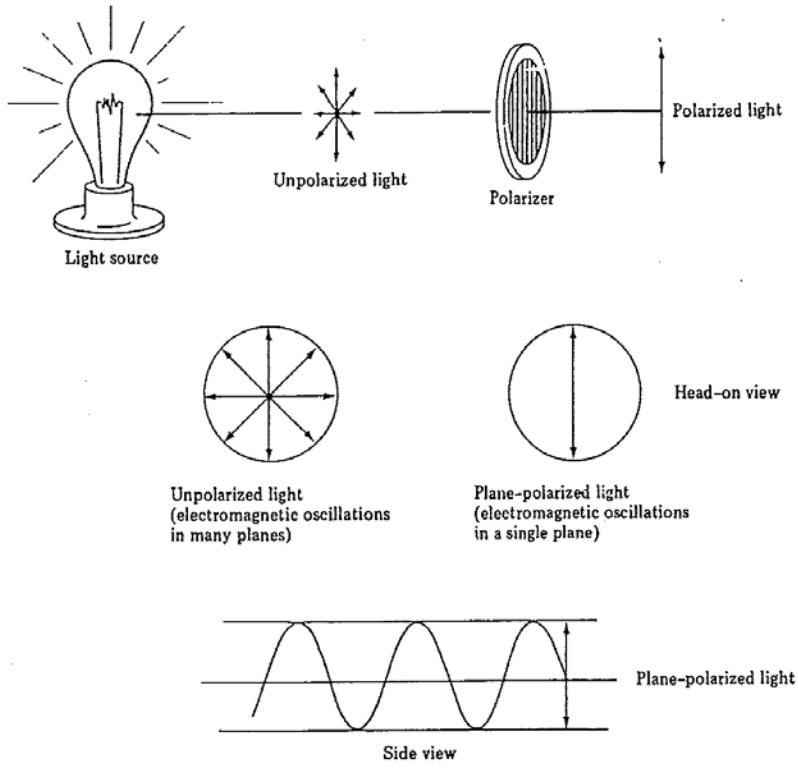


Figure 9.5 Plane-polarized light. Oscillation of the electromagnetic field occurs in a single plane.

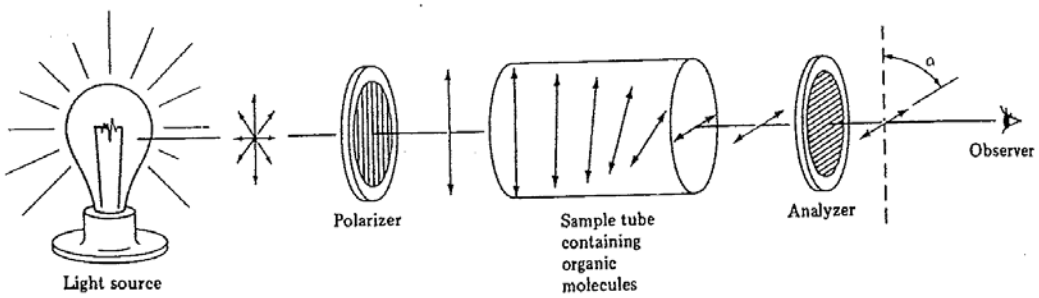
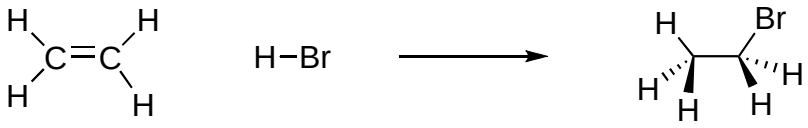
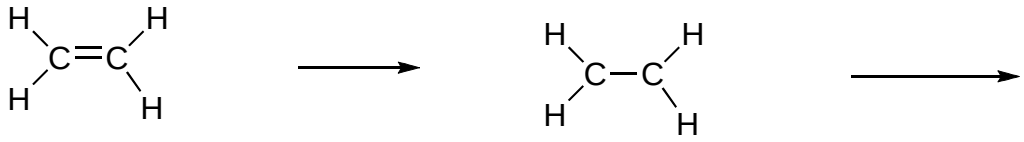


Figure 9.6 Schematic representation of a polarimeter. Plane-polarized light passes through a solution of optically active molecules, which rotate the plane of polarization.

Draw a stepwise mechanism for the following reaction:



Mechanism:

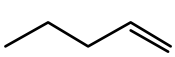


Draw a Reaction Coordinate for the above reaction:

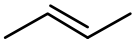
Label DG for the reaction, DG of Activation and the Transition State(s)

Draw any Transition State Structure(s):

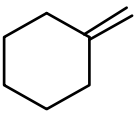
Alkene Addition Practice:



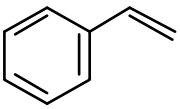
HBr →



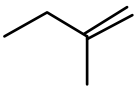
HBr →



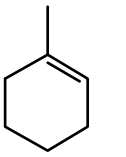
HBr →



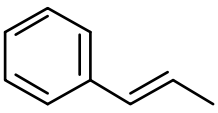
HI →



HBr →

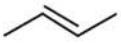


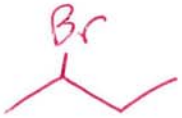
HCl →

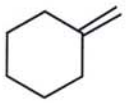


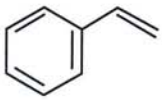
HBr →

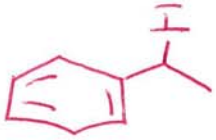
Alkene Addition Practice: Just draw major product

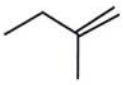


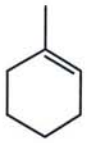


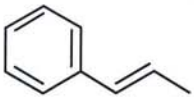


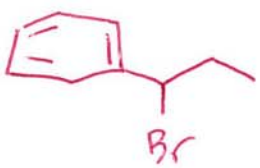








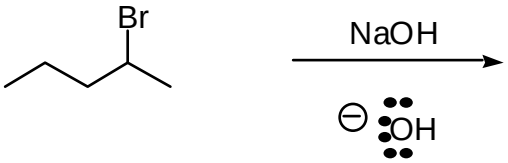


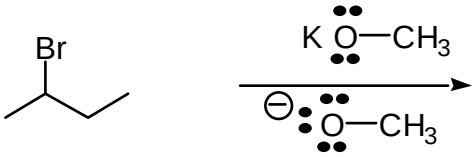


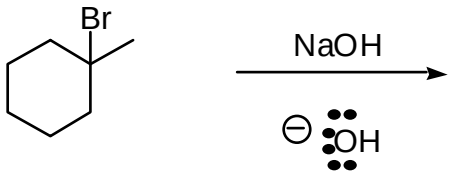
(

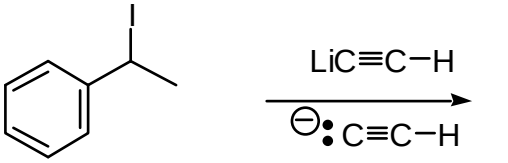
minor)

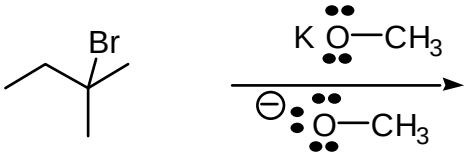
Elimination Reaction Practice:

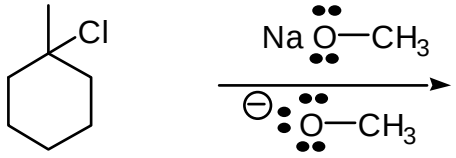


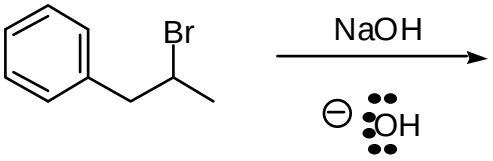




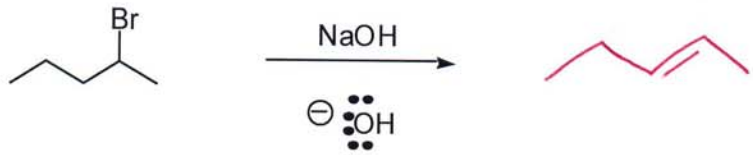




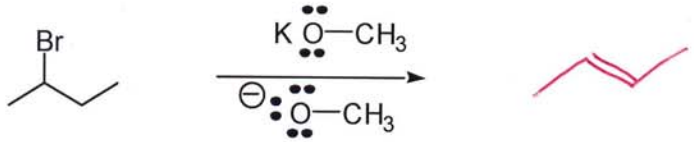




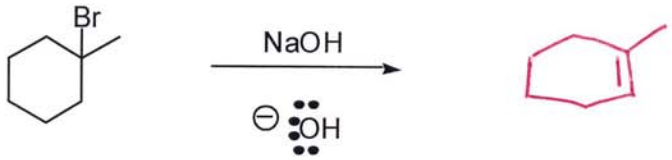
Elimination Reaction Practice: All E2 Major Products (note $t\text{-}O^{\ominus}K^{\oplus}$ would give least sub alkene)



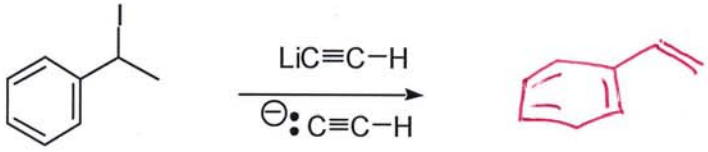
most sub alkene



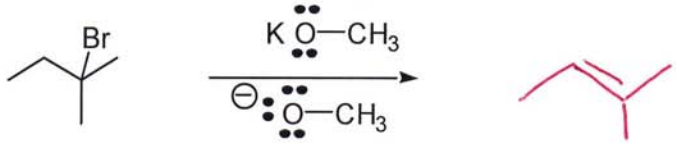
most sub alkene



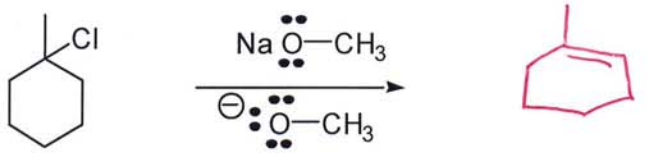
most sub alkene



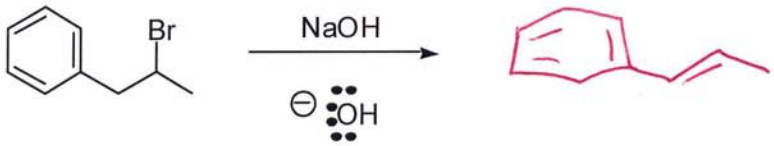
only possible product



most sub alkene

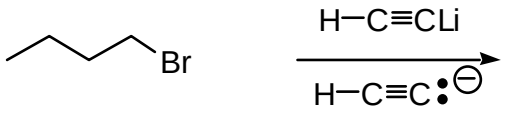


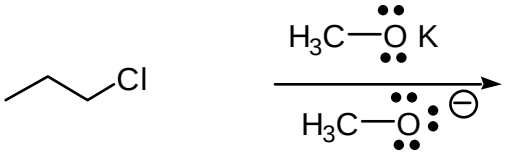
most sub alkene

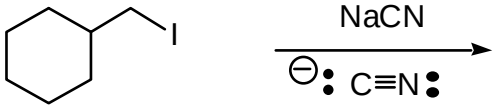


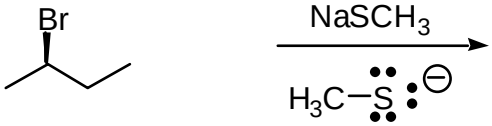
most sub and conjugated

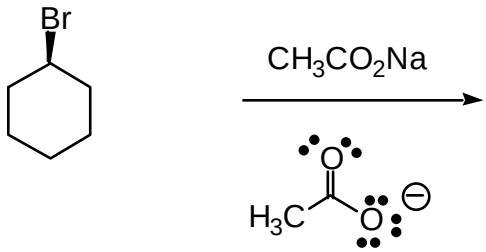
Substitution Practice:

