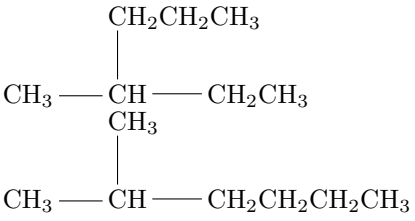
Show all work leading up to **all** responses. You may attach additional pages if needed.

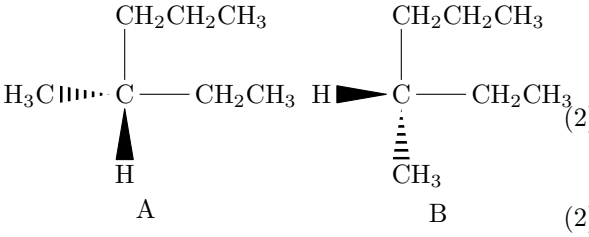
1. Identify and explain the isomeric relationship between the following pairs of compounds.

(3) (a) 2,2-Dimethylpentane and 2-Methylhexane

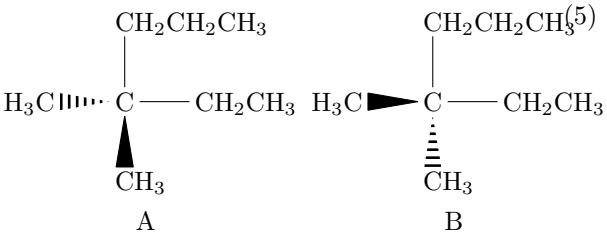
(3) (b)



(3) (c)



(3) (d)



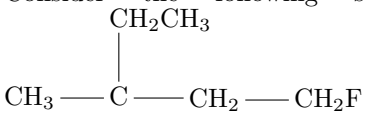
2. Represent ethane using the following kinds of diagrams:

(2) (a) Lewis-Dot Diagram

(2) (b) Line-bond Diagram

(3) (c) Condensed structural formula

3. Consider the following structural formula:



(2) (a) Identify the parent alkane.

(2) (b) Identify all functional groups in the compound.

(5) (c) Write the IUPAC name of the compound.

4. Consider 3-ethyl-2-methylhexane:

(2) (a) Identify the parent alkane.

(2) (b) Identify all functional groups in the compound.

(5) (c) Draw the chemical structure of the compound.

5. Consider the bond between the 2nd and 3rd carbon of butane.

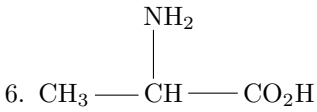
(5) (a) Draw the Newman projections for all possible conformations. Label them with letters such as A, B, C, etc.

Points earned: _____ out of a possible 42 points

(3) (b) Which conformers are eclipsed? Which are staggered?

(4) (c) Draw a rough potential energy diagram for rotating around the bond.

(3) (d) Explain your reasons for identifying the highest and lowest energy conformers.

6. 

Alanine

(2) (a) Draw a 3D line-bond diagrams of both stereoisomers.

(2) (b) Draw Fisher projections of each steroisomer.

(3) (c) Use the Cahn-Ingold-Prelog Rules to determine the configuration of each steroisomer (R or S).

(1) (d) Compare and constrast the stereoisomers physical properties.

(1) (e) Compare and constrast the stereoisomers chemical activity.

7. Draw a reaction energy diagram for a two-step reaction with $K_{\text{eq}} > 1$.

(5) (a) Label the parts of the diagram corresponding tor reactants, products, transition state, ΔG°, and $\Delta G^{\ddagger}$.

(2) (b) Is ΔG° positive or negative?

Points earned: _____ out of a possible 26 points

8. Draw a reaction energy diagram for a two-step reaction with $K_{eq} > 1$, whose second step is faster than the first step of the reaction.

(5) (a) Label the parts of the diagram corresponding tor reactants, products, transition state, ΔG°, and $\Delta G^{\ddagger}$.

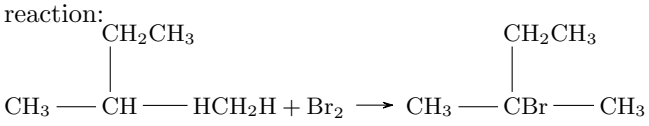
(2) (b) Is ΔG° positive or negative?

(2) (c) Why is the second step as you have drawn it faster than the first step?

(8) 9. Predict the products of the following reaction and balance the resulting equation:
$C_3H_8 + O_2 \longrightarrow$

(10) 10. Predict the products and draw the mechanism for the following reaction:
$CH_3CH_3 + Cl_2 \longrightarrow$

(5) 11. Explain the lack of side reactions for the following reaction:



Assigning Abs. Config. to Wedge/Dashed 3D Structures

1. Prioritize the four groups around a chiral center according to atomic number. The highest atomic number is assigned priority #1, and the lowest atomic number is assigned priority #4.[1]
2. Orient the chiral centre such that the #4 priority substituent is pointing away from the viewer.
3. Trace the path of priorities #1, #2 and #3. (For this part you ignore #4).
4. If the path traced from 1-2-3 is clockwise, the chiral center is assigned (R) (from Latin, rectus)
5. If the path traced is counter clockwise, the chiral center is assigned (S) (from the Latin sinister)

Assigning Abs. Cong. to Fischer Proj.

1. Prioritize the four groups around a chiral center according to atomic number. The highest atomic number is assigned priority #1, and the lowest atomic number is assigned priority #4.[1]
2. Perform the two allowed manipulations of the Fischer projection to place the lowest priority group on one of the vertical positions (either top or bottom).
3. If the priorities of the other three groups (1-2-3) proceed clockwise, the stereogenic center is assigned as R. If the priorities of the other three groups (1-2-3) proceed counter clockwise, the stereogenic center is assigned as S.

[1] If two adjacent atoms are tied then you go to the next atom away from the center until the tie is broken.

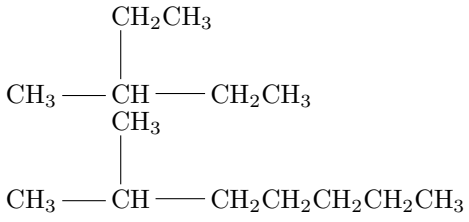
Points earned: _____ out of a possible 32 points

Show all work leading up to **all** responses. You may attach additional pages if needed.

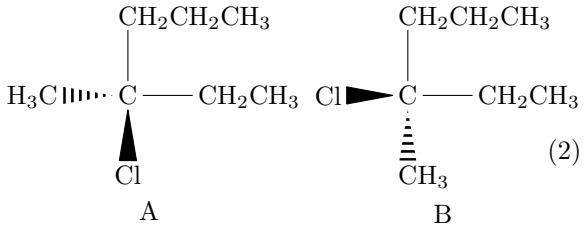
1. Identify and explain the isomeric relationship between the following pairs of compounds.

(3) (a) 2,3-Dimethylbutane and 2-Methylpentane

(3) (b)

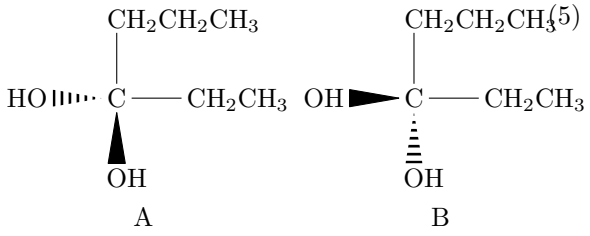


(3) (c)



A B

(3) (d)



A B

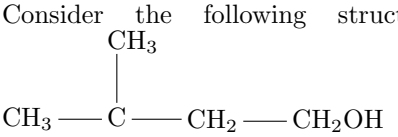
2. Represent 2-methylbutane using the following kinds of diagrams:

(2) (a) Lewis-Dot Diagram

(2) (b) Line-bond Diagram

(3) (c) Condensed structural formula

3. Consider the following structural formula:



(2) (a) Identify the parent alkane.

(2) (b) Identify all functional groups in the compound.

(5) (c) Write the IUPAC name of the compound.

4. Consider 2-methyl-4-propylhexane:

(2) (a) Identify the parent alkane.

(2) (b) Identify all functional groups in the compound.

(5) (c) Draw the chemical structure of the compound.

5. Consider the bond between the 2nd and 3rd carbon of 2-methylbutane.

(5) (a) Draw the Newman projections for all possible conformations. Label them with letters such as A, B, C, etc.

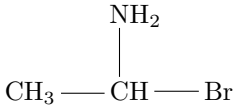
Points earned: _____ out of a possible 42 points

(3) (b) Which conformers are eclipsed? Which are staggered?

(4) (c) Draw a rough potential energy diagram for rotating around the bond.

(3) (d) Explain your reasons for identifying the highest and lowest energy conformers.

6. Consider the following



(2) (a) Draw a 3D line-bond diagrams of both stereoisomers.

(2) (b) Draw Fisher projections of each steroisomer.

(3) (c) Use the Cahn-Ingold-Prelog Rules to determine the configuration of each steroisomer (R or S).

(1) (d) Compare and constrast the stereoisomers physical properties.

(1) (e) Compare and constrast the stereoisomers chemical activity.

Points earned: _____ out of a possible 19 points

7. Draw a reaction energy diagram for a reaction with $K_{eq} = 1$.

(5) (a) Label the parts of the diagram corresponding tor reactants, products, transition state,$\Delta G^{\ominus}$, and $\Delta G^{\ddagger}$.

(2) (b) Is $\Delta G^{\ominus}$ positive or negative?

8. Draw a reaction energy diagram for a one-step reaction with $K_{eq} < 1$.

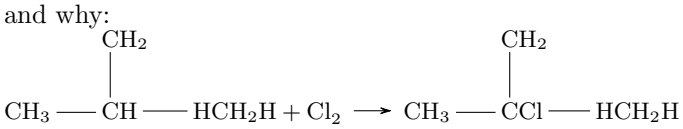
(5) (a) Label the parts of the diagram corresponding tor reactants, products, transition state,$\Delta G^{\ominus}$, and $\Delta G^{\ddagger}$.

(2) (b) Is $\Delta G^{\ominus}$ positive or negative?

(10) 9. Predict the products of the following reaction and balance the resulting equation:
$CH_3CH_2CH_2CH_3 + O_2 \longrightarrow$

(10) 10. Predict the products and draw the mechanism for the following reaction:
$CH_3CH_3 + Cl_2 \longrightarrow$

(5) 11. What side reactions would exist for the following and why:



Assigning Abs. Config. to Wedge/Dashed 3D Structures

1. Prioritize the four groups around a chiral center according to atomic number. The highest atomic number is assigned priority #1, and the lowest atomic number is assigned priority #4.[1]
2. Orient the chiral centre such that the #4 priority substituent is pointing away from the viewer.
3. Trace the path of priorities #1, #2 and #3. (For this part you ignore #4).
4. If the path traced from 1-2-3 is clockwise, the chiral center is assigned (R) (from Latin, rectus)
5. If the path traced is counter clockwise, the chiral center is assigned (S) (from the Latin sinister)

[1] If two adjacent atoms are tied then you go to the next atom away from the center until the tie is broken.

Assigning Abs. Cong. to Fischer Proj.

1. Prioritize the four groups around a chiral center according to atomic number. The highest atomic number is assigned priority #1, and the lowest atomic number is assigned priority #4.[1]
2. Perform the two allowed manipulations of the Fischer projection to place the lowest priority group on one of the vertical positions (either top or bottom).
3. If the priorities of the other three groups (1-2-3) proceed clockwise, the stereogenic center is assigned as R. If the priorities of the other three groups (1-2-3) proceed counter clockwise, the stereogenic center is assigned as S.

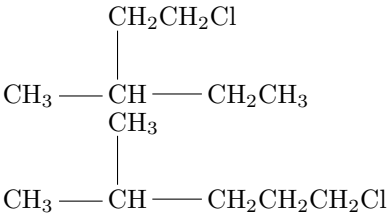
Points earned: _____ out of a possible 0 points

Show all work leading up to **all** responses. You may attach additional pages if needed.

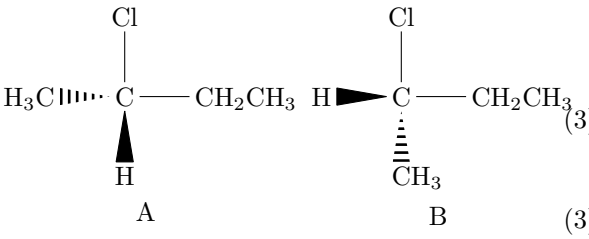
1. Identify and explain the isomeric relationship between the following pairs of compounds.

(3) (a) 2,2-Dibromopentane and 2,3-Dibromopentane

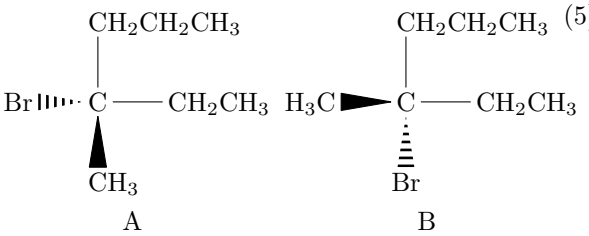
(3) (b)



(3) (c)



(3) (d)



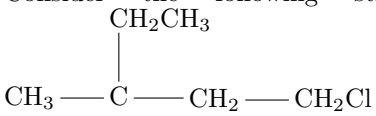
2. Represent bromomethane using the following kinds of diagrams:

(3) (a) Lewis-Dot Diagram

(3) (b) Line-bond Diagram

(3) (c) Condensed structural formula

3. Consider the following structural formula:



(3) (a) Identify the parent alkane.

(3) (b) Identify all functional groups in the compound.

(5) (c) Write the IUPAC name of the compound.

4. Consider 2-bromo-4-ethylhexane:

(3) (a) Identify the parent alkane.

(3) (b) Identify all functional groups in the compound.

(5) (c) Draw the chemical structure of the compound.

5. Consider the bond between the 2nd and 3rd carbon of 2-chlorobutane. $CH_3 - CH_2 - CHCl - CH_3$

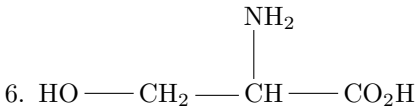
(5) (a) Draw the Newman projections for all possible conformations. Label them with letters such as A, B, C, etc.

Points earned: _____ out of a possible 48 points

(3) (b) Which conformers are eclipsed? Which are staggered?

(4) (c) Draw a rough potential energy diagram for rotating around the bond.

(3) (d) Explain your reasons for identifying the highest and lowest energy conformers.

6. 

Serine

(2) (a) Draw a 3D line-bond diagrams of both stereoisomers.

(2) (b) Draw Fisher projections of each steroisomer.

(3) (c) Use the Cahn-Ingold-Prelog Rules to determine the configuration of each steroisomer (R or S).

(1) (d) Compare and constrast the stereoisomers physical properties.

(1) (e) Compare and constrast the stereoisomers chemical activity.

7. Draw a reaction energy diagram for a two-step reaction with $K_{eq} > 1$, whose second step is faster than the first step of the reaction.

(5) (a) Label the parts of the diagram corresponding tor reactants, products, transition state, ΔG°, and $\Delta G^{\ddagger}$.

(2) (b) Is ΔG° positive or negative?

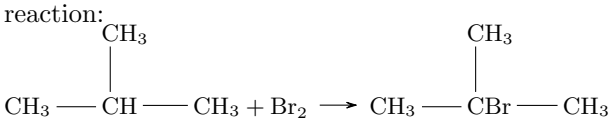
(2) (c) Why is the second step as you have drawn it faster than the first step?

Points earned: _____ out of a possible 28 points

(8) 8. Predict the products of the following reaction and balance the resulting equation:
$CH_4 + O_2 \longrightarrow$

(10) 9. Predict the products and draw the mechanism for the following reaction:
$CH_3CH_3 + Br_2 \longrightarrow$

(6) 10. Explain the lack of side reactions for the following reaction:



Points earned: _____ out of a possible 24 points

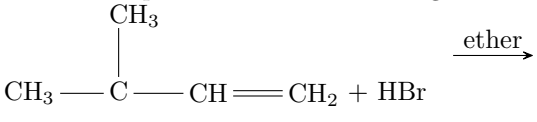
Show all work leading up to **all** responses. You may attach additional pages if needed. If you do so, then list the question number next to any work.

(8) 1. Draw the mechanism for the following reaction:
$CH_3CH{=}CH_2 + HCl \longrightarrow CH_3CH_2CH_2Cl$

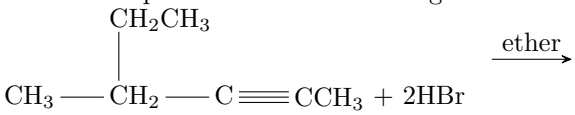
(8) 2. Draw the mechanism for the following reaction:
$CH_3CH_2CH_2OH + H_3O^+ \longrightarrow CH_3CH{=}CH_2$

(8) 3. Predict the products for the following reaction:
$CH_3CH{=}CHCH_3 + H_3O^+ \longrightarrow$

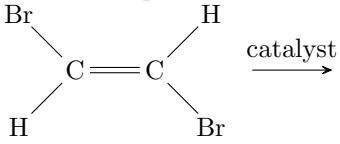
(8) 4. Predict the products for the following reaction:



(8) 5. Predict the products for the following reaction:

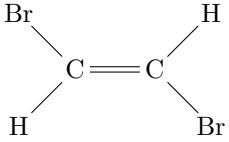


(8) 6. Predict the products for the following reaction:



(8) 7. Predict the products for the following reaction:
$CH3CCl_2CH_2CH3 \xrightarrow{2KOH}$

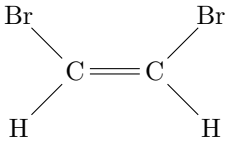
8. Consider the following compound:



(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*)designation?

(6) (b) How many $\sigma$and π-bonds are in this compound?

9. Consider the following compound:

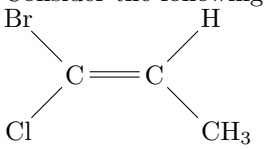


(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*)designation?

