

Name: _____

Date: _____

Exam #1

CHEM 211 - Practice Exam

Dr. M. Nerz

Starting Time: _____

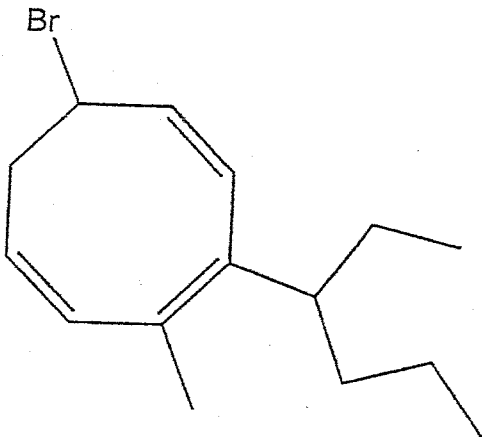
Finishing Time: _____

THOROUGHLY ANSWER THE FOLLOWING QUESTIONS IN THE PROVIDED BLUEBOOKS. WORK RAPIDLY AND DIVIDE YOUR TIME ACCORDING TO THE POINT VALUE OF EACH QUESTION. YOUR ANSWERS DO NOT HAVE TO BE MASTERPIECES OF ART AND LITERATURE, JUST LEGIBLE AND CLEAR.

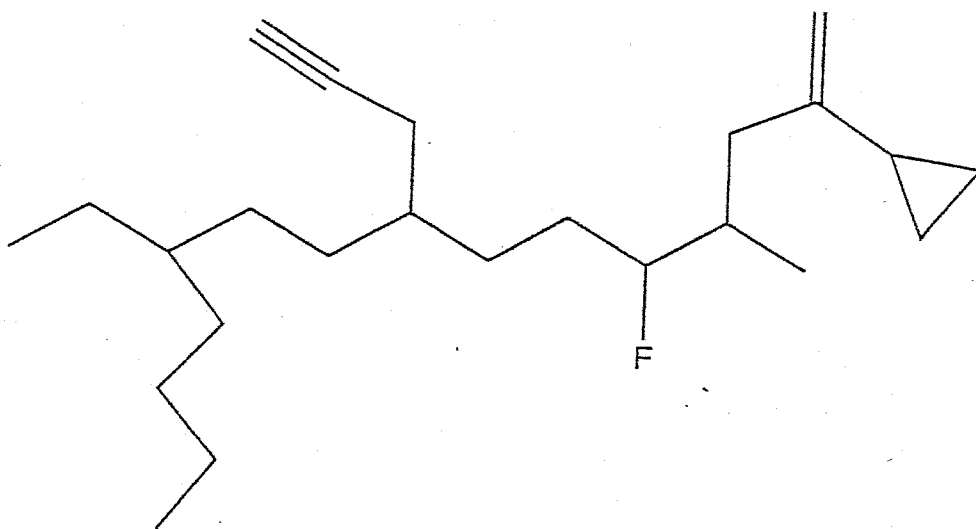
GOOD LUCK!!!! WHEN IN DOUBT, RELY ON LOGIC, NOT MEMORY!!!

1. Write acceptable IUPAC names for each of the following structures. 20 points

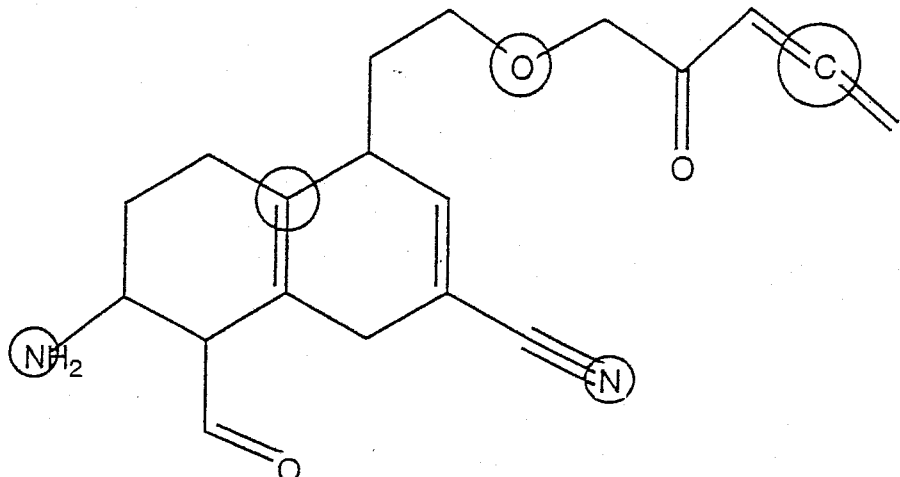
a.



b.



2. Consider the following molecule:

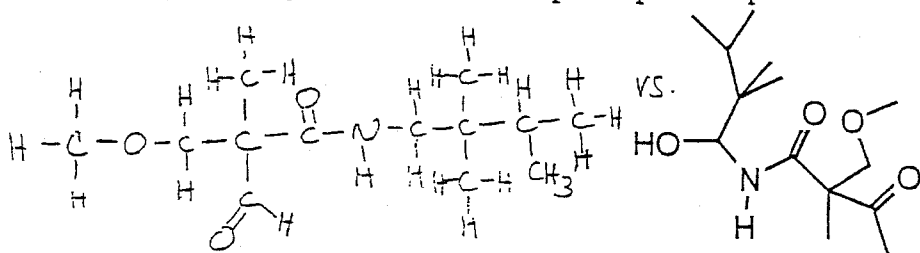


- Specify the hybridization and geometry at each of the circled atoms. 10 points
- Draw an orbital representation of the aldehyde functional group in terms of overlapping atomic and hybrid orbitals. Label all of the overlapping orbitals (p, s, sp, etc.) and include all electrons. 20 points
- What is the index of hydrogen deficiency for the given molecule? 4 points
- How many pi bonds are found in the given molecule? 4 points
- How many of the sigma bonds in the given molecule involve hydrogen atoms? 4 points

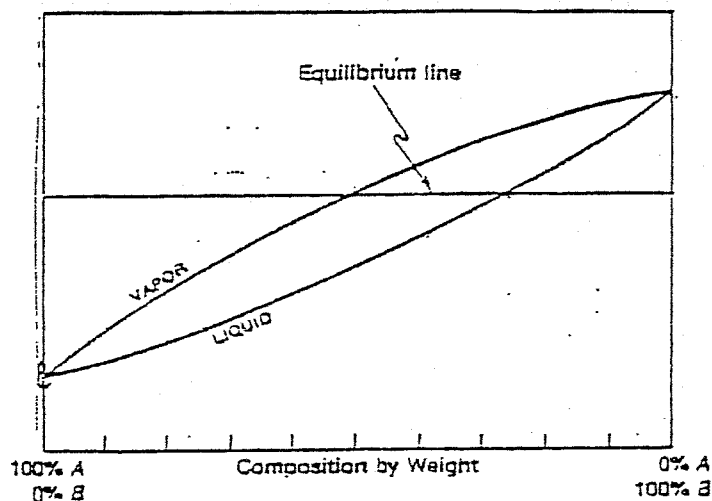
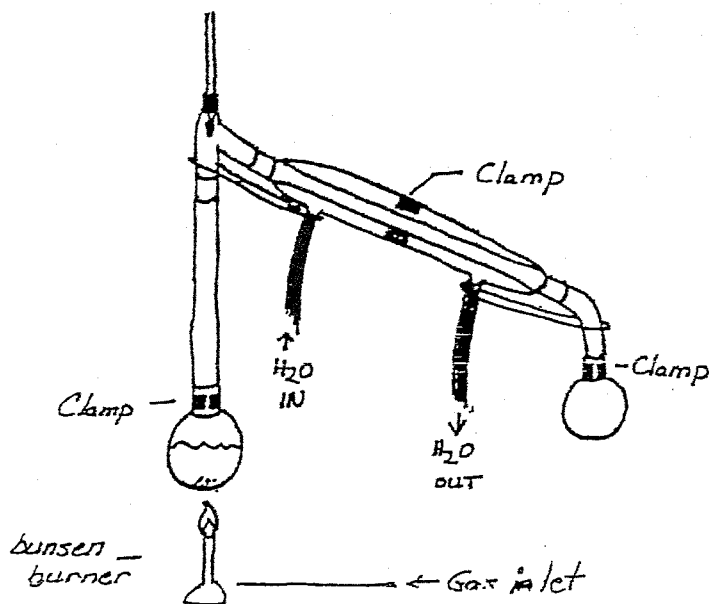
3. Consider the molecular formula, $\text{C}_{12}\text{H}_{13}\text{N}_2\text{O}_3\text{Br}$

- Calculate the index of hydrogen deficiency for this formula. 8 points
- In your own words, explain the meaning and usefulness of the index of hydrogen deficiency. 8 points
- Write a structure consistent with the given formula having a tertiary amine and an aromatic ring among other functional groups. 8 points
- Write a structural isomer of that written in part c having a secondary alcohol and a cyclic amide among other functional groups. 8 points
- Using bond-line notation, i.e., , write a third isomer having an alkyne, an ester and an ether among other functional groups. 8 points

4. State the relationship between the following molecules. Are they structural isomers, the same molecule or do they have no relationship? Explain. 8 points



5. Frederica Fractionation and Harry Hydrocarbon have a solution that is 30% by weight heptane (b.p. = 98°C), 60% by weight octane (b.p. = 126°C) and 10% by weight phenanthrene (b.p. = 340°C , m.p. = 101°C). They wish to separate the components by distillation so they build the illustrated apparatus. It should be noticed that their distilling column has three theoretical plates and they have available to them the accompanying boiling point composition diagram which describes heptane/octane solutions.



Freda and Harry begin their distillation, maintaining a distillation rate of 1 drop per second. They collect four fractions. Fraction A consists of the first few drops of distillate which are collected at 99°C . Fraction B is collected from 99°C to 102°C , Fraction C from 103°C to 124°C and Fraction D from 125°C to 126°C .

After an additional hour of heating at the highest rate possible, it becomes apparent to Freda and Harry that no more material will distill. They decide to remove the heat source and allow the apparatus to cool, whereupon a solid mass forms in the still pot. They break up the mass with a spatula and vacuum filter it to remove residual liquids.

Freda and Harry analyze each of the four collected fractions by gas chromatography. For each of the four injections they observe two peaks in varying proportions. One peak is consistently at 1.8 minutes and the other at 2.3 minutes. They also take a small amount of the isolated solid, dissolve it in cyclohexane (b.p. = 81°C) and analyze it by G.C. After this injection, they observe three peaks, one at 1.3 minutes, the next at 1.8 minutes and the last at 2.3 minutes.

- Cite any significant errors Freda and Harry have made and explain the chemical and/or physical consequences of each error. 18 points
- Fully explain their G.C. results. Make an educated guess as to the identities of the various peaks they observed. 10 points
- Predict the composition of the first few drops of distillate they collected. How did you arrive at your ratio? 6 points
- Did Freda and Harry ever isolate phenanthrene? If so, did they isolate pure phenanthrene? How can it be obtained in higher purity? 6 points

Name: _____

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Exam #2

CHEM 211 -Practice Exam

Dr. M. Nerz

Starting Time: _____

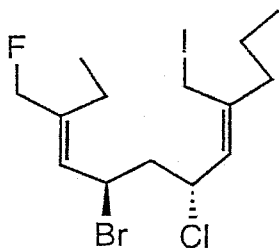
Finishing Time: _____

4

THOROUGHLY ANSWER THE FOLLOWING QUESTIONS IN THE PROVIDED BLUEBOOKS. WORK RAPIDLY AND DIVIDE YOUR TIME ACCORDING TO THE POINT VALUE OF EACH QUESTION. YOUR ANSWERS DO NOT HAVE TO BE MASTERPIECES OF ART AND LITERATURE, JUST LEGIBLE AND CLEAR.

GOOD LUCK!!!! WHEN IN DOUBT, RELY ON LOGIC, NOT MEMORY!!!!

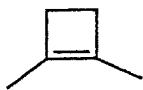
1. Write a complete and acceptable IUPAC name for the following molecule. Include Cahn-Ingold-Prelog stereochemical designations if appropriate. 12 points



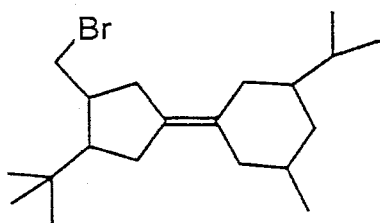
2. Consider the following molecules.

Which of these compounds can be represented as two or more geometric isomers. In cases where geometric isomerism is possible, clearly draw all geometric isomers and label them cis or trans (Z or E). In cases where geometric isomerism is not possible, briefly explain your reasoning. 24 points

a)

b) $(\text{CH}_3)\text{CHCHCH}(\text{CH}_3)\text{CH}_2\text{CH}_3$

c)



d) 2-methyl-2-hexen-4-yne

3. An unknown compound, X, has the formula, $C_{10}H_{18}$. The infrared spectrum of X is measured and three significant absorptions are observed in the functional group region, i.e., 3040 cm^{-1} , 2900 cm^{-1} , and 1660 cm^{-1} (weak). X is also found to have an optical rotation of $+32.6^\circ$.

X is converted by a chemical reaction into Y which has the formula $C_{10}H_{20}$. Y shows only one significant absorption in the functional group region at 2900 cm^{-1} and exhibits no optical rotation. Y is known to exist in exclusively one conformation.

- Propose reasonable structures for X and Y. 12 points
 - Explain the I.R. data. Include in your answers the reason for two types of high frequency absorption (3040 cm^{-1} and 2900 cm^{-1}) observed for X and the reason why the absorption at 1600 cm^{-1} is weak. 8 points
 - Draw two Newman projections that illustrate the two lowest energy conformers of Y and explain the dominance of one of these conformers in the molecular population. Identify all important interactions raising the energy of one conformer with respect to the other. 20 points
 - Explain the difference in optical rotation between X and Y. 10 points
 - Can the absolute configuration of X be assigned? If so, assign it a configuration. If not, explain why it cannot be assigned. 8 points
4. Carry out a conformational analysis of (3R), (4S)-4-(1-methylethyl)-2,3-dimethyloctane using Newman projections. The Newman projections should be drawn so that the stereogenic carbons are the atoms "projected".