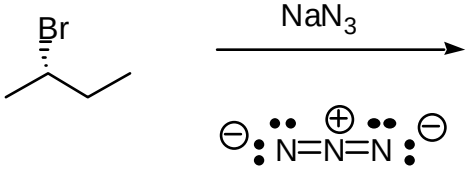




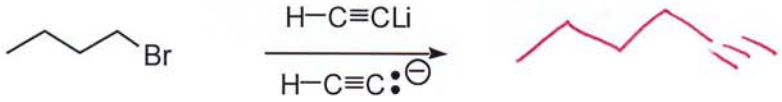


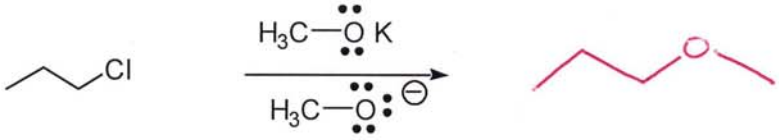


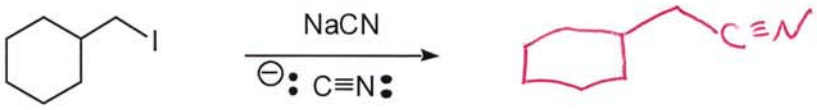


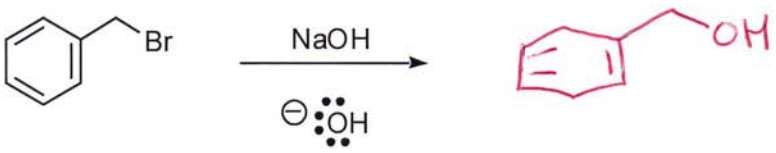


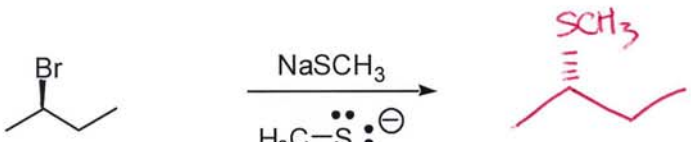
Substitution Practice: All S_N2

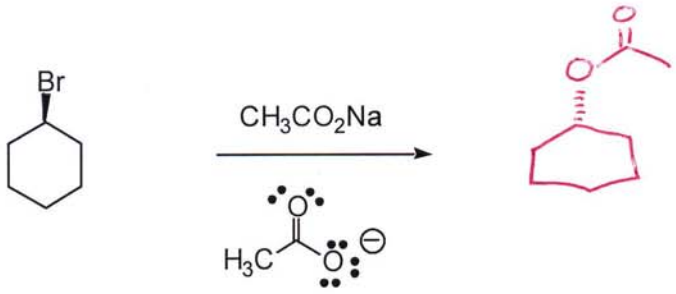


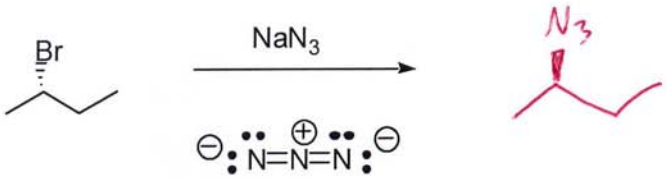






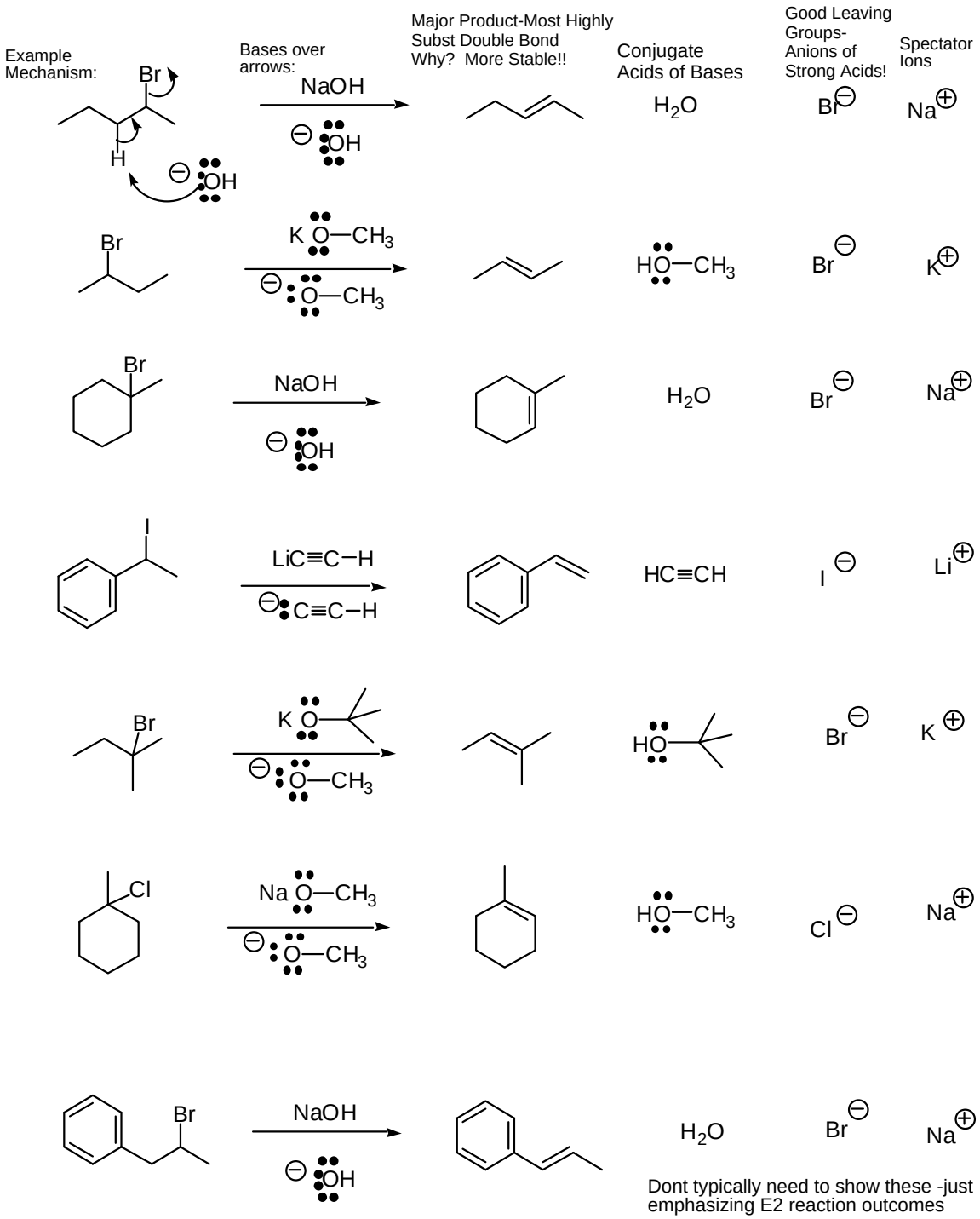






Elimination (E2) Reaction Practice:

Draw a mechanism for each reaction use the example mechanism for first reaction



Elimination versus Substitution Reactions:

The basicity of the base/nucleophile and the structure of the alkyl halide are the most important factors to consider when deciding whether a reaction proceeds by a Substitution or Elimination mechanism. Also the structure of the base can be important when bulky bases are used to effect an E2 elimination.

1. Primary Alkyl Halides:

a. SN2 reaction is favored, even with strong bases/nucleophiles such as CH_3CH_2ONa or NaOH. They will not act as bases in the reaction but as a Nucleophile and attack the primary halide, and do a SN2 displacement.

b. The only time you get an elimination reaction is with a bulky base such as $(H_3C)_3CONa$ (sodium t-butoxide). With added steric bulk, t-butoxide can not act as a nucleophile, therefore only an elimination process (E2) can occur.

c. Even with a poor nucleophiles such as H_2O, ROH or H_2S, any substitution reaction that will occur will proceed via an SN2 mechanism.

2. Secondary Alkyl Halides:

a. With Bases/Nucleophiles that are strongly basic, such as NaOH (pKa of H_2O=15) and RONa (pKa of alcohols=16-18) elimination will predominate. Other bases that could lead to elimination with secondary alkyl halides : Acetylene anion($HC{\equiv}CNa$) $NaNH_2$ and other conjugate bases of acids with a pKa>15.

b. With weakly basic but good nucleophiles (NaCN, NaO_2CCH_3, NaN_3, NH_3) SN2 will predominate (pKa range 5-12 for the above bases/nucleophiles). A polar aprotic solvent will improve conditions for an SN2 process.

c. For the above two scenarios (**a** and **b**) one must realize that although we are predicting the major product in these reactions, SN2 and E2 reactions are competitive processes. Both products most likely will be observed, with one compound in a greater proportion. We would have to do the chemistry to test accuracy and usefulness of our predictions. (i.e. Good desired product ratio such as 80:20 vs a poor ratio such as 60:40)

d. With poor nucleophiles such as H_2O or ROH, an SN1 reaction process would predominate, with the accompanying minor product being the E1 product. Anything that might stabilize the intermediate cation (Resonance) such as the cation being allylic (or benzylic) or the use of a polar protic solvent would increase the likelihood of and SN1 reaction.

3. Tertiary Alkyl Halides:

a. With Bases/Nucleophiles that are strongly basic, such as NaOH and RONa elimination (E2) will predominate. Other bases that could lead to elimination : Acetylene anion, $HC{\equiv}CNa$, $NaNH_2$ and other conjugate bases of acids with a pKa$\geq$15.

b. With poor nucleophiles such as H_2O or ROH, an SN1 reaction process would predominate, with the accompanying minor product being the E1 product. The SN1 process is aided by the use of a polar protic solvent.

c. SN1 reactions also occur with tertiary alcohols with treatment with a mineral acid (HX such as: HCl, HBr etc.) to form tertiary alkyl halides.

Nature of Nucleophiles:

Strongly Basic/Nucleophilic:
General Rule: pKa>15

NaOH, RONa, $NaNH_2$

$HC{\equiv}CNa$

Moderately Nucleophilic, Weakly Basic:

General Rule: 5<pKa<12

$NaCN$, NaN_3, NH_3

NaO_2CCH_3 (Sodium Acetate)

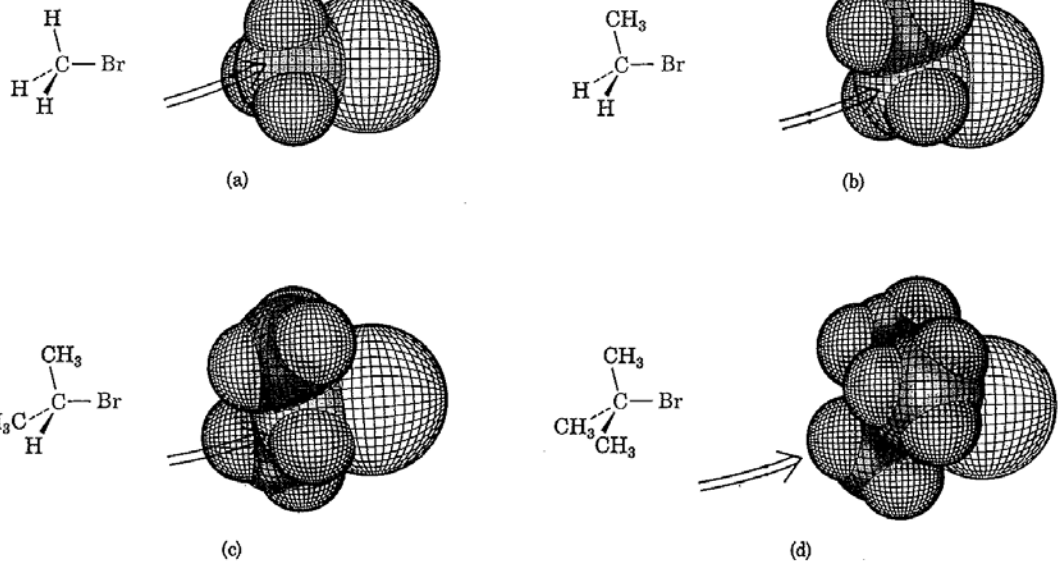
$NaSR$

Non-Basic, Weakly Nucleophilic:

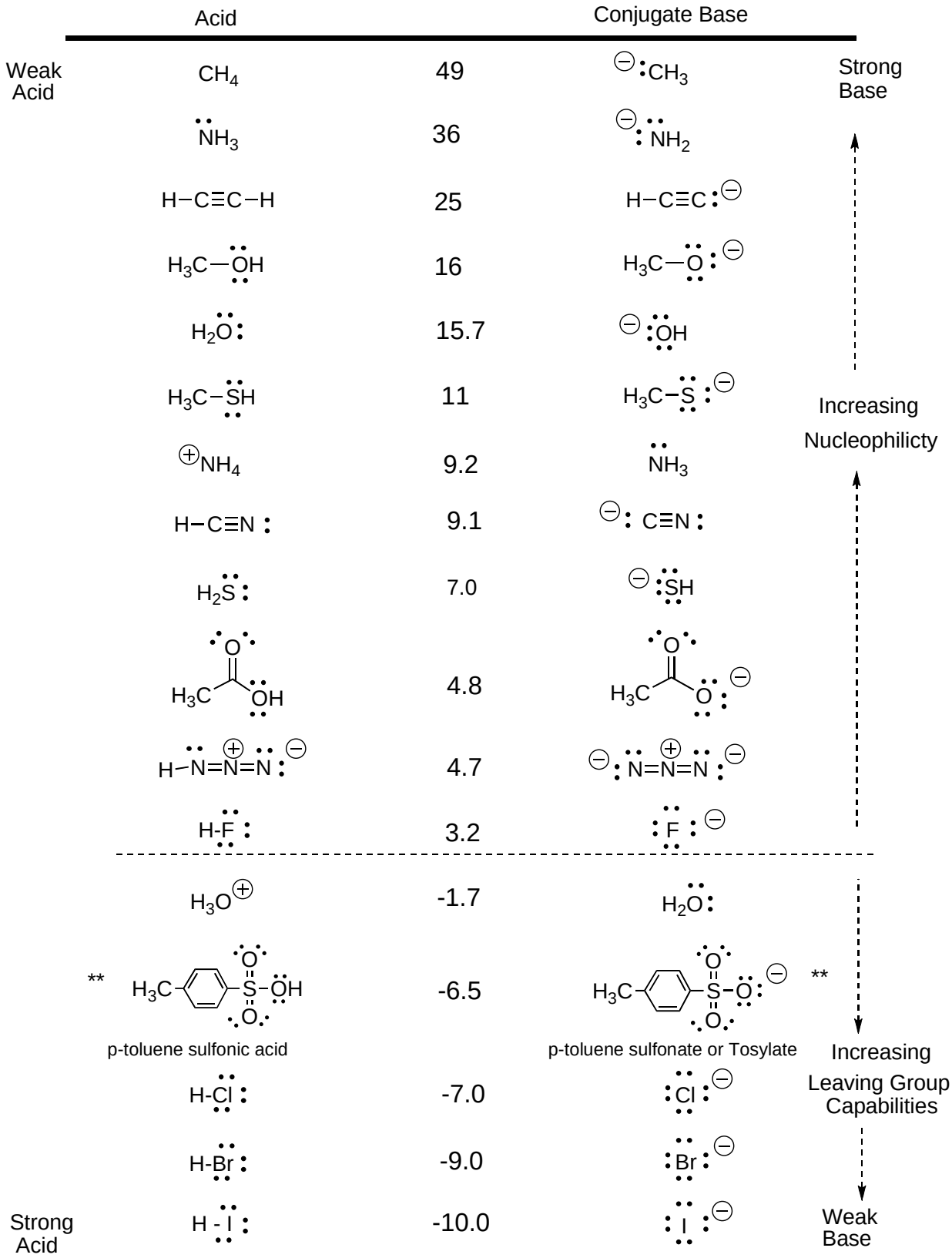
General Rule: pKa<5

H_2O, ROH

Steric hindrance of S_N2 reactions



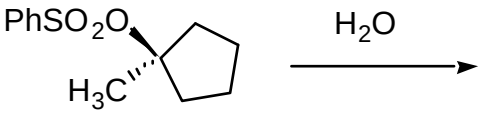
pKa Table: Acidity and Basicity



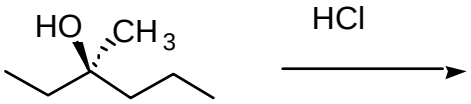
Substitution vs Elimination Practice Problems:

For the following reactions give the major product of the reaction and the mechanism (SN1, SN2, E1, E2). Be sure to include the stereochemical outcome.