(6) (b) How many $\sigma$and π-bonds are in this compound?

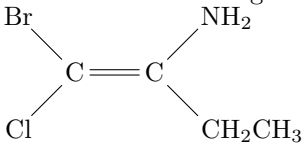
Points earned: _____ out of a possible 80 points

10. Consider the following compound:



(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*) designation?

11. Consider the following compound:



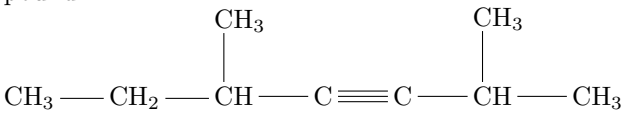
(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*) designation?

(8) 12. Compare and contrast the following two addition reactions.

$HC \equiv CH + HCl$

$HC \equiv CH + HCl$

13. Write the name of the following chemical compound:



(1) (a) Identify the parent alkyne.

(1) (b) Identify all functional groups in the compound.

(3) (c) Write the IUPAC name of the compound.

14. Draw the structure of 2-Methylhexa-1,5-diene.

(1) (a) Identify the parent alkene.

(1) (b) Identify all functional groups in the compound.

(3) (c) Draw the chemical structure of the compound.

Naming Alkenes/Alkynes

1. Name the parent hydrocarbon. Find the longest hydrocarbon chain that contains the double or triple bond. Triple bonds take precedence over double bonds.

2. Number the carbon atoms in the chain. Begin numbering the parent hydrocarbon at the end nearer the double or triple bond. (Again triple bonds recieve precedence.) The numbering should be such that the double/triple bonds recieve the lowest number possible. If there is a tie, then use the numbering that gives other substituents the lowest numbers possible.

3. Write the full name. Number the substituents using the carbon atom that the substituent is attached to. Note the first alkene/yne carbon and place it before the -ene suffix. For an example, hex-2-ene.

Points earned: _____ out of a possible 30 points

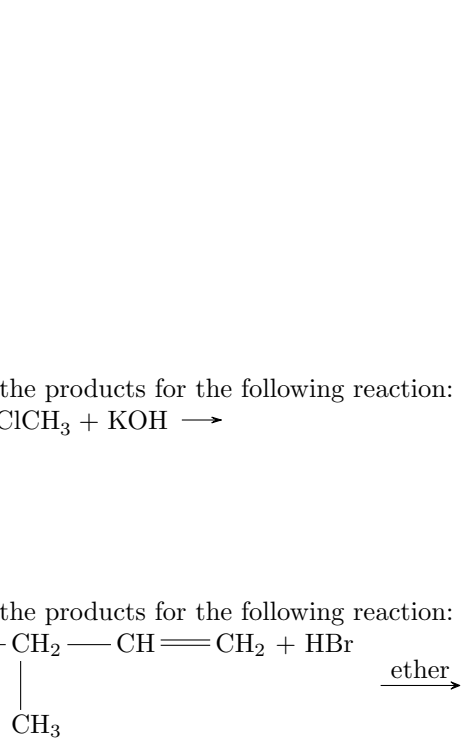
Show all work leading up to **all** responses. You may attach additional pages if needed. If you do so, then list the question number next to any work.

(8) 1. Draw the mechanism for the following reaction:
$CH_3CH{=}CHCH_3 + HCl \longrightarrow CH_3CH_2CH_2CH_2Cl$

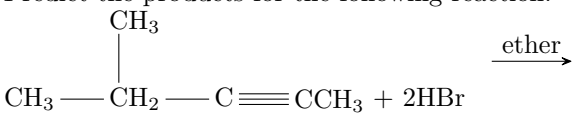
(8) 2. Draw the mechanism for the following reaction:
$CH_3CH_2OH + H_3O^+ \longrightarrow CH_2{=}CH_2$

(8) 3. Predict the products for the following reaction:
$CH_3CHClCH_3 + KOH \longrightarrow$

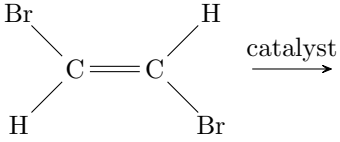
(8) 4. Predict the products for the following reaction:



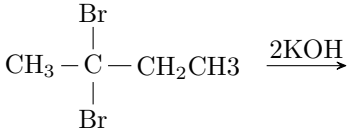
(8) 5. Predict the products for the following reaction:



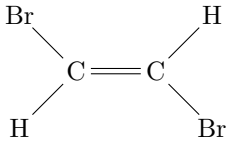
(8) 6. Predict the products for the following reaction:



(8) 7. Predict the products for the following reaction:



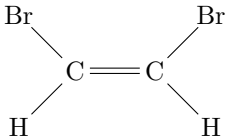
8. Consider the following compound:



(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*)designation?

(6) (b) How many $\sigma$and π-bonds are in this compound?

9. Consider the following compound:



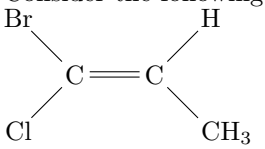
(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*)designation?

(6) (b) How many $\sigma$and π-bonds are in this compound?

Points earned: _____ out of a possible 80 points

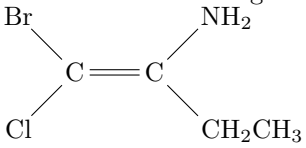
Points earned: _____ out of a possible 0 points

10. Consider the following compound:



(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*) designation?

11. Consider the following compound:



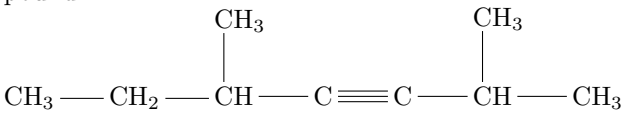
(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*) designation?

(8) 12. Compare and contrast the following two addition reactions.

$HC \equiv CH + HCl$

$HC \equiv CH + HCl$

13. Write the name of the following chemical compound:



(1) (a) Identify the parent alkyne.

(1) (b) Identify all functional groups in the compound.

(3) (c) Write the IUPAC name of the compound.

14. Draw the structure of 2-Methylhexa-1,5-diene.

(1) (a) Identify the parent alkene.

(1) (b) Identify all functional groups in the compound.

(3) (c) Draw the chemical structure of the compound.

Naming Alkenes/Alkynes

1. Name the parent hydrocarbon. Find the longest hydrocarbon chain that contains the double or triple bond. Triple bonds take precedence over double bonds.

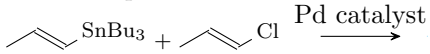
2. Number the carbon atoms in the chain. Begin numbering the parent hydrocarbon at the end nearer the double or triple bond. (Again triple bonds recieve precedence.) The numbering should be such that the double/triple bonds recieve the lowest number possible. If there is a tie, then use the numbering that gives other substituents the lowest numbers possible.

3. Write the full name. Number the substituents using the carbon atom that the substituent is attached to. Note the first alkene/yne carbon and place it before the -ene suffix. For an example, hex-2-ene.

Points earned: _____ out of a possible 30 points

Show all work leading up to **all** responses. You may attach additional pages if needed. If you do so, then list the question number next to any work.

(6) 1. Write the product of this reaction.



(6) 2. Write the product of this reaction.

$CH_3CH_2CH_2OH \xrightarrow[CH_2Cl_2]{\text{Periodinane}}$

(6) 3. Write the product of this reaction.

$CH_3CH_2CH_2OH \xrightarrow[H_3O^+,\ \text{acetone}]{CrO_3}$

(6) 4. Write the product of this reaction.

$CH_3CHOHCH_2CH_3 \xrightarrow[CH_2Cl_2]{\text{Periodinane}}$

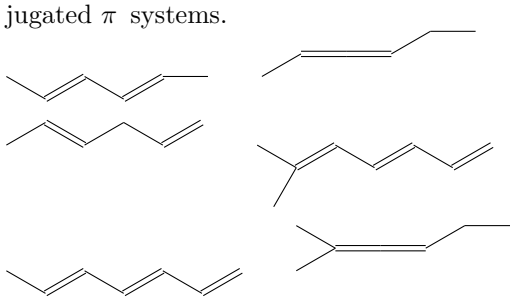
(6) 5. Write the product of this reaction.

$NH_3 + CH_3CH_2CH_2Cl \xrightarrow{NaOH}$

(10) 6. Write the mechanism of this reaction

$CH_3CH_2OH \xrightarrow[\text{heat}]{H_3O^+} H_2C{=}CH_2 + H_2O$

(8) 7. Circle the chemical structures that represent conjugated π systems.



8. Consider the ion SCN^- and the molecule SCNH. The electrognegativity of the elements involved are: S, 2.5; C, 2.5; N, 3.0.

(5) (a) Draw all the resonance structures for the ion SCN^-.

(5) (b) Draw all the resonance structures for the molecule SCNH.

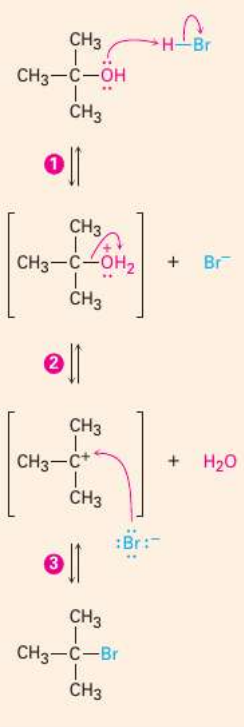
(5) (c) Draw in above or list the partial charges on all atoms for each resonance structure.

(4) (d) Determine which resonance structure is the most stable. And, explain why it is the most stable.

(4) (e) SCN^- can act as a base by accepting a proton to make SCNH. How do the resonance structures explain that SCNH is a weak acid, but stronger than acetic acid (for an example)?

Points earned: _____ out of a possible 71 points

9. Consider the following mechanism.



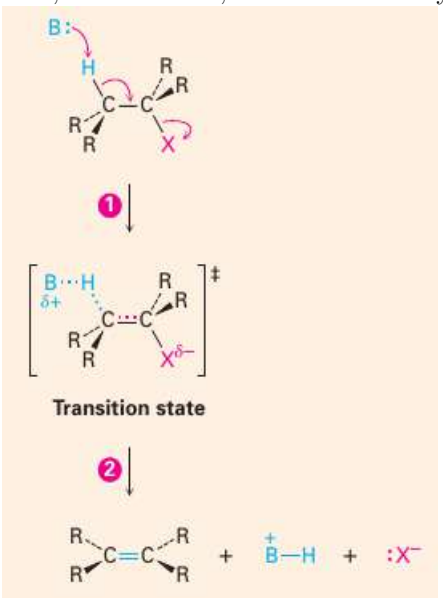
(3) (a) Identify the above reaction as either SN_1, SN_2, E_1, or E_2.

(3) (b) If the OH^- was replaced by a NH_2^-, would the reaction occur more or less quickly? Explain.

(3) (c) What effects could occur by changing the nucleophile (HBr) to something else?

(3) (d) What kind of solvents are required for the polar protic, polar aprotic and/or nonpolar reaction? Explain.

10. Consider the following mechanism, where B is a base, X is a halide, and R can be alkyl groups.



(3) (a) Identify the above reaction as either SN_1, SN_2, E_1, or E_2.

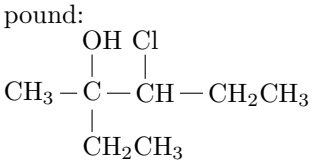
(3) (b) Would the reaction be faster or slower with a weaker base compared to a strong base?

(3) (c) Which would have a faster reaction? A chloride (Cl^-) or bromide (Br^-) as the X.

(8) 11. Compare and contrast the above mechanisims, and in particular consider, the nucleophile, leaving group, and solvent. Which effect how quickly these reactions occur?

Points earned: _____ out of a possible 29 points

12. Write the name of the following chemical compound:



(1) (a) Identify the parent alkyne.

(1) (b) Identify all functional groups in the compound.

(3) (c) Write the IUPAC name of the compound.

13. Draw the structure of 2-amino-2-methylpropane

(1) (a) Identify the parent alkene.

(1) (b) Identify all functional groups in the compound.

(3) (c) Draw the chemical structure of the compound.

IUPAC Naming Rules[1]

1. Find the longest continuous carbon chain containing the highest priority functional group. Determine the root name for this parent chain.[2] Assign the parent name using the root name and the functional group. Note that the position number will need to go before the ending with dashes if the ending is anything other than -ane.

2. Number the chain in the direction such that the position number of the first substituent is the smaller number. If the first substituents from either end have the same number, then number so that the second substituent has the smaller number, etc.

3. Determine the name and position number of each substituent.

4. Indicate the number of identical groups by the prefixes di, tri, tetra, etc.

5. Place the position numbers and names of the substituent groups, in alphabetical order, before the root name. In alphabetizing, ignore prefixes like sec-, tert-, di, tri, etc. and include the iso-prefix. Always include a position number for each substituent, regardless of redundancies.

[1] Derived and adjusted for this course from `https://www.angelo.edu/faculty/kboudrea/organic/IUPAC_Handout.pdf` Note that this version will not work for cyclic compounds.

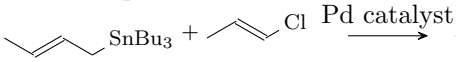
[2] When there are two longest chains of equal length, use the chain with the greater number of substituents.

Points earned: _____ out of a possible 10 points

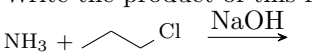
Show all work leading up to **all** responses. You may attach additional pages if needed. If you do so, then list the question number next to any work.

(6) 1. Write the product of this reaction.

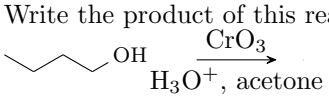
(6) 2. Write the product of this reaction.



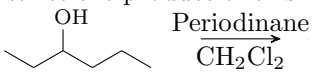
(6) 3. Write the product of this reaction.



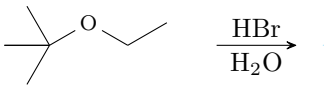
(6) 4. Write the product of this reaction.



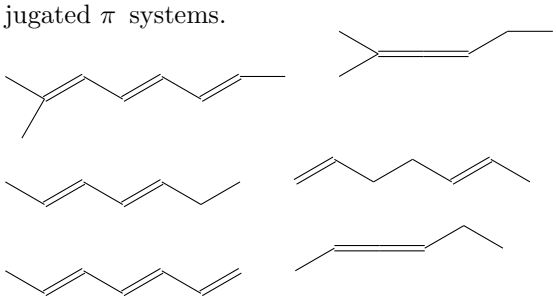
(6) 5. Write the product of this reaction.



(10) 6. Write the mechanism of this reaction



(8) 7. Circle the chemical structures that represent conjugated π systems.



8. Consider the ion $NH_2CH_2COO^-$ and the molecule NH_2CH_2COOH. The electrognegativity of the elements involved are: O, 3.5; C, 2.5; N, 3.0; H, 2.1.

(5) (a) Draw all the resonance structures for the ion $NH_2CH_2COO^-$.

(5) (b) Draw all the resonance structures for the molecule NH_2CH_2COOH.

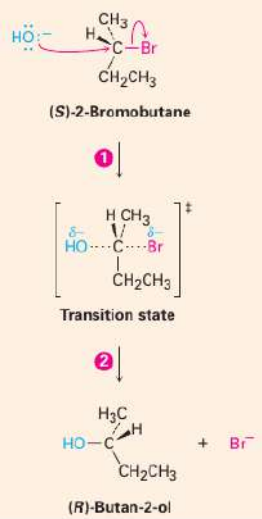
(5) (c) Draw in above or list the formal charges on all atoms for each resonance structure.

(4) (d) Determine which resonance structure is the most stable. And, explain why it is the most stable.

(4) (e) $NH_2CH_2COO^-$ can act as a base by accepting a proton to make NH_2CH_2COOH. How do the resonance structures explain that NH_2CH_2COOH is a weak acid, but stronger than acetic acid (for an example)?

Points earned: _____ out of a possible 71 points

9. Consider the following mechanism.



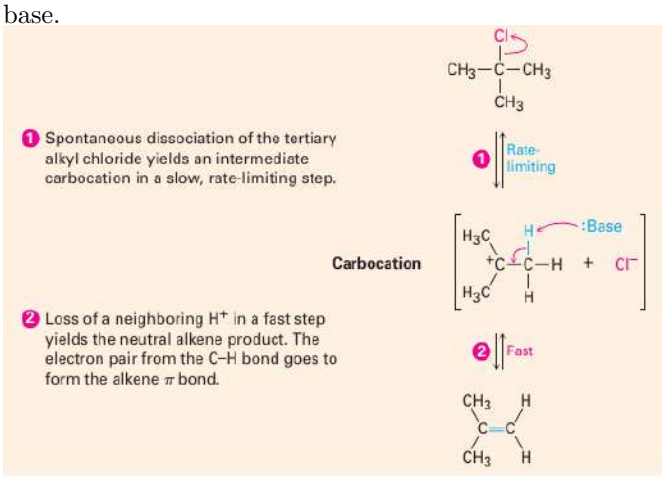
(3) (a) Identify the above reaction as either SN_1, SN_2, E_1, or E_2.

(3) (b) If the Br^- was replaced by a Cl^-, would the reaction occur more or less quickly? Explain.

(3) (c) What effects could occur by changing the nucleophile (OH^-) to something else?

(3) (d) What kind of solvents are required for the polar protic, polar aprotic and/or nonpolar reaction? Explain.

10. Consider the following mechanism, where B is a base.



(3) (a) Identify the above reaction as either SN_1, SN_2, E_1, or E_2.

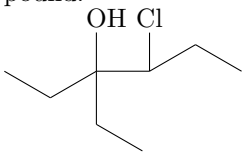
(3) (b) Would the reaction be faster or slower with a weaker base compared to a strong base?

(3) (c) Which would have a faster reaction? A chloride (Cl^-) or bromide (Br^-) as the leaving group?