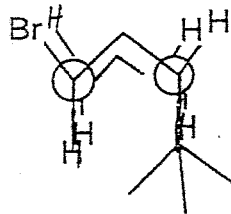
Rank the conformers in terms of energy (I = lowest energy, VI = highest energy). Explain your ranking in terms of steric and torsional interactions existing for the various conformers. 24 points

5. Establish the relationship (if any) that exists between the following pairs of molecules. Are they - structural isomers, geometric isomers, diastereomers, enantiomers, conformers or do they have no relationship. Wherever possible, assign the absolute configuration to stereogenic centers and classify each molecule as chiral or achiral. 16 points

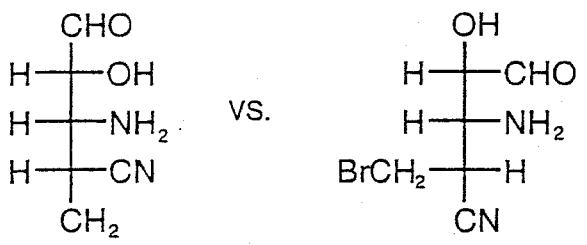
a)



vs.



b)

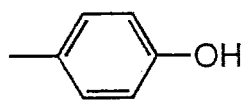


Just draw structures

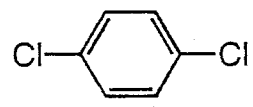
6. Draw the two lowest energy conformations of (1S), (3S)-1-ethyl-3-(1-ethylpropyl)-1,3-dimethyl cyclohexane. Which of these conformations is lower in energy. Explain your reasoning in terms of numbers and types of steric and torsional interactions. 24 points

7. A mixture of 2 grams of 4-methylphenol (structure and physical properties shown below) and 1 gram of 1,4-dichlorobenzene (structure and physical properties shown below) were dissolved in 125 mL of CHCl₃. The resulting solution was extracted once with 25 mL of 7 M HCl (K = 4, favoring aqueous layer). After separation, the organic layer was distilled giving rise to one fraction (b.p. = 61-63°C). Upon cooling, the pot residue solidified and was allowed to dry in a 50°C oven overnight. The resulting solid mass was ground into a fine powder and then its melting point was measured and found to be 32-33°C. The aqueous layer was also subjected to distillation and also gave rise to one fraction, boiling at 100°C. The resulting pot residue was dried and its melting point was determined.

- a) Write a "mechanism" or equation explaining the reaction of 4-methylphenol with NaOH solution. 4 points
- b) Fully explain the melting point range of the "organic layer" pot residue. 8 points
- c) What do you predict with regard to the melting point of the "aqueous" pot residue? Will it be higher, lower or the same as the melting point of 4-methylphenol? Explain. 8 points
- d) What major errors were made in the procedure. What are the chemical/physical consequences of the errors. 18 points
- e) How can the experiment be salvaged? 8 points



4-methylphenol
 b.p. = 173°C
 m.p. = 35°C



1,4-dichlorobenzene
 b.p. = 173°C
 m.p. = 53°C

Name: _____

Date: _____

Exam #3

CHEM 211 *Practice Exam*

Starting Time: _____

Dr. M. Nerz

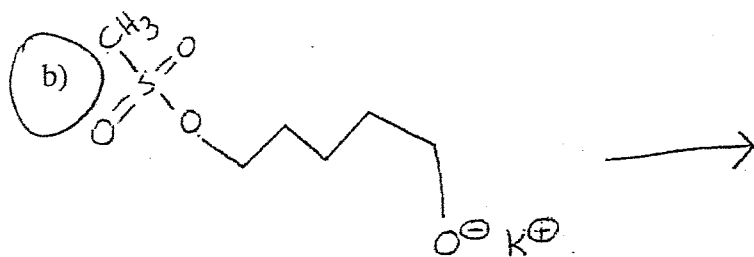
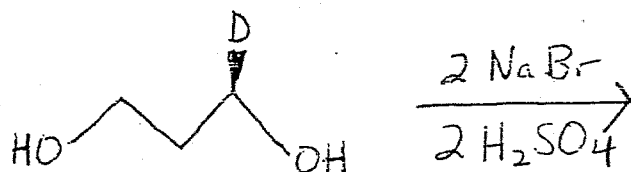
Finishing Time: _____

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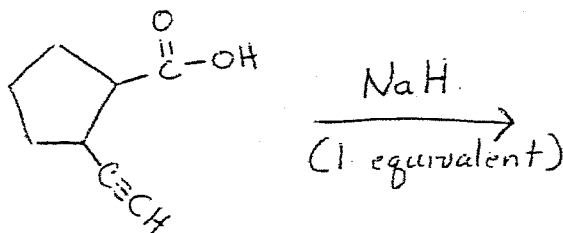
THOROUGHLY ANSWER THE FOLLOWING QUESTIONS IN THE PROVIDED SPACES/BLUEBOOKS. WORK RAPIDLY AND DIVIDE YOUR TIME ACCORDING TO THE POINT VALUE OF EACH QUESTION. KEEP YOUR EXPLANATIONS AS BRIEF AND TO THE POINT AS POSSIBLE.

1. Using the arrow formalism, predict products for each of the following proposed reactions. If you do not believe a reaction will work, write "no reaction" and explain briefly. Identify all S_N2 reactions and show the stereochemistry of products where appropriate. 8 points each

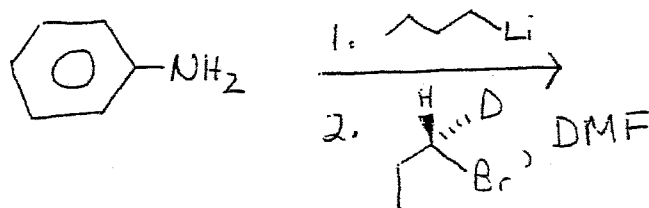
a)



c)

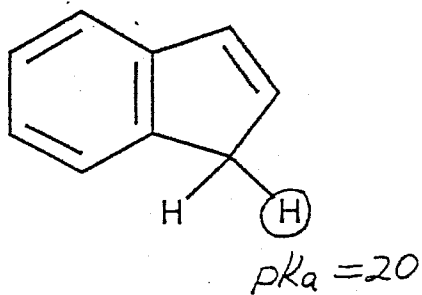


d)

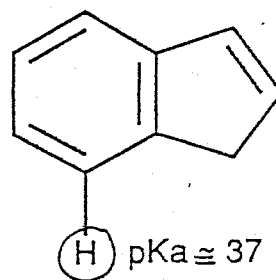


2. Using resonance theory, explain the following differences in pKa values.

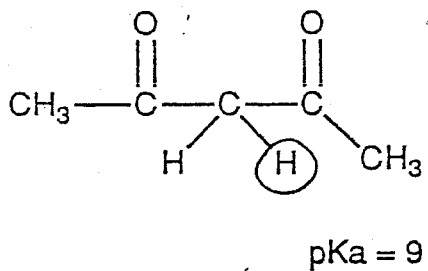
a)



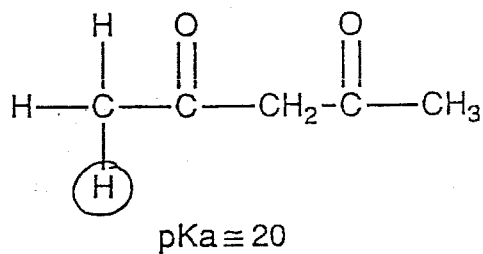
vs.



b)



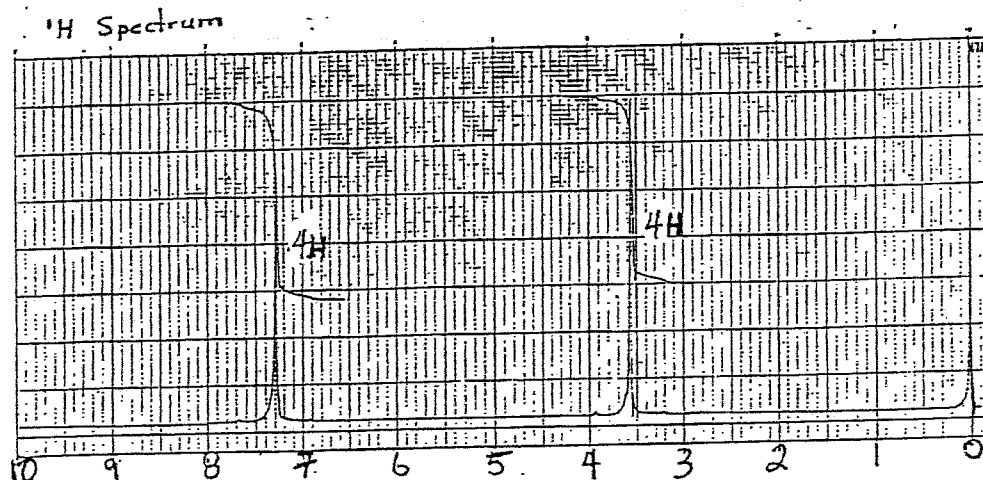
vs.



Write all appropriate resonance structures. Where possible, evaluate the relative contribution of structures to the hybrid. 12 points each

3. Compound X has the formula C_9H_8O . When the 1H NMR spectra is measured, the following spectrum is obtained. When the IR spectrum of X is measured a strong absorption at 1710 cm^{-1} is observed. Fully interpret the IR and 1H NMR data and proposed a reasonable structure for X.

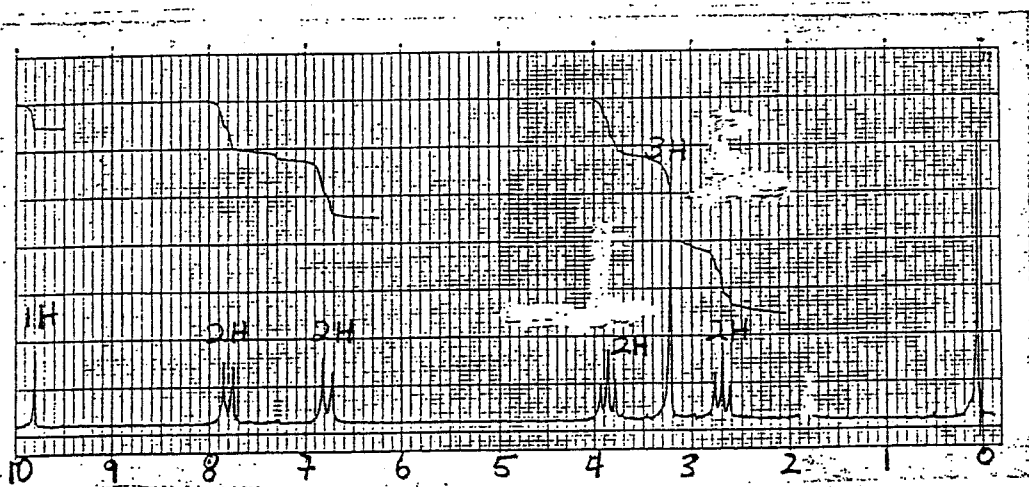
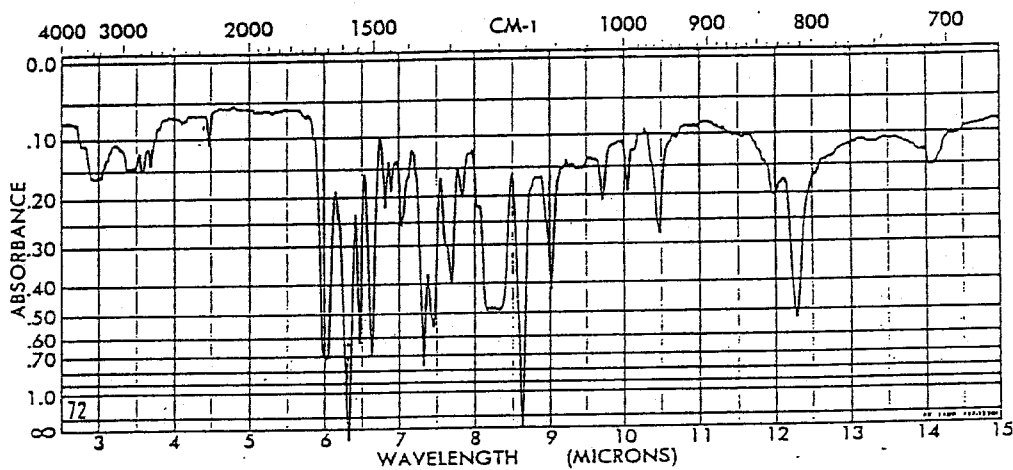
To maximize your score, please show all work. Generous credit will be given for partial structures. 24 points



4. Compound Y has the formula $C_{11}H_{12}N_2O$. When the 1H NMR spectrum of Y is measured the following IR and 1H NMR spectra are obtained, respectively. Fully interpret the spectra and propose a reasonable structure for Y. Hints: N is similar to O in its effect on chemical shift, but it deshields local hydrogens to a slightly lesser extent. Also the weak IR absorption at 2200 cm^{-1} is significant.

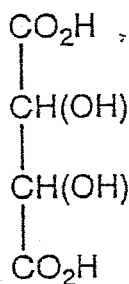
To maximize your score, please show your work. Generous credit will be given for partial structures. 24 points

10

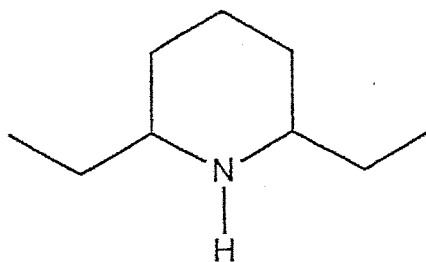


5. Consider the separation of racemic tartaric acid using 2,6-diethylpiperidine as a resolving agent. 11

- Draw a three dimensional representation of the two molecules comprising racemic tartaric acid. 4 points
- Draw a three dimensional representation of a 2,6-diethylpiperidine that would be a suitable resolving agent for this separation. 4 points
- Outline an approximate procedure for this proposed resolution. In your outline, delineate how both stereoisomers of tartaric acid can be obtained and how the resolving agent can be recycled. 20 points
- Suppose that after one resolution, a 3:1, -:+ mixture of tartaric acid is obtained. If the theoretical specific rotation for the tartaric acid is 12.4° , what is the experimental specific rotation and the optical purity of this mixture? 8 points
- When the optical rotation of another mixture of tartaric acid enantiomers was measured, two different readings were obtained, i.e., one positive and one negative. If the positive rotation was found to be $+173^\circ$, what was the negative reading? How can one determine which rotation is the correct reading?



tartaric acid



2,6-diethylpiperidine

Name: _____
Exam #4 - Final
CHEM 211 - Practice
Dr. M. Nerz

Date: _____

Starting Time: 10:00 AM
Finishing Time: 12:00 AM

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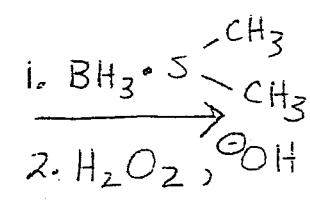
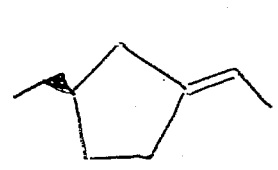
THIS IS A SELF-ADMINISTERED, CLOSED BOOK/NOTES EXAM. THE EXAM IS TO BE TAKEN IN THE PHYSICS LECTURE HALL. YOU HAVE EXACTLY 120 MINUTES TO COMPLETE THE EXAM. AT THE END OF THIS TIME, PLACE YOUR EXAM IN THE ACCORDION FILE AT THE FRONT OF THE ROOM.