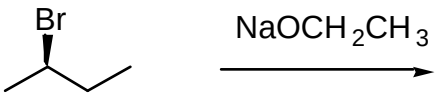
a.



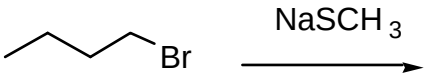
b.



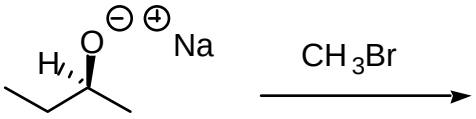
c



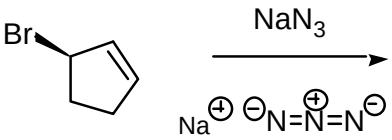
d.



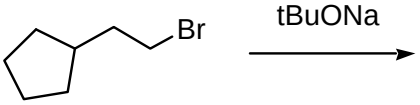
e.



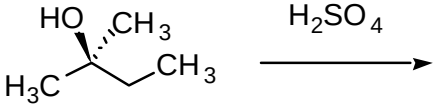
f.



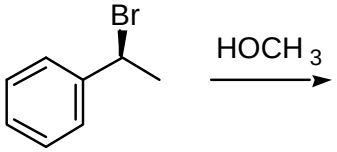
g.



h.



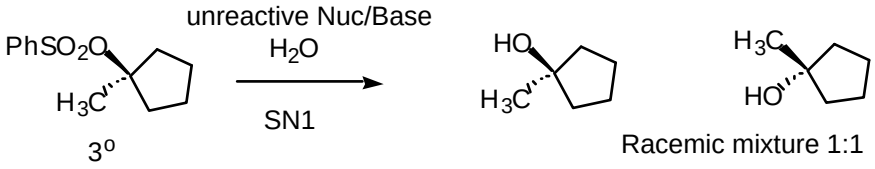
i.



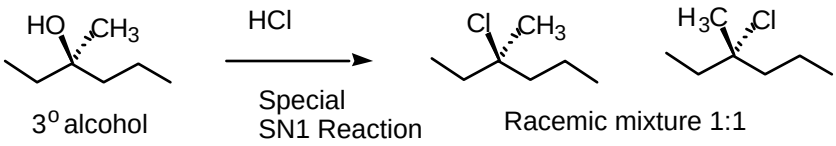
Substitution vs Elimination Practice Problems:

For the following reactions give the major product of the reaction and the mechanism (SN1, SN2, E1, E2). Be sure to include the stereochemical outcome.

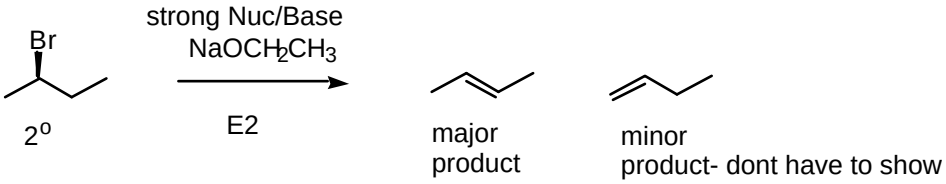
a.


unreactive Nuc/Base
H_2O
SN1
$PhSO_2O$
H_3C
3°
HO
H_3C
H_3C
HO
Racemic mixture 1:1

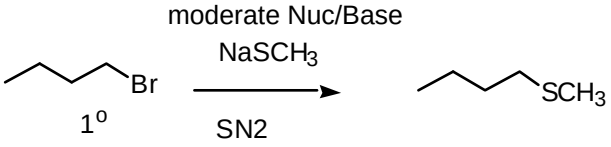
b.


HO CH_3
3° alcohol
HCl
Special
SN1 Reaction
Cl CH_3
H_3C Cl
Racemic mixture 1:1

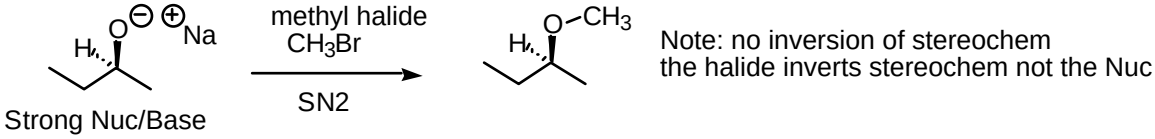
c


strong Nuc/Base
$NaOCH_2CH_3$
Br
2°
E2
major
product
minor
product- dont have to show

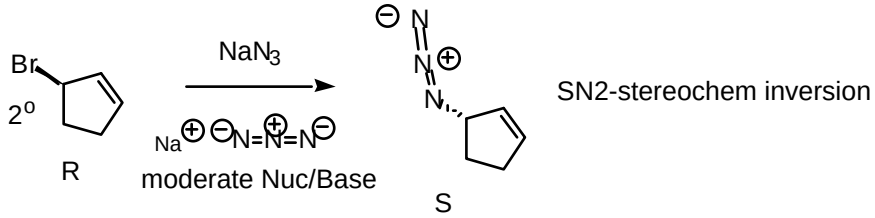
d.


moderate Nuc/Base
$NaSCH_3$
Br
1°
SN2
SCH_3

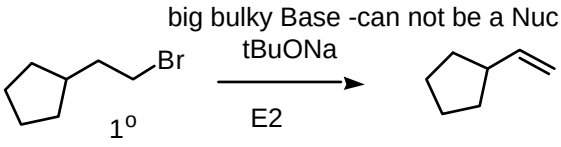
e.


methyl halide
CH_3Br
O Na
H
Strong Nuc/Base
SN2
O CH_3
H
Note: no inversion of stereochem
the halide inverts stereochem not the Nuc

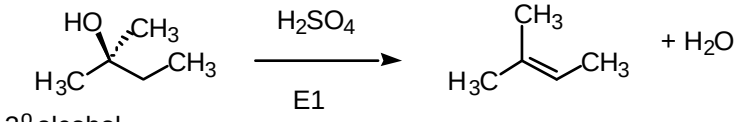
f.


Br
2°
R
NaN_3
$Na^{\oplus}\ ^{\ominus}N=N^{\oplus}=N^{\ominus}$
moderate Nuc/Base
N
N
N
S
SN2-stereochem inversion

g.


big bulky Base -can not be a Nuc
tBuONa
Br
1°
E2

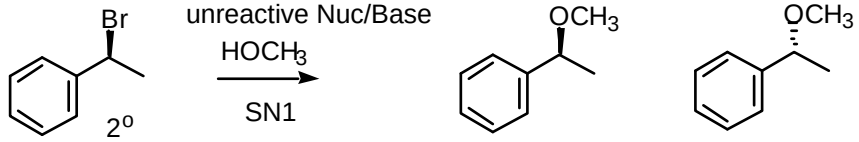
h.



3^o alcohol

only time we have E1
mechanism leading to the product

i.



2^o

but with resonance
so cation is more stable

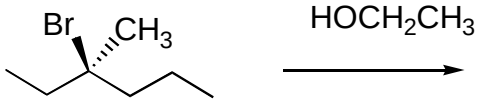
Racemic mixture 1:1

Substitution vs Elimination Practice Problems: In Class Problems 2

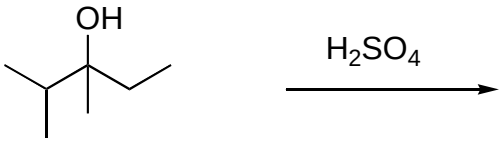
For the following reactions give the major product of the reaction and the mechanism (SN1, SN2, E1, E2). Be sure to include the stereochemical outcome.

a.

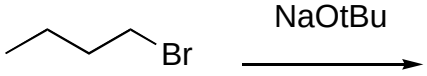
b.



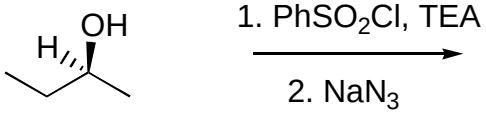
c



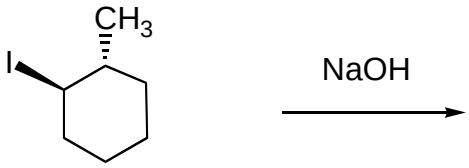
d.



e.



f.

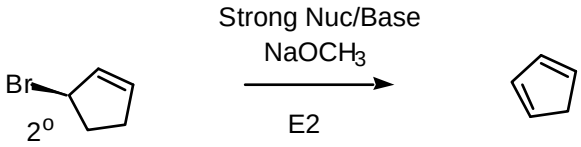


g.

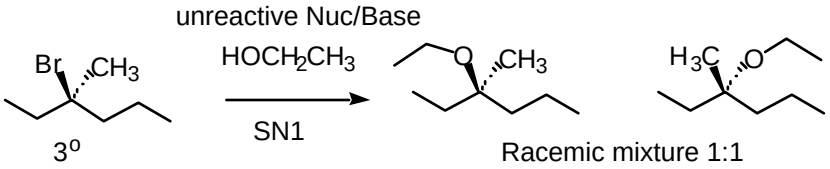
Substitution vs Elimination Practice Problems: In Class Problems 2

For the following reactions give the major product of the reaction and the mechanism (SN1, SN2, E1, E2). Be sure to include the stereochemical outcome.

a.

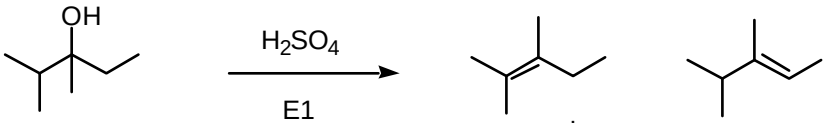


b.



Racemic mixture 1:1

c



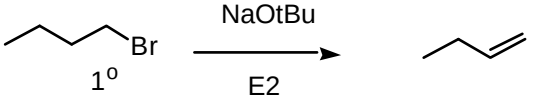
3° alcohol

major product

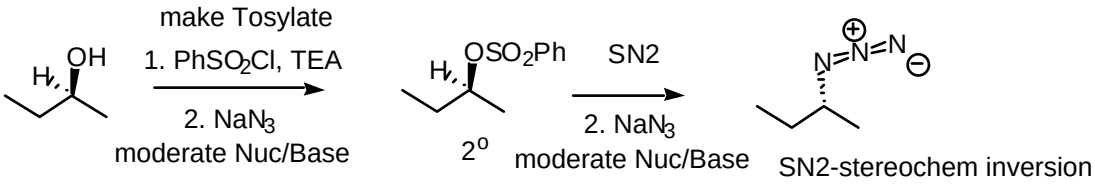
minor product- dont have to show

only time we have E1 mechanism leading to the product

d.

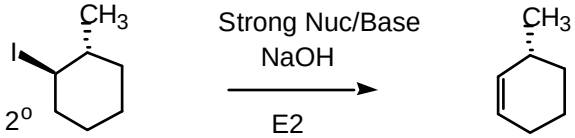


e.



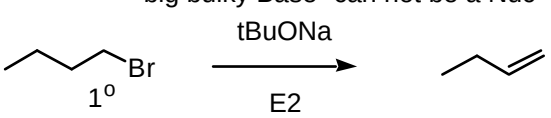
SN2-stereochem inversion

f.



Anti -H and leaving group required for E2

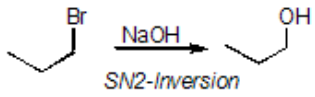
g.