(8) 11. Compare and contrast the above mechanisims, and in particular consider, the nucleophile, leaving group, and solvent. Which effect how quickly these reactions occur?

Points earned: _____ out of a possible 29 points

12. Write the name of the following chemical compound:



(1) (a) Identify the parent alkyne.

(1) (b) Identify all functional groups in the compound.

(3) (c) Write the IUPAC name of the compound.

13. Draw the structure of 2-methylpent-3-thiol

(1) (a) Identify the parent alkane.

(1) (b) Identify all functional groups in the compound.

(3) (c) Draw the chemical structure of the compound.

IUPAC Naming Rules[1]

1. Find the longest continuous carbon chain containing the highest priority functional group. Determine the root name for this parent chain.[2] Assign the parent name using the root name and the functional group. Note that the position number will need to go before the ending with dashes if the ending is anything other than -ane.

2. Number the chain in the direction such that the position number of the first substituent is the smaller number. If the first substituents from either end have the same number, then number so that the second substituent has the smaller number, etc.

3. Determine the name and position number of each substituent.

4. Indicate the number of identical groups by the prefixes di, tri, tetra, etc.

5. Place the position numbers and names of the substituent groups, in alphabetical order, before the root name. In alphabetizing, ignore prefixes like sec-, tert-, di, tri, etc. and include the iso-prefix. Always include a position number for each substituent, regardless of redundancies.

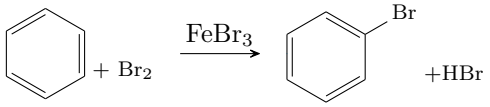
[1] Derived and adjusted for this course from `https://www.angelo.edu/faculty/kboudrea/organic/IUPAC_Handout.pdf` Note that this version will not work for cyclic compounds.

[2] When there are two longest chains of equal length, use the chain with the greater number of substituents.

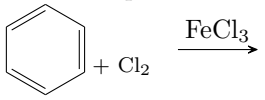
Points earned: _____ out of a possible 10 points

Show all work leading up to **all** responses. You may attach additional pages if needed. If you do so, then list the question number next to any work.

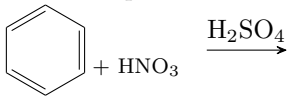
(13) 1. Write the mechanism for this reaction.



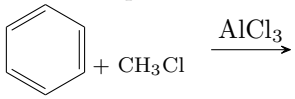
(9) 2. Write the product of this reaction.

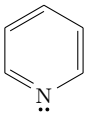


(9) 3. Write the product of this reaction.



(9) 4. Write the product of this reaction.



5. Pyridine 

(7) (a) Draw all major resonance structures.

(4) (b) Using Huckel's Rule, determine whether the molecule is aromatic, anti-aromatic, or non-aromatic.

(7) (c) Explain your answer to part (b)

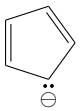
_____

_____

_____

_____

_____

6. Cyclopentadienyl anion 

(7) (a) Draw all major resonance structures.

(4) (b) Using Huckel's Rule, determine whether the molecule is aromatic, anti-aromatic, or non-aromatic.

(7) (c) Explain your answer to part (b)

_____

_____

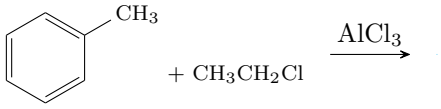
_____

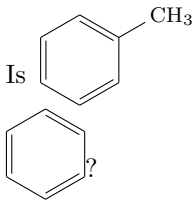
_____

_____

Points earned: _____ out of a possible 76 points

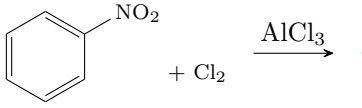
7. Consider the reactants below:

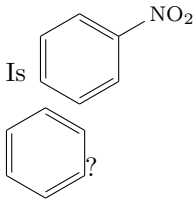


(4) (a) Is  more or less reactive than ?

(4) (b) Draw the major product(s) of the reaction.

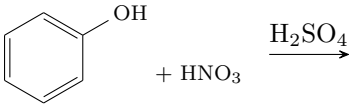
8. Consider the reactants below:

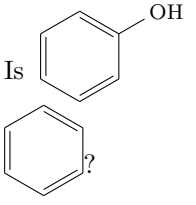


(4) (a) Is  more or less reactive than ?

(5) (b) Draw the major product(s) of the reaction.

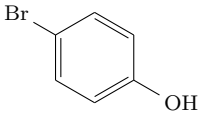
9. Consider the reactants below:



(4) (a) Is  more or less reactive than ?

(5) (b) Draw the major product(s) of the reaction.

10. Write the name of the following chemical compound:



(2) (a) Identify all functional groups in the compound.

(2) (b) Write the IUPAC name of the compound.

11. Draw the structure of 1-Chloro-3,5-dimethylbenzene

(2) (a) Identify all functional groups in the compound.

(2) (b) Draw the chemical structure of the compound.

IUPAC Naming for Aromatic Compounds

Monosubstituted Aromatic Rings Monosubstituted benzenes are systematically named in the same manner as other hydrocarbons, with -benzene as the parent name. Also, many monosubstituted benzene rings go by their common names. If the benzene ring is considered to be a substituent, then the name phenyl sometimes abbreviated as Ph.

Disubstituted Aromatic Rings

ortho- (o-) next to each other in a benzene ring

meta- (m) separated by one carbon in a benzene ring

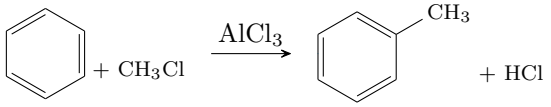
para- (p) across from each other in a benzene ring

Trisubstituted Aromatic Rings benzenes with more than two substituents are named by choosing a point of attachment as carbon 1 and numbering the substituents on the ring so that the second substituent has as low a number as possible. The substituents are listed alphabetically when writing the name.

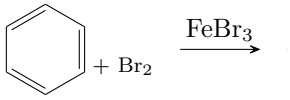
Points earned: _____ out of a possible 34 points

Show all work leading up to **all** responses. You may attach additional pages if needed. If you do so, then list the question number next to any work.

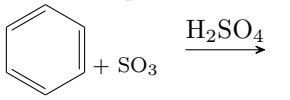
(13) 1. Write the mechanism for this reaction.



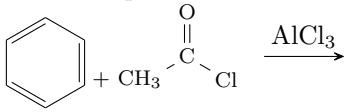
(9) 2. Write the product of this reaction.

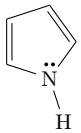


(9) 3. Write the product of this reaction.



(9) 4. Write the product of this reaction.



5. Pyrrole 

(7) (a) Draw all major resonance structures.

(4) (b) Using Huckel's Rule, determine whether the molecule is aromatic, anti-aromatic, or non-aromatic.

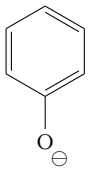
(7) (c) Explain your answer to part (b)

_____

_____

_____

_____

6. Phenolate anion 

(7) (a) Draw all major resonance structures.

(4) (b) Using Huckel's Rule, determine whether the molecule is aromatic, anti-aromatic, or non-aromatic.

(7) (c) Explain your answer to part (b)

_____

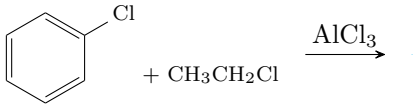
_____

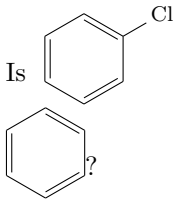
_____

_____

Points earned: _____ out of a possible 0 points

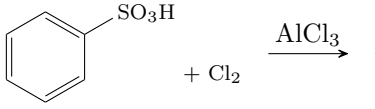
7. Consider the reactants below:

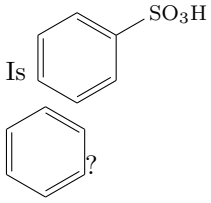


(4) (a) Is  more or less reactive than ?

(4) (b) Draw the major product(s) of the reaction.

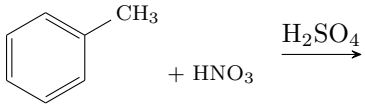
8. Consider the reactants below:

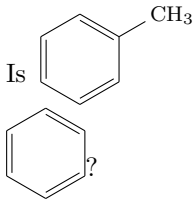


(4) (a) Is  more or less reactive than ?

(5) (b) Draw the major product(s) of the reaction.

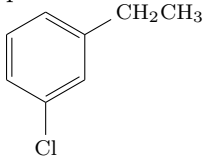
9. Consider the reactants below:



(4) (a) Is  more or less reactive than ?

(5) (b) Draw the major product(s) of the reaction.

10. Write the name of the following chemical compound:



(2) (a) Identify all functional groups in the compound.

(2) (b) Write the IUPAC name of the compound.

11. Draw the structure of 1-Nitro-2,4,5-trimethylbenzene

(2) (a) Identify all functional groups in the compound.

(2) (b) Draw the chemical structure of the compound.

IUPAC Naming for Aromatic Compounds

Monosubstituted Aromatic Rings Monosubstituted benzenes are systematically named in the same manner as other hydrocarbons, with -benzene as the parent name. Also, many monosubstituted benzene rings go by their common names. If the benzene ring is considered to be a substituent, then the name phenyl sometimes abbreviated as Ph.

Disubstituted Aromatic Rings

ortho- (o-) next to each other in a benzene ring

meta- (m) separated by one carbon in a benzene ring

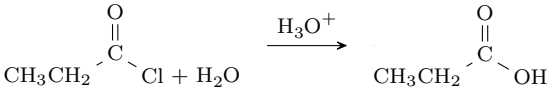
para- (p) across from each other in a benzene ring

Trisubstituted Aromatic Rings benzenes with more than two substituents are named by choosing a point of attachment as carbon 1 and numbering the substituents on the ring so that the second substituent has as low a number as possible. The substituents are listed alphabetically when writing the name.

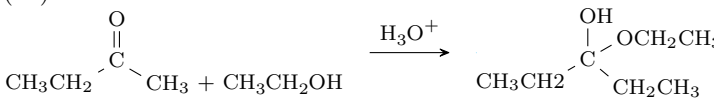
Points earned: _____ out of a possible 0 points

Show all work leading up to **all** responses. You may attach additional pages if needed. If you do so, then list the question number next to any work.

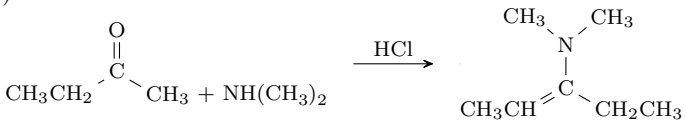
(13) 1. Write the mechanism for this reaction.



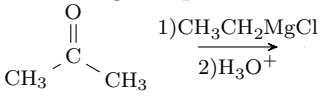
(13) 2. Write the mechanism for this reaction.



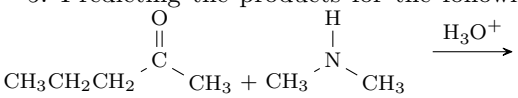
(13) 3. Write the mechanism for this reaction.



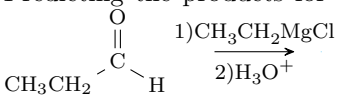
(10) 4. Predicting the products for the following reaction:



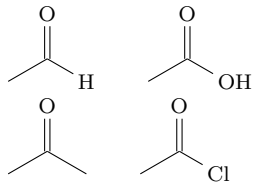
(10) 5. Predicting the products for the following reaction:



(10) 6. Predicting the products for the following reaction:



Points earned: _____ out of a possible 69 points

7. 

(5) (a) Circle the alpha proton in each of the following structures.

(6) (b) Order the molecules above from least acidic to most acidic.

(4) (c) Explain your choice for most and least acidic molecules.

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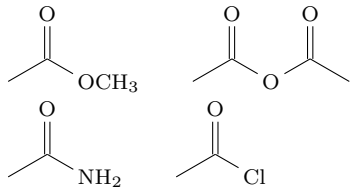
8. 

(7) (a) Order the molecules above from least reactive to most reactive.

(9) (b) Explain your choice for most and least reactive carbocyclic acid derivatives.

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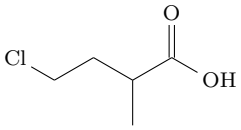
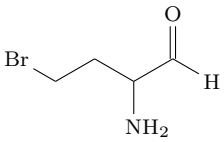
9. Write the name of the following chemical compound:



(1) (a) Identify all functional groups in the compound.

(2) (b) Write the IUPAC name of the compound.

10. Write the name of the following chemical compound:



(2) (a) Identify all functional groups in the compound.

(2) (b) Write the IUPAC name of the compound.

11. Draw the structure of 3,3,5,5-Tetramethyl-4-heptanone

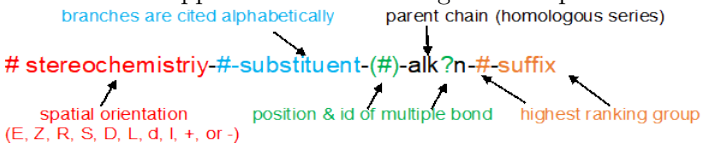
(1) (a) Identify all functional groups in the compound.

(2) (b) Draw the chemical structure of the compound.

IUPAC Naming for Ketones, Aldehydes, and Carboxylic acids Be able to name aldehydes (-al), ketones (-one), and carboxylic acids (-ic acid). These ending take precendence over the others that we've learned.

1. Recognize and prioritize the functional group(s) present.
2. Identify and number the longest continuous carbon chain to give the highest ranking group the lowest possible number.
3. Cite the substituents (branches) alphabetically using the numbering determined above.
4. Recognize an classify any stereochemistry (E/Z, R/S, cis/trans, etc).

With these four pieces of information, the IUPAC name is written using the format below. This same format applies to ALL the organic compounds.



Points earned: _____ out of a possible 41 points

Give complete answers for **all** responses.

(4) 1. Why does he encourage you not to wear contact lenses to an organic chemistry lab?

(7) 2. Why is it good to be careful of touching your skin during the lab?

(6) 3. What does he mean by "drive defensively"?

(5) 4. Which would be a better choice to wear to the Organic Chemistry Lab, a cotton t-shirt or a polyester polo shirt? Explain.

(7) 5. Why are bunsen burners generally not used in the organic chemistry lab?

(7) 6. If you have spill some acid on your hand (but not clothing), what two actions should you take?

7. Look up the information for vinyl formate in the CRC Handbook.

(2) (a) Chemical formula:

(2) (b) Chemical structure:

(2) (c) Physical form:

(1) (d) Molecular weight:

(2) (e) Melting point:

(2) (f) Boiling point:

(2) (g) Density:

8. Look up the information for 2-Vinylnaphthalene in the CRC Handbook..

(2) (a) Chemical formula:

(2) (b) Chemical structure:

(2) (c) Insoluble in:

(2) (d) Soluble in:

9. Look up capsaicin in the Aldrich Catlaog.

(2) (a) IUPAC name.

(2) (b) Chemical formula

(2) (c) Formula/Molecular weight

(2) (d) Melting Point:

(4) (e) Name 4 Hazards that are listed:

(1) (f) The cost for 1 g in its natural form.

(7) 10. Should a lab notebook be written in pencil or pen? If you make a mistake what do you do? Why?

(7) 11. The lab book (or manual) tells you to measure 24 g of sodium bromide. You measure out 24.123 g of sodium bromide. What do you write in your lab notebook?

Points earned: _____ out of a possible 84 points

12. Describe what makes each of these elements of the lab notes for a technique experiment important.

(1) (a) Date of Introductory Notes:

(4) (b) Diagrams of the apparatus:

(3) (c) Description of what actually occured in the lab:

(1) (d) Date the lab was done:

(3) (e) What observations do you write in your lab notebook. Do you write any tenative explanations in as well?

(4) 13. Differentiate between clear, cloudy and colorless.

▶ powder

(S)-(+)-Camptothecin binds irreversibly to the DNA-topoisomerase I complex, inhibiting the reassociation of DNA after cleavage by topoisomerase I and traps the enzyme in a covalent linkage with DNA. The enzyme complex is ubiquinated and destroyed by the 26S proteasome, thus depleting cellular topoisomerase I.

20S isomer

soluble in chloroform/methanol (4:1) (4 mg/mL)
color yellow

Danger H301 store at 2-8°C

C9911-100MG	glass btl	100 mg	80.00
C9911-250MG	glass btl	250 mg	175.00
C9911-1G	glass btl	1 g	477.00

Canada balsam

Balsam Canada
[8007-47-4]

density 0.99 g/mL, 25 °C
n_D^{20} 1.522

▶ Mounting medium for microscopy

Canada Balsam is a natural mounting medium obtained from balsam fir trees. The optical properties are nearly identical with those of glass. Specimens must be dehydrated. Permanent slides mounted with Canada Balsam have been stored for over a century.