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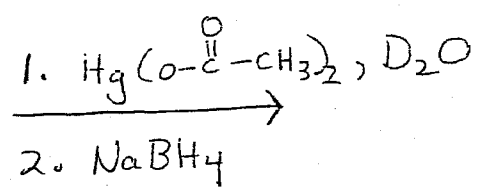
1. Write the major product or products to each of the following reactions. Mechanisms are not necessary here, but you should include the stereochemistry of your products. 8 points each

a)

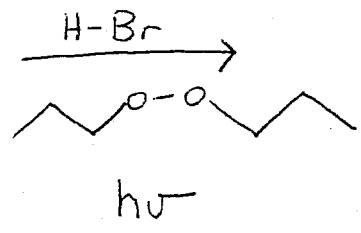
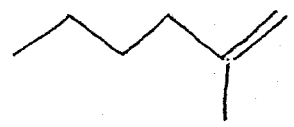


b)

(2E), (5S)-5-methyl-5-isopropyl-2-octene



c)



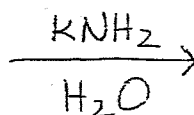
2. Write complete mechanisms (arrow formalism) leading to major product(s) for each of the following reactions. Include conformational analysis when it is necessary to determine the major product. Include the specific stereochemistry of products where it is appropriate. Do not abbreviate stereoisomers by writing M.I. for mirror image. 12 points each

a)

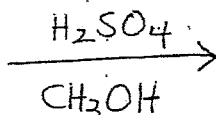
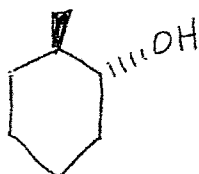


b)

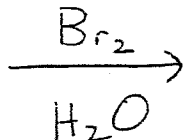
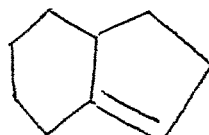
(3R), (4R)-3-bromo-3,4-dimethylhexane



c)

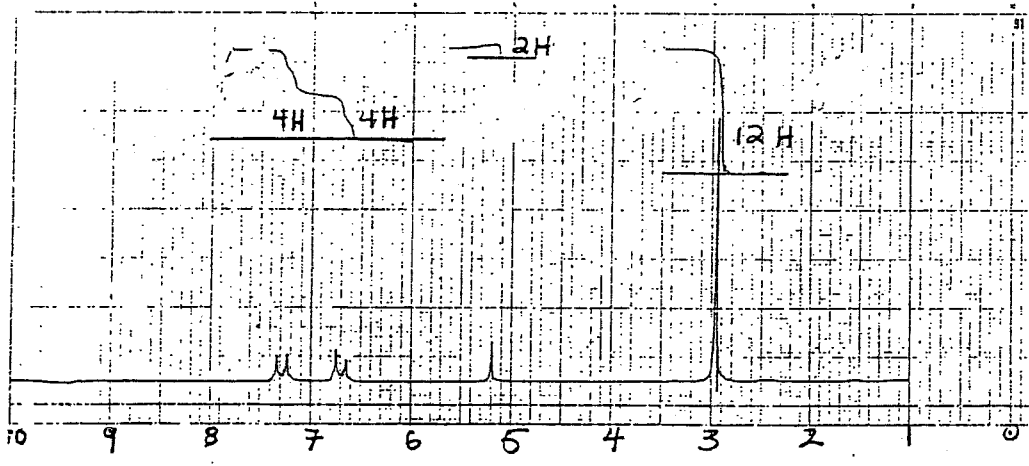
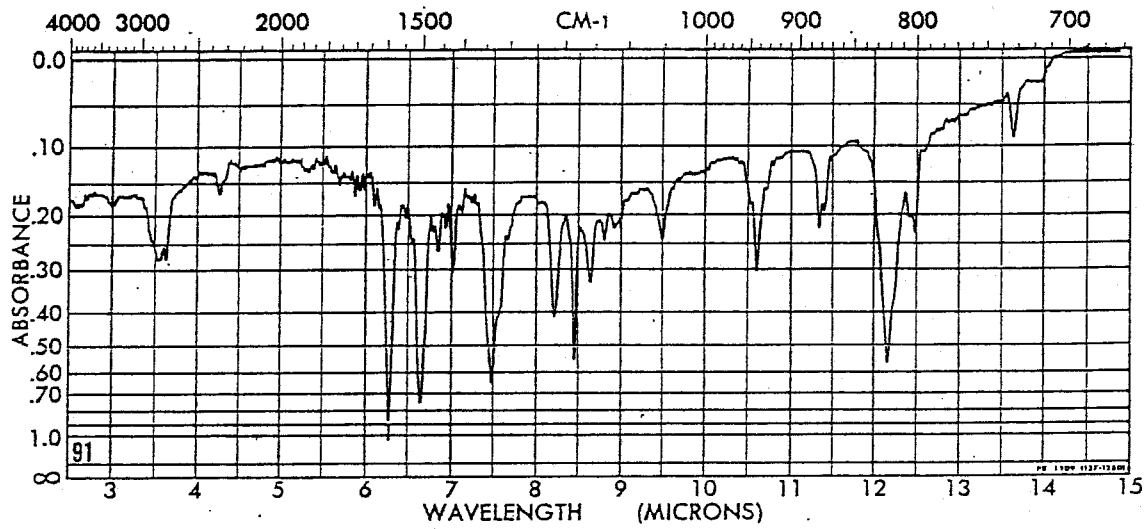


d)

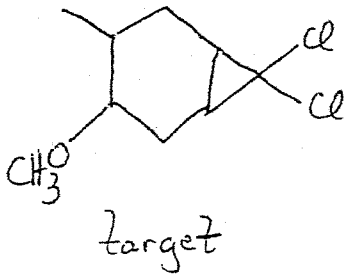


3. Compound X has the formula $C_{18}H_{22}N_2$. When compound X is treated with cold, basic permanganate solution a clear solution having a brown precipitate results. When compound X is treated with hot, basic permanganate solution, a gas is evolved. The IR and 1H NMR spectra are given below. Fully interpret the IR and NMR spectra and propose a structure for X. Write equations describing the two reactions of X with cold and hot, basic permanganate, respectively. 30 points.

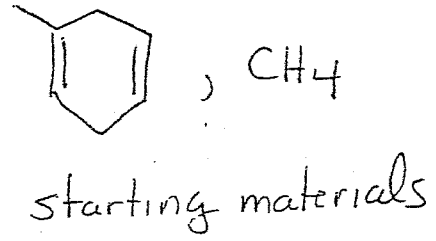
M



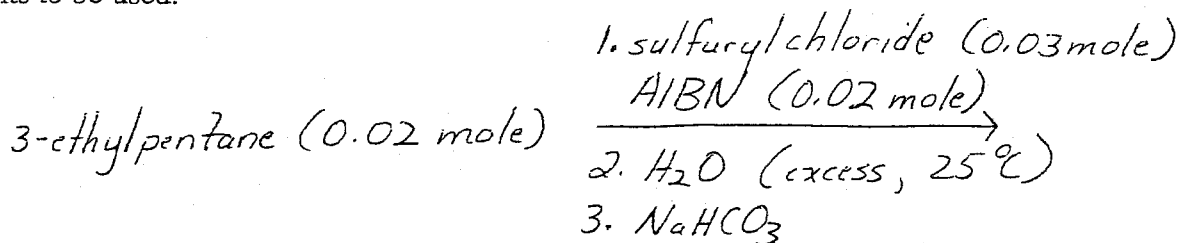
4. Outline a reasonable synthesis of the following target molecule using the given starting materials and any needed inorganic reagents needed. 16 points



FROM



5. Helen Homolytic and Ralph Radical have decided to study the chlorination of 3-ethylpentane. Consider the following equation describing their proposed reactions and the quantities of reagents to be used.



- a) Write equations describing the chemistry of each step of the proposed sequence. 16 points
- b) Limiting your remarks to the steps listed, cite any major errors in the proposed reaction sequence. Briefly state the chemical/physical consequences of each error. Do not comment on apparatus or steps not mentioned!!!!!!! 12 points
- c) Helen and Ralph know that the relative reactivity of hydrogens to free radical chlorination is 5.0:3.5:1.0, 3°:2°:1°. Calculate the theoretical percent of each monochlorination product they should obtain from chlorination of 3-ethylpentane. 8 points

Atom	Common Stable States	Transient, Unstable States
Carbon		
Hydrogen		
Halogen (F, Cl, Br, I)		
Oxygen, Sulfur		
Nitrogen		

19

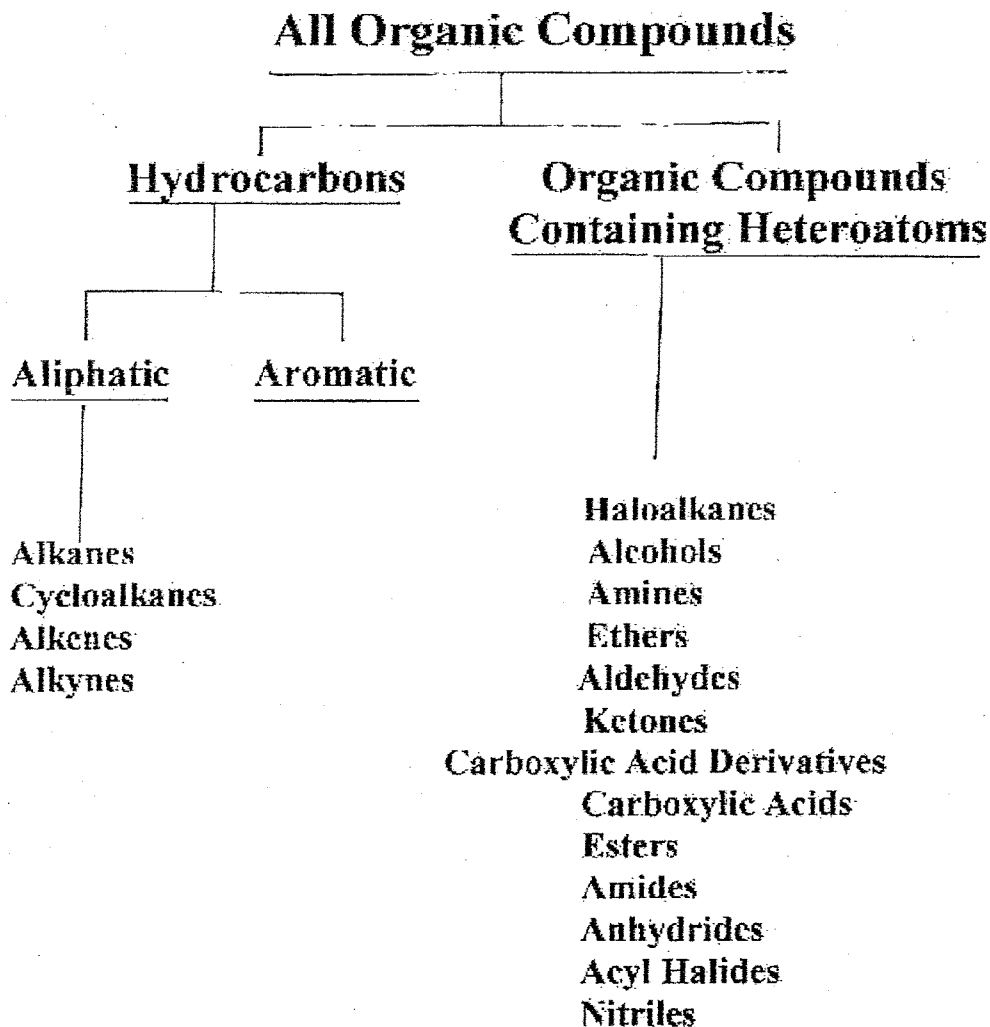
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[Return to Learning Tools](#)

Functional Group Overview

Functional Group: A group of atoms bonded in a particular arrangement that undergoes characteristic chemistry.



Hydrocarbon: Molecules made only of hydrogen and carbon.

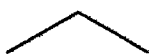
Heteroatom: Atoms other than carbon or hydrogen.

Functional Group Overview Continued - Specific Examples

20

1. Alkanes : General Formula C_nH_{2n+2}

Examples:



methane

ethane

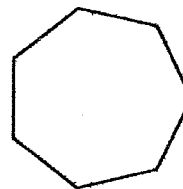
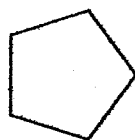
propane

heptane

Write the structure of octane:

2. Cycloalkanes: General Formula C_nH_{2n}

Examples

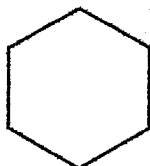


cyclopropane

cyclopentane

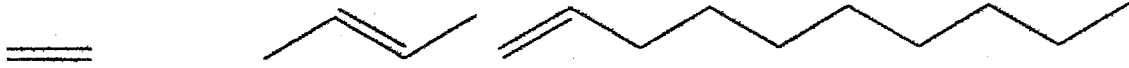
cycloheptane

What is the name of the following compound?



3. Alkenes: General Formula C_nH_{2n}

Examples:

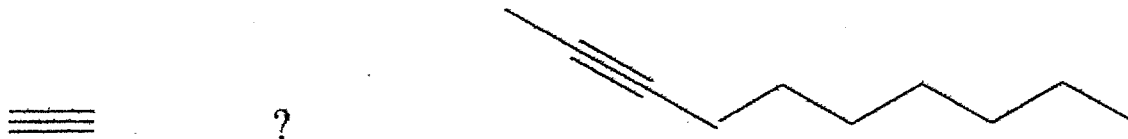


ethene(ethylene) 2-butene 1-nonene

Write the structure of 2-pentene.

4. Alkynes: General Formula C_nH_{2n-2}

Examples:



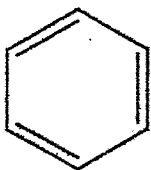
ethyne 3-hexyne 2-decyne
(acetylene)

What is the name of the following compound?

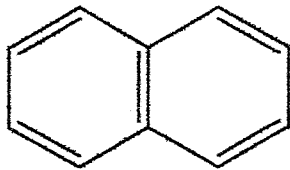


5. Aromatics:

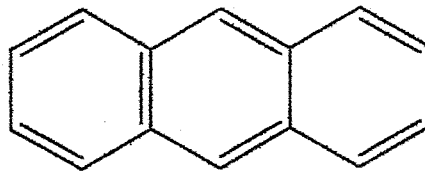
Examples



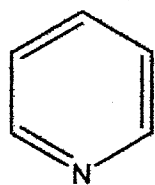
benzene



naphthalene



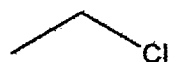
anthracene



pyridine

6. Haloalkanes (alkyl halides):

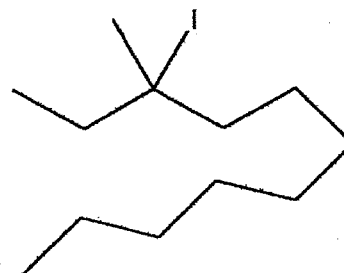
Examples:



chloroethane
 1°

?

2-bromopentane
 2°

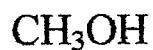


3-iodo-3methylundecane
 3°

The order of a haloalkane and an alcohol has to do with the number of carbons directly attached to the carbon bearing the heteroatom. If that carbon has three carbons the haloalkane (or alcohol) is 3° or tertiary, if it has two carbons it is 2° or secondary, etc. It is noteworthy that carbons in alkanes can be designated similarly. There is even a designation 4° or quaternary for a carbon bearing four directly attached carbons. These designations are useful when communicating specific information about regions of the molecules. There is also a variation in reactivity that relates to order.