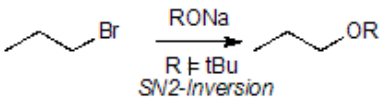
opps-same as above

ORGANIC REVIEW SHEET- SUBSTITUTION, ELIMINATION AND ALKENE ADDITION RXNS

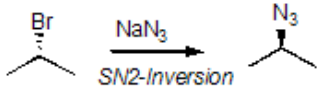
Substitution Reactions: Some Examples



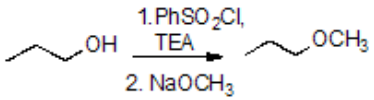
SN2-Inversion



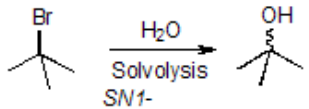
SN2-Inversion



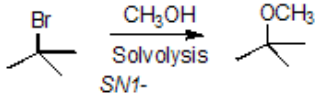
SN2-Inversion



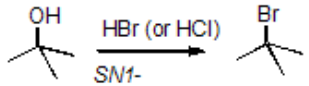
SN2-Inversion



SN1-
Racemic

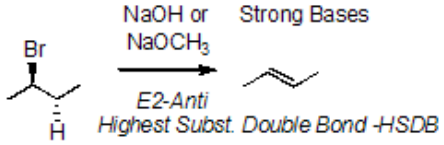


SN1-
Racemic

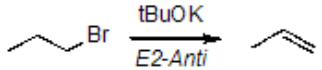


SN1-
Racemic

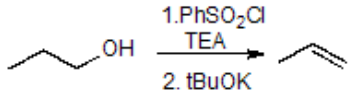
Alkene Synthesis, Elimination Rxns: Some Examples

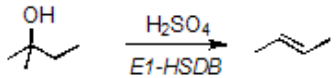


E2-Anti
Highest Subst. Double Bond -HSDB



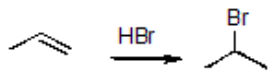
E2-Anti
HSDB

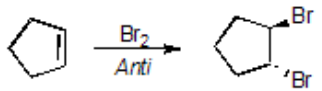


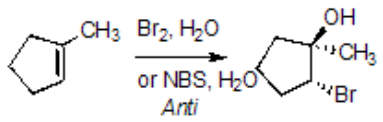


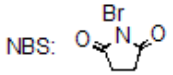
E1-HSDB

HBr and Br_2 Addition Reactions

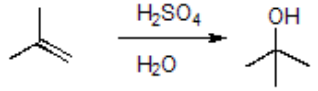


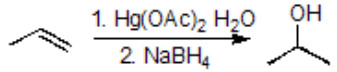


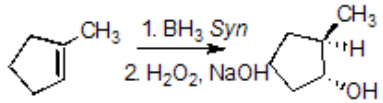




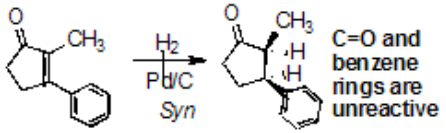
Hydration Reactions: Addition of H_2O





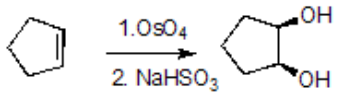


Reduction of Alkenes, Hydrogenation: Addtion of H_2

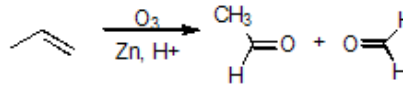


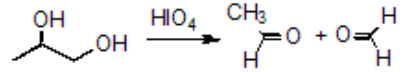
C=O and benzene rings are unreactive

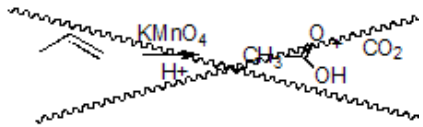
Dihydroxylation Reaction: Addition of 2 -OH Grou



Oxidative Cleavage Reactions



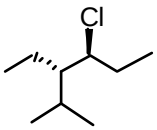




Organic Chemistry I **KEY** **Chemistry 31**
Sample Exam I **100 points**

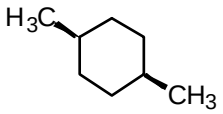
1 . Name the following structures including cis, trans and/or R, S designations when appropriate.

a.



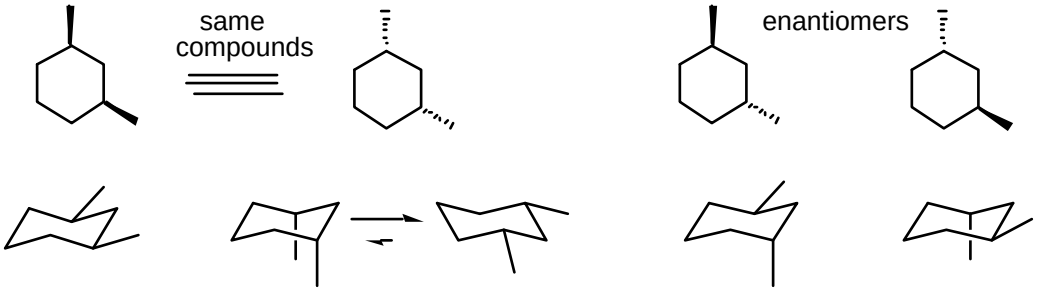
3S, 4S 4-chloro-3-ethyl-2-methylhexane

b.

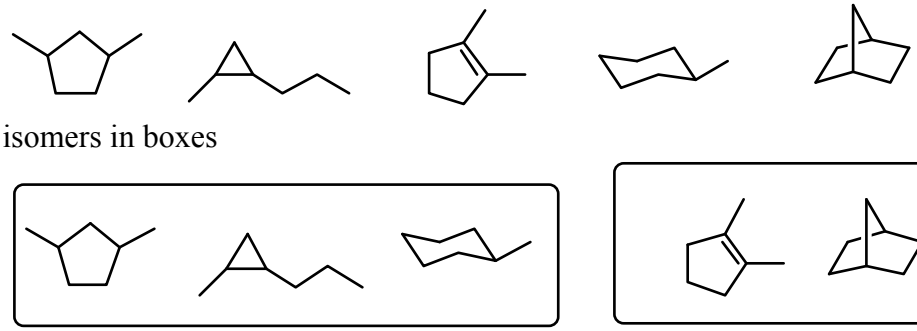


cis 1,4 dimethylcyclohexane

2. Draw all the possible stereoisomers isomers of 1, 3 dimethylcyclohexane. Draw the most stable chair conformations of these isomers.



3. For the following set of compounds below, circle the compounds that are isomers of each other.

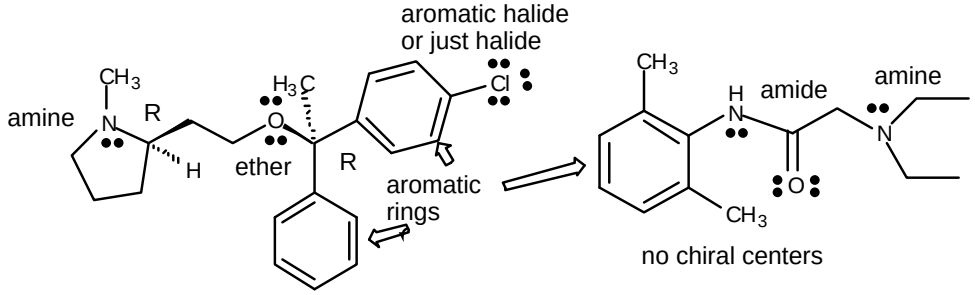


isomers in boxes

4. a. For molecules below, label the functional groups and fill in any nonbonding electrons.

b. What is the total number of sp^2 oxygen atoms below? ___1_____ Total number of sp^2 carbons?___19_____

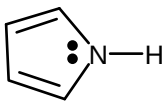
c. Label all the chiral centers in the following compounds and assign R and S configuration



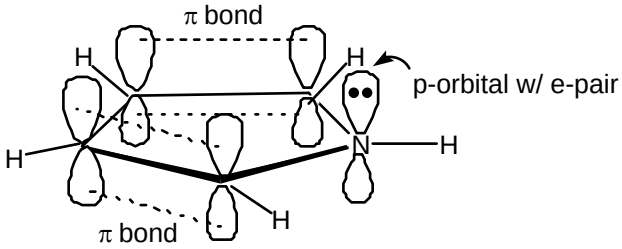
Tavist D (An OTC Antihistamine) **Lidocaine (Local Anesthetic)**

5. Pyrrole has an interesting structure. The nitrogen is sp2 hybridized so the nonbonding electrons are placed in an orbital that is properly oriented to be shared with the other adjacent π-bonds. What kind of orbital is that? To the right of the pyrrole's structure below is a side view of this compound showing the main σ-bonds only. Add the appropriate orbitals and bonds to complete the structure that are consistent with pyrrole's structure and hybridization at each atom. As always, assume the appropriate number of hydrogens on carbon.

Pyrrole



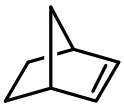
Side View of Pyrrole --just fill in the orbitals to complete the structure



all p-orbitals shown making π-bonds; e-pair in p-orbital too since sp2 hybrid.
All atoms sp2 hybridized

6. For the following pairs of molecules, determine the relationship between the two: enantiomers, diastereomers, identical or structural isomers.

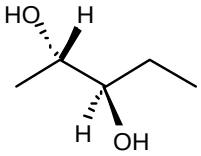
a.



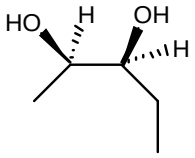
identical compounds

compounds are not chiral, mirror plane bisects both

b.



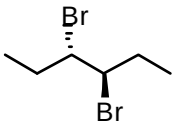
S,R



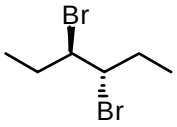
R,S

enantiomers: S,R relects to R,S
Note: second structure is just rotated funny
Rotate it 180° and you can see that both chiral centers are inverted from SR to RS in the second structure

c.



S, R

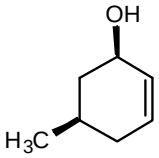


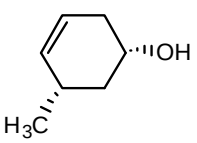
R, S

identical compounds

molecules with chiral centers but are not chiral-meso

d.





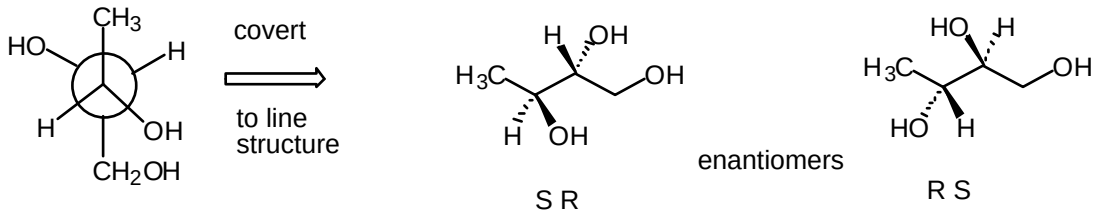
structural isomers

look carefully at the postion of the pi bond, adjacent to -OH in first compound,
2 Cs away in the second compound

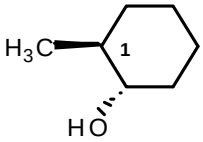
e.

identical compounds, superimposible

f. This one is pretty tough-a little combination Newman projection and chirality. Write the Newman like a regular line bond structure and then compare to the second structure.



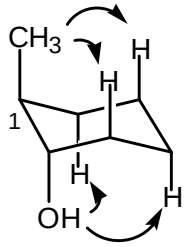
7. For the following molecule, perform a complete conformational analysis using the data provided in Table 1.



3. Draw the two chair conformations possible for the compound. Fill in the appropriate substituents on the chairs below.

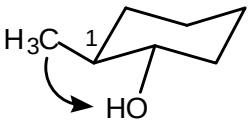
Conformation A

2 x 1,3 Diaxial
CH3-H interactions



2 x1,3 Diaxial
OH - H interactions

Conformation B



1 x CH3-OH Gauch interaction

No 1,3 Diaxial interactions

b. Calculate the energy difference between the two chair conformations drawn above. For gauche interactions between a methyl (-CH_3) and some other group, use the value for the 1,3 Diaxial interaction of that group from Table 1. For example a gauche interaction between a methyl (-CH_3) and a ethyl (-CH_2CH_3) group would be 0.95 kcal/mol.

And likewise, gauche interaction between a methyl (-CH_3) and a hydroxyl (-OH) group would be 0.5 kcal/mol

2 x 0.9 + 2 x 0.5 = 2.8 kcal/mol

1 x 0.5 = 0.5 kcal/mol

c. Estimate the ratio of most stable to least stable conformation that could be found in a sample of this compound at 25°C.

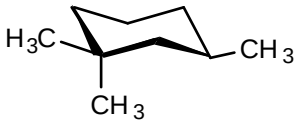
Energy difference: Conformation A is 2.3 kcal/mol higher in energy
A:B is about 2:98

d. Briefly explain why we can use the 1,3 Diaxial interaction values to approximate the gauche interactions between a methyl and other groups?

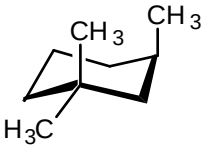
Since 1,3 diaxial interactions are just like 60° staggered interaction with two groups, the 1,3 diaxial interactions with a group in the axial position is really a Y-CH2 interaction. Since when Y=CH3 the energy is exactly 0.9, just like the gauge interaction in butane, this Y-CH2 staggered interaction is a good approximation of a Y-CH3 gauche, where Y=substituents in Table 1

8. Determine which molecule is more stable or if they are equal in energy in each of the following pairs and **<u>explain your answer briefly</u>**.

a.

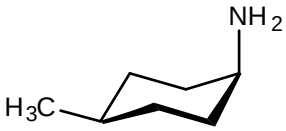


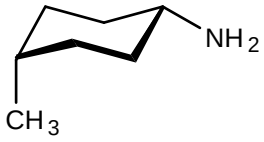
more stable
2 groups equatorial



two groups axial
and 2 axial CH3s interacting

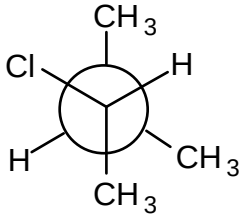
b.



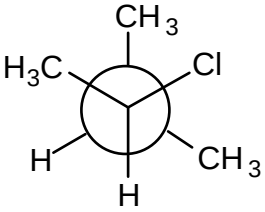


more stable
bigger -CH3 group equatorial

c.

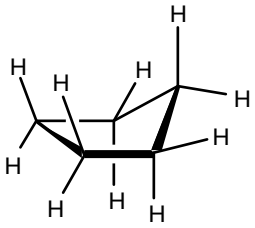


more stable
2 staggered interactions

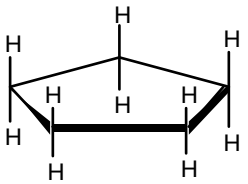


3 staggered interactions

d.