Warning H227

C1795-25ML	glass btl	25 mL	63.00
C1795-100ML	glass btl	100 mL	201.50

L-(+)-Canavanine sulfate salt monohydrate, 98%

[206996-57-8] *Beil.* 4,III,1637
$H_2NC(=NH)NHOCH_2CH_2CH(NH_2)CO_2H·H_2SO_4·H_2O$ FW 292.27
$[\alpha]_D^{20}$ +17.3°, c = 2 in H_2O

Warning H302 + H312-H332 P280

861839-1G	glass btl	1 g	155.50

Candelilla wax

[8006-44-8] *Merck* 14,1738

mp 68 to 72 °C density 0.988 g/mL, 25 °C
bp >240 °C

soluble in ethanol, benzene and petroleum ether (hot)
saponification value 44 mg KOH/g iodine value 19-44
acid number 11-19 mg KOH/g ester number 40-47

432288-250G	glass btl	250 g	34.90
432288-1KG	glass btl	1 kg	88.40

(A-^{Cy}Phos)$_2$PdCl$_2$, see Bis[(dicyclohexyl)(4-dimethylaminophenyl)phosphine] palladium(II) chloride Page 313
Capric acid, see Decanoic acid Page 838
Capric anhydride, see Decanoic anhydride Page 838
Caproic acid, see Hexanoic acid Page 1435

ε-Caprolactam, 99%

Aza-2-cycloheptanone; 2-Oxohexamethyleneimine
[105-60-2] *Merck* 14,1761; *Beil.* 21,V,6,444; *Fieser* 9,316
$C_6H_{11}NO$ FW 113.16

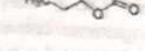
mp 68 to 71 °C vp <0.01 mmHg (20 °C)
bp 136-138 °C/10 mmHg ait 707 °F

Warning H302 + H332-H313-H315-H317-H319-H335 P261-P305 + P351 + P338

C2204-5G	glass btl	5 g	19.40
C2204-250G	poly btl	250 g	22.40
C2204-1KG	poly btl	1 kg	31.00

γ-Caprolactone, 98%

γ-Ethyl-γ-butyrolactone
[695-06-7] *Beil.* 17,238 $C_6H_{10}O_2$ FW 114.14



bp 219 °C n_D^{20} 1.439
density 1.023 g/mL, 25 °C

Warning H316-H319 P305 + P351 + P338

303836-25G	glass btl	25 g	26.00

ε-Caprolactone, 97%

NEW

6-Caprolactone monomer; 2-Oxepanone; 6-Hexanolactone
[502-44-3] *Beil.* 17,V,9,34 $C_6H_{10}O_2$ FW 114.14

bp 97-98 °C/15 mmHg vd 3.9 (vs air)
density 1.03 g/mL, 25 °C vp 0.01 mmHg (20 °C)
n_D^{20} 1.463

Danger H303-H315-H318-H335 P261-P280-P305 + P351 + P338

704067-100G	glass btl	100 g	23.40
704067-500G	glass btl	500 g	76.20

6-Caprolactone polymer, see Polycaprolactone Page 2095
Caproyl chloride, see Hexanoyl chloride Page 1436
Capryl alcohol, see 1-Octanol Page 1945
Caprylamine, see Octylamine Page 1948
Caprylic acid, see Octanoic acid Page 1945
sec-Caprylic alcohol, see 2-Octanol Page 1946
Caprylolactam, see 2-Azacyclononanone Page 208
Caprylolyl chloride, see Octanoyl chloride Page 1947
Capryloyl-2,4,6,8-$^{13}C_4$ coenzyme A, lithium salt, see Octanoyl-2,4,6,8-$^{13}C_4$ Coenzyme A, lithium salt Page 1947

CAPS, ≥98.0%

3-(Cyclohexylamino)-1-propanesulfonic acid
[1135-40-6] *Merck* 14,1767 $C_6H_{11}NH(CH_2)_3SO_3H$ FW 221.32

pKa 10.4 useful pH range 9.7 - 11.1
mp >300 °C

pKa (25 °C) 10.4
pH range 9.7 - 11.1

Warning H302

C2632-25G	poly btl	25 g	21.30
C2632-100G	poly btl	100 g	55.20
C2632-6X100G		6 × 100 g	258.00
C2632-250G	poly btl	250 g	136.00
C2632-1KG	poly drum	1 kg	413.00

Capsaicin

8-Methyl-N-vanillyl-*trans*-6-nonenamide
[404-86-4] *Merck* 14,1768; *Beil.* 13,IV,2588
$(CH_3)_2CHCH=CH(CH_2)_4CONHCH_2C_6H_3$-4-(OH)-3-($OCH_3$) FW 305.41
Prototype vanilloid receptor agonist; neurotoxin.
Active component of cayenne pepper

mp 62 to 65 °C

Danger H301 + H311-H315-H317-H318-H334-H335 P261-P280-P301 + P310-P305 + P351 + P338-P342 + P311

▶ natural

composition
capsaicin 65%
dihydrocapsaicin 35%

360376-250MG	glass btl	250 mg	45.00
360376-1G	glass btl	1 g	136.00

▶ from *Capsicum* sp., ≥50% (HPLC)

dihydrocapsaicin ~35%
store at 2-8°C

21750-100MG-F	glass btl	100 mg	34.00
21750-1G-F	glass btl	1 g	175.50
21750-5G-F	glass btl	5 g	627.00

PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS

The basic physical constants and structure diagrams for about 10,900 organic compounds are presented in this table. An effort has been made to include the compounds most frequently encountered in the laboratory, the workplace, and the environment. Particular emphasis has been given to substances that are considered environmental or human health hazards. In making the selection of compounds for the table, added weight was assigned to the appearance of a compound in various lists or reference sources such as:

- Laboratory reagent lists, e.g., the ACS *Reagent Chemicals* volume (Ref. 1)
- The DIPPR list of industrially important compounds (Ref. 2) and the (much larger) TSCA Inventory of chemicals used in commerce.
- The Hazardous Substance Data Bank (Ref. 3)
- The UNEP list of Persistent Organic Pollutants (Ref. 4)
- Chemicals on Reporting Rules (CORR), a database of about 7500 regulated compounds prepared by the Environmental Protection Agency (Ref. 5)
- The EPA Integrated Risk Information System (IRIS), a database of human health effects of exposure to chemicals in the environment (Ref. 6)
- Compendia of chemicals of biochemical or medical importance, such as *The Merck Index* (Ref. 10)
- Specialized tables in this *Handbook*

It should be noted that the above lists vary widely in their choice of chemical names, and even in the use of Chemical Abstracts Registry Numbers. To the extent possible, we have attempted to systematize the names and registry numbers for this table.

Clearly, criteria of this type are somewhat subjective, and compounds considered important by some users have undoubtedly been omitted. Suggestions for additional compounds or other improvements are welcomed.

The data in the table have been derived from many sources, including both the primary literature and evaluated compilations. The *Handbook of Data on Organic Compounds, Third Edition* (Ref. 7) and the *Combined Chemical Dictionary* (Ref. 8) were important sources. Other useful sources of physical property data on organic compounds are listed in Refs. 9-19. The values in the table for the normal boiling point and the melting point that are accompanied with uncertainties (in parentheses) have been critically evaluated using the NIST ThermoData Engine (TDE, Ref. 20), designed to implement the dynamic data evaluation concept (Refs. 21-24). This concept requires large electronic databases capable of storing essentially all relevant experimental data known to date with detailed descriptions of metadata and uncertainties. The combination of these electronic databases with expert-system software, designed to automatically generate recommended property values based on available experimental and predicted data, leads to the ability to produce critically evaluated data dynamically or "to order." The uncertainties listed are combined expanded uncertainties (level of confidence, approximately 95 %) representing the most comprehensive measure of the overall data reliability (Refs. 25-28).

The table is arranged alphabetically by substance name, which generally is either an IUPAC systematic name or, in the case of pesticides, pharmaceuticals, and other complex compounds, a simple trivial name. Names in ubiquitous use, such as acetic acid and formaldehyde, are adopted rather than their systematic equivalents. Synonyms are given in the column following the primary name, and structure diagrams are given on the page facing the data listing. The explanation of the data columns follows:

No.: An identification number used in the indexes.

Name: Primary name of the substance

Synonym: A synonym in common use. When the primary name is non-systematic, a systematic name may appear here.

Mol. Form.: The molecular formula written in the Hill convention.

CAS RN.: The Chemical Abstracts Service Registry Number for the compound.

Mol. Wt: Molecular weight (relative molar mass) as calculated with the 2001 IUPAC Standard Atomic Weights.

Physical Form: A notation of the physical phase, color, crystal type, or other features of the compound at ambient temperature. Abbreviations are given below.

mp: Normal melting point in °C. A value is sometimes followed by "dec", indicating decomposition is observed at the stated temperature (so that it is probably not a true melting point). The notation "tp" indicates a triple point, where solid, liquid, and gas are in equilibrium. A number in parentheses following the melting point value is the combined expanded uncertainty (see above).

bp: Normal boiling point in °C, if it is available. This is the temperature at which the liquid phase is in equilibrium with the vapor at a pressure of 760 mmHg (101.325 kPa). A number in parentheses following the boiling point value is the combined expanded uncertainty (see above). A notation "sp" following the value indicates a sublimation point, where the vapor pressure of the solid phase reaches 760 mmHg. When a notation such as "dec" (decomposes) or "exp" (explodes) follows the value, the temperature may not be a true boiling point. A simply entry "sub" indicates the solid has a significant sublimation pressure at ambient temperatures. When the normal boiling point is not available, a boiling point at reduced pressure may be listed with a superscript indicating the pressure in mmHg.

den: Density (mass per unit volume) in g/cm^3. The temperature in °C is indicated by a superscript. Values refer to the liquid or solid phase, and all values are true densities, not specific gravities. The number of decimal places gives a rough estimate of the accuracy of the value.

n_D: Refractive index, at the temperature in °C indicated by the superscript. Unless otherwise indicated, all values refer to a wavelength of 589 nm (sodium D line). Values are given only for liquids and solids.

Solubility: Qualitative indication of solubility in common solvents. Abbreviations are:
i insoluble
sl slightly soluble
s soluble
vs very soluble
msc miscible
dec decomposes

Abbreviations for solvents are given below.

In order to facilitate the location of compounds in the table, an index to synonyms follows the main table. Indexes to Molecular Formulas and CAS Registry Numbers are available in the electronic versions of the *Handbook* or as pdf files by request via e-mail (fiona.macdonald@taylorandfrancis.com).

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List of Abbreviations

Ac	acetyl
Ac_2O	acetic anhydride
AcOEt	ethyl acetate
ac	acid
ace	acetone
al	alcohol (ethanol)
alk	alkali
amor	amorphous
anh	anhydrous
aq	aqueous
bipym	bipyramidal
bl	blue
blk	black
bp	boiling point
br	brown
bt	bright
Bu	butyl
BuOH	1-butanol
bz	benzene
chl	chloroform
col	colorless
con, conc	concentrated
cry	crystals
ctc	carbon tetrachloride
cy, cyhex	cyclohexane
dec	decomposes
den	density
dil	dilute
diox	dioxane
dk	dark
DMF	dimethylformamide
DMSO	dimethyl sulfoxide
efflor	efflorescent
Et	ethyl
EtOH	ethanol
eth	diethyl ether
exp	explodes
fl	flakes
flr	fluorescent
fum	fumes, fuming
gl	glacial
gr	gray
gran	granular
grn	green
hex	hexagonal
HOAc	acetic acid
hp	heptane
hx	hexane
hyd	hydrate
hyg	hygroscopic
i	insoluble
i-	iso-
iso	isooctane
lf	leaves
lig	ligroin
liq	liquid
lo	long
mcl	monoclinic
Me	methyl
MeCN	acetonitrile
MeOH	methanol
misc	miscible
mp	melting point
n	refractive index
nd	needles
oct	octahedra, octahedral
oran	orange
orth	orthorhombic
os	organic solvents
pa	pale
peth	petroleum ether
Ph	phenyl
PhCl	chlorobenzene
$PhNH_2$	aniline
$PhNO_2$	nitrobenzene
pl	plates
pow	powder
Pr	propyl
PrOH	1-propanol
pr	prisms
purp	purple
py	pyridine
pym	pyramids, pyramidal
reac	reacts
rhom	rhombic
s	soluble
sat	saturated
sc	scales
sl	slightly soluble
soln	solution
sp	sublimation point
stab	stable
sub	sublimes
sulf	sulfuric acid
syr	syrup
tab	tablets
tcl	triclinic
tetr	tetragonal
tfa	trifluoroacetic acid
thf, THF	tetrahydrofuran
tol	toluene
tp	triple point
trg	trigonal
unstab	unstable
vap	vapor
viol	violet
visc	viscous
vol	volatile
vs	very soluble
w	water
wh	white
xyl	xylene
ye	yellow

No.	Name	Synonym	Mol. Form.	CAS RN	Mol. Wt.	Physical Form	mp/°C	bp/°C	den g cm^{-3}	n_D	Solubility
10794	Vinyl butanoate		$C_6H_{10}O_2$	123-20-6	114.142			116.7	0.9006^{20}		
10795	Vinyl *trans*-2-butenoate	Vinyl crotonate	$C_6H_8O_2$	3234-54-6	112.127						s ctc
10796	9-Vinyl-9*H*-carbazole		$C_{14}H_{11}N$	1484-13-5	193.244	cry (al)	66				i H_2O; sl EtOH; vs eth
10797	Vinylcyclohexane		C_8H_{14}	695-12-5	110.197			127(6)	0.8166^{19}	1.455^{19}	
10798	1-Vinylcyclohexene		C_8H_{12}	2622-21-1	108.181			144(7)	0.8623^{15}	1.4915^{20}	i H_2O; s eth, bz; vs MeOH
10799	4-Vinylcyclohexene		C_8H_{12}	100-40-3	108.181	liq	-108.9	130(4)	0.8299^{20}	1.4639^{20}	i H_2O; s eth, bz, peth
10800	Vinylcyclopentane		C_7H_{12}	3742-34-5	96.170	liq	-126.4(0.2)	99(3)	0.7834^{20}	1.4360^{20}	
10801	Vinyldiethoxymethylsilane		$C_7H_{16}O_2Si$	5507-44-8	160.287			133	0.8620^{20}	1.4001^{20}	
10802	Vinylethoxydimethylsilane		$C_6H_{14}OSi$	5356-83-2	130.260			99	0.790^{20}	1.3983^{20}	
10803	1-Vinyl-4-fluorobenzene		C_8H_7F	405-99-2	122.140		-34.5	67.4^{50}	1.0220^{20}	1.5150^{20}	i H_2O; s EtOH, eth, bz
10804	Vinyl formate		$C_3H_4O_2$	692-45-5	72.063	visc liq	-78	42(18)	0.965^{20}	1.3842^{20}	
10805	2-Vinylfuran		C_6H_6O	1487-18-9	94.111	liq	-94(4)	101(3)	0.9445^{19}	1.4992^{19}	
10806	1-Vinyl-2-methoxybenzene		$C_9H_{10}O$	612-15-7	134.174	nd	29	215(18)	1.0049^{17}	1.5388^{20}	vs ace, bz, eth, EtOH
10807	1-Vinyl-3-methoxybenzene		$C_9H_{10}O$	626-20-0	134.174			91^{15}	0.9919^{20}	1.5586^{23}	i H_2O; s EtOH, eth, bz
10808	1-Vinyl-4-methoxybenzene		$C_9H_{10}O$	637-69-4	134.174		2.0	208(19)	1.0001^{13}	1.5642^{13}	i H_2O; s EtOH, eth, bz; sl ctc
10809	6-Vinyl-6-methyl-1-isopropyl-3-(1-methylethylidene)-cyclohexene, (*S*)-		$C_{15}H_{24}$	5951-67-7	204.352			125^{8}	0.8782^{20}	1.5130^{26}	vs ace, bz
10810	1-Vinylnaphthalene		$C_{12}H_{10}$	826-74-4	154.207			124^{15}	1.0656^{20}	1.644^{20}	
10811	2-Vinylnaphthalene		$C_{12}H_{10}$	827-54-3	154.207		65(2)	135^{18}			i H_2O; s EtOH, ace, bz
10812	1-Vinyl-3-nitrobenzene		$C_8H_7NO_2$	586-39-0	149.148		-10	120^{11}	1.1552^{32}	1.5836^{20}	i H_2O; s EtOH, eth, bz, chl, lig, HOAc
10813	1-Vinyl-4-nitrobenzene		$C_8H_7NO_2$	100-13-0	149.148	pr (lig)	29	dec			vs EtOH, eth; s chl, HOAc, lig
10814	5-Vinyl-2-norbornene	5-Vinylbicyclo[2.2.1]hept-2-ene	C_9H_{12}	3048-64-4	120.191	liq	-80	140.7(0.5)	0.841	1.4810^{20}	
10815	Vinyl octadecanoate	Vinyl stearate	$C_{20}H_{38}O_2$	111-63-7	310.515		29	167^{2}	0.8517^{20}		sl chl
10816	3-Vinyl-7-oxabicyclo[4.1.0]-heptane		$C_8H_{12}O$	106-86-5	124.180		<-100	169	0.9581^{20}	1.4700^{20}	
10817	Vinyloxirane		C_4H_6O	930-22-3	70.090			68(2)	0.9006^{25}	1.4168^{20}	s EtOH, eth, bz
10818	2-(Vinyloxy)ethanol	Ethylene glycol monovinyl ether	$C_4H_8O_2$	764-48-7	88.106			139(4)	0.9821^{20}	1.4564^{17}	s H_2O, EtOH, eth, bz; i lig
10819	Vinyl propanoate	Vinyl propionate	$C_5H_8O_2$	105-38-4	100.117			94.8(0.2)			
10820	2-Vinylpyridine		C_7H_7N	100-69-6	105.138			159.5	0.9983^{20}	1.5495^{20}	sl H_2O; vs EtOH, eth, ace, chl
10821	3-Vinylpyridine		C_7H_7N	1121-55-7	105.138			162	0.9879^{20}	1.5530^{20}	sl H_2O; s EtOH, eth
10822	4-Vinylpyridine		C_7H_7N	100-43-6	105.138	red to dk-br		121^{150}	0.9879^{20}	1.5449^{20}	s H_2O, EtOH, chl; sl eth
10823	1-Vinyl-2-pyrrolidinone		C_6H_9NO	88-12-0	111.141		13.5	193^{400}	1.04^{20}		
10824	Vinylsilane		C_2H_6Si	7291-09-0	58.155	col gas	-171.6	-22.8			
10825	Vinyl sulfoxide	Divinyl sulfoxide	C_4H_6OS	1115-15-7	102.155	liq		86^{18}			
10826	Vinyltriacetoxysilane	Vinylsilanetriol, triacetate	$C_8H_{12}O_6Si$	4130-08-9	232.263			115^{10}	1.169^{20}	1.4226^{20}	
10827	Vinyltriethoxysilane		$C_8H_{18}O_3Si$	78-08-0	190.313			160.0(0.8)	0.901^{20}	1.3960^{25}	s chl
10828	Vinyltrimethylsilane		$C_5H_{12}Si$	754-05-2	100.235			55.3(0.2)	0.65^{20}	1.3914^{20}	i H_2O
10829	Violaxanthin		$C_{40}H_{56}O_4$	126-29-4	600.871	red pr (MeOH, al-eth)	208				s EtOH, eth, CS_2; i peth
10830	Viquidil		$C_{20}H_{24}N_2O_2$	84-55-9	324.417	red ye amor	60				vs eth, EtOH, chl
10831	Visnadine		$C_{21}H_{24}O_7$	477-32-7	388.412	nd	85.5				i H_2O; s EtOH, eth
10832	Visnagin	4-Methoxy-7-methyl-5*H*-furo[3,2-*g*][1]benzopyran-5-one	$C_{13}H_{10}O_4$	82-57-5	230.216	nd (w, MeOH)	144.5				sl H_2O, EtOH; vs chl
10833	Vitamin B12	Cyanocobalamin	$C_{63}H_{88}CoN_{14}O_{14}P$	68-19-9	1355.365		>300				
10834	Vitamin D2		$C_{28}H_{44}O$	50-14-6	396.648	pr (ace)	116.5	sub			i H_2O; s EtOH, eth, ace, chl
10835	Vitamin D3	9,10-Secocholesta-5,7,10(19)-trien-3-ol, (3β,5*Z*,7*E*)-	$C_{27}H_{44}O$	67-97-0	384.637		84.5				i H_2O; s os
10836	Vitamin E	α-Tocopherol	$C_{29}H_{50}O_2$	59-02-9	430.706	pale ye oil	3.0	210$^{0.1}$	0.950^{25}	1.5045^{25}	i H_2O; s EtOH, eth, ace, chl

▸ **powder**

(S)-(+)-Camptothecin binds irreversibly to the DNA-topoisomerase I complex, inhibiting the reassociation of DNA after cleavage by topoisomerase I and traps the enzyme in a covalent linkage with DNA. The enzyme complex is ubiquinated and destroyed by the 26S proteasome, thus depleting cellular topoisomerase I.