7. Alcohols

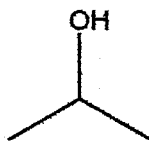
Examples:



methanol
 0°



ethanol
 1°



2-propanol
 2°

?

3-methyl-3-pentanol
 3°

8. Amines

Examples:

?



?

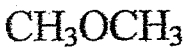
ethylamine

dipropylamine

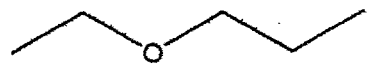
trimethylamine

9. Ethers:

Examples:



?



dimethyl ether

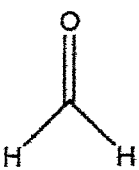
diethyl ether

ethylpropyl ether

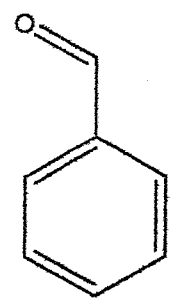
Since nitrogen is a central atom, the order of the amine is defined by the number of carbons directly attached to the nitrogen. What is the order of each the above amines?

10. Aldehydes

Examples:



?



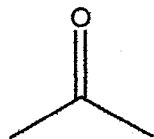
methanal (formaldehyde)

propanal

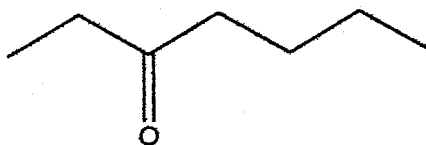
benzaldehyde

11. Ketones:

Examples:



2-propanone (acetone)



3-heptanone

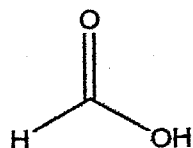
?

4-dodecanone

12. Carboxylic Acid Derivatives

a. Carboxylic Acid

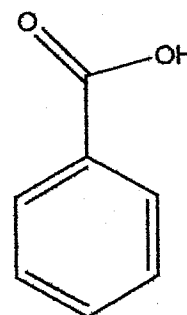
Examples:



methanoic acid (formic acid)

?

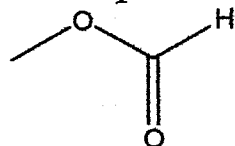
ethanoic acid (acetic acid)



benzoic acid

b. Esters

Examples:



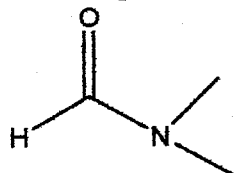
methyl formate (methyl methanoate)

?

ethyl hexanoate

c. Amides

Examples:

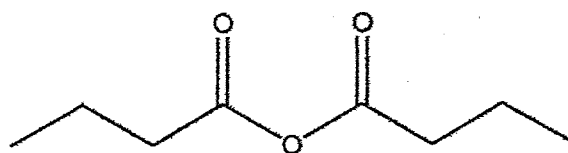


dimethyl formate (DMF, N,N-dimethyl methanoate)

d. Anhydrides:

Examples:

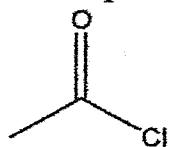
?

acetic anhydride
(ethanoic anhydride)

butanoic anhydride

e. Acyl Halides:

Examples:



acetylchloride (ethanoyl chloride)

?

propanoyl bromide

f. Nitriles:

Examples:

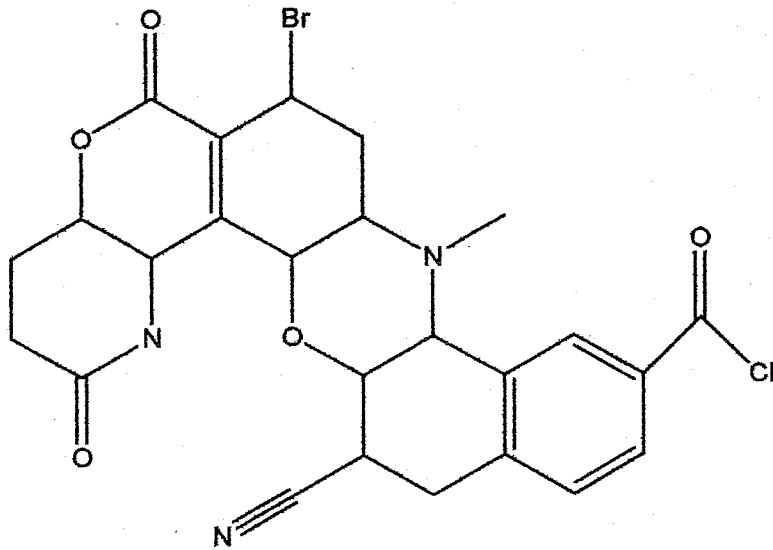
?



acetonitrile (ethanenitrile)

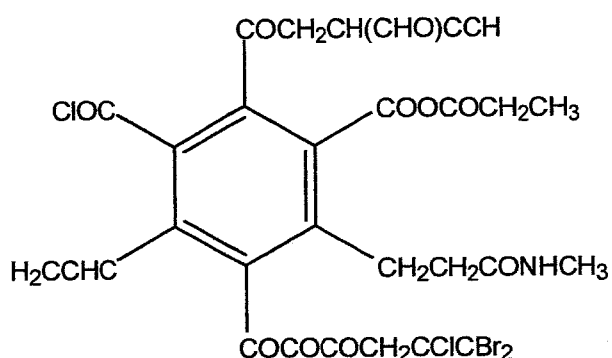
butanenitrile

Identify all the functional groups in the following molecule....

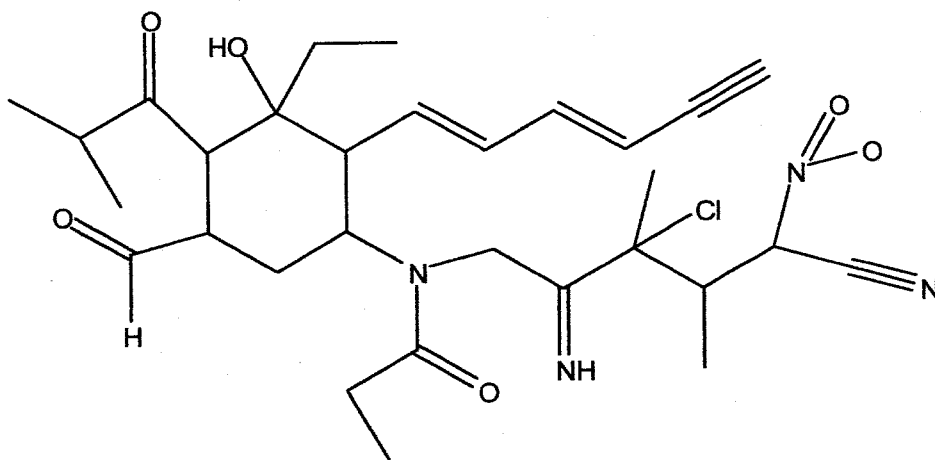


Additional Exercises

I call this one the wheel of difficult functional groups - try to convert them all to Lewis Dash and then to bond line (note the middle ring is in bond-line). It is not easy.



Convert the following to Lewis Structure and then to condensed formul (not the ring of course). Using your handout, can you name all the functional groups? There should be two that you cannot. Classify all amines, halides and alcohols as primary, secondary and tertiary.



Write the following simple structures in Lewis and then in bond-line

methylethylbutylamine

pentanaal

3-methyl-2,3-decanediol (diol means two alcohol groups)

pentanenitrile

butanoic anhydride

hexanoyl bromide

pentyl-octyl ether

4,5-diethyl-1-undecene

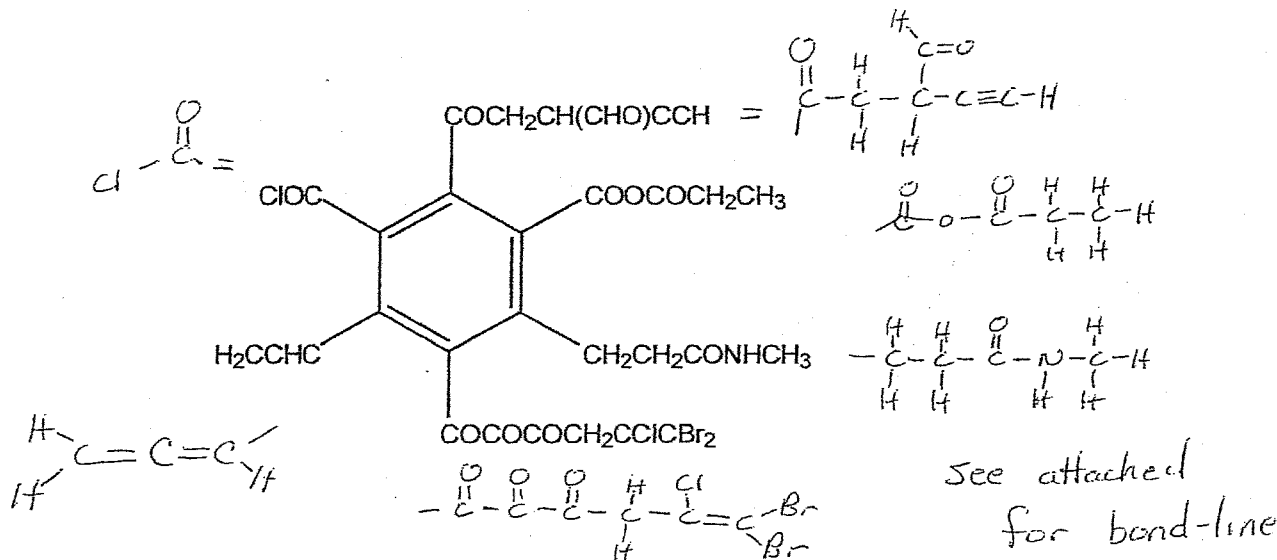
SOLUTIONS

1/4

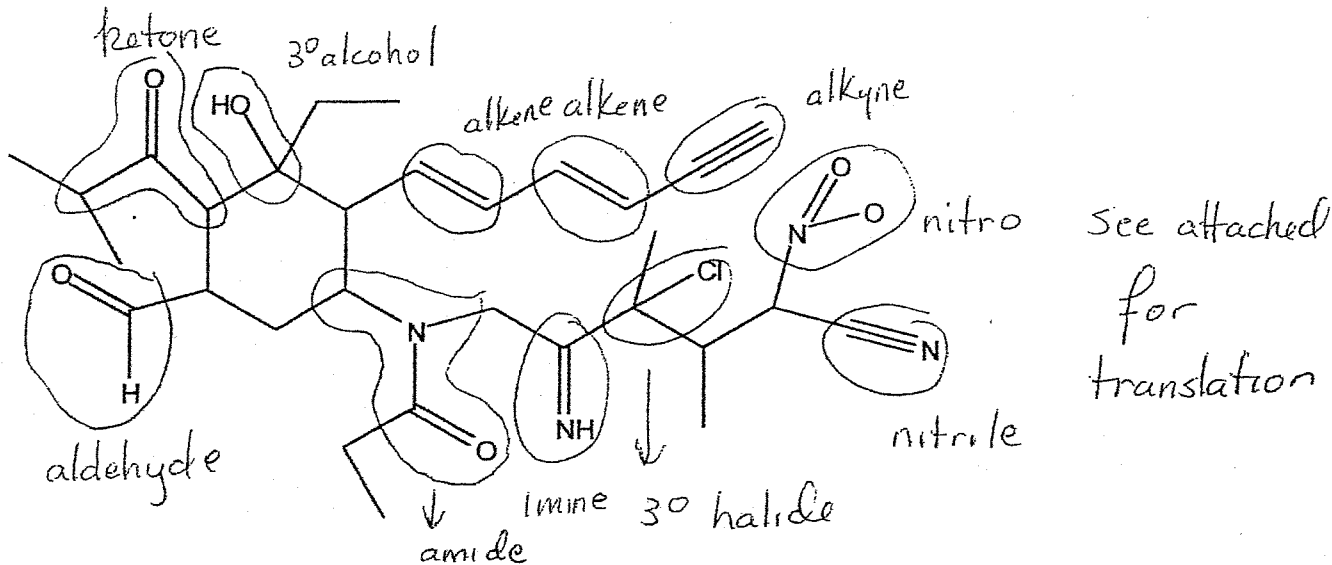
28

Additional Exercises for translation of molecules - Answers to be posted in 24 hours Fall 2002 M. Nerz

I call this one the wheel of difficult functional groups - try to convert them all to Lewis Dash and then to bond line (note the middle ring is in bond-line). It is not easy.



Convert the following to Lewis Structure and then to condensed formula (not the ring of course). Using your handout, can you name all the functional groups? There should be two that you cannot. Classify all amines, halides and alcohols as primary, secondary and tertiary.



Write the following simple structures in Lewis and then in bond-line

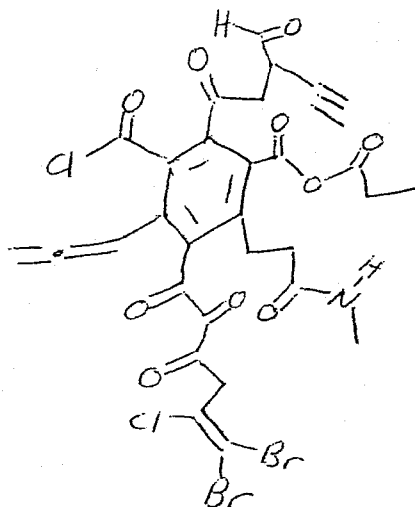
- 1 methylethylbutylamine
- 2 pentanal
- 3 3-methyl-2,3-decanediol (diol means two alcohol groups)
- 4 pentanenitrile
- 5 butanoic anhydride
- 6 hexanoyl bromide
- 7 pentyloctyl ether
- 8 4,5-diethyl-1-undecene

See attached

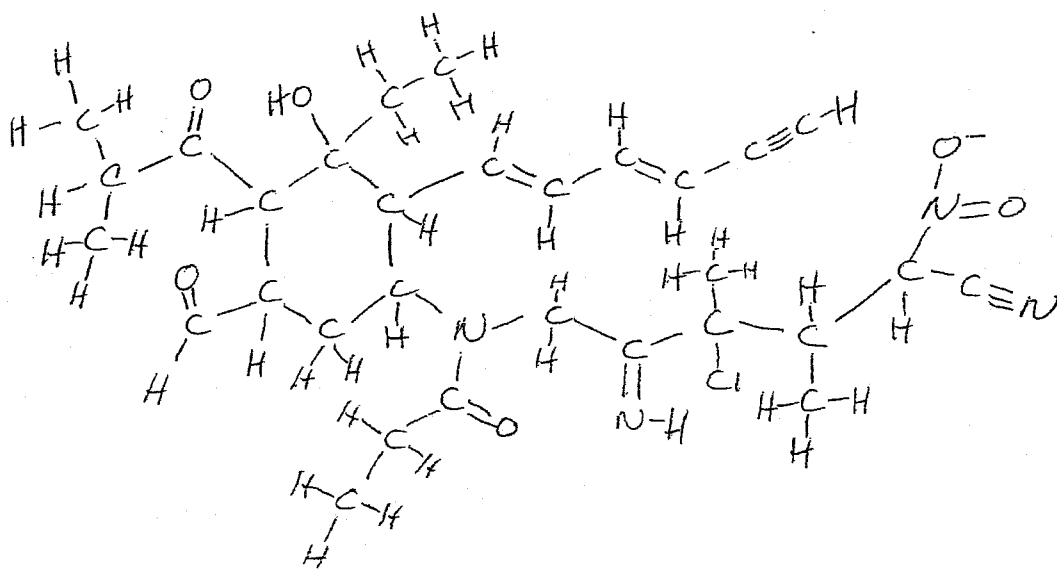
Translation Solutions - 2

20 2/4

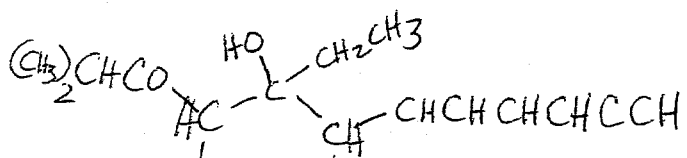
Bond Line of "wheel of difficult functional groups"