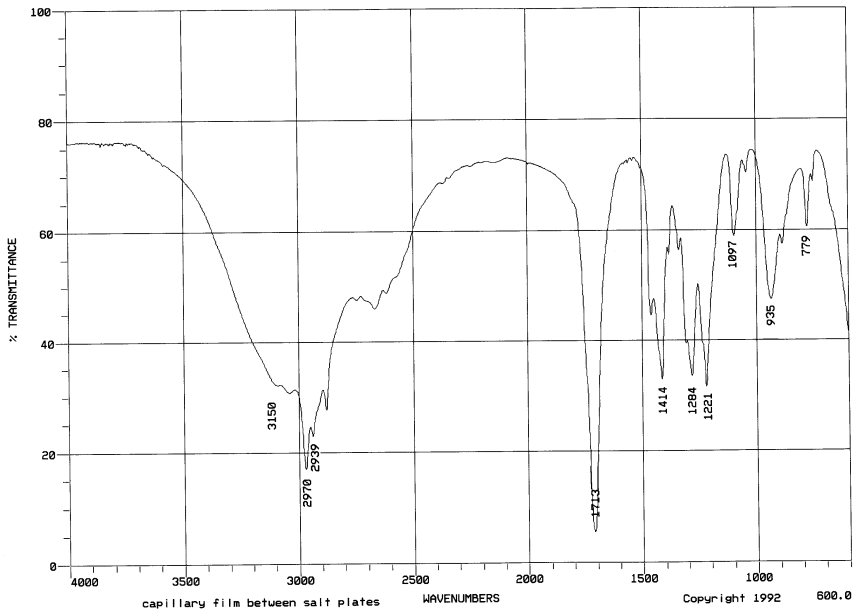


more stable
less eclipsing interactions



all eclipsing interactions

9. You are trying to determine the identity of a compound that you have unexpectedly produced in your laboratory. You determine that the compounds molecular formula is $C_4H_8O_2$. You take an IR spectrum, which is shown below and a ^{13}CNMR and determine there are 4 peaks in the spectrum. Answer the questions below to determine the structure.

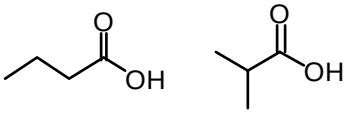


big carboxylic acid peak ^ ^ C=O peak

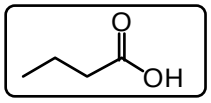
a. What is the major functional group in this molecule?

Carboxylic acid!!!

b. Knowing the functional group and molecular formula, draw all of the possible isomers for this compound? (There are at most 2 isomers if you have the functional group correct).

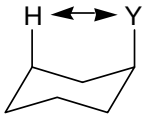


c. Which of the above structures is consistent with the ^{13}CNMR data?



4 peaks in CNMR; second structure above has 3 peaks in CNMR

Table 1: Steric Strain Due to 1,3-Diaxial Interactions



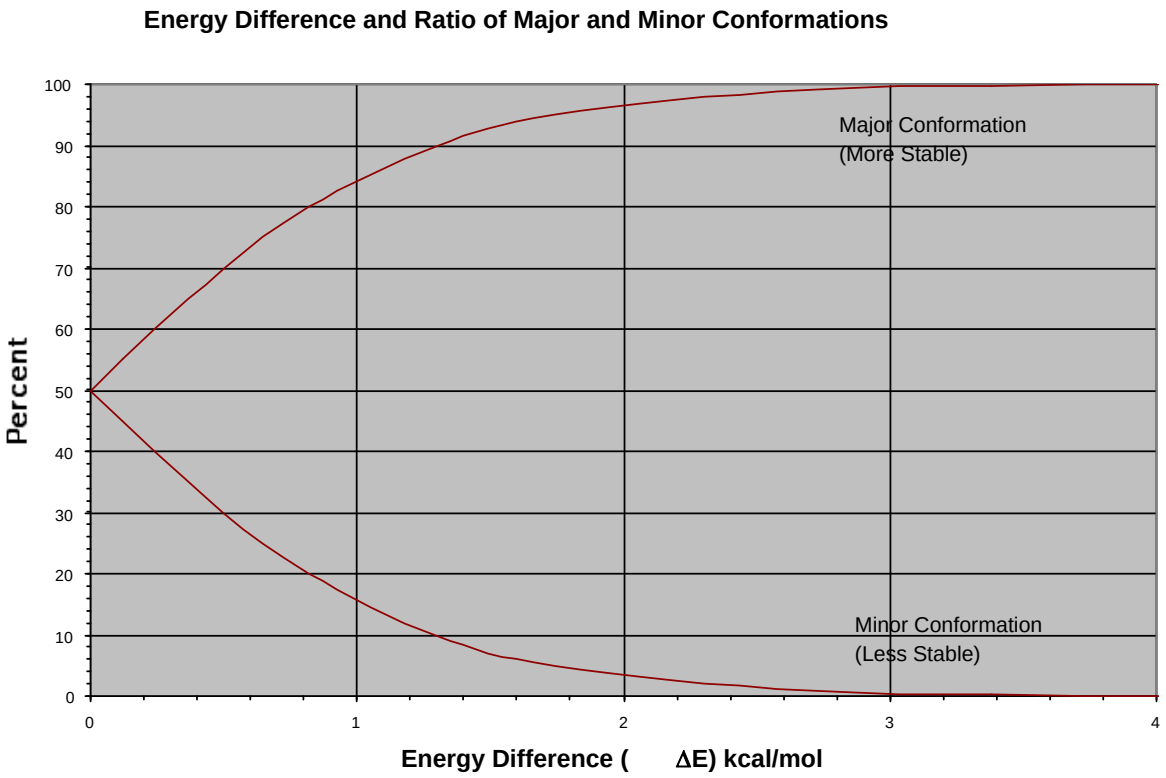
Strain of one H-Y 1,3-Diaxial Interaction		
Y	(kcal/mol)	(kJ/mol)
-F	0.12	0.5
-Cl	0.25	1.4
-Br	0.25	1.4
-OH	0.5	2.1
$-CH_3$	0.9	3.8
$-CH_2CH_3$	0.95	4.0
$-CH(CH_3)_2$	1.1	4.6

$-C(CH_3)_3$	2.7	11.3
$-C_6H_5$	1.5	6.3
-COOH	0.7	2.9
-CN	0.1	0.4

Relationship Between Stability and Isomer Percentages at Equilibrium**

More stable isomer (%)	Less stable isomer (%)	Energy difference at 25˚C (kcal/mol)	(kJ/mol)
50	50	0	0
75	25	0.651	2.72
90	10	1.302	5.45
95	5	1.744	7.29
99	1	2.722	11.38
99.9	0.1	4.092	17.11

**The values in this table are calculated from the equation $K = e^{-(\Delta E/RT)}$, where K is the equilibrium constant between isomers; e ≈ 2.718 (the base of natural logarithms); ΔE = energy difference between isomers; T = absolute temperature (in kelvins); and R = 1.986 cal/mol •K (the gas constant).

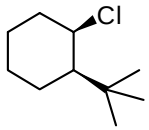


Infrared Spectroscopy: Simplified Correlation Table

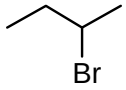
	Frequency	Intensity
O-H	3400 cm^{-1}	Large, Broad
Carboxylic Acids	3200-2500 cm^{-1}	Large, Broad
C-H		
Aliphatic	Below 3000 cm^{-1}	Large
Aromatic & Vinyl	Above 3000 cm^{-1}	Medium
Aldehyde	2850, 2750 cm^{-1}	Medium (Two)
C=O	1690 cm^{-1} - 1715 cm^{-1}	Large, Sharp
Ester	1735 cm^{-1}	Large, Sharp
Conjugation	1690 cm^{-1}	Large, Sharp
C≡C	2250-2100 cm-1	Small
C≡N	2250 cm-1	Medium
$-NO_2$	1600, 1500 cm^{-1}	Large (Two)

Organic Chemistry I Chemistry 31
Sample Exam II **Key - short version, I wanted to get it out quickly** 100 points

1. Name the following compounds.



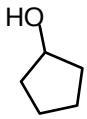
1-*tert*-Butyl-2-chloro-cyclohexane

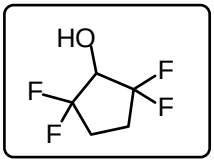


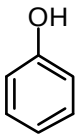
2-bromobutane

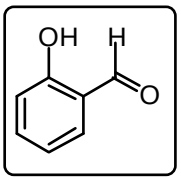
2. Decide which of the following sets of compounds are more acidic and estimate the pKa for both acids. Briefly explain why the compound you chose is more acidic. See pKa numbers rationale below.

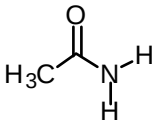
16 10-12, inductive effects 10 7-8, resonance stabilized anion (by C=O)

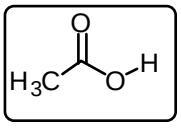


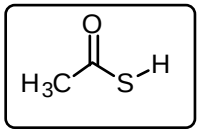


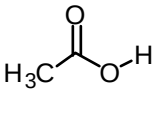








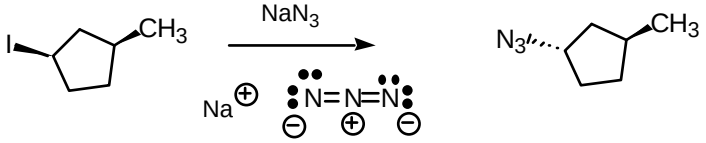




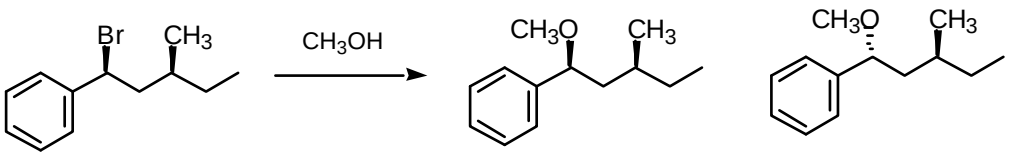
4. 5, anion on more electronegative atom-oxygen about 3 charge on S, larger, more stable anion

3. For the following reactions give the major product of the reaction and the mechanism (SN1, SN2, E1, E2). Be sure to include the stereochemical outcome.

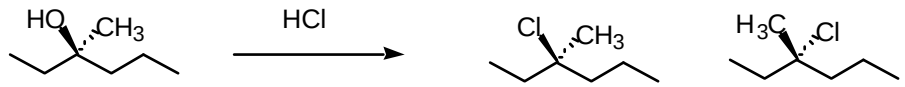
a. 2^o , moderate nuc/base, SN2, inversion



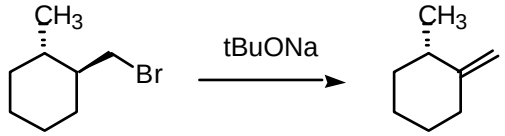
b. 2^o with resonance possibility, poor nuc/base -SN1, racemic mixture (actually here the products are diastereomers, since there was a chiral center in the starting compound)



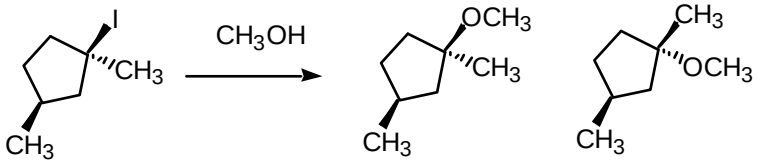
c. 3° alcohol with strong acid, HCl- SN1, racemic mixture



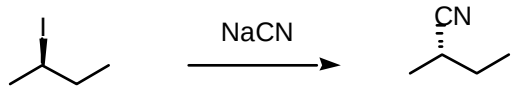
d. 1°, bulky base-E2



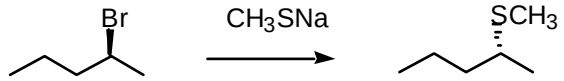
e. 3°, poor nuc/base -SN1, racemic mixture (actually here the products are diastereomers, since there was a chiral center in the starting compound)



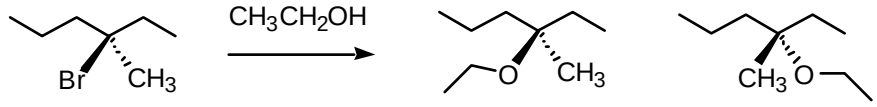
f. . 2° , moderate nuc/base, SN2, inversion



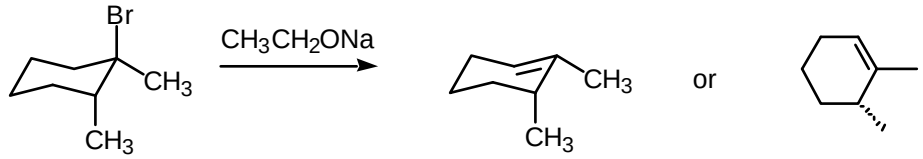
g. . 2° , moderate nuc/base, SN2, inversion



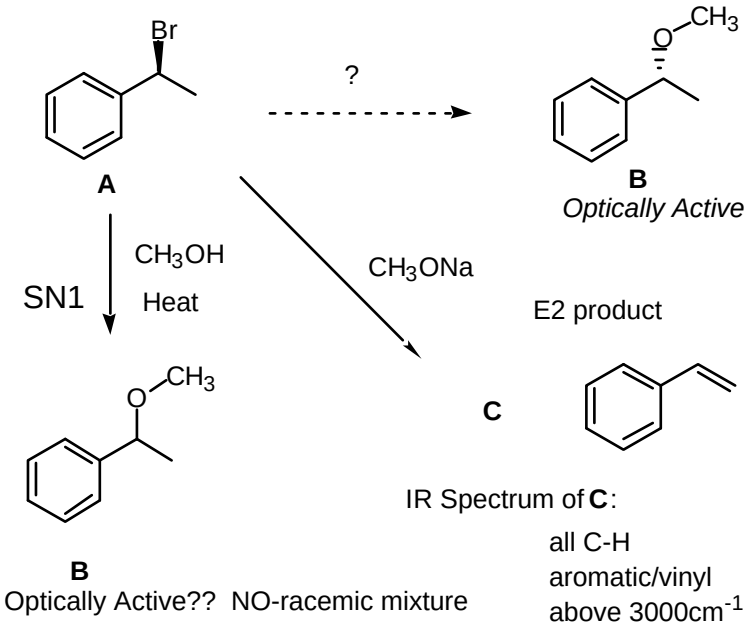
h. 3°, poor nuc/base -SN1, racemic mixture



i. 3°, strong nuc/base-E2



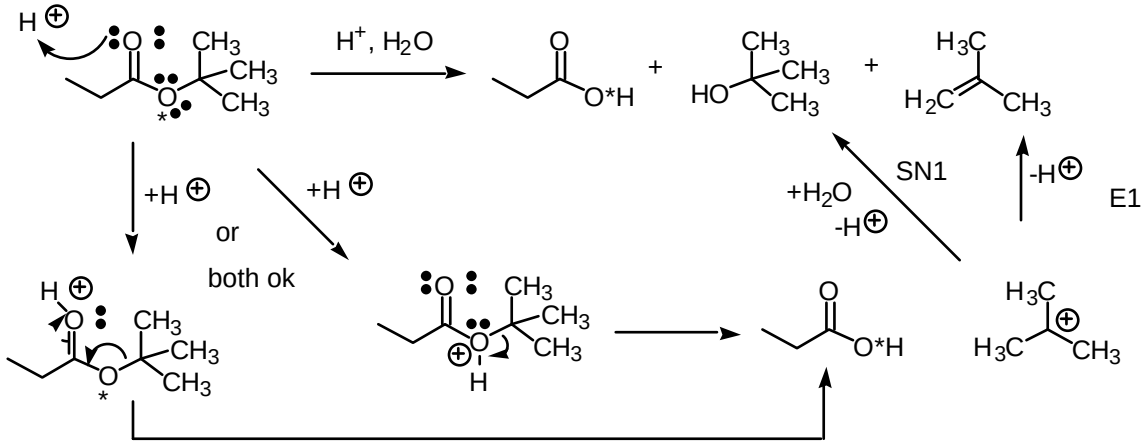
4. **Compound A**, a chiral alkyl halide, was reacted with $NaOCH_3$ in an attempt to form the optically active ether, **Compound B**. The major product obtained after purification was **Compound C**. Determine the structure of **Compound C** from the major peaks in the IR spectrum provided. **Compound A** was also treated with CH_3OH and heat. Subsequent spectroscopic analysis of the reaction product (IR and NMR) it appeared that **Compound B** was produced. Was optically active **Compound B** obtained? Explain your answer and give the mechanism (SN2, SN1, E2, or E1) for each of the reactions shown below.