20S isomer

soluble in chloroform/methanol (4:1) (4 mg/mL)

color yellow

Danger H301 store at 2-8°C

C9911-100MG	glass btl	100 mg	80.00
C9911-250MG	glass btl	250 mg	175.00
C9911-1G	glass btl	1 g	477.00

Canada balsam

Balsam Canada

[8007-47-4]

density 0.99 g/mL, 25 °C

n_D^{20} 1.522

▸ **Mounting medium for microscopy**

Canada Balsam is a natural mounting medium obtained from balsam fir trees. The optical properties are nearly identical with those of glass. Specimens must be dehydrated. Permanent slides mounted with Canada Balsam have been stored for over a century.

Warning H227

C1795-25ML	glass btl	25 mL	63.00
C1795-100ML	glass btl	100 mL	201.50

L-(+)-Canavanine sulfate salt monohydrate, 98%

[206996-57-8] *Beil.* 4,III,1637

$H_2NC(=NH)NHOCH_2CH_2CH(NH_2)CO_2H·H_2SO_4·H_2O$ FW 292.27

$[\alpha]_D^{20}$ +17.3°, c = 2 in H_2O

Warning H302 + H312-H332 P280

861839-1G	glass btl	1 g	155.50

Candelilla wax

[8006-44-8] *Merck* 14,1738

mp 68 to 72 °C density 0.988 g/mL, 25 °C

bp >240 °C

soluble in ethanol, benzene and petroleum ether (hot)

saponification value 44 mg KOH/g iodine value 19-44

acid number 11-19 mg KOH/g ester number 40-47

432288-250G	glass btl	250 g	34.90
432288-1KG	glass btl	1 kg	88.40

(A-^{ca}Phos)$_2$PdCl$_2$, see Bis[(dicyclohexyl)(4-dimethylaminophenyl)phosphine] palladium(II) chloride Page 313

Capric acid, see Decanoic acid Page 838

Capric anhydride, see Decanoic anhydride Page 838

Caproic acid, see Hexanoic acid Page 1435

ε-Caprolactam, 99%

Aza-2-cycloheptanone; 2-Oxohexamethyleneimine

[105-60-2] *Merck* 14,1761; *Beil.* 21,V,6,444; *Fieser* 9,316

$C_6H_{11}NO$ FW 113.16

mp 68 to 71 °C vp <0.01 mmHg (20 °C)

bp 136-138 °C/10 mmHg ait 707 °F

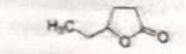
Warning H302 + H332-H313-H315-H317-H319-H335 P261-P305 + P351 + P338

C2204-5G	glass btl	5 g	19.40
C2204-250G	poly btl	250 g	22.40
C2204-1KG	poly btl	1 kg	31.00

γ-Caprolactone, 98%

γ-Ethyl-γ-butyrolactone

[695-06-7] *Beil.* 17,238 $C_6H_{10}O_2$ FW 114.14



bp 219 °C n_D^{20} 1.439

density 1.023 g/mL, 25 °C

Warning H316-H319 P305 + P351 + P338

303836-25G	glass btl	25 g	26.00

ε-Caprolactone, 97%

NEW

6-Caprolactone monomer; 2-Oxepanone; 6-Hexanolactone

[502-44-3] *Beil.* 17,V,9,34 $C_6H_{10}O_2$ FW 114.14

bp 97-98 °C/15 mmHg vd 3.9 (vs air)

density 1.03 g/mL, 25 °C vp 0.01 mmHg (20 °C)

n_D^{20} 1.463

Danger H303-H315-H318-H335 P261-P280-P305 + P351 + P338

704067-100G	glass btl	100 g	23.40
704067-500G	glass btl	500 g	76.20

6-Caprolactone polymer, see Polycaprolactone Page 2095

Caproyl chloride, see Hexanoyl chloride Page 1436

Capryl alcohol, see 1-Octanol Page 1945

Caprylamine, see Octylamine Page 1948

Caprylic acid, see Octanoic acid Page 1945

sec-Caprylic alcohol, see 2-Octanol Page 1946

Caprylolactam, see 2-Azacyclononanone Page 208

Capryloyl chloride, see Octanoyl chloride Page 1947

Capryloyl-2,4,6,8-$^{13}C_4$ coenzyme A, lithium salt, see Octanoyl-2,4,6,8-$^{13}C_4$ Coenzyme A, lithium salt Page 1947

CAPS, ≥98.0%

3-(Cyclohexylamino)-1-propanesulfonic acid

[1135-40-6] *Merck* 14,1767 $C_6H_{11}NH(CH_2)_3SO_3H$ FW 221.32

pKa 10.4 useful pH range 9.7 - 11.1

mp >300 °C

pKa (25 °C) 10.4

pH range 9.7 - 11.1

Warning H302

C2632-25G	poly btl	25 g	21.30
C2632-100G	poly btl	100 g	55.20
C2632-6X100G		6 × 100 g	258.00
C2632-250G	poly btl	250 g	136.00
C2632-1KG	poly drum	1 kg	413.00

Capsaicin

8-Methyl-N-vanillyl-*trans*-6-nonenamide

[404-86-4] *Merck* 14,1768; *Beil.* 13,IV,2588

$(CH_3)_2CHCH{=}CH(CH_2)_4CONHCH_2C_6H_3$-4-(OH)-3-($OCH_3$) FW 305.41

Prototype vanilloid receptor agonist; neurotoxin.

Active component of cayenne pepper

mp 62 to 65 °C

Danger H301 + H311-H315-H317-H318-H334-H335 P261-P280-P301 + P310-P305 + P351 + P338-P342 + P311

▸ **natural**

composition

capsaicin 65%

dihydrocapsaicin 35%

360376-250MG	glass btl	250 mg	45.00
360376-1G	glass btl	1 g	136.00

▸ **from *Capsicum* sp., ≥50% (HPLC)**

dihydrocapsaicin ~35%

store at 2-8°C

21750-100MG-F	glass btl	100 mg	34.00
21750-1G-F	glass btl	1 g	175.50
21750-5G-F	glass btl	5 g	627.00

H

Hydrogen [4-di-*tert*-butylphosphino-2,3,5,6-tetrafluorophenyl]hydrobis(2,3,4,5,6-pentafluorophenyl) borate, 97%

NEW

Frustrated phosphonium borate 1

[952208-49-0] H^+ $[((CH_3)^3C)_2PC_6F_4)B(H)(C_6F_5)_2]^-$ FW 640.20

mp 222 to 227 °C

Frustrated phosphonium borate for metal-free catalytic hydrogenation of imines. Activates dihydrogen under mild conditions.[1,2]

Lit. cited: 1. Chase, P. A. et al., *Angew. Chem. Int. Ed. Engl.* **46**, 8050 (2007)
2. Welch, G. C. et al., *Science* **314**, 1124 (2006)

Warning H315-H319-H335 P261-P305 + P351 + P338

703087-250MG	glass btl	250 mg	55.10
703087-1G	glass btl	1 g	181.00

Hydrogen fluoride pyridine

HF-Pyridine; Pyridine hydrofluoride

[62778-11-4] *Merck* **14**,6821; *Fieser* **9**,399; **5**,538; **12**,419; **16**,286; **6**,473 $C_5H_5N \cdot (HF)_x$ FW 20.01

density 1.1 g/mL, 20 °C

▶ **pyridine: ~30%, hydrogen fluoride: ~70%**

Used together with hypervalent iodine(III) reagents for *ipso*-fluorination of *para*-substituted phenols providing cyclohexadienones.[1] Employed with Selectfluor® (Catalog No. 439479) for geminal fluorination of 2,2-diaryl-1,3-dithiolanes.[2]

May contain or form low levels of calcium fluoride during storage. Presence of this does not impact the specification values.

Lit. cited: 1. *Tetrahedron* **60**, 6629 (2004)
2. *Chem. Commun. (Camb.)* 654 (2005)

Danger H300-H310-H314-H330 P260-P264-P280-P284-P301 + P310-P302 + P350

184225-25G	poly btl	25 g	38.70
184225-100G	poly btl	100 g	71.30

Hydrogen hexabromoplatinate(IV) hydrate, 99.9% trace metals basis

Platinic bromide; Bromoplatinic acid

[207386-85-4] $H_2PtBr_6 \cdot xH_2O$ FW 676.52 (Anh)

powder and chunks

composition

Pt 24-26%

Danger H314-H334 P261-P280-P305 + P351 + P338-P310

398357-2G	glass btl	2 g	140.00

Hydrogen hexachloroiridate(IV) hydrate

[110802-84-1] *Fieser* **5**,119; **3**,47; **1**,131; **2**,67; **4**,93 $H_2Cl_6Ir \cdot xH_2O$ FW 406.95 (Anh)

Features and Benefits

Catalyzes the electrochemical synthesis of polyaniline on the surface of non-noble metal electrodes.[1] Utilized in the formation of iridium-substituted Dawson-[2] and Keggin-type polyoxometallates by refilling the vacant site of the lacunary precursors.[3]

mp 65 °C

density 1.02 g/mL, 25 °C

Lit. cited: 1. Abalyaeva, V.V.; Efimov, O.N., *Polym. Adv. Technol.* **8**, 517 (1997)
2. Liu, H. et al., *Transition Met. Chem. (London)* **22**, 321 (1997)
3. Liu, H. et al., *Synth. React. Inorg. Met.-Org. Chem.* **27**, 551 (1997)

Danger H302 + H312-H314-H332-H351 P280-P305 + P351 + P338-P310

▶ **99.98% trace metals basis**

455962-1G	glass btl	1 g	179.50

powder

208973-1G	glass btl	1 g	151.50
208973-5G	glass btl	5 g	466.00

Hydrogen hexahydroxyplatinate(IV), 99.9% trace metals basis

[51850-20-5] $H_2Pt(OH)_6$ FW 299.14

powder and chunks

Warning H315-H319-H332-H335 P261-P305 + P351 + P338

334472-500MG	glass btl	500 mg	
334472-2.5G	glass btl	2.5 g	

Hydrogen ionophore I, see Tridodecylamine Page 2483

Hydrogen ionophore III, ≥99.0% (NT)

N,N-Dioctadecylmethylamine; Proton ionophore III

[4088-22-6] *Beil.* **4**,III,435 $[CH_3(CH_2)_{17}]_2NCH_3$ FW 536.01

▶ **Selectophore®**

Visit our Sensor Applications portal to learn more.

Neutral ionophore for proton-sensitive solvent polymeric membrane electrodes used in biological studies[1]

mp 48 to 49 °C

Lit. cited: 1. H.L. Wu, R. Yu, *Talanta* **34**, 577 (1987)

Warning H315-H319-H335 P261-P305 + P351 + P338

95298-50MG	glass btl	50 mg	

Hydrogen peroxide solution

[7722-84-1] *Merck* **14**,4798; *Fieser* **6**,286; **8**,247; **10**,201; **13**,145; **5**,337; **7**,174; **14**,176; **4**,253; **15**,166; **1**,457; **9**,241; **12**,242; **2**,216; **3**,154; **16**,177; **17**,146 H_2O_2 FW 34.01

vp 23.3 mmHg (30 °C)

▶ **contains potassium stannate as inhibitor, 30-32 wt. % in water, semiconductor grade, 99.999% trace metals basis**

contains stabilizer

density 1.11 g/mL, 25 °C

vd 1 (vs air)

Danger H271-H302-H314-H333-H402 P280-P305 + P351 + P338

316989-3.7L		3.7 L	

▶ **contains inhibitor, 30 wt. % in H_2O, ACS reagent**

29.0-32.0% (ACS specification)

contains stabilizer

Titr. acid			≤0.0006 meq/g
APHA color	≤10	phosphate (PO_4^{3-})	≤2 ppm
evapn. residue	≤0.002%	sulfate (SO_4^{2-})	≤5 ppm
vd	1 (vs air)	Fe	≤0.5 ppm
chloride (Cl^-)	≤3 ppm	heavy metals (as Pb)	≤1 ppm
nitrate (NO_3^-)	≤2 ppm	NH_4^+	≤5 ppm

Danger H271-H302-H314-H333-H402 P280-P305 + P351 + P338

216763-100ML	poly btl	100 mL	
216763-500ML	poly btl	500 mL	
216763-4L	poly btl	4 L	

▶ **50 wt. % in H_2O, stabilized**

Contains proprietary inorganic tin-based stabilizer

mp −40 °C

density 1.197 g/mL, 20 °C

Danger H271-H302-H314-H333-H402 P220-P261-P280-P305 + P351 + P338-P310

516813-500ML	poly btl	500 mL	
516813-4L	poly btl	4 L	

▶ **35 wt. % in H_2O**

contains stabilizer

mp −40 °C

bp 126 °C

density 1.13 g/mL, 25 °C

n_D^{20} 1.387

349887-500ML	poly btl	500 mL	
349887-4L	poly btl	4 L	

Lithium bis(trimethylsilyl)amide, 97%

Hexamethyldisilazane lithium salt

[4039-32-1] *Fieser* **5**,393; **12**,280; **7**,197; **4**,296; **14**,194 $[(CH_3)_3Si]_2NLi$ FW 167.33

density ..... 0.860 g/mL, 25 °C

Used to catalyze the addition of phosphine P-H bonds to carbodiimides leading to phosphaguanidines.[1] Also used in a novel three-step synthesis of disubstituted 1,2,5-thiadiazoles.[2]

Lit. cited: 1. *Chem. Commun. (Camb.)* 3812 (2006)
2. *Tetrahedron Lett.* **47**, 8285 (2006)

Danger H228-H314 P210-P280-P305 + P351 + P338-P310

324620-10G	glass btl	10 g	25.10
324620-50G	glass btl	50 g	70.90
324620-250G	glass btl	250 g	255.00

Lithium bis(trimethylsilyl)amide solution

Hexamethyldisilazane lithium salt

[4039-32-1] *Fieser* **4**,296; **12**,280; **5**,393; **14**,194; **7**,197 $[(CH_3)_3Si]_2NLi$ FW 167.33

▸ 1 M in *tert*-butyl methyl ether

577014-100ML	Sure/Seal™	100 mL	134.50
577014-800ML	Sure/Seal™	800 mL	768.00

▸ 1.0 M in hexanes

Significantly accelerated the polymerization of phenylacetylene in conjunction with rhodium (I) catalysis.[1]

bp ..... 55-56 °C
density ..... 0.707 g/mL, 25 °C

Lit. cited: 1. *Macromolecules* **39**, 5347 (2006)

Danger H225-H304-H314-H336-H361-H371-H401 P210-P261-P273-P280-P301 + P310-P305 + P351 + P338

224367-100ML	Sure/Seal™	100 mL	58.60
224367-800ML	Sure/Seal™	800 mL	325.00
224367-8L	Kilo-Lab®	8 L	734.00

▸ 1.0 M in THF

Significantly accelerated the polymerization of phenylacetylene in conjunction with rhodium(I) catalysis.[1]

density ..... 0.891 g/mL, 25 °C

Lit. cited: 1. *Macromolecules* **39**, 5347 (2006)

Danger H225-H303-H314-H371 P210-P261-P280-P305 + P351 + P338-P310

225770-4X10ML	Sure/Seal™	4 × 10 mL	40.00
225770-100ML	Sure/Seal™	100 mL	42.10
225770-800ML	Sure/Seal™	800 mL	203.00
225770-1L	Sure/Seal™	1 L	239.50
225770-8L	Kilo-Lab®	8 L	961.00
225770-18L	Kilo-Lab®	18 L	1,835.00
225770-100L	steel drum	100 L	Inquire
225770-200L	steel drum	200 L	Inquire

▸ 1 M in toluene

density ..... 0.860 g/mL, 25 °C

Danger H225-H304-H314-H336-H361d-H373 P210-P261-P280-P301 + P310-P305 + P351 + P338-P310

577928-100ML	Sure/Seal™	100 mL	34.70
577928-800ML	Sure/Seal™	800 mL	209.00

Lithium borodeuteride, ≥95%

Lithium borohydride-d_4

[15246-28-3] $LiBD_4$ FW 25.81

Danger H260-H301 + H311-H314-H331 P223-P231 + P232-P261-P280-P370 + P378-P422

685917-500MG	glass btl	500 mg	365.00

Lithium borohydride

[16949-15-8] *Merck* **14**,5525; *Fieser* **12**,276; **1**,603; **4**,296; **14**,191; **11**,293; **15**,186 $LiBH_4$ FW 21.78

mp ..... 275 °C (dec.)
density ..... 0.666 g/mL, 25 °C

Danger P223-P231 + P232-P261-P280-P370 + P378-P422

▸ ≥95.0%

Review[1]; Smooth reduction of esters[2,3]; Reduction of acids and other functional groups with $LiBH_4/Me_3SiCl$[4]

Lit. cited: 1. H.C. Brown, S. Krishnamurthy, *Tetrahedron* **35**, 567 (1979)
2. H.C. Brown, S. Narasimhan, *J. Org. Chem.* **47**, 1604 (1982)
3. H.C. Brown et al., *J. Org. Chem.* **47**, 4702 (1982)
4. A. Giannis, K. Sandhoff, *Angew. Chem.* **101**, 220 (1989)

H260-H302-H311-H314-H330

62460-5G-F	glass btl	5 g	79.70
62460-25G-F		25 g	274.50

▸ ≥90%

H260-H301 + H311-H314-H331

222356-1G	glass btl	1 g	24.30
222356-10G	poly btl	10 g	121.50
222356-50G	poly btl	50 g	395.50

▸ hydrogen-storage grade, ≥90%

Hydrogen content, XRD plots and metal purity data are available upon request.