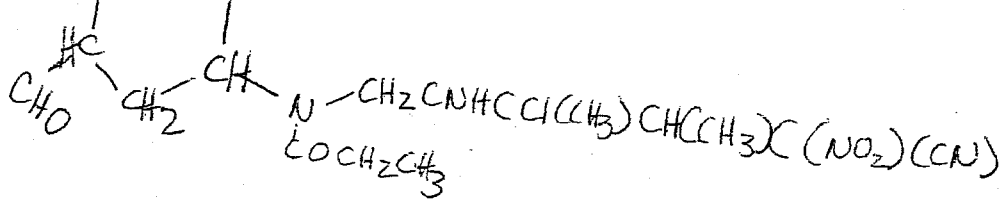
Lewis Dash and Condensed of Large Structure



Lewis DASH



Condensed



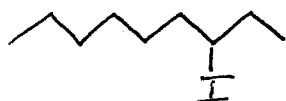
Nerz

32

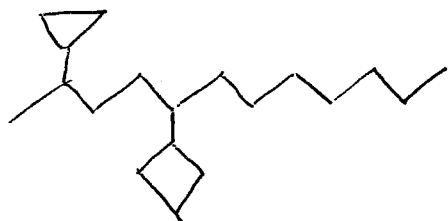
email - basic things about nomenclature

-1-

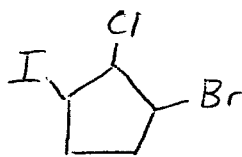
① Mini exercise: 3-iodononane



② Mini exercise: 2-cyclopropyl-5-cyclobutyldecane
1,2,3,4,5,6-hexachlorocycloheptane



③ Mini exercise 1-iodo-2-chloro-3-bromocyclopentane



This is wrong
should be

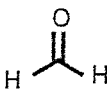

1-bromo-2-chloro-1-iodocyclopentane

④ Mini-exercise: 3,4,6-trimethyl-3,5-octatrien-1-yl
1-ethyl-5,6-di(2-methyl-3-hexenyl)cyclohexene
(next page)

Organic Nomenclature Needed For The First Semester

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Organic chemists use a combination of IUPAC (International Union of Pure and Applied Chemistry) and trivial nomenclature when referring to compounds. IUPAC nomenclature is a systematic method of naming compounds on which much of this discussion will focus. Chemists also frequently use common or trivial names. To be able to communicate effectively, some trivial names must also be known. Some examples of commonly used trivial names and their corresponding systematic names are given below.



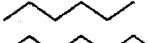


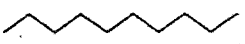

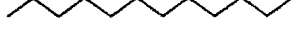
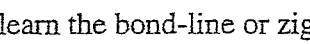
CH_3COOH		$\text{H}-\text{C}\equiv\text{C}-\text{H}$	
trivial name: acetic acid	formaldehyde	acetylene	acetone
IUPAC name: ethanoic acid	methanal	ethyne	2-propanone

By the end of this unit, you will be able to name systematically the following classes of compounds.

Alkanes
Cycloalkanes
Haloalkanes
Alkenes
Alkynes
Aromatic Compounds

In addition to studying these notes, it is very important to read the assigned sections for unit one and to do the corresponding assigned problems in McMurry

Fundamental to naming all molecules systematically is learning the names of the straight chain alkanes. For this course it is expected that you will learn the names and structures for alkanes having one carbon through twelve carbons. These names and structures are given below.

# c's	name	structure
1	methane	CH_4
2	ethane	CH_3CH_3
3	propane	$\text{CH}_3\text{CH}_2\text{CH}_3$
4	butane	
5	pentane	
6	hexane	
7	heptane	
8	octane	
9	nonane	
10	decane	
11	undecane	
12	dodecane	

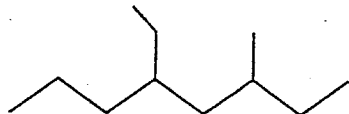
From the above it is clear why we learn the bond-line or zigzag method of writing structures.

Not all alkanes are straight chain compounds. Many have branches. To handle these the following rules are used.

A. Naming Branched Alkanes

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e.g. this is a branched alkane



Branched alkanes are named using the straight chain or root names listed above combined with special names for the branches. Branch positions are indicated by a number.

The correct IUPAC name for the above compound is.....

above: 5-ethyl-3-methyl octane

↑ ↑
branch name
prefix

↑
root name

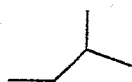
The following are the names chemists give to the branches. The arrow to the left indicates the point of attachment to the main chain. Notice that most of the names are related to the straight chain names, but several of them are trivial. The trivial names given are accepted by IUPAC. The systematic naming of branched side chains (yes, sometimes even the branches have branches) will be covered shortly.

—CH_3 = methyl (based on methane)
 $\text{—CH}_2\text{CH}_3$ = ethyl (based on ethane)
 $\text{—CH}_2\text{CH}_2\text{CH}_3$ = propyl (based on propane)
 $\text{—CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ = butyl

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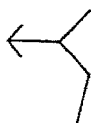
$\begin{array}{c} \text{CH}_3 \\ | \\ \text{—C—H} \\ | \\ \text{CH}_3 \end{array}$ = isopropyl (trivial accepted by IUPAC)
 or - (1- methylethyl) systematic

—(1-methylethyl) systematic



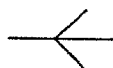
= isobutyl (trivial)

OR -(2-methylpropyl) = IUPAC



= sec butyl (trivial)

OR -(1-methylpropyl) = IUPAC



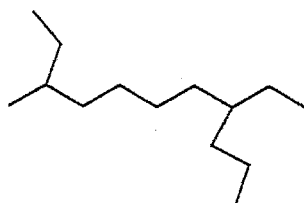
= t-butyl = tertiary butyl

OR (1,1-dimethyl ethyl)

With the above basic information we can name many organic compounds using the following rules.

Rules

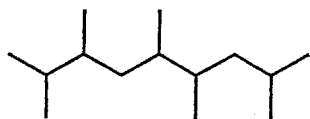
1. Locate the longest continuous chain of carbons. If two or more chains of equal length exist, pick the one with the greatest number of branch points. Notice the longest chain is not always the one going from left to right or from right to left. You need to count carbons in all different directions, from terminus to terminus until you find the longest continuous chain. Consider the following example.



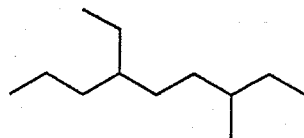
8-ethyl-3-methylundecane

2. Give the longest continuous chain an appropriate base name. For the above compound it would be undecane.

3. Number the parent chain so that each branch (substituent) has a number associated with it. In numbering the "parent" chain start at whichever end of chain that gives rise to lowest numbers at branches. This can be a little tricky at times. When the direction does not seem obvious (as when there are multiple branches), choose the direction which has the lowest number at the first point of difference. Sometimes numbering in either direction gives rise to the same combination of numbers. When this occurs, number the branches in the order in which they will occur in the name, i.e., alphabetically. The following two examples illustrate these two points.



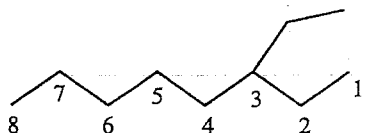
2,3,5,6,8-pentamethylnonane



4-ethyl-7-methyldecane

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4. Name each branch (side chain), i.e., give the branch one of the branch names above.
5. Combine the number with the branch name, putting a dash between the number and branch name. This is put directly in front of (to the left of) the main chain name. The following examples illustrates rules 1-5 for a simple compound.



3-ethyloctane

6. When 2 or more branches are on the same carbon of the main chain, use the number as many times as there are substituents. Consider the following example illustrating this point.



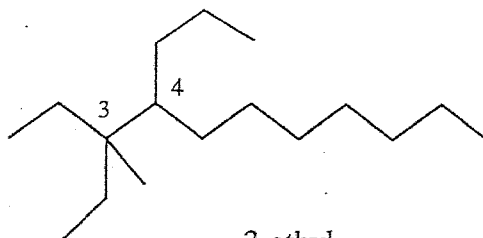
4-ethyl-4-methyloctane

7. If some alkyl group occurs more than once in chain, indicate and abbreviate this by using a prefix: di, tri, tetra. Notice that all the numbers are used even though the branch name is abbreviated. Also notice that commas are used between the numbers.



2,2,4,4-tetramethylheptane

8. If there are several different substituents on parent chain, put them in alphabetical order in name. When alphabetizing ignore prefixes such as, sec-t-, di-, tri-, etc. The only prefixes that should be considered when alphabetizing are iso and neo.



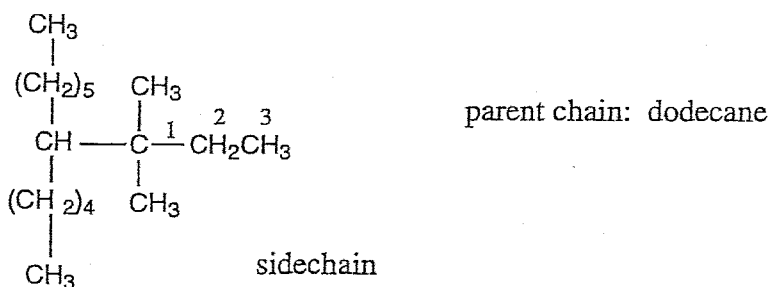
3-ethyl
3-methyl
4-propyl

3-ethyl-3-methyl-4-propylundecane

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Please note the punctuation used in the above name. Dashes are used around numbers and commas between adjacent numbers.

There are many other possible side chains than the ones listed above. When naming side chains that contain branches that are more complex than those given it is best to use the IUPAC method. Consider the following example and the listed rules.



1. Identify the complex side chain. In this case the parent or main chain is dodecane. The side chain has a total of five carbons but it is branched.
2. Find the longest continuous chain of carbons within this side chain always starting at the carbon that is attached directly to the parent chain. In this case the longest continuous chain consists of three carbons.
3. This "main" side chain is given the appropriate alkyl name. In this case it is propyl.
4. the "main" side chain is always numbered from the parent chain out. There is no decision when it comes to numbering. The numbering is given on the structure above.
5. The branches off the "main" side chain are given appropriate alkyl names. In this case there are two subbranches and both are methyl groups.
6. The sub-branch numbers and names are combined with the "main" branch name as follows.

1,1-dimethylpropyl

7. When combined with the main chain name, the entire complex side chain name is put in parenthesis and given a parent chain number as follows for our example.

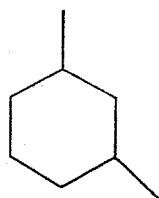
6-(1,1-dimethylpropyl)dodecane

B. NOMENCLATURE OF CYCLOALKANES

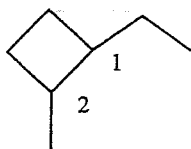
Rules

1. Normally the **cycloalkane** part of molecule is root or parent name. Therefore, count **c's** in ring and give it an appropriate alkane parent name prefixed with **cyclo**.
2. Number the ring so that the substituents have the lowest combination of numbers. A substituent must be number one on the ring.
3. When two or more different alkyl groups are present they are numbered alphabetically.

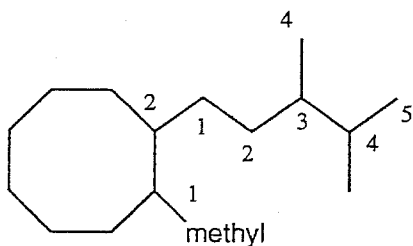
The following examples illustrate the basics of naming of ring compounds.



1,3-dimethyl cyclohexane



1-ethyl-2-methylcyclobutane

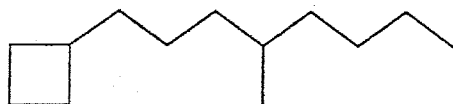


1-methyl-2-(3,4-dimethylpentyl)cyclooctane



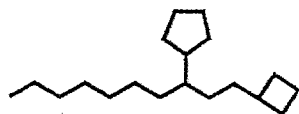
4. Occasionally, it is more appropriate to name a compound containing a ring so that the ring is the substituent. This is done when an alkyl chain has more carbons than the attached ring or when there are multiple rings attached to a chain.

e.g.



1-cyclobutyl-4-methyloctane

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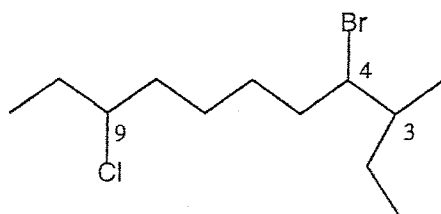


1-cyclobutyl-3-cyclopentyldecane

C. Naming Haloalkanes or Alkyl Halides

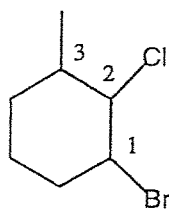
Organic compounds containing halogens are named as "haloalkanes". The halogen atoms are viewed as substituents or branches on the main chain and are given the branch names fluoro, chloro, bromo and iodo. Halogen substituents are treated the same as alkyl substituents in terms of numbering, i.e., they are viewed as equal in priority to alkyl groups.

e.g.



Cl - chloro Br - bromo
F - fluoro I - iodo

4-bromo-9-chloro-3-methyl undecane



1-bromo-2-chloro-3-methylcyclohexane

D. Naming Alkenes (Olefins) and Polyenes

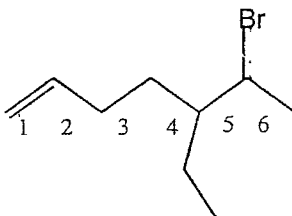
At this point, it is important to realize that some functional groups take priority over others in terms of numbering. When naming alkenes the position of the double bond or double bonds must be specified. The numbering of the double bond takes priority over the numbering of the substituents. So given the choice between a double bond having a lower number or the substituents having a lower number, the double bond will win out.

Rules

40

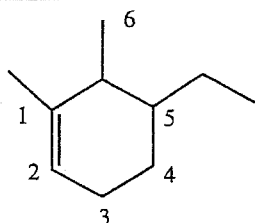
1. Find the longest continuous chain containing the double bond or double bonds.
2. Give this parent chain (which may not be the longest chain) an appropriate alkane root name. Drop the "ane" ending and substitute the "ene" ending.
3. Number chain so that double bond is in the lowest possible position (regardless of the positions of other halogens or alkyl groups). The numbering must include both carbons of the double bond!
4. Name the halo and alkyl groups as usual, giving them the position numbers as dictated by alkene position

e.g.