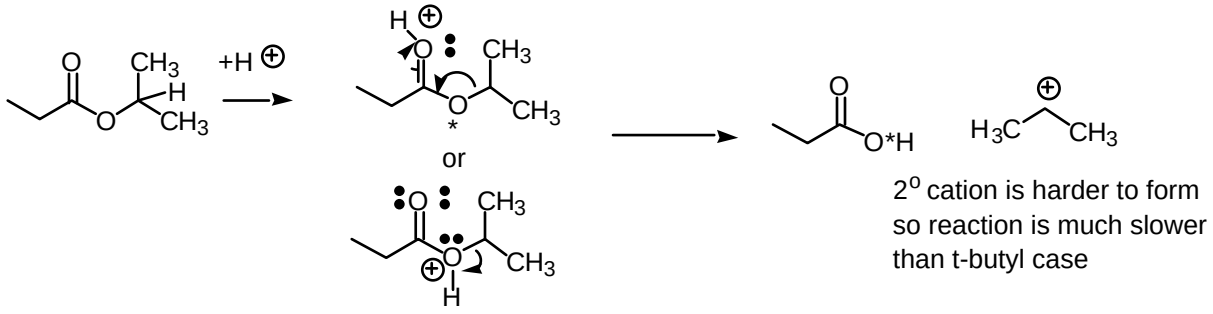
IR spectral data of C:

Large peak just above 3000 cm^{-1}
No peaks: 3400, just below 3000,
1720 cm^{-1}

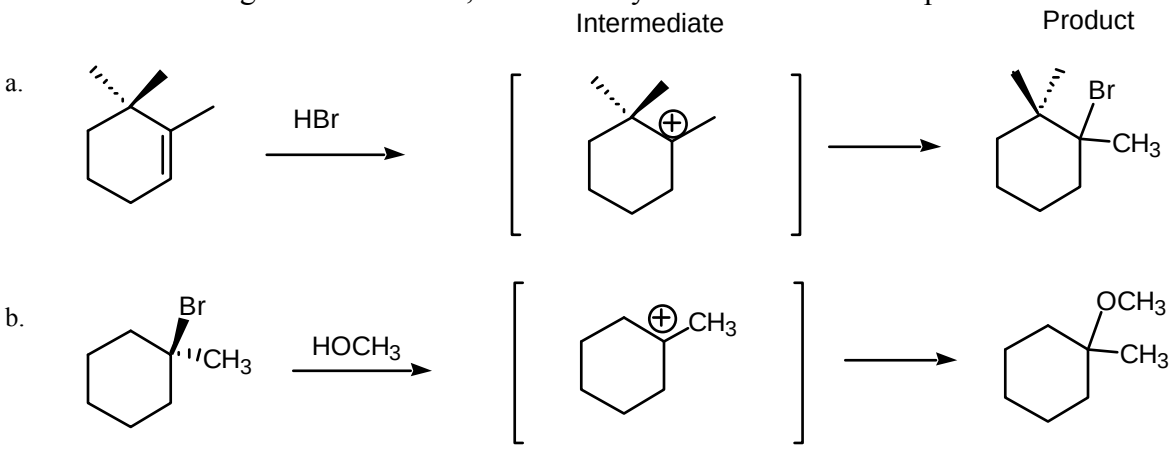
5. t-Butyl esters are synthetically useful protecting groups for carboxylic acids. They can be cleaved quite readily using aqueous acids such as H_2SO_4 to yield the carboxylic acid and t-butanol plus small amounts of 2-methylpropene. Draw a reasonable mechanism that explains this reaction, including the formation of both t-butanol and 2-methylpropene. (Note where the oxygen with the asterisk (O*) is in the starting material and the product)



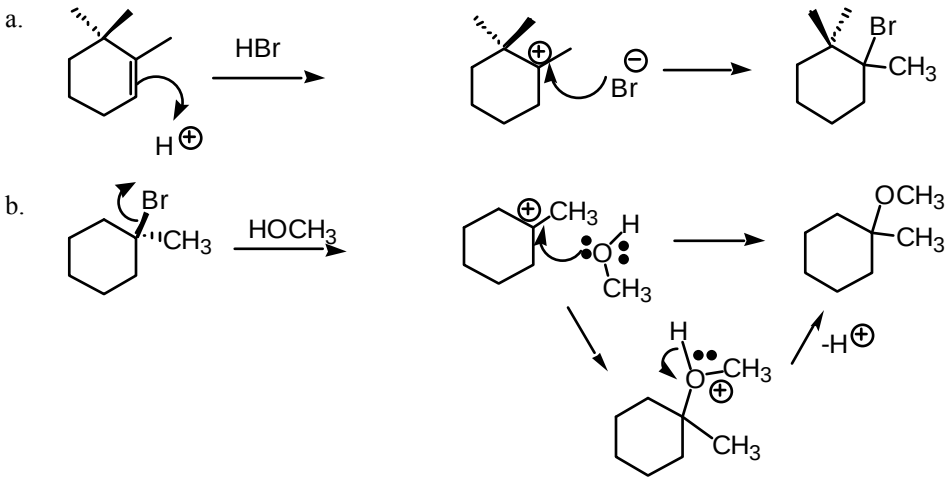
b. Isopropyl esters are not as easily cleaved with acid as t-butyl esters. Explain.



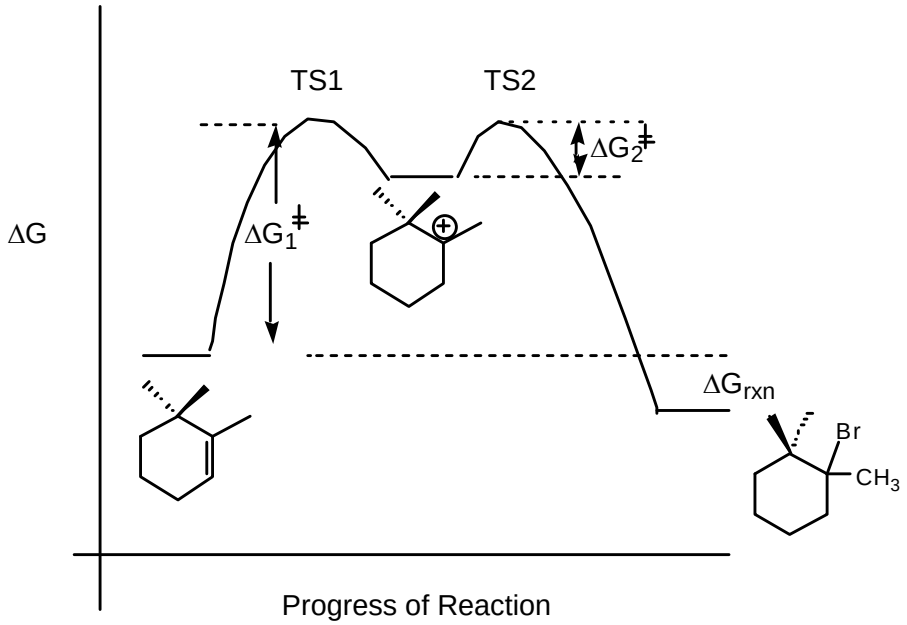
6. For the following reactions below, draw the key intermediate and the product structures



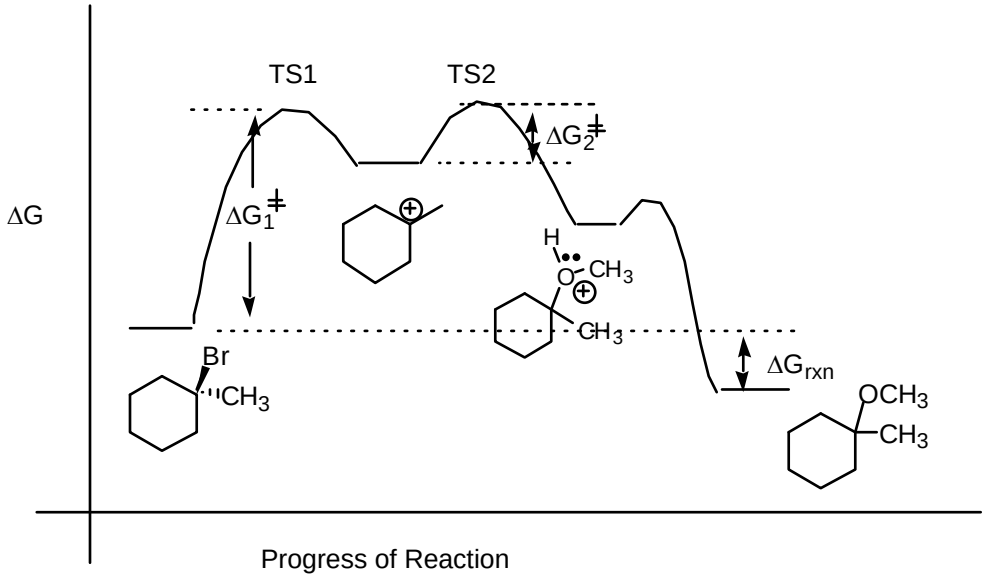
c. For each of the above reactions, draw a reasonable mechanism that accounts for the observed product, showing all steps and intermediates.



d. Draw a reaction coordinate diagram for each reaction. Be sure to label the transition state(s), intermediate(s) and the energy of activation(s) and energy of reaction.
Reaction a:

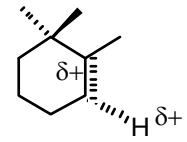


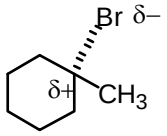
Reaction b:



e. For the transition state(s) draw the structure(s) of the transition state(s) using the conventions for drawing such structures.

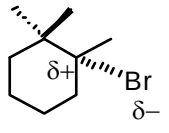
TS1

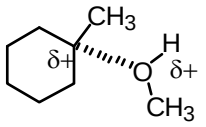




TS1

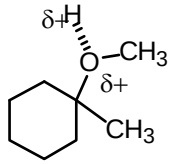
TS2





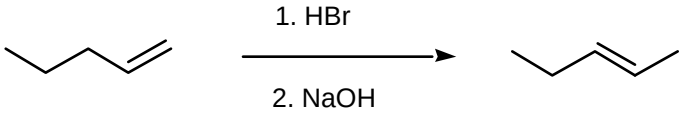
TS2

TS3-for fun

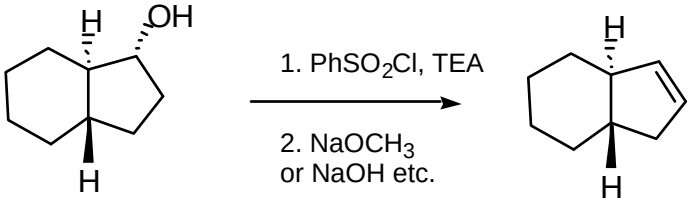


7. For the following multistep transformations, show what reagents would be used to synthesize the desired products in a practical manner. Show all your steps.

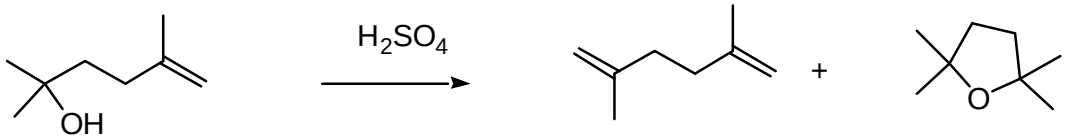
a.



b.

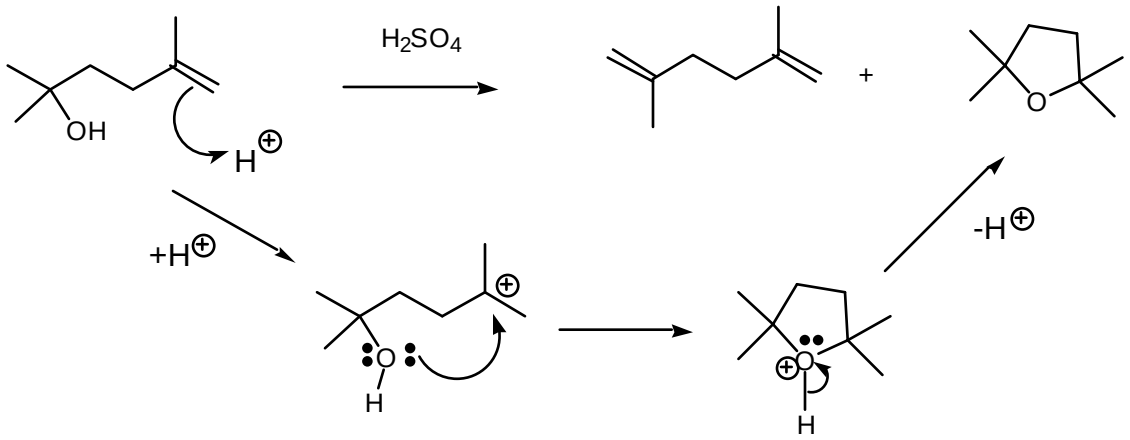


8. In the following elimination reaction to form the di-alkene product an ether side product was formed. Draw a reasonable mechanism to explain this result. Just need to explain the formation of the ether.