H260-H302-H311-H314-H330

686026-10G	glass btl	10 g	141.00

Lithium borohydride solution

[16949-15-8] *Merck* **14**,5525; *Fieser* **1**,603; **4**,296; **14**,191; **12**,276; **15**,186; **11**,293 $LiBH_4$ FW 21.78

Danger

▸ 2.0 M in THF

density ..... 0.896 g/mL, 25 °C

H225-H260-H302 + H312-H314-H332-H335 + H336 P210-P223-P231 + P232-P261-P370 + P378-P422

230200-4X10ML	Sure/Seal™	4 × 10 mL	40.00
230200-100ML	Sure/Seal™	100 mL	88.80
230200-800ML	Sure/Seal™	800 mL	451.50

▸ 0.5 M in diethyl ether NEW

Material may form precipitate on standing, which does not affect its use

density ..... 0.719 g/mL, 25 °C

H224-H302 + H332-H315-H319-H336 P210-P261-P305 + P351 + P338

702714-100ML	Sure/Seal™	100 mL	90.00
702714-800ML	Sure/Seal™	800 mL	623.00

Lithium borohydride-d_4, see Lithium borodeuteride Page 1613

Lithium bromide

[7550-35-8] *Merck* **14**,5526; *Fieser* **13**,332; **4**,297; **2**,245; **1**,604 LiBr FW 86.85

mp ..... 550 °C

Warning

▸ anhydrous, beads, −10 mesh, 99.999% trace metals basis

H302

429465-5G	ampule	5 g	52.90
429465-25G	ampule	25 g	170.00

▸ anhydrous, beads, −10 mesh, ≥99.9% trace metals basis

H302

449873-25G	ampule	25 g	82.60
449873-100G	ampule	100 g	268.00

PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS

The basic physical constants and structure diagrams for about 10,900 organic compounds are presented in this table. An effort has been made to include the compounds most frequently encountered in the laboratory, the workplace, and the environment. Particular emphasis has been given to substances that are considered environmental or human health hazards. In making the selection of compounds for the table, added weight was assigned to the appearance of a compound in various lists or reference sources such as:

- Laboratory reagent lists, e.g., the ACS *Reagent Chemicals* volume (Ref. 1)
- The DIPPR list of industrially important compounds (Ref. 2) and the (much larger) TSCA Inventory of chemicals used in commerce.
- The Hazardous Substance Data Bank (Ref. 3)
- The UNEP list of Persistent Organic Pollutants (Ref. 4)
- Chemicals on Reporting Rules (CORR), a database of about 7500 regulated compounds prepared by the Environmental Protection Agency (Ref. 5)
- The EPA Integrated Risk Information System (IRIS), a database of human health effects of exposure to chemicals in the environment (Ref. 6)
- Compendia of chemicals of biochemical or medical importance, such as *The Merck Index* (Ref. 10)
- Specialized tables in this *Handbook*

It should be noted that the above lists vary widely in their choice of chemical names, and even in the use of Chemical Abstracts Registry Numbers. To the extent possible, we have attempted to systematize the names and registry numbers for this table.

Clearly, criteria of this type are somewhat subjective, and compounds considered important by some users have undoubtedly been omitted. Suggestions for additional compounds or other improvements are welcomed.

The data in the table have been derived from many sources, including both the primary literature and evaluated compilations. The *Handbook of Data on Organic Compounds, Third Edition* (Ref. 7) and the *Combined Chemical Dictionary* (Ref. 8) were important sources. Other useful sources of physical property data on organic compounds are listed in Refs. 9-19. The values in the table for the normal boiling point and the melting point that are accompanied with uncertainties (in parentheses) have been critically evaluated using the NIST ThermoData Engine (TDE, Ref. 20), designed to implement the dynamic data evaluation concept (Refs. 21-24). This concept requires large electronic databases capable of storing essentially all relevant experimental data known to date with detailed descriptions of metadata and uncertainties. The combination of these electronic databases with expert-system software, designed to automatically generate recommended property values based on available experimental and predicted data, leads to the ability to produce critically evaluated data dynamically or "to order." The uncertainties listed are combined expanded uncertainties (level of confidence, approximately 95 %) representing the most comprehensive measure of the overall data reliability (Refs. 25-28).

The table is arranged alphabetically by substance name, which generally is either an IUPAC systematic name or, in the case of pesticides, pharmaceuticals, and other complex compounds, a simple trivial name. Names in ubiquitous use, such as acetic acid and formaldehyde, are adopted rather than their systematic equivalents. Synonyms are given in the column following the primary name, and structure diagrams are given on the page facing the data listing. The explanation of the data columns follows:

No.: An identification number used in the indexes.
Name: Primary name of the substance
Synonym: A synonym in common use. When the primary name is non-systematic, a systematic name may appear here.
Mol. Form.: The molecular formula written in the Hill convention.
CAS RN.: The Chemical Abstracts Service Registry Number for the compound.
Mol. Wt: Molecular weight (relative molar mass) as calculated with the 2001 IUPAC Standard Atomic Weights.
Physical Form: A notation of the physical phase, color, crystal type, or other features of the compound at ambient temperature. Abbreviations are given below.
mp: Normal melting point in °C. A value is sometimes followed by "dec", indicating decomposition is observed at the stated temperature (so that it is probably not a true melting point). The notation "tp" indicates a triple point, where solid, liquid, and gas are in equilibrium. A number in parentheses following the melting point value is the combined expanded uncertainty (see above).
bp: Normal boiling point in °C, if it is available. This is the temperature at which the liquid phase is in equilibrium with the vapor at a pressure of 760 mmHg (101.325 kPa). A number in parentheses following the boiling point value is the combined expanded uncertainty (see above). A notation "sp" following the value indicates a sublimation point, where the vapor pressure of the solid phase reaches 760 mmHg. When a notation such as "dec" (decomposes) or "exp" (explodes) follows the value, the temperature may not be a true boiling point. A simply entry "sub" indicates the solid has a significant sublimation pressure at ambient temperatures. When the normal boiling point is not available, a boiling point at reduced pressure may be listed with a superscript indicating the pressure in mmHg.
den: Density (mass per unit volume) in g/cm^3. The temperature in °C is indicated by a superscript. Values refer to the liquid or solid phase, and all values are true densities, not specific gravities. The number of decimal places gives a rough estimate of the accuracy of the value.
n_D: Refractive index, at the temperature in °C indicated by the superscript. Unless otherwise indicated, all values refer to a wavelength of 589 nm (sodium D line). Values are given only for liquids and solids.
Solubility: Qualitative indication of solubility in common solvents. Abbreviations are:
i insoluble
sl slightly soluble
s soluble
vs very soluble
msc miscible
dec decomposes

Abbreviations for solvents are given below.

In order to facilitate the location of compounds in the table, an index to synonyms follows the main table. Indexes to Molecular Formulas and CAS Registry Numbers are available in the electronic versions of the *Handbook* or as pdf files by request via e-mail (fiona.macdonald@taylorandfrancis.com).

The assistance of members of the Thermodynamics Research Center (TRC) of the National Institute of Standards and Technology (Vladimir Diky, Rob Chirico, Andrei Kazakov) and especially Chris Muzny and Michael Frenkel in the determination of values of the normal-boiling-point and melting-point temperatures with uncertainties is greatly appreciated. The editors of the Handbook are much indebted to Chris Muzny who spent countless hours in producing these critically evaluated results. The assistance of Fiona Macdonald in checking names and formulas is gratefully acknowledged, as well as the efforts of Janice Shackleton, Trupti Desai, Nazila Kamaly, Matt Griffiths, and Lawrence Braschi in preparing the structure diagrams.

List of Abbreviations

Ac	acetyl	flr	fluorescent	pow	powder
Ac_2O	acetic anhydride	fum	fumes, fuming	Pr	propyl
AcOEt	ethyl acetate	gl	glacial	PrOH	1-propanol
ac	acid	gr	gray	pr	prisms
ace	acetone	gran	granular	purp	purple
al	alcohol (ethanol)	grn	green	py	pyridine
alk	alkali	hex	hexagonal	pym	pyramids, pyramidal
amor	amorphous	HOAc	acetic acid	reac	reacts
anh	anhydrous	hp	heptane	rhom	rhombic
aq	aqueous	hx	hexane	s	soluble
bipym	bipyramidal	hyd	hydrate	sat	saturated
bl	blue	hyg	hygroscopic	sc	scales
blk	black	i	insoluble	sl	slightly soluble
bp	boiling point	i-	iso-	soln	solution
br	brown	iso	isooctane	sp	sublimation point
bt	bright	lf	leaves	stab	stable
Bu	butyl	lig	ligroin	sub	sublimes
BuOH	1-butanol	liq	liquid	sulf	sulfuric acid
bz	benzene	lo	long	syr	syrup
chl	chloroform	mcl	monoclinic	tab	tablets
col	colorless	Me	methyl	tcl	triclinic
con, conc	concentrated	MeCN	acetonitrile	tetr	tetragonal
cry	crystals	MeOH	methanol	tfa	trifluoroacetic acid
ctc	carbon tetrachloride	misc	miscible	thf, THF	tetrahydrofuran
cy, cyhex	cyclohexane	mp	melting point	tol	toluene
dec	decomposes	n	refractive index	tp	triple point
den	density	nd	needles	trg	trigonal
dil	dilute	oct	octahedra, octahedral	unstab	unstable
diox	dioxane	oran	orange	vap	vapor
dk	dark	orth	orthorhombic	viol	violet
DMF	dimethylformamide	os	organic solvents	visc	viscous
DMSO	dimethyl sulfoxide	pa	pale	vol	volatile
efflor	efflorescent	peth	petroleum ether	vs	very soluble
Et	ethyl	Ph	phenyl	w	water
EtOH	ethanol	PhCl	chlorobenzene	wh	white
eth	diethyl ether	$PhNH_2$	aniline	xyl	xylene
exp	explodes	$PhNO_2$	nitrobenzene	ye	yellow
fl	flakes	pl	plates		

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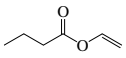
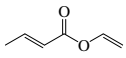
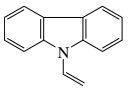
No.	Name	Synonym	Mol. Form.	CAS RN	Mol. Wt.	Physical Form	mp/°C	bp/°C	den g cm^{-3}	n_D	Solubility
10794	Vinyl butanoate		$C_6H_{10}O_2$	123-20-6	114.142			116.7	0.9006^{20}		
10795	Vinyl *trans*-2-butenoate	Vinyl crotonate	$C_6H_8O_2$	3234-54-6	112.127						s ctc
10796	9-Vinyl-9*H*-carbazole		$C_{14}H_{11}N$	1484-13-5	193.244	cry (al)	66				i H_2O; sl EtOH; vs eth
10797	Vinylcyclohexane		C_8H_{14}	695-12-5	110.197			127(6)	0.8166^{19}	1.455^{19}	
10798	1-Vinylcyclohexene		C_8H_{12}	2622-21-1	108.181			144(7)	0.8623^{15}	1.4915^{20}	i H_2O; s eth, bz; vs MeOH
10799	4-Vinylcyclohexene		C_8H_{12}	100-40-3	108.181	liq	-108.9	130(4)	0.8299^{20}	1.4639^{20}	i H_2O; s eth, bz, peth
10800	Vinylcyclopentane		C_7H_{12}	3742-34-5	96.170	liq	-126.4(0.2)	99(3)	0.7834^{20}	1.4360^{20}	
10801	Vinyldiethoxymethylsilane		$C_7H_{16}O_2Si$	5507-44-8	160.287			133	0.8620^{20}	1.4001^{20}	
10802	Vinylethoxydimethylsilane		$C_6H_{14}OSi$	5356-83-2	130.260			99	0.790^{20}	1.3983^{20}	
10803	1-Vinyl-4-fluorobenzene		C_8H_7F	405-99-2	122.140		-34.5	67.4^{50}	1.0220^{20}	1.5150^{20}	i H_2O; s EtOH, eth, bz
10804	Vinyl formate		$C_3H_4O_2$	692-45-5	72.063	visc liq	-78	42(18)	0.965^{20}	1.3842^{20}	
10805	2-Vinylfuran		C_6H_6O	1487-18-9	94.111	liq	-94(4)	101(3)	0.9445^{19}	1.4992^{19}	
10806	1-Vinyl-2-methoxybenzene		$C_9H_{10}O$	612-15-7	134.174	nd	29	215(18)	1.0049^{17}	1.5388^{20}	vs ace, bz, eth, EtOH
10807	1-Vinyl-3-methoxybenzene		$C_9H_{10}O$	626-20-0	134.174			91^{15}	0.9919^{20}	1.5586^{23}	i H_2O; s EtOH, eth, bz
10808	1-Vinyl-4-methoxybenzene		$C_9H_{10}O$	637-69-4	134.174		2.0	208(19)	1.0001^{13}	1.5642^{13}	i H_2O; s EtOH, eth, bz; sl ctc
10809	6-Vinyl-6-methyl-1-isopropyl-3-(1-methylethylidene)-cyclohexene, (*S*)-		$C_{15}H_{24}$	5951-67-7	204.352			125^{8}	0.8782^{20}	1.5130^{26}	vs ace, bz
10810	1-Vinylnaphthalene		$C_{12}H_{10}$	826-74-4	154.207			124^{15}	1.0656^{20}	1.644^{20}	
10811	2-Vinylnaphthalene		$C_{12}H_{10}$	827-54-3	154.207		65(2)	135^{18}			i H_2O; s EtOH, ace, bz
10812	1-Vinyl-3-nitrobenzene		$C_8H_7NO_2$	586-39-0	149.148		-10	120^{11}	1.1552^{32}	1.5836^{20}	i H_2O; s EtOH, eth, bz, chl, lig, HOAc
10813	1-Vinyl-4-nitrobenzene		$C_8H_7NO_2$	100-13-0	149.148	pr (lig)	29	dec			vs EtOH, eth; s chl, HOAc, lig
10814	5-Vinyl-2-norbornene	5-Vinylbicyclo[2.2.1]hept-2-ene	C_9H_{12}	3048-64-4	120.191	liq	-80	140.7(0.5)	0.841	1.4810^{20}	
10815	Vinyl octadecanoate	Vinyl stearate	$C_{20}H_{38}O_2$	111-63-7	310.515		29	167^{2}	0.8517^{20}		sl chl
10816	3-Vinyl-7-oxabicyclo[4.1.0]-heptane		$C_8H_{12}O$	106-86-5	124.180		<-100	169	0.9581^{20}	1.4700^{20}	
10817	Vinyloxirane		C_4H_6O	930-22-3	70.090			68(2)	0.9006^{25}	1.4168^{20}	s EtOH, eth, bz
10818	2-(Vinyloxy)ethanol	Ethylene glycol monovinyl ether	$C_4H_8O_2$	764-48-7	88.106			139(4)	0.9821^{20}	1.4564^{17}	s H_2O, EtOH, eth, bz; i lig
10819	Vinyl propanoate	Vinyl propionate	$C_5H_8O_2$	105-38-4	100.117			94.8(0.2)			
10820	2-Vinylpyridine		C_7H_7N	100-69-6	105.138			159.5	0.9983^{20}	1.5495^{20}	sl H_2O; vs EtOH, eth, ace, chl
10821	3-Vinylpyridine		C_7H_7N	1121-55-7	105.138			162	0.9879^{20}	1.5530^{20}	sl H_2O; s EtOH, eth
10822	4-Vinylpyridine		C_7H_7N	100-43-6	105.138	red to dk-br		121^{150}	0.9879^{20}	1.5449^{20}	s H_2O, EtOH, chl; sl eth
10823	1-Vinyl-2-pyrrolidinone		C_6H_9NO	88-12-0	111.141		13.5	193^{400}	1.04^{20}		
10824	Vinylsilane		C_2H_6Si	7291-09-0	58.155	col gas	-171.6	-22.8			
10825	Vinyl sulfoxide	Divinyl sulfoxide	C_4H_6OS	1115-15-7	102.155	liq		86^{18}			
10826	Vinyltriacetoxysilane	Vinylsilanetriol, triacetate	$C_8H_{12}O_6Si$	4130-08-9	232.263			115^{10}	1.169^{20}	1.4226^{20}	
10827	Vinyltriethoxysilane		$C_8H_{18}O_3Si$	78-08-0	190.313			160.0(0.8)	0.901^{20}	1.3960^{25}	s chl
10828	Vinyltrimethylsilane		$C_5H_{12}Si$	754-05-2	100.235			55.3(0.2)	0.65^{20}	1.3914^{20}	i H_2O
10829	Violaxanthin		$C_{40}H_{56}O_4$	126-29-4	600.871	red pr (MeOH, al-eth)	208				s EtOH, eth, CS_2; i peth
10830	Viquidil		$C_{20}H_{24}N_2O_2$	84-55-9	324.417	red ye amor	60				vs eth, EtOH, chl
10831	Visnadine		$C_{21}H_{24}O_7$	477-32-7	388.412	nd	85.5				i H_2O; s EtOH, eth
10832	Visnagin	4-Methoxy-7-methyl-5*H*-furo[3,2-*g*][1]benzopyran-5-one	$C_{13}H_{10}O_4$	82-57-5	230.216	nd (w, MeOH)	144.5				sl H_2O, EtOH; vs chl
10833	Vitamin B12	Cyanocobalamin	$C_{63}H_{88}CoN_{14}O_{14}P$	68-19-9	1355.365		>300				
10834	Vitamin D2		$C_{28}H_{44}O$	50-14-6	396.648	pr (ace)	116.5	sub			i H_2O; s EtOH, eth, ace, chl
10835	Vitamin D3	9,10-Secocholesta-5,7,10(19)-trien-3-ol, (3β,5*Z*,7*E*)-	$C_{27}H_{44}O$	67-97-0	384.637		84.5				i H_2O; s os
10836	Vitamin E	α-Tocopherol	$C_{29}H_{50}O_2$	59-02-9	430.706	pale ye oil	3.0	210$^{0.1}$	0.950^{25}	1.5045^{25}	i H_2O; s EtOH, eth, ace, chl