6-bromo-5-ethyl-1-heptene

N.B. d.b. position: d.b. given no. 1 if between carbons 1 & 2
d.b. given no 2 if between carbons 2 & 3



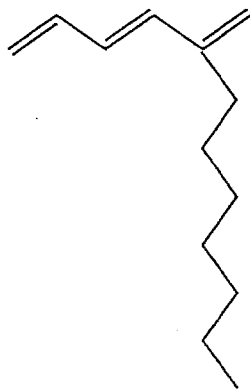
5-ethyl-1,6-dimethyl cyclohexene

Notice in the above example that when numbering the positions of the double bond, the site bearing the substituent is given number one.

Multiple Double Bonds

For molecules having multiple double bonds the rules are basically the same but the root name becomes "alkadiene" or "alkatriene"

e.g.



2-heptyl-1,3,5-hexatriene

E. Naming Alkynes

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Alkynes are named in the same way as alkenes, but the "yne" ending is used for monoalkynes. The "diyne, triyne, etc." endings are used for polyynes.

e.g.,



6-methyl-1,3-decadiyne

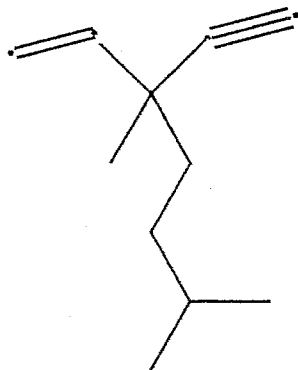
F. Naming Molecules With Different Types of Functional Groups

Generally, the functional group having the highest priority dictates the numbering. For example, the position of a ketone would take priority over the position of an alkene. When it comes to alkenes versus alkynes, they are considered to be of almost equal priority. When an alkene and an alkyne are in the same chain the following rules apply.

Rules

1. Choose the chain having both functional groups.
2. Number the chain so that you get the lowest combination of bond position. There is no concern about which bond receives the lower number.
3. If the number pattern is the same in either direction along the chain, then number to give the alkene the lower number.
4. The chain is given an appropriate #-alken-#-yne ending. The first number in the name refers to the position of the double bond. The second number refers to the position of the triple bond.
5. The substituents are named in the usual way.

e.g.



3-methyl-3(3-methylbutyl)1-penten-4-yne

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G. Naming Aromatic Compounds

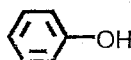
The following names and associated structures of aromatics should be committed to memory. The simple aromatics that you will be studying are these and some derivative of the listed compounds. The names of the derivatives are usually based on the listed names.



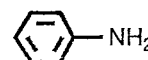
benzene



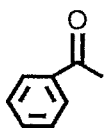
toluene



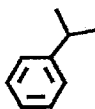
phenol



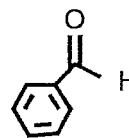
aniline



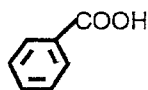
acetophenone



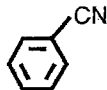
cumene



benzaldehyde



benzoic acid



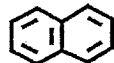
benzonitrile



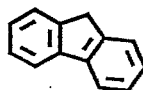
xylene (regiochemistry not specified)



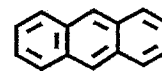
styrene



naphthalene



fluorene



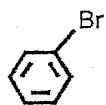
anthracene



phenanthrene

Rules

1. The benzene ring is usually viewed as the root name so many simple aromatics are named as substituted benzenes. Substituents are named as you have learned earlier in these notes. If an attached alkyl chain is larger than the benzene ring, then the compound may be named as a substituted alkyl chain with the aromatic ring being incorporated into the name as a phenyl group. The following examples illustrate this point.

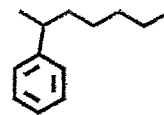


bromobenzene



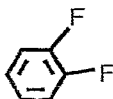
propylbenzene

43

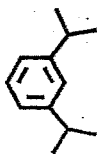


2-phenylheptane

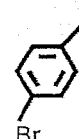
2. When two substituents are on a benzene ring, the prefixes ortho, meta and para are used to designate relative positions. Ortho refers to 1,2 disubstitution, meta to 1,3 -disubstitution and para to 1,4 disubstitution. These prefixes are usually abbreviated o, m and p, respectively at the beginning of the name. The following examples illustrate the use of ortho, meta and para.



ortho-difluorobenzene

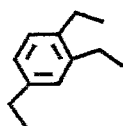


meta-diisopropylbenzene

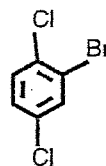


para-bromoiodobenzene

3. When more than two substituents are on a benzene ring the positions are numbered so that the lowest numbers are used. As you learned with the other classes of compounds, the substituents are alphabetized in the name. Consider the following examples.

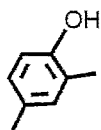


1,2,4 - triethylbenzene



2-bromo-1,4-dichlorobenzene

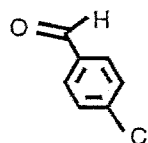
4. Any of the names given in the general table on page ten are commonly used as root names. For example, if one was naming a benzene ring with a methyl group and nitro (NO_2) group attached and these groups were ortho with respect to one another, the compound would most likely be called ortho-nitrotoluene. Calling it ortho-methylnitrobenzene makes sense, but you won't find it written that way very often in the chemical literature. The following examples further illustrate this idea.



2,4-dimethylphenol



meta-xylene



para-chlorobenzaldehyde

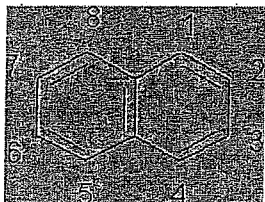
44

[BacktoStudyAids]

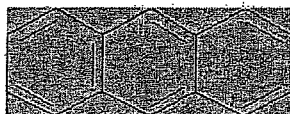
Nomenclature Needed for the Second Semester Course

H. Nomenclature of Polycyclic Aromatic and Aromatic Heterocycles

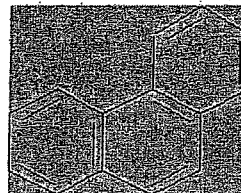
The following fundamental structures should be learned for the course. You should be able to name the base structure as well as simply substituted derivatives. If numbers are not given, you will not have to name substituted derivatives.



naphthalene



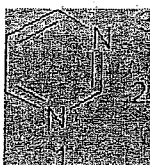
anthracene



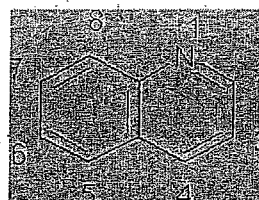
phenanthrene



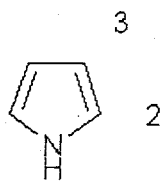
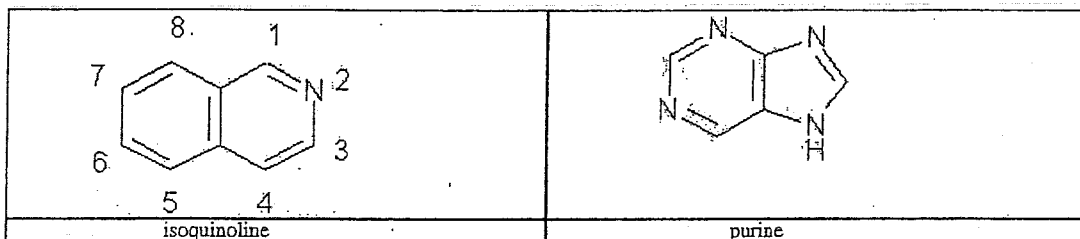
pyridine



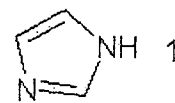
pyrimidine



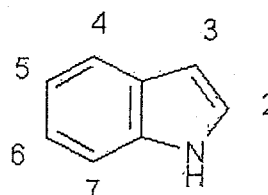
quinoline



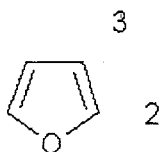
pyrrole



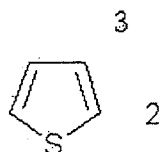
imidazole



indole

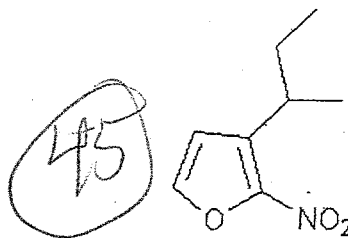
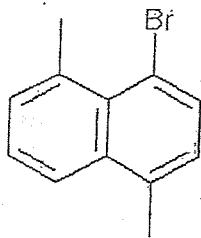


furan



thiophene

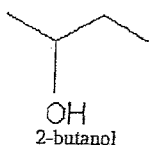
Try to name the following substituted, aromatic heterocycles.....



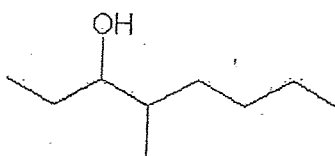
I. Nomenclature of Alcohols

Alcohols are named using the alkane root name, but the *e* is dropped and replaced with the alcohol ending *-ol*. A number is placed just ahead of the revised root name specifying the position of the $-OH$ group. It is important to note that the alcohol functional group is considered to be higher priority than the alkene or alkyne group. This means that when a molecule has multiple functional groups including hydroxyls, double bonds and triple bonds, you pick the longest continuous chain containing the alcohol or alcohol groups and you number the chain so that the alcohol groups have the lowest positions possible.

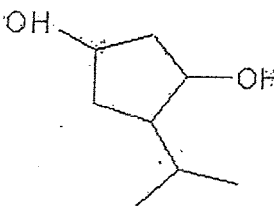
Consider the following examples.



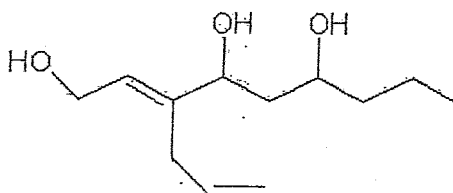
2-butanol



4-methyl-3-heptanol



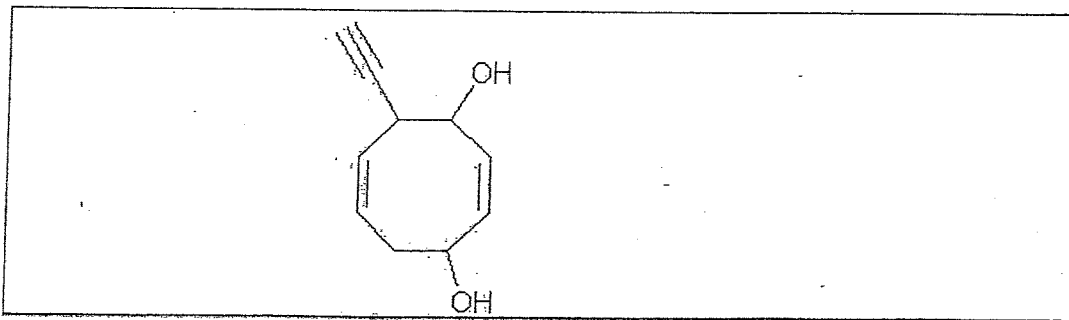
4-isopropyl-1,3-cyclopentanediol



3-(2-propenyl)-2-nonene-1,4,6-triol

Notice in the third example that the numbering in the ring must start at an alcohol position and pay particular attention to the nomenclature in the last example. The side chain is a complex side chain and since the main chain has two different types of functional groups both are incorporated into the root name as shown. The number for the alkene functional group in the main chain appears just before the root name while the numbers for the hydroxyl groups appear just before the alcohol suffix.

Try to name the following compound.

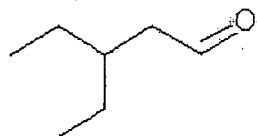


I. Nomenclature of Aldehydes and Ketones

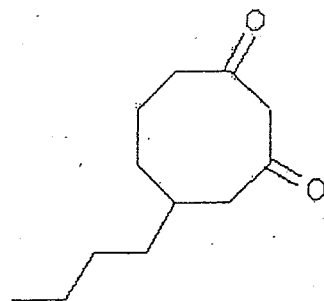
Simple aldehydes and ketones are named similarly to alcohols. The fundamental alkane names are used, but the *e* is dropped and replaced with *-al* and *-one*, depending on the situation. In terms of priority, both groups are higher than alcohols, but between the two, the aldehyde is highest. This means that if the aldehyde and ketone appeared in the same molecule, you would give chain and numbering preference to the aldehyde.

You will note that the aldehyde group is always a terminal group so in most structures numbering is redundant and can be left out.

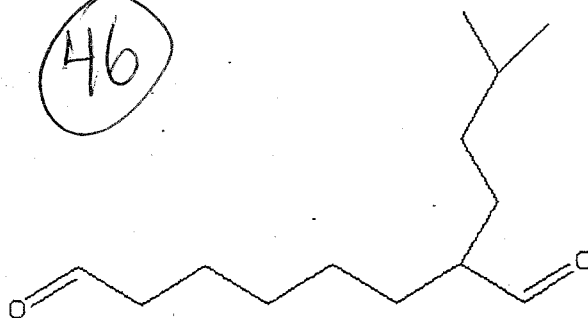
Study the following examples.



3-ethylpentanal

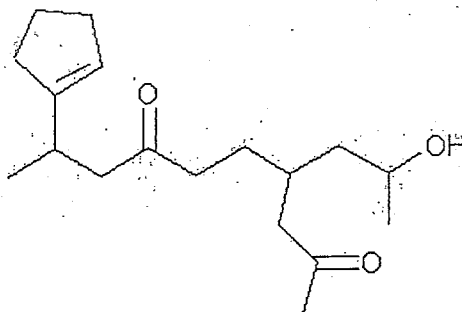
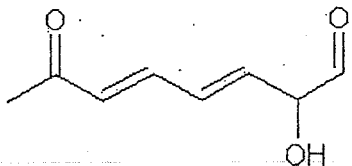


5-butyl-1,3-cyclooctanedione



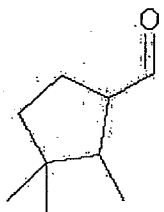
2-(3-methylbutyl)-octanedial

Try to name the following structures

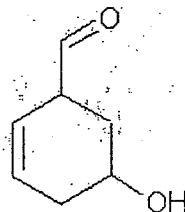


Sometimes an aldehyde appears on a ring. Given its high priority the ring is named as a cycloalkanecarbaldehyde.

Please consider the following examples.



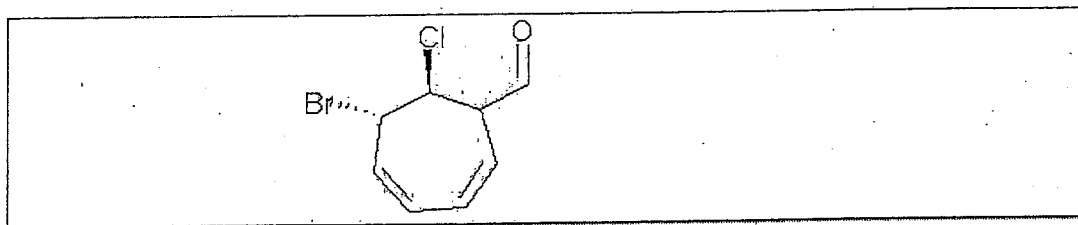
2,3,3-trimethyl-cyclopentanecarbaldehyde.