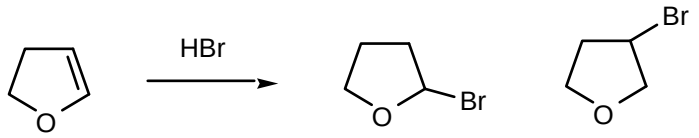


di-alkene product ether side product

Mechanism for #8



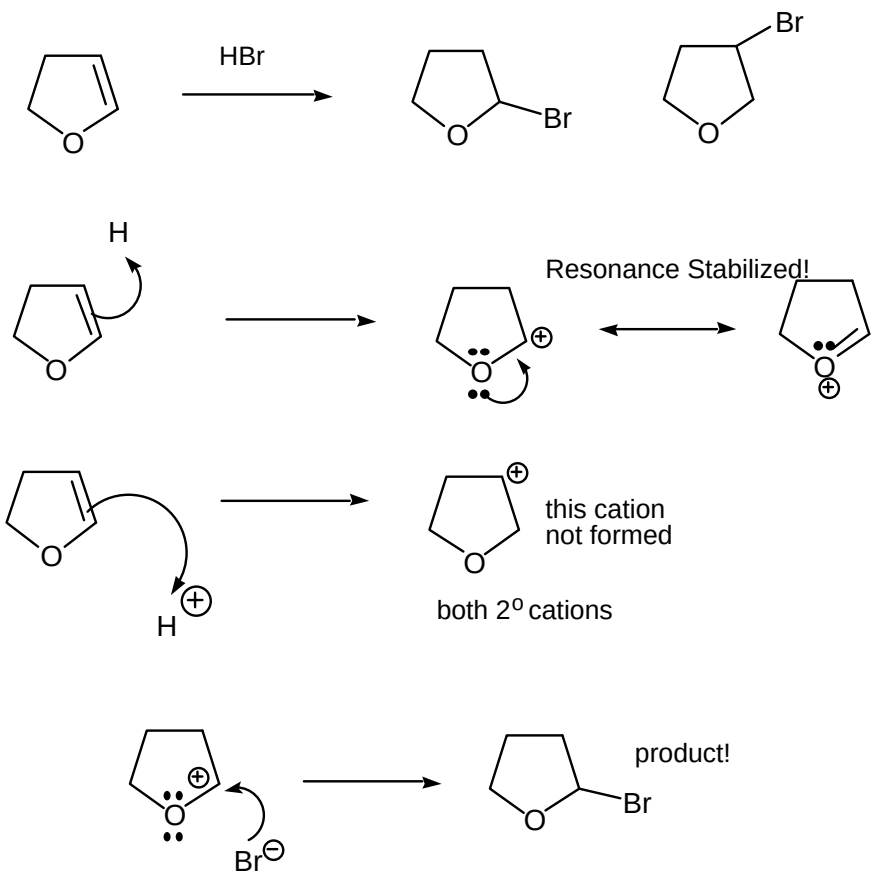
9. Explain the following reaction outcome. When compound **1** is reacted with HBr only **2** is observed and none of compound **3**.



1 **2** **3**

(Not Observed)

Mechanism:


HBr
Br
O
Br
O
H
O
Resonance Stabilized!
O
O
O
H
this cation
not formed
O
both 2° cations
O
Br
product!
Br
O

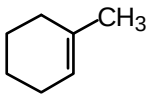
Infrared Spectroscopy: Simplified Correlation Table

	Frequency	Intensity
O-H	3400 cm^{-1}	Large, Broad
Carboxylic Acids	3200-2500 cm^{-1}	Large, Broad
C-H		
Aliphatic	Below 3000 cm^{-1}	Large
Aromatic & Vinyl	Above 3000 cm^{-1}	Medium
Aldehyde	2850, 2750 cm^{-1}	Medium (Two)
C=O	1690 cm^{-1} - 1715 cm^{-1}	Large, Sharp
Ester	1735 cm^{-1}	Large, Sharp
Conjugation	1690 cm^{-1}	Large, Sharp
C=C	2250-2100 cm-1	Small
C≡N	2250 cm-1	Medium
-NO_2	1600, 1500 cm^{-1}	Large (Two)

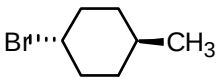
Organic Chemistry I — Chemistry 31
Sample Final Exam — 200 points

1. Name the following structures, including R,S and E,Z designations.

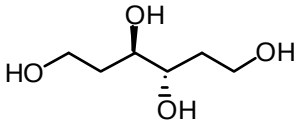
a.



b.



2. a. Label each chiral center and assign R,S designations.

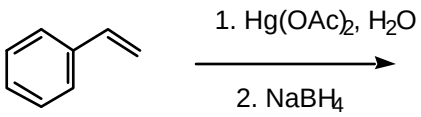


b. Is the molecule chiral?

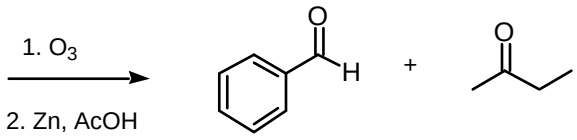
c. Would a sample of this compound rotate plane polarized light?

3. For the following reactions supply the missing reagent reactant or product. For stereoselective reactions, indicate the relative stereochemistry of the products.

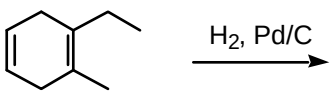
a.



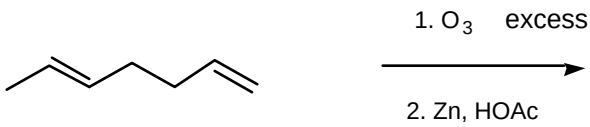
b.



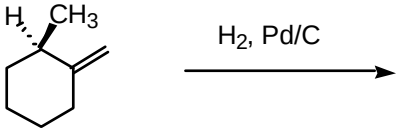
c.



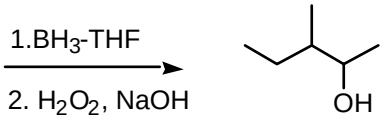
d.



e.

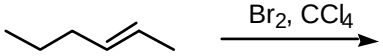


f.

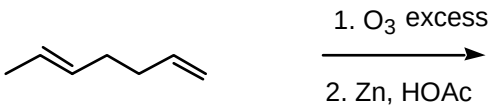


As the only product

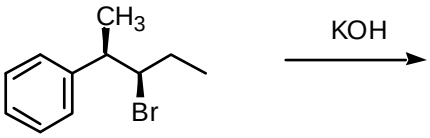
g.



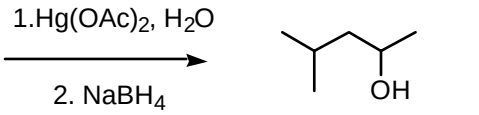
h.



i

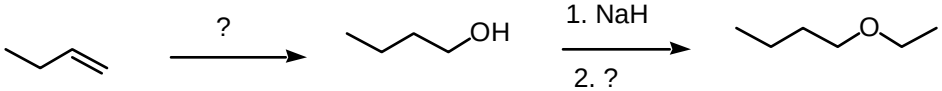


j.

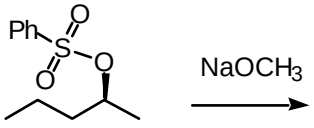


As the only product

k.

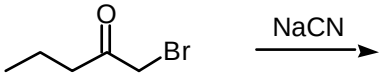


l.

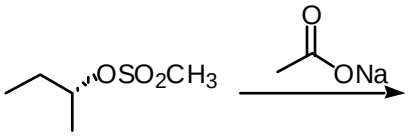


4. Give the expected major products for the following reactions, and indicate the type of mechanism by which the reaction proceeds for cases of SN1, SN2, E1, and E2.

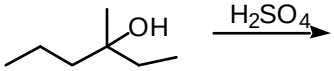
a.



b.



c.



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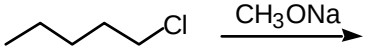
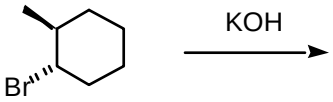
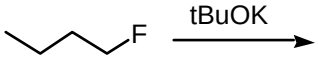


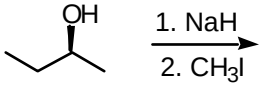
e.



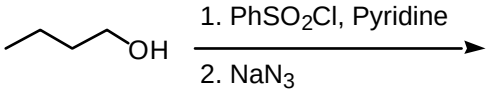
f.



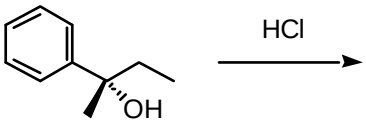
g.



h.

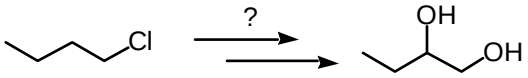


i.

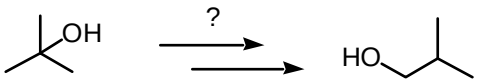


5. Propose syntheses to accomplish the following transformations.

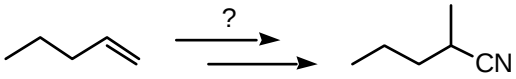
a.



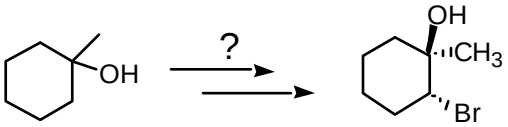
b.



c.



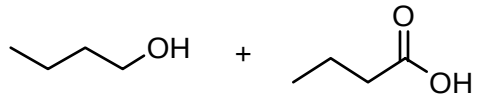
d.



6. Acid-base reactions are important to the understanding of organic chemistry, in both reaction mechanism and in the separation of organic compounds via extraction. Below are a number of questions (a-d) that test your knowledge of acid-base chemistry and it's use in organic chemistry.

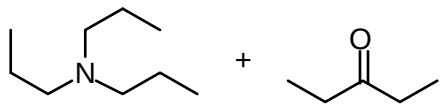
a. Below are two sets of compounds: using acid (HCl) or base (NaOH) show how you might effect a separation of one compound from the other. In each case, show the acid-base reaction, and explain how this reaction facilitates the requisite separation. For each set of compounds **i.** and **ii.** your should demonstrate how using acid or base allows for a separation of the two compounds. *(Note: You are trying to show how **1** and **2** could be separated and how **3** and **4** could be separated. However there is no need to go into detail concerning the specifics of extraction)*

i.



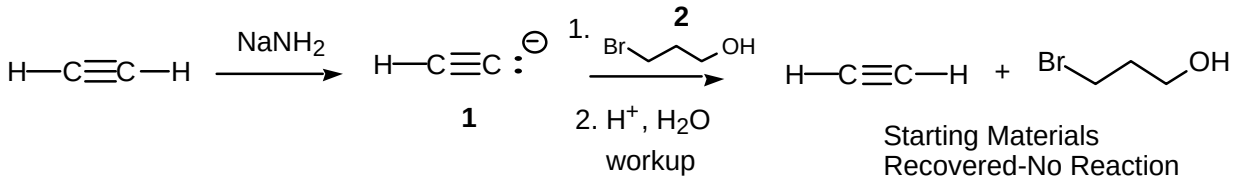
1 **2**

ii.

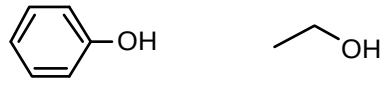


3 **4**

b. In the reaction below, a student tried to alkylate acetylene anion **1**, with an alcohol containing a primary alkyl halide **2**, and no product was observed after workup of the reaction. What went wrong with the reaction? Explain by showing any side reactions that may have interfered with the intended reaction.

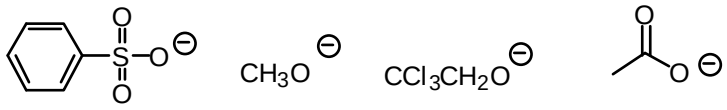


c. Explain why compound **1** (pKa= 10) is more acidic than **2** (pKa=16). Hint: You may want to consider the conjugate base stability of each acid. Be sure to clearly and completely explain your answer.

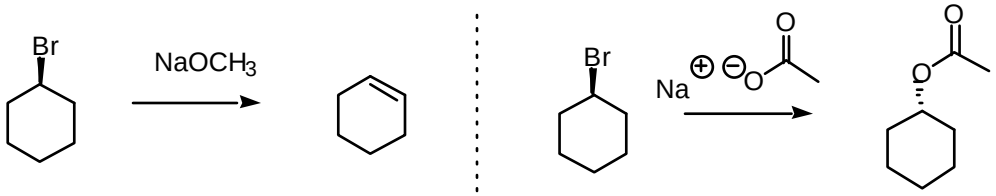


1 **2**

d. Rank the following species in order of their strength as nucleophiles.



7. When 1-bromocyclohexane is treated with sodium methoxide the major product is cyclohexene, however, if sodium acetate is used the product is 1-acetoxycyclohexane. Explain these results and determine the mechanism (SN1, SN2, E1 or E2) for each reaction.



8. For the following pairs of molecules, determine the relationship between the two: enantiomers, diastereomers, identical or structural/constitutional isomers.