10794
Vinyl butanoate


10795
Vinyl *trans*-2-butenoate

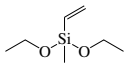

10796
9-Vinyl-9*H*-carbazole


10797
Vinylcyclohexane

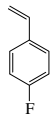

10798
1-Vinylcyclohexene


10799
4-Vinylcyclohexene


10800
Vinylcyclopentane


10801
Vinyldiethoxymethylsilane


10802
Vinylethoxydimethylsilane

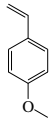

10803
1-Vinyl-4-fluorobenzene

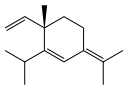

10804
Vinyl formate


10805
2-Vinylfuran

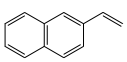

10806
1-Vinyl-2-methoxybenzene


10807
1-Vinyl-3-methoxybenzene


10808
1-Vinyl-4-methoxybenzene


10809
6-Vinyl-6-methyl-1-isopropyl-3-(1-methylethylidene)cyclohexene, (*S*)-


10810
1-Vinylnaphthalene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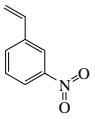
2-Vinylnaphthalene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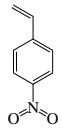
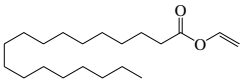
1-Vinyl-3-nitrobenzene


10813
1-Vinyl-4-nitrobenzene


10814
5-Vinyl-2-norbornene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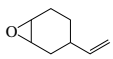
Vinyl octadecanoate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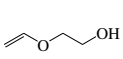
3-Vinyl-7-oxabicyclo[4.1.0]heptane


10817
Vinyloxirane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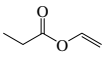
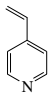
2-(Vinyloxy)ethanol


10819
Vinyl propanoate


10820
2-Vinylpyridine

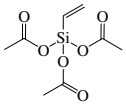

10821
3-Vinylpyridine

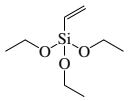

10822
4-Vinylpyridine


10823
1-Vinyl-2-pyrrolidinone

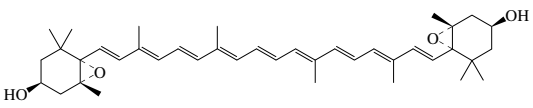

10824
Vinylsilane


10825
Vinyl sulfoxide


10826
Vinyltriacetoxysilane


10827
Vinyltriethoxysilane


10828
Vinyltrimethylsilane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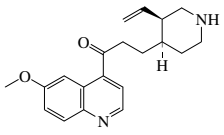
Violaxanthin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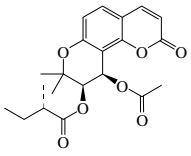
Viquidil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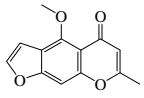
Visnadine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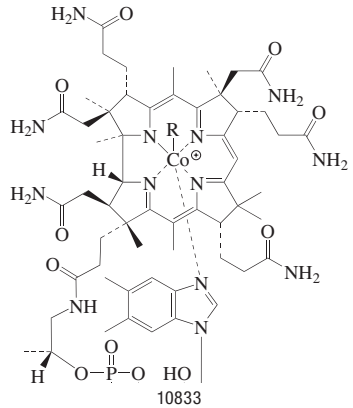
Visnagin


10833
Vitamin B12

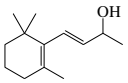
10834
Vitamin D2

10835
Vitamin D3

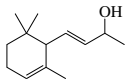
10836
Vitamin E

No.	Name	Synonym	Mol. Form.	CAS RN	Mol. Wt.	Physical Form	mp/°C	bp/°C	den g cm^{-3}	n_D	Solubility
10540	3,5,5-Trimethyl-2-cyclohexen-1-ol	Isophorol	$C_9H_{16}O$	470-99-5	140.222			69^{5}	0.914^{20}	1.4717^{20}	
10541	4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-ol	β-Ionol	$C_{13}H_{22}O$	22029-76-1	194.313			130^{14}	0.9243^{20}	1.4969^{20}	s EtOH, eth, ace
10542	4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-ol	α-Ionol	$C_{13}H_{22}O$	25312-34-9	194.313	oil		127^{14}	0.9189^{20}	1.4735^{20}	
10543	1,1,2-Trimethylcyclopentane		C_8H_{16}	4259-00-1	112.213	liq	-21.7(0.2)	113.7(0.2)	0.7660^{20}	1.4199^{20}	
10544	1,1,3-Trimethylcyclopentane		C_8H_{16}	4516-69-2	112.213	liq	-142.5(0.2)	104.9(0.6)	0.7439^{25}	1.4112^{20}	i H_2O
10545	1α,2α,4β-1,2,4-Trimethylcyclopentane		C_8H_{16}	4850-28-6	112.213	liq	-131(5)	116.7(0.6)	0.7592^{25}	1.4186^{20}	
10546	1α,2β,4α-1,2,4-Trimethylcyclopentane		C_8H_{16}	16883-48-0	112.213	liq	-130.8(0.3)	110(3)	0.7430^{25}	1.4106^{20}	
10547	*cis*-1,2,2-Trimethyl-1,3-cyclopentanedicarboxylic acid, (1*R*)		$C_{10}H_{16}O_4$	124-83-4	200.232	pr, lf (w)	187		1.186^{20}		sl H_2O; vs EtOH, eth; s ace; i bz, chl
10548	2,2,4-Trimethylcyclopentanone		$C_8H_{14}O$	28056-54-4	126.196	liq	-40.6	158	0.877^{25}	1.4300^{20}	
10549	2,4,4-Trimethylcyclopentanone		$C_8H_{14}O$	4694-12-6	126.196	liq	-25.6	160.5	0.8785^{18}	1.433^{18}	
10550	1,1,2-Trimethylcyclopropane		C_6H_{12}	4127-45-1	84.159	liq	-138.2(0.1)	53(1)	0.6897^{25}	1.3864^{20}	
10551	3,7,11-Trimethyl-2,6,10-dodecatrienal		$C_{15}H_{24}O$	19317-11-4	220.351			172^{14}	0.893^{18}	1.4995	
10552	Trimethylgallium		C_3H_9Ga	1445-79-0	114.826			55.7			dec H_2O (exp)
10553	2,2,6-Trimethylheptane		$C_{10}H_{22}$	1190-83-6	142.282	liq	-105(1)	149(4)	0.7200^{25}	1.4078^{20}	
10554	2,5,5-Trimethylheptane		$C_{10}H_{22}$	1189-99-7	142.282			153(3)	0.7362^{25}	1.4149^{20}	
10555	3,3,5-Trimethylheptane		$C_{10}H_{22}$	7154-80-5	142.282			157(3)	0.7248^{20}	1.4170^{20}	i H_2O; s bz, ctc, chl
10556	3,4,5-Trimethylheptane		$C_{10}H_{22}$	20278-89-1	142.282			162.5	0.7519^{25}	1.4229^{20}	
10557	2,2,3-Trimethylhexane		C_9H_{20}	16747-25-4	128.255			134(2)	0.7257^{25}	1.4106^{20}	
10558	2,2,4-Trimethylhexane		C_9H_{20}	16747-26-5	128.255	liq	-122(4)	127(2)	0.711^{20}	1.4033^{20}	
10559	2,2,5-Trimethylhexane		C_9H_{20}	3522-94-9	128.255	liq	-105.9(0.1)	124(2)	0.7072^{20}	1.3997^{20}	i H_2O; vs EtOH, eth, ace, bz; s ctc
10560	2,3,3-Trimethylhexane		C_9H_{20}	16747-28-7	128.255	liq	-116.8(0.2)	137(3)	0.7345^{25}	1.4141^{20}	
10561	2,3,4-Trimethylhexane		C_9H_{20}	921-47-1	128.255			139(3)	0.7354^{25}	1.4144^{20}	
10562	2,3,5-Trimethylhexane		C_9H_{20}	1069-53-0	128.255	liq	-127.9(0.2)	131(2)	0.7218^{20}	1.4051^{20}	
10563	2,4,4-Trimethylhexane		C_9H_{20}	16747-30-1	128.255	liq	-113.4(0.1)	130.6(0.7)	0.7201^{25}	1.4074^{20}	
10564	3,3,4-Trimethylhexane		C_9H_{20}	16747-31-2	128.255	liq	-101.2(0.2)	139(4)	0.7414^{25}	1.4178^{20}	
10565	3,5,5-Trimethylhexanoic acid	Isononanoic acid	$C_9H_{18}O_2$	3302-10-1	158.238	liq		121^{10}			
10566	3,5,5-Trimethyl-1-hexanol		$C_9H_{20}O$	3452-97-9	144.254			193(5)	0.8236^{25}	1.4300^{25}	
10567	1,2,3-Trimethylindene		$C_{12}H_{14}$	4773-83-5	158.239	liq		100.5^{10}	0.9714^{20}	1.5521^{20}	
10568	Trimethylindium	Indium trimethyl	C_3H_9In	3385-78-2	159.921			135.7	1.568^{19}		
10569	2,3,3-Trimethyl-3*H*-indole		$C_{11}H_{13}N$	1640-39-7	159.228			107^{11}			
10570	Trimethyl(4-methylphenyl)-silane		$C_{10}H_{16}Si$	3728-43-6	164.320		38	192	0.8666^{20}	1.4900^{20}	
10571	1,4,5-Trimethylnaphthalene		$C_{13}H_{14}$	2131-41-1	170.250	lf (MeOH)	64.0(0.6)	145^{12}			i H_2O
10572	1,3,5-Trimethyl-2-nitrobenzene		$C_9H_{11}NO_2$	603-71-4	165.189	orth pr (al)	44(2)	255	1.51^{25}		vs EtOH
10573	2,6,8-Trimethyl-4-nonanol		$C_{12}H_{26}O$	123-17-1	186.333			225.4	0.8178^{20}		sl ctc
10574	2,4,7-Trimethyloctane		$C_{11}H_{24}$	62016-38-0	156.309			170(5)			
10575	Trimethylolpropane		$C_6H_{14}O_3$	77-99-6	134.173	wh pow or pl	60.2(0.2)	160^{5}			vs H_2O, EtOH
10576	3,5,5-Trimethyl-2,4-oxazolidinedione	Trimethadione	$C_6H_9NO_3$	127-48-0	143.140		46	79^{5}			s H_2O; vs EtOH, eth, ace, bz; i peth
10577	Trimethyloxonium fluoborate		$C_3H_9BF_4O$	420-37-1	147.907	hyg nd	148 dec				vs ace, chl
10578	2,4,4-Trimethyl-2-pentanamine		$C_8H_{19}N$	107-45-9	129.244						s chl
10579	2,2,3-Trimethylpentane	2-*tert*-Butylbutane	C_8H_{18}	564-02-3	114.229	liq	-112.4(0.3)	109.8(0.4)	0.7161^{20}	1.4030^{20}	i H_2O; msc EtOH, eth, ace, hp; s bz
10580	2,2,4-Trimethylpentane	Isooctane	C_8H_{18}	540-84-1	114.229	liq	-107.36(0.04)	99.2(0.2)	0.6878^{25}	1.3884^{25}	i H_2O; msc EtOH, ace, hp; s eth, ctc
10581	2,3,3-Trimethylpentane		C_8H_{18}	560-21-4	114.229	liq	-101.2(0.3)	114.7(0.3)	0.7262^{20}	1.4075^{20}	i H_2O; vs EtOH; msc eth, ace, bz, hp
10582	2,3,4-Trimethylpentane		C_8H_{18}	565-75-3	114.229	liq	-109.3(0.2)	113.4(0.3)	0.7191^{20}	1.4042^{20}	i H_2O; vs EtOH; msc eth, ace, bz; sl ctc
10583	2,2,4-Trimethyl-1,3-pentanediol		$C_8H_{18}O_2$	144-19-4	146.228	pl (bz)	55.2(0.5)	230.1(0.3)	0.936^{15}	1.4513^{15}	sl H_2O; vs EtOH, eth; s bz, chl

10540
3,5,5-Trimethyl-2-cyclohexen-1-ol



10541
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-ol



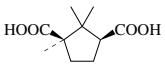
10542
4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-ol

10543
1,1,2-Trimethylcyclopentane

10544
1,1,3-Trimethylcyclopentane

10545
1α,2α,4β-1,2,4-Trimethylcyclopentane

10546
1α,2β,4α-1,2,4-Trimethylcyclopentane

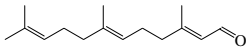


10547
cis-1,2,2-Trimethyl-1,3-cyclopentanedicarboxylic acid, (1*R*)

10548
2,2,4-Trimethylcyclopentanone

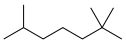
10549
2,4,4-Trimethylcyclopentanone

10550
1,1,2-Trimethylcyclopropane

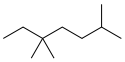


10551
3,7,11-Trimethyl-2,6,10-dodecatrienal

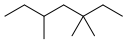
10552
Trimethylgallium



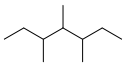
10553
2,2,6-Trimethylheptane



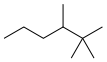
10554
2,5,5-Trimethylheptane



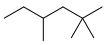
10555
3,3,5-Trimethylheptane



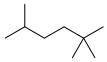
10556
3,4,5-Trimethylheptane



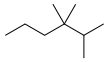
10557
2,2,3-Trimethylhexane



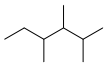
10558
2,2,4-Trimethylhexane



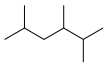
10559
2,2,5-Trimethylhexane



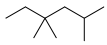
10560
2,3,3-Trimethylhexane



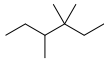
10561
2,3,4-Trimethylhexane



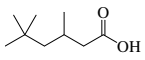
10562
2,3,5-Trimethylhexane



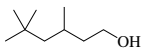
10563
2,4,4-Trimethylhexane



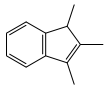
10564
3,3,4-Trimethylhexane



10565
3,5,5-Trimethylhexanoic acid

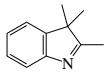


10566
3,5,5-Trimethyl-1-hexanol

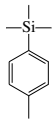


10567
1,2,3-Trimethylindene

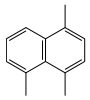
10568
Trimethylindium



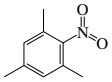
10569
2,3,3-Trimethyl-3*H*-indole



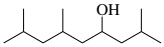
10570
Trimethyl(4-methylphenyl)silane



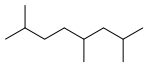
10571
1,4,5-Trimethylnaphthalene



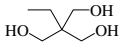
10572
1,3,5-Trimethyl-2-nitrobenzene



10573
2,6,8-Trimethyl-4-nonanol

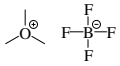


10574
2,4,7-Trimethyloctane

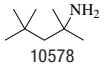


10575
Trimethylolpropane

10576
3,5,5-Trimethyl-2,4-oxazolidinedione



10577
Trimethyloxonium fluoborate



10578
2,4,4-Trimethyl-2-pentanamine

10579
2,2,3-Trimethylpentane

10580
2,2,4-Trimethylpentane

10581
2,3,3-Trimethylpentane

10582
2,3,4-Trimethylpentane

10583
2,2,4-Trimethyl-1,3-pentanediol

Give complete answers for **all** responses.

(15) 1. Do you **need** to write a description of the apparatus or techniques used in a synthesis experiment? Explain, why or why not.

(10) 2. What determines whether to write out the side reactions or not? How do you make this determination?

(10) 3. Why would you measure the melting point of a product in the lab?

(10) 4. Lab group A measures the melting point of a product presumed to be isatin to be between 188 C° and 193 C°. Lab group B measures the melting point of a product also presumed to be isatin to be between 190 C° and 194 C°. The Aldrich catalog lists the melting point of isatin to be between 193 C° and 195 C°. Whose product is more pure? Explain.

5. You synthesize asprin ($C_9H_8O_4$) from salicyclic acid ($C_7H_6O_3$) and acetic anhydride ($C_4H_8O_3$) using 3.00 g of salicyclic acid and 6.00 grams of acetic anhydride. After the reaction and filtration, you recover 3.10 g of aspirin. The reaction is as follows:

$$C_7H_6O_3 + C_4H_8O_3 \longrightarrow C_9H_8O_4 + C_2H_4O_2$$

(5) (a) What is the theoretical yield for the above reaction?

(3) (b) What is the experimental yield for the reaction?

(4) (c) What is the percent yield for the reaction?

(10) 6. What would you include in the lab notebook of a synthesis experiment? List and describe as many elements as you can.