3-hydroxy-5-cyclohexenecarbaldehyde ...

Notice in the second example that the alcohol group is called a hydroxy because it is lower priority than the aldehyde. Also please note that the alkene is given last consideration in terms of numbering.

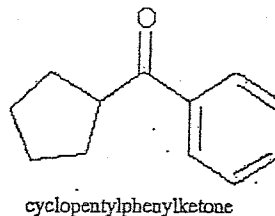
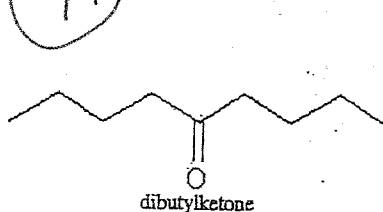
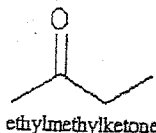
Please attempt to name the following compound.



As a review try to designate the absolute stereochemistry of the stereocenters.

Ketones are frequently named using their common names which involves simply giving alkyl-type names to the two chains coming off the ketone and following those names with the word . ketone. . The following examples illustrate this trivial, but acceptable nomenclature.

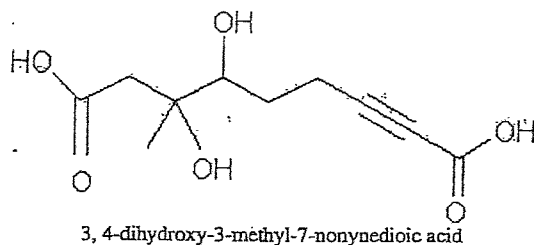
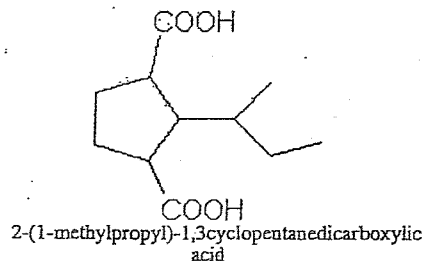
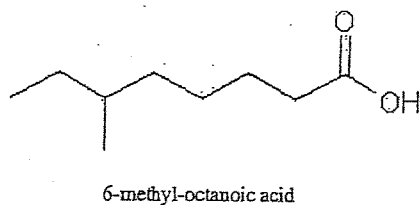
47



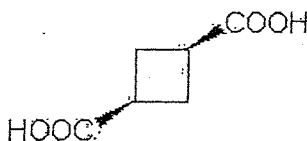
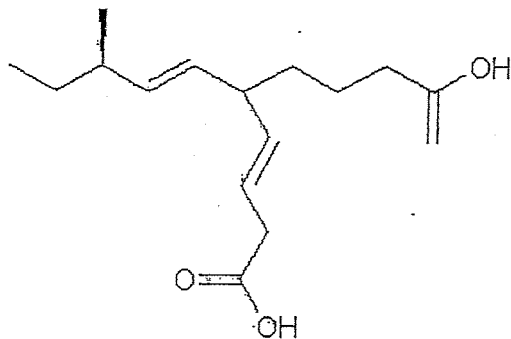
Please note that the two substituents are ordered alphabetically in the common name. - In alphabetizing, the prefixes: t-, sec-, di-, tri-, etc. are ignored. The prefixes neo-, iso-, cyclo- are considered. In complex side chain names (the ones in parenthesis), the first letter encountered is used in the ordering.

K. Nomenclature of Carboxylic Acids

Carboxylic Acids have a lot in common with aldehydes since they are terminal groups and by structural necessity must be peripheral on rings. The one difference to note is that they are higher priority than aldehydes. At this point, I figure you can get the drift of carboxylic acid nomenclature by just absorbing a few good examples.....



Try your hand at naming these carboxylic acids.



Please include the absolute configuration of any stereocenters.

Nomenclature of Carboxylic Acid Derivatives

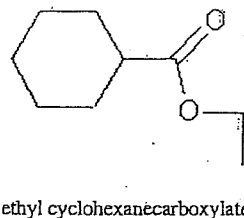
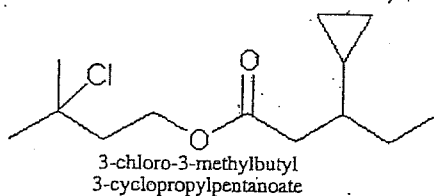
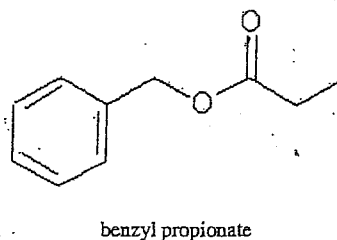
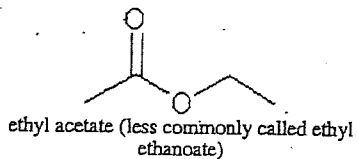
You will not be expected to be supreme experts on these derivatives, but you do need to know the basics of naming them. The esters are the most important so these will be covered the most rigorously.

esters

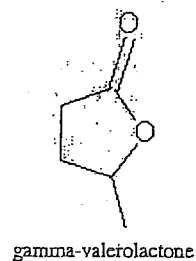
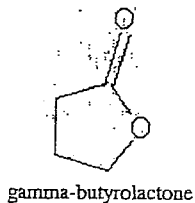
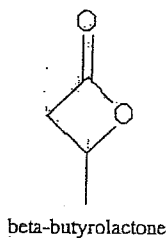
Esters are named the way salts are named. Think about the sodium salt of acetic acid. It is called sodium acetate. For an ester, the sodium would be replaced by the appropriate alkyl name for the substituent on the oxygen of the ester functional group.

48

Please consider the following examples....



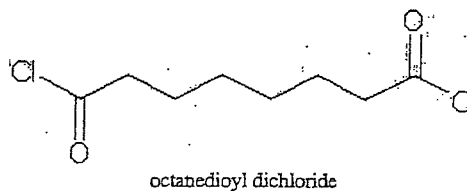
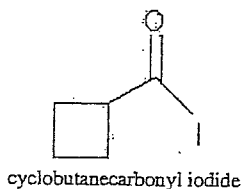
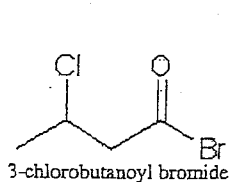
Cyclic esters are called lactones. A few examples are given below. You will not be responsible for the specific nomenclature of this subclass.



Acid (Acyl Halides)

Acid halides are named taking the .ic. ending off the corresponding carboxylic acid name and replacing it with .yl. and then adding the appropriate halide ending.

A few simple examples.....

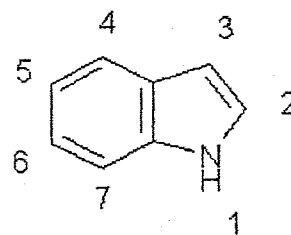
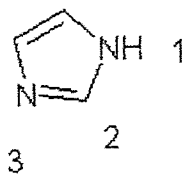
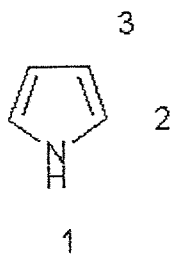
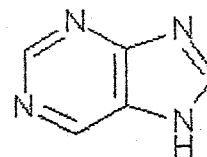
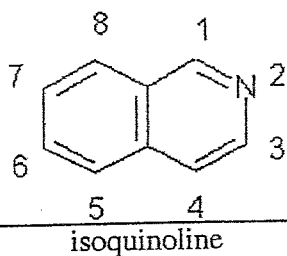
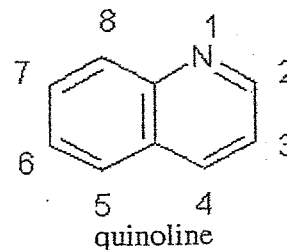
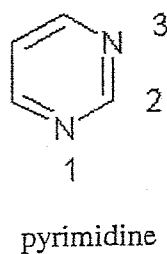
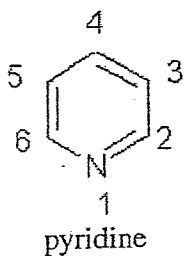
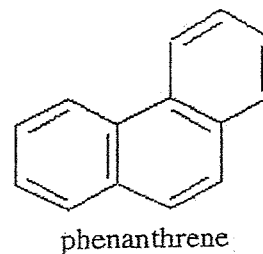
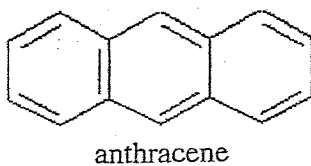
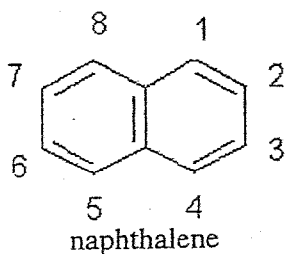


[BacktoStudyAids]

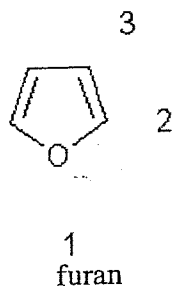
49

Nomenclature Needed for the Second Semester Course**H. Nomenclature of Polycyclic Aromatic and Aromatic Heterocycles**

The following fundamental structures should be learned for the course. You should be able to name the base structure as well as simply substituted derivatives. If numbers are not given, you will not have to name substituted derivatives.



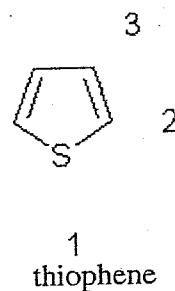
pyrrole



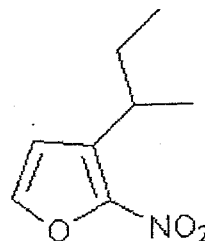
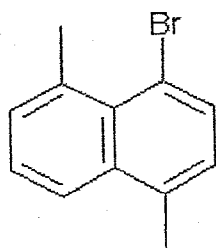
imidazole

50

indole



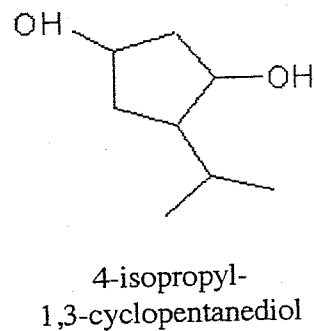
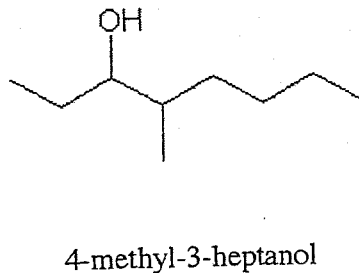
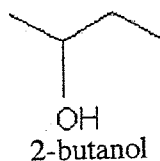
Try to name the following substituted, aromatic heterocycles.....

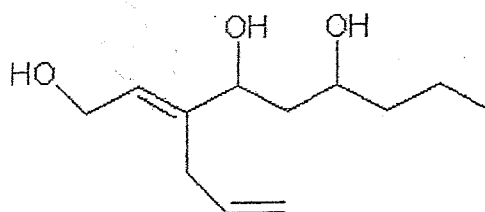


I. Nomenclature of Alcohols

Alcohols are named using the alkane root name, but the . e. is dropped and replaced with the alcohol ending . -ol. . A number is placed just ahead of the revised root name specifying the position of the -OH group. It is important to note that the alcohol functional group is considered to be higher priority than the alkene or alkyne group. This means that when a molecule has multiple functional groups including hydroxyls, double bonds and triple bonds, you pick the longest continuous chain containing the alcohol or alcohol groups and you number the chain so that the alcohol groups have the lowest positions possible.

Consider the following examples.



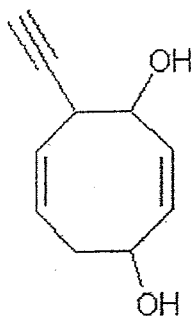


3-(2-propenyl)-2-nonen-1,4,6-triol

(57)

Notice in the third example that the numbering in the ring must start at an alcohol position and pay particular attention to the nomenclature in the last example. The side chain is a complex side chain and since the main chain has two different types of functional groups both are incorporated into the root name as shown. The number for the alkene functional group in the main chain appears just before the root name while the numbers for the hydroxyl groups appear just before the alcohol suffix.

Try to name the following compound.

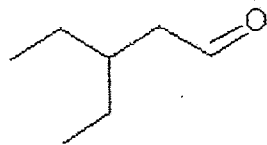


J. Nomenclature of Aldehydes and Ketones

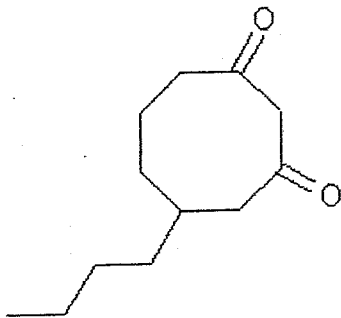
Simple aldehydes and ketones are named similarly to alcohols. The fundamental alkane names are used, but the .e. is dropped and replaced with .al. and .one., depending on the situation. In terms of priority, both groups are higher than alcohols, but between the two, the aldehyde is highest. This means that if the aldehyde and ketone appeared in the same molecule, you would give chain and numbering preference to the aldehyde.

You will note that the aldehyde group is always a terminal group so in most structures numbering is redundant and can be left out.

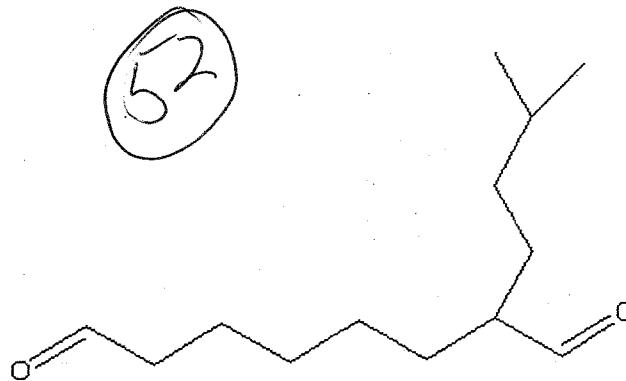
Please study the following examples.



3-ethylpentanal

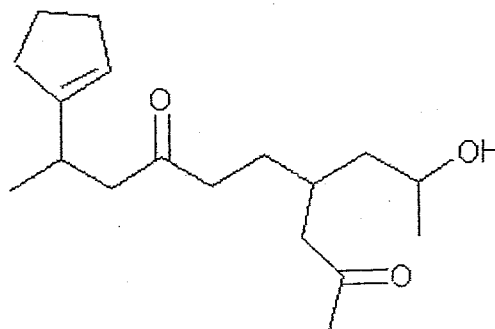
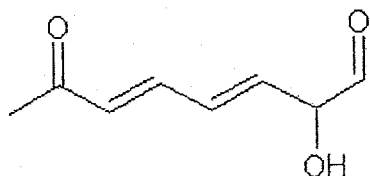


5-butyl-
1,3-cyclooctanedione



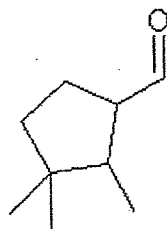
2-(3-methylbutyl)-octanal

Try to name the following structures

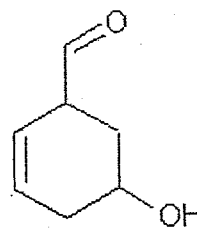


Sometimes an aldehyde appears on a ring. Given its high priority the ring is named as a cycloalkanecarbaldehyde.