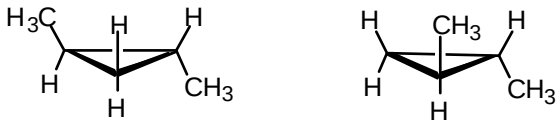
a.

b.

c.

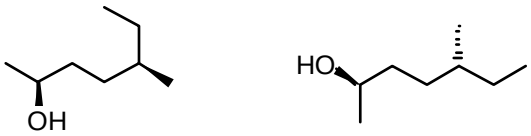
d.

e.

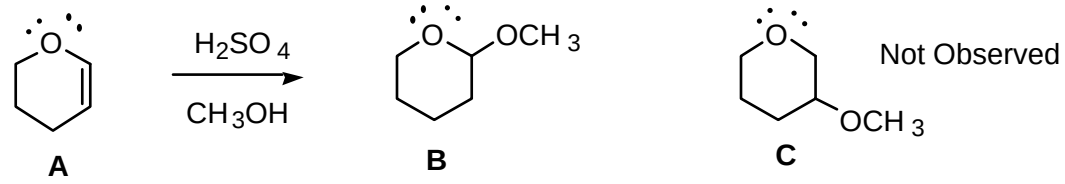


f.

g.

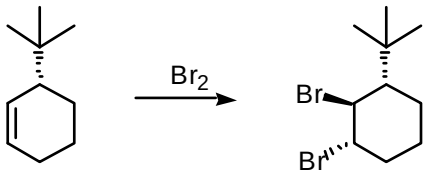


9. For the following reaction of Compound **A** with H_2SO_4 and H_2O, only product **B** is formed and none of the other regiochemical addition product, **C**, is observed. Explain these results.



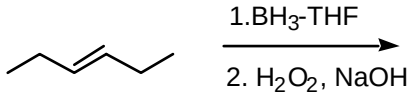
A **B** **C**

10. In the following reaction, the only product had the relative stereochemistry shown. Why? You may want to use what you know about this mechanism to explain the reaction outcome

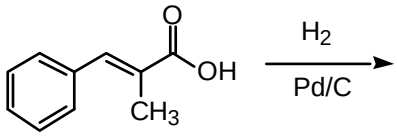


11. For each of the following reactions draw all the possible stereoisomers formed in each reaction and give the stereochemical relationship between the products (i.e. enantiomers, diastereomers, etc.). The mechanism of these reactions may help in your predictions of the products. (Recall, draw both products from top or bottom face attack on the alkene and determine their stereochemical relationship)

a.

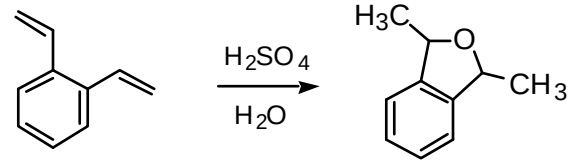


b.

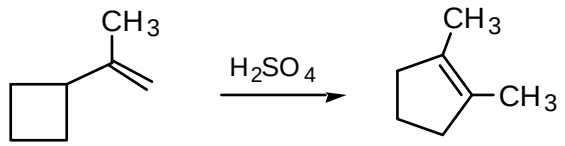


12. Draw a mechanism that would explain the products in the following reactions.

a.



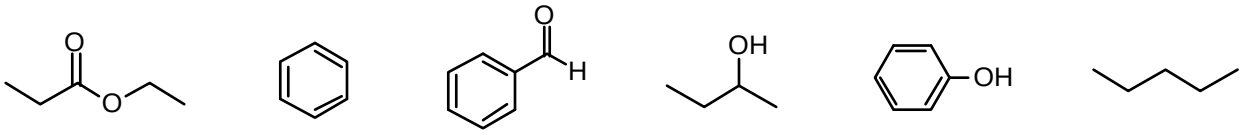
b.



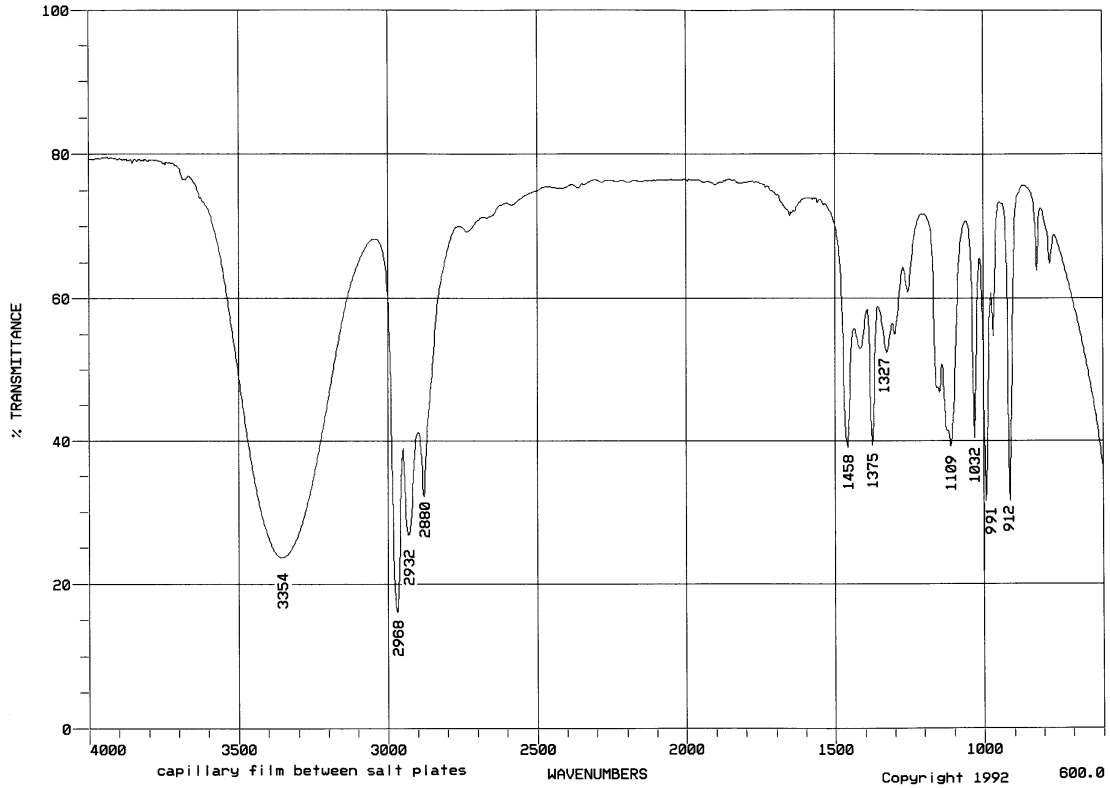
Note: the following question is a challenging type of question called a "road map". I included one of these here and on the problem set so you would get some practice with these. I don't always include this kind of question on the final, but just in case….

13. Compound **A** ($C_8H_{17}Cl$) is a **chiral** primary (1^o) chloride. Treatment of Compound **A** with NaOtBu converts **A** to Compound **B** (C_8H_{16}) which is also **chiral**. Compound **B** absorbs 1 molar equivalent (meaning 1 mole of **B** would add 1 mole of H_2 gas) of H_2 gas on catalytic hydrogenation with Pd on carbon to form Compound **C** (C_8H_{18}) which is an **achiral** compound (i.e. it did not rotate plan polarized light). Using alternative spectroscopic methods, **C** was found to be 3, 4-dimethylhexane. What are the structures of **A**, **B** and **C**? Be sure to clearly indicate the configuration of all chiral centers in each compound.

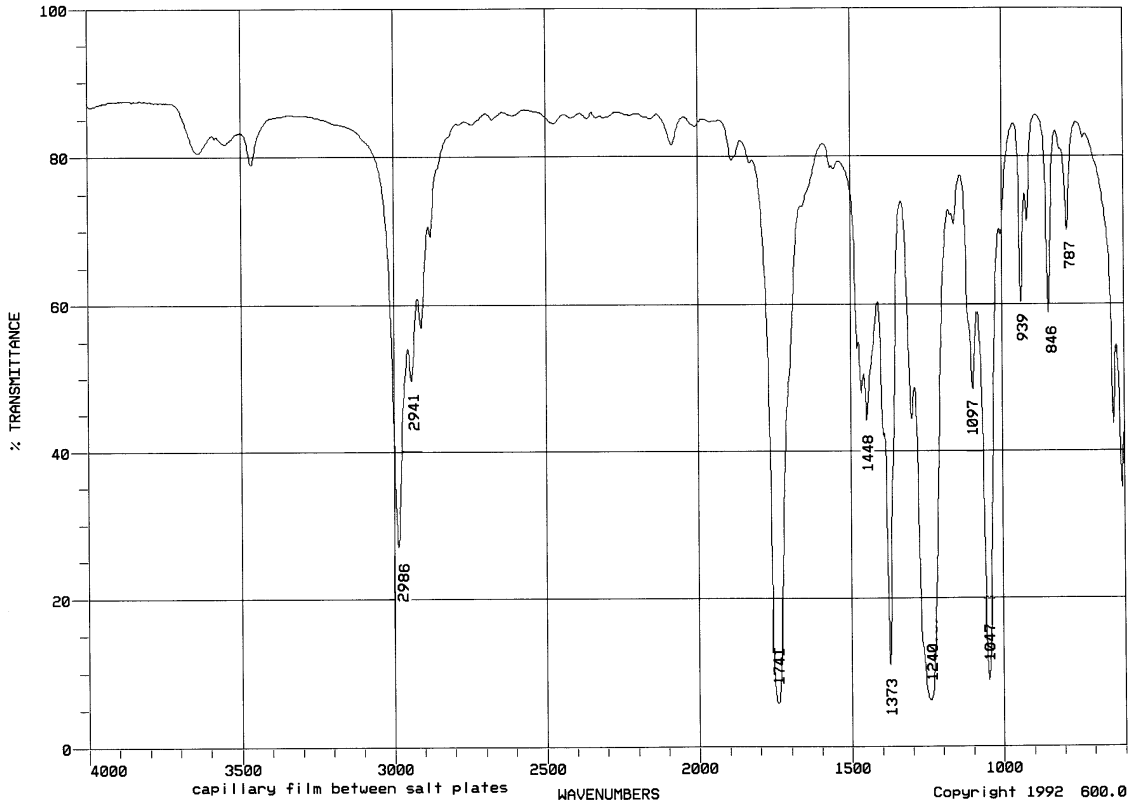
14. For the following compounds below, match the spectra to the structure. There are more molecules given than spectra so you have to rule out two of the molecules. Write the letter of the spectra next to the appropriate molecule.



a.



b.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80
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capillary film between salt plates
WAVENUMBERS
Copyright 1992
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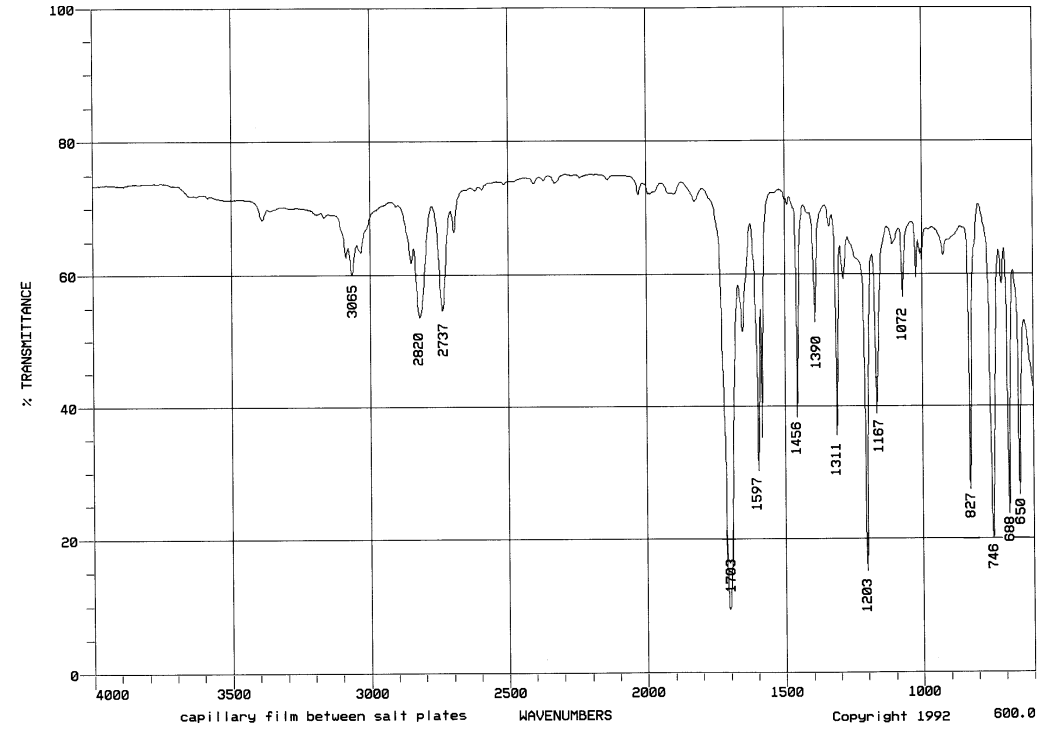
C.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827
746
698
650
4000
3500
3000
2500
2000
1500
1000
capillary film between salt plates
WAVENUMBERS
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Infrared Spectroscopy: Simplified Correlation Table

	Frequency	Intensity
O-H	3400 cm^{-1}	Large, Broad
Carboxylic Acids	3200-2500 cm^{-1}	Large, Broad
C-H		
Aliphatic	Below 3000 cm^{-1}	Large
Aromatic & Vinyl	Above 3000 cm^{-1}	Medium
Aldehyde	2850, 2750 cm^{-1}	Medium (Two)
C=O	1690 cm^{-1} - 1715 cm^{-1}	Large, Sharp
Ester	1735 cm^{-1}	Large, Sharp
Conjugation	1690 cm^{-1}	Large, Sharp
C≡C	2250-2100 cm-1	Small
C≡N	2250 cm-1	Medium
$-NO_2$	1600, 1500 cm^{-1}	Large (Two)