Please consider the following examples.



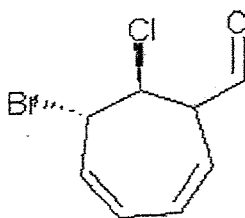
2,3,3-trimethyl-cyclopentanecarbaldehyde



3-hydroxy-5-cyclohexenecarbaldehyde

Notice in the second example that the alcohol group is called a hydroxy because it is lower priority than the aldehyde. Also please note that the alkene is given last consideration in terms of numbering.

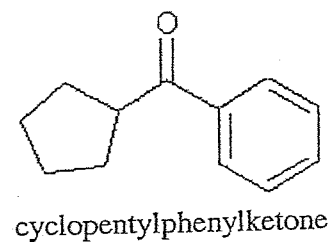
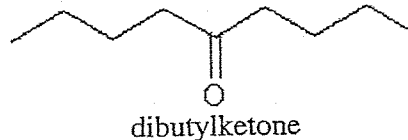
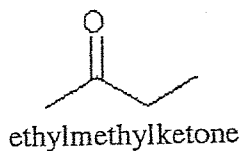
Please attempt to name the following compound.



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As a review try to designate the absolute stereochemistry of the stereocenters.

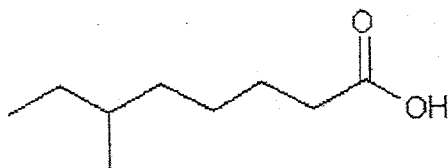
Ketones are frequently named using their common names which involves simply giving alkyl-type names to the two chains coming off the ketone and following those names with the word . ketone. . The following examples illustrate this trivial, but acceptable nomenclature.



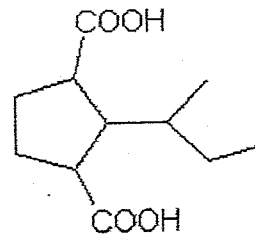
Please note that the two substituents are ordered alphabetically in the common name. In alphabetizing, the prefixes: t-, sec-, di-, tri-, etc. are ignored. The prefixes neo-, iso-, cyclo- are considered. In complex side chain names (the ones in parenthesis), the first letter encountered is used in the ordering.

K. Nomenclature of Carboxylic Acids

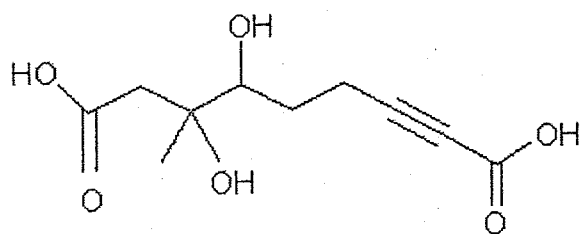
Carboxylic Acids have a lot in common with aldehydes since they are terminal groups and by structural necessity must be peripheral on rings. The one difference to note is that they are higher priority than aldehydes. At this point, I figure you can get the drift of carboxylic acid nomenclature by just absorbing a few good examples.....



6-methyl-octanoic acid



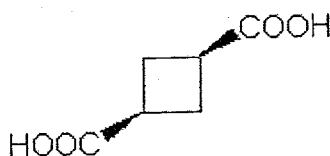
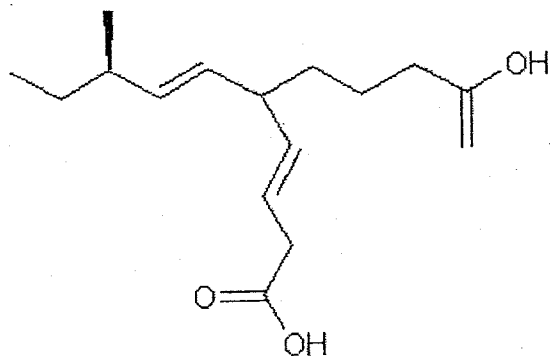
2-(1-methylpropyl)-1,3cyclopentanedicarboxylic acid



3,4-dihydroxy-3-methyl-7-nonynedioic acid

54

Try your hand at naming these carboxylic acids.



Please include the absolute configuration of any stereocenters.

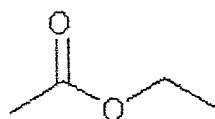
L. Nomenclature of Carboxylic Acid Derivatives

You will not be expected to be supreme experts on these derivatives, but you do need to know the basics of naming them. The esters are the most important so these will be covered the most rigorously.

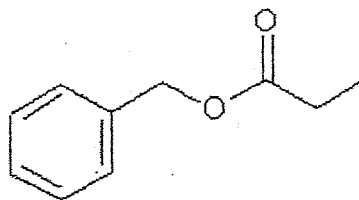
Esters

Esters are named the way salts are named. Think about the sodium salt of acetic acid. It is called sodium acetate. For an ester, the sodium would be replaced by the appropriate alkyl name for the substituent on the oxygen of the ester functional group.

Please consider the following examples....

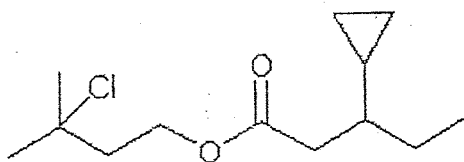
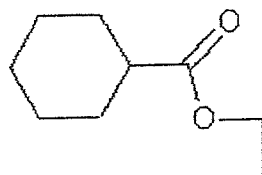


ethyl acetate (less commonly called ethyl ethanoate)



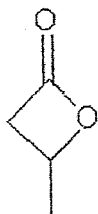
benzyl propionate

4/12
55

3-chloro-3-methylbutyl
3-cyclopropylpentanoate

ethyl cyclohexanecarboxylate

Cyclic esters are called lactones. A few examples are given below. You will not be responsible for the specific nomenclature of this subclass.



beta-butyrolactone



gamma-butyrolactone

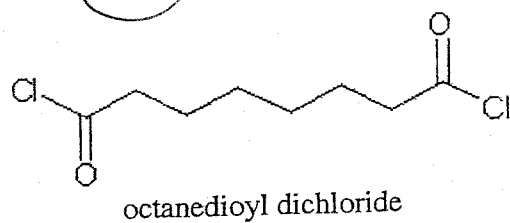
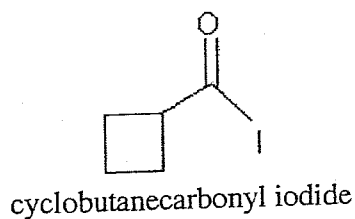
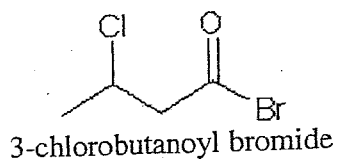


gamma-valerolactone

Acid (Acyl Halides)

Acid halides are named taking the .ic. ending off the corresponding carboxylic acid name and replacing it with .yl. and then adding the appropriate halide ending.

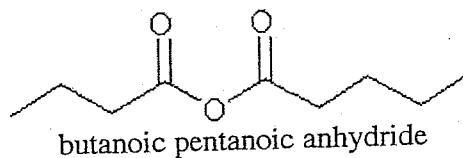
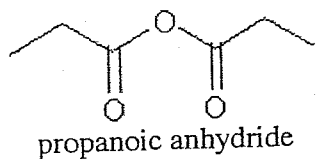
A few simple examples.....



Anhydrides

Anhydrides are named in a manner similar to the trivial method for ketones. The two parent acids are given names and that is followed by the word anhydride.

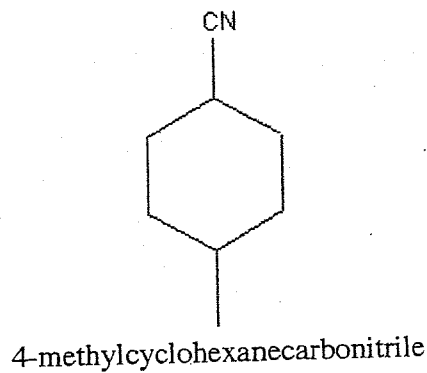
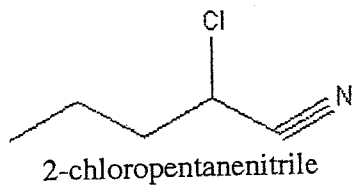
Here are a few examples...

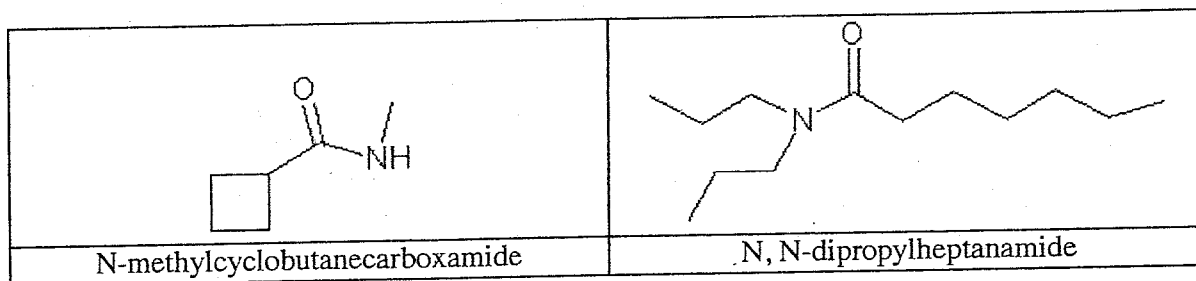


Notice that the two acid names are alphabetized when they are different and that when the anhydride is symmetrical, no di- prefix is used.

Nitriles and Amides

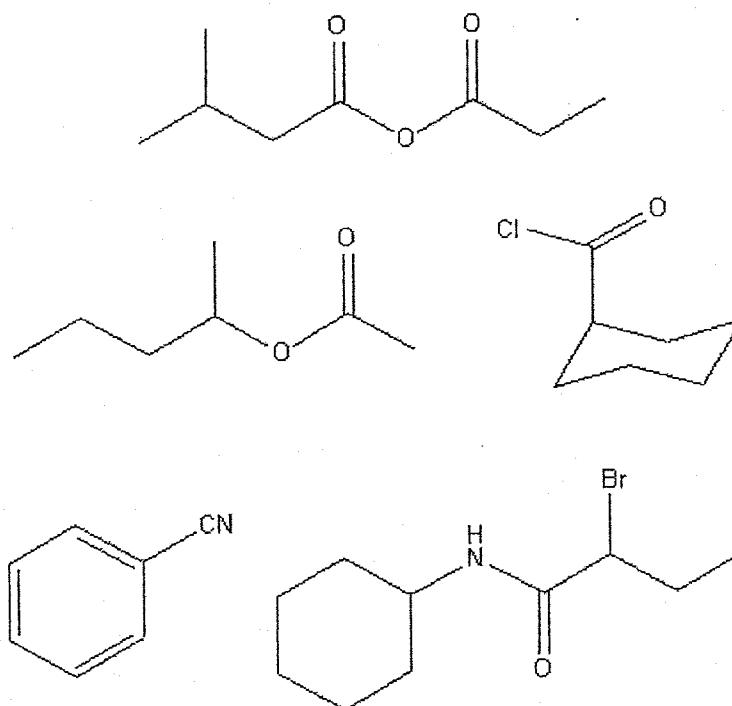
Please study the following examples.....





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Try to name these carboxylic acid derivatives

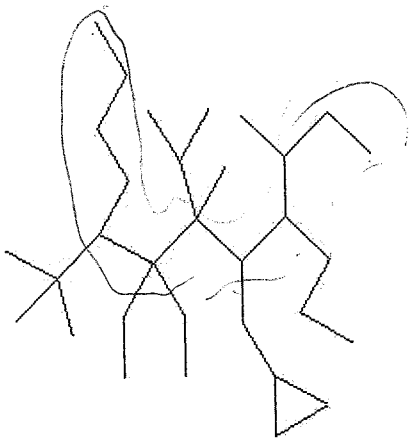


M. Amines

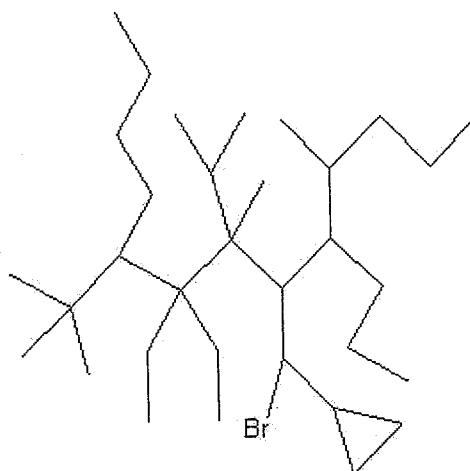
Amines are named like ethers. You give the chains attached to the nitrogen the normal alkyl names and follow them by . amine. . You should alphabetize the alkyl names and use multiple prefixes as needed. Try to name the following compounds.

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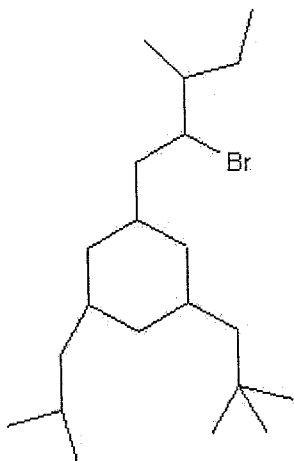
Nomenclature Workshop



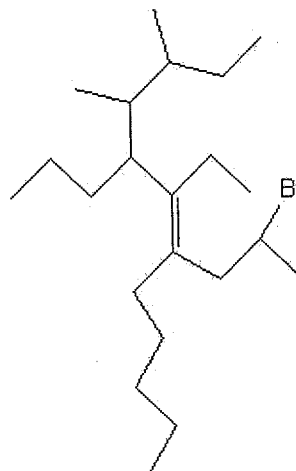
Problem 1a



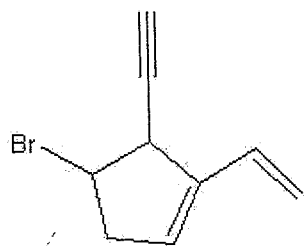
Problem 1b



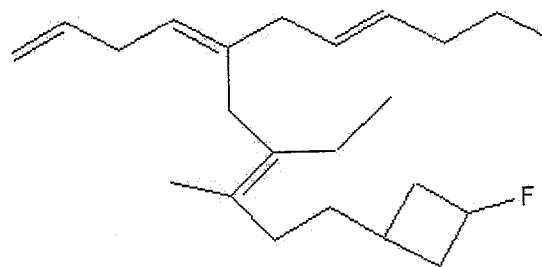
Problem 2



Problem 3



Problem 4



Problem 5