Points earned: _____ out of a possible 0 points

Give complete answers for **all** responses and feel free to draw diagrams.

(10) 1. Demonstrate how to fold filter paper and take a picture to submit along with your responses.

(5) 2. Draw a diagram of the gravity filtration setup.

(5) 3. Draw a diagram of the vacuum filtration setup with Buchner flask.

4. A good solvent for the recrystalization process used for purification of a product.

(2) (a) Dissolves the solid while _____.

(4) (b) The same solvent does not dissolve the solid when _____ and does not dissolve the _____ for forever.

5. Describe the process of recrystalization. Assuming your solvent has been selected.

(2) (a) Put the solid in an _____ _____.

(2) (b) Heat the solvent on a _____ _____.

(2) (c) Add the hot _____ to the solid until it is just _____

(2) (d) Add _____ of excess solvent to the the solid.

(2) (e) If there is obvious trash in the sample, then use _____.

(3) (f) Examine the sample mixture for _____ If it looks like there is more product to be dissolved, then add more hot _____.

(4) (g) _____ the solution down slowly. Once it is warm to the touch, cool with an _____.

(3) (h) When the flask is cooling down in its bath, watch out for (1) the flask _____, and (2) a flask that is too hot _____

(4) (i) After the product is cool, use _____ and take a _____.

Points earned: _____ out of a possible 0 points

Give complete answers for **all** responses and feel free to draw diagrams.

(8) 1. The distillation process seperates liquids on the basis of what?

.....

2. Concerning simple and vacuum distillation:

(4) (a) What is the difference between these methods?

.....

.....

.....

(3) (b) When is it appropriate to use vacuum distillation rather than simple?

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.....

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3. Concerning simple and fractional distillation:

(4) (a) What is the difference between these methods?

.....

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(3) (b) When is it appropriate to use fractional distillation rather than simple?

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4. Concerning simple and steam distillation:

(4) (a) What is the difference between these methods?

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(3) (b) When is it appropriate to use steam distillation rather than simple?

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5. Concerning simple distillation:

(5) (a) Describe the process of simple distillation.

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(8) (b) Draw a diagram of the setup and label the parts.

6. Concerning fractional distillation:

(5) (a) Describe the process of fractional distillation.

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(8) (b) Draw a diagram of the setup and label the parts.

Points earned: _____ out of a possible 55 points

Give complete answers for **all** responses and feel free to draw diagrams.

(8) 1. The purpose of the reflux setup is to allow a reaction to occur at _____ temperature for an extended period of time. The temperature of the reaction is always the _____ point of the solvent.

2. Concerning the reflux setup:

(14) (a) Draw a diagram of a standard reflux setup. Label all of the parts.

(7) (b) How does the reflux setup keep the mixture boiling without losing solvent?

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(7) 3. When do you start the timer on a refluxing reaction?

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(7) 4. What is the difference between a dry and a wet reflux?

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(7) 5. Why would you do an addition and reflux setup?

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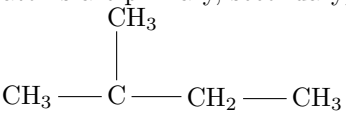
.....

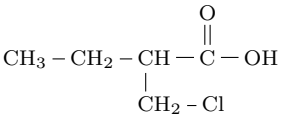
Points earned: _____ out of a possible 50 points

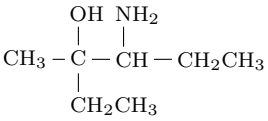
Show all work leading up to **all** responses. You may attach additional pages if needed. If you do so, then list the question number next to any work.

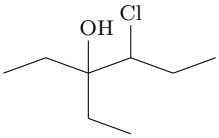
(4) 1. Given the structure below label the Carbon atoms as 1, 2, 3 and 4. Then, indicate which carbon atoms are primary, secondary, and tertiary.



2. Identify all the functional groups in the following compounds:

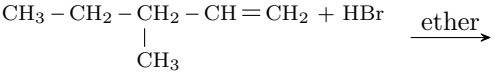
(3) (a) 

(3) (b) 

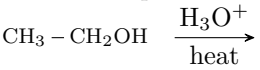
(3) (c) 

(3) (d) $CH_3OCH_2CH_2CH_2CH_3$

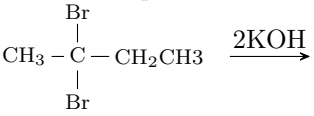
(8) 3. Predict the products for the following reaction:



(8) 4. Predict the products for the following reaction:



(8) 5. Predict the products for the following reaction:

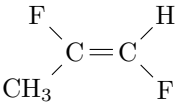


6. Draw a reaction energy diagram for a two-step reaction with $K_{eq} > 1$.

(5) (a) Label the parts of the diagram corresponding tor reactants, products, transition state, ΔG°, and $\Delta G^{\ddagger}$.

(2) (b) Is ΔG° positive or negative?

7. Consider the following compound:

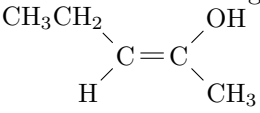


(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*)designation?

(5) (b) How many $\sigma$and π-bonds are in this compound?

Points earned: _____ out of a possible 58 points

8. Consider the following compound:



(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*)designation?

(5) (b) How many $\sigma$and π-bonds are in this compound?

9. Consider the ion NO_2^- and the molecule NO_3^-. The electrognegativity of the elements involved are: O, 3.5 and N, 3.0.

(6) (a) Draw all the resonance structures for the ion NO_2^-.

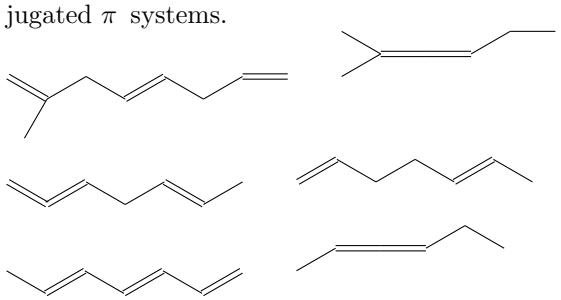
(6) (b) Draw all the resonance structures for the molecule NO_3^-.

(4) (c) Draw in above the formal charges on all atoms for each resonance structure.

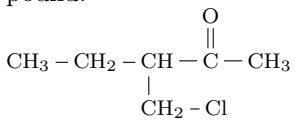
(4) (d) Determine which resonance structure is the most stable. And, explain why it is the most stable.

(4) (e) Would you predict adding an oxygen atom making (oxidizing) to NO_2^- result in a less or more energetic form in NO_3^-? Explain why using your resonance structures and formal charges.

(7) 10. Circle the chemical structures that represent conjugated π systems.



11. Write the name of the following chemical compound:



(1) (a) Identify the parent alkane.

(1) (b) Identify all functional groups in the compound.

(3) (c) Write the IUPAC name of the compound.

12. Draw the structure of 2-Chloro-3-methylhex-4-one

(1) (a) Identify the parent alkane.

(1) (b) Identify all functional groups in the compound.

(3) (c) Draw the chemical structure of the compound.

Points earned: _____ out of a possible 52 points

IUPAC Naming Rules

1. Find the longest continuous carbon chain containing the highest priority functional group. Determine the root name for this parent chain.[1] Assign the parent name using the root name and the functional group. Note that the position number will need to go before the ending with dashes if the ending is anything other than -ane.

2. Number the chain in the direction such that the position number of the first substituent is the smaller number. If the first substituents from either end have the same number, then number so that the second substituent has the smaller number, etc.

3. Determine the name and position number of each substituent.

4. Indicate the number of identical groups by the prefixes di, tri, tetra, etc.

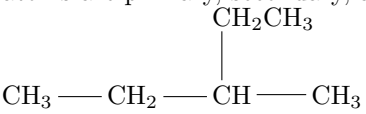
5. Place the position numbers and names of the substituent groups, in alphabetical order, before the root name. In alphabetizing, ignore prefixes like sec-, tert-, di, tri, etc. and include the iso- prefix. Always include a position number for each substituent, regardless of redundancies.

[1] When there are two longest chains of equal length, use the chain with the greater number of substituents.

Points earned: _____ out of a possible 0 points

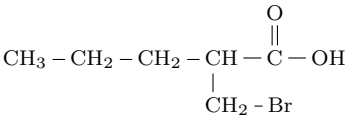
Show all work leading up to **all** responses. You may attach additional pages if needed. If you do so, then list the question number next to any work.

(4) 1. Given the structure below label the Carbon atoms as 1, 2, 3 and 4. Then, indicate which carbon atoms are primary, secondary, and tertiary.

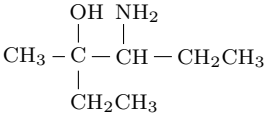


2. Identify all the functional groups in the following compounds:

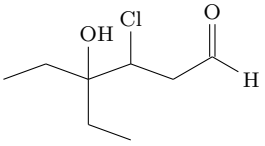
(3) (a)



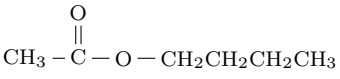
(3) (b)



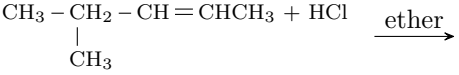
(3) (c)



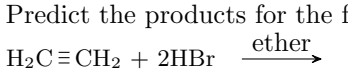
(3) (d)



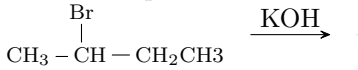
(8) 3. Predict the products for the following reaction:



(8) 4. Predict the products for the following reaction:



(8) 5. Predict the products for the following reaction:

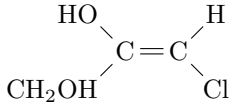


6. Draw a reaction energy diagram for a two-step reaction with $K_{eq} = 1$.

(5) (a) Label the parts of the diagram corresponding tor reactants, products, transition state, ΔG°, and $\Delta G^{\ddagger}$.

(2) (b) Is ΔG° positive, negative or zero?

7. Consider the following compound:

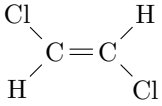


(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*)designation?

(5) (b) How many $\sigma$and π-bonds are in this compound?

Points earned: _____ out of a possible 58 points

8. Consider the following compound:



(6) (a) Would this compound need a *cis*, *trans*, (*Z*), or (*E*) designation?

(5) (b) How many $\sigma$and π-bonds are in this compound?

9. Consider the ion HCO_3^- and the molecule CO_3^{2-}. The electrognegativity of the elements involved are: O, 3.5; C, 2.5; and H, 2.1.

(6) (a) Draw all the resonance structures for the ion CO_3^{2-}.

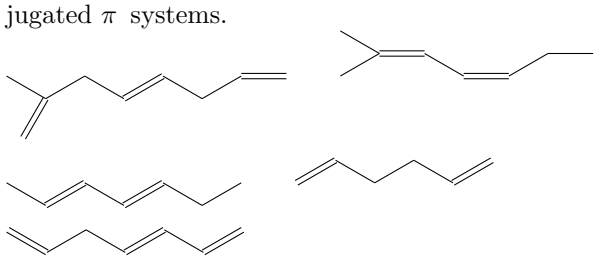
(6) (b) Draw all the resonance structures for the ion HCO_3^-.

(4) (c) Draw in above the formal charges on all atoms for each resonance structure.

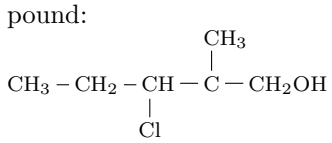
(4) (d) Determine which resonance structure is the most stable. And, explain why it is the most stable.

(4) (e) Is CO_3^{2-} a good base by being able to accept a proton (H^+)? Explain why using your resonance structures and formal charges.

(7) 10. Circle the chemical structures that represent conjugated π systems.



11. Write the name of the following chemical compound:



(1) (a) Identify the parent alkane.

(1) (b) Identify all functional groups in the compound.

(3) (c) Write the IUPAC name of the compound.

12. Draw the structure of 2-Bromo-3-methylpental

(1) (a) Identify the parent alkane.

(1) (b) Identify all functional groups in the compound.

(3) (c) Draw the chemical structure of the compound.

Points earned: _____ out of a possible 52 points

IUPAC Naming Rules

1. Find the longest continuous carbon chain containing the highest priority functional group. Determine the root name for this parent chain.[1] Assign the parent name using the root name and the functional group. Note that the position number will need to go before the ending with dashes if the ending is anything other than -ane.

2. Number the chain in the direction such that the position number of the first substituent is the smaller number. If the first substituents from either end have the same number, then number so that the second substituent has the smaller number, etc.

3. Determine the name and position number of each substituent.

4. Indicate the number of identical groups by the prefixes di, tri, tetra, etc.

5. Place the position numbers and names of the substituent groups, in alphabetical order, before the root name. In alphabetizing, ignore prefixes like sec-, tert-, di, tri, etc. and include the iso- prefix. Always include a position number for each substituent, regardless of redundancies.

[1] When there are two longest chains of equal length, use the chain with the greater number of substituents.

Points earned: _____ out of a possible 0 points

Memorize

1. Names, structures of the common Alkanes: methane, ethane, propane, butane, pentane, hexane.

2. Names, endings and structures of the common Alkyl groups: methane, ethane, propane, butane.

3. Names, structures and endings of common functional groups: halide, alkene, alkyne, aldehyde, ketone, carboxylic acid, amine.

Reaction Patterns

1. Addition Reactions: Two reactants add together to give a single new product. The reactions also follow Markovnikov's Rule.

   Markovnikov's Rule In the addition of HX to an alkene, the H attaches to the carbon with fewer alkyl substituents and the X attaches to the carbon with more alkyl substituents.

   $$H_2C{=}CH_2 + H{-}X \xrightarrow{\text{ether}} \begin{matrix} H & X \\ | & | \\ CH_2 & - & CH_2 \end{matrix}$$

   where X=Cl, Br, or I.

   $$H_2C{\equiv}CH_2 + H{-}X \xrightarrow{\text{ether}} \begin{matrix} & & & X \\ & & CH & = & CH \\ H & \diagup & & \diagdown & \end{matrix}$$

   $$HC{\equiv}CH + 2H{-}X \xrightarrow{\text{ether}} \begin{matrix} X & & X \\ | & & | \\ CH_2 & - & CH_2 \end{matrix}$$

   where X=Cl or Br.

2. Elimination Reaction: One reactant splits into two products. Typically one product is a small molecule such as H_2O or HCl.

   $$\begin{matrix} H & & OH \\ | & & | \\ CH_2 & - & CH_2 \end{matrix} \xrightarrow[\text{heat}]{H_3O^+} H_2C{=}CH_2 + H_2O$$

   $$\begin{matrix} H & & X \\ | & & | \\ CH_2 & - & CH_2 \end{matrix} \xrightarrow{KOH} H_2C{=}CH_2 + KX + H_2O$$

   $$\begin{matrix} H & & X \\ | & & | \\ CH & - & CH \\ | & & | \\ H & & X \end{matrix} \xrightarrow{2KOH} HC{\equiv}CH + 2KX + 2H_2O$$

   $$\begin{matrix} H & & H \\ | & & | \\ CH & - & CH \\ | & & | \\ X & & X \end{matrix} \xrightarrow{2KOH} HC{\equiv}CH + 2KX + 2H_2O$$

   where X=Cl, Br, or I.

   $$\begin{matrix} H & & X \\ | & & | \\ CH_2 & - & CH_2 \end{matrix} \xrightarrow{KOH} H_2C{=}CH_2 + KX + H_2O$$

   where X=Cl, Br, or I.

3. Substitution Reaction: Two reactants exhange parts to give two new products. (X=Cl, Br, or I)

   $$\begin{matrix} H \\ | \\ CH_3 \end{matrix} + X_2 \xrightarrow{h\nu} \begin{matrix} X \\ | \\ CH_3 \end{matrix} + HCl$$

4. Rearrangement Reaction: One reactant undergoes a reorganiziation to yield a single isomeric product.

   $$\begin{matrix} Br & & H \\ & \diagdown\diagup & \\ & C{=}C & \\ & \diagup\diagdown & \\ H & & Br \end{matrix} \xrightarrow{\text{catalyst}} \begin{matrix} Br & & Br \\ & \diagdown\diagup & \\ & C{=}C & \\ & \diagup\diagdown & \\ H & & H \end{matrix}$$

Alcohols

- Dehydration to produce an alkene.

  $$CH_3CH_2OH \xrightarrow[\text{heat}]{H_3O^+} H_2C{=}CH_2 + H_2O$$

- Primary alcohols with periodinane to produce an aldehyde.

  $$CH_3CH_2OH \xrightarrow[CH_2Cl_2]{\text{Periodinane}} \begin{matrix} & & O \\ & & \| \\ CH_3 & - & CH \end{matrix}$$

- Primary alcohols with CrO_3 to produce a carbocylic acid.

  $$CH_3CH_2OH \xrightarrow[H_3O^+,\ \text{acetone}]{CrO_3} \begin{matrix} & & O \\ & & \| \\ CH_3 & - & C \\ & & \diagdown \\ & & OH \end{matrix}$$

- Secondary alcohols with periodinane to produce a ketone.

  $$CH_3CHOHCH_3 \xrightarrow[CH_2Cl_2]{\text{Periodinane}} \begin{matrix} & & O \\ & & \| \\ CH_3 & - & C & - & CH_3 \end{matrix}$$

Ethers and Epoxides

- Acidic cleaveage of an ether with HBr or HI

  $$CH_3OCH_2CH_3 \xrightarrow[H_2O]{HX} CH_3X + CH_2CH_3OH$$

- Epoxide opening with aqueous acid.

  $$\begin{matrix} & \diagup\diagdown \\ O & \end{matrix} \xrightarrow{H_3O^+} \begin{matrix} & & & & OH \\ & & CH_2 & - & CH_2 & \diagup \\ OH & \diagup & & & & \end{matrix}$$

Skills Needed

1. Be able to draw chemical structures given a name.
2. Be able to determine the IUPAC name given the chemical structure.
3. Be able to identify common functional groups.
4. Be able to determine whether a carbon atom is primary, secondary, or tertiary.
5. Be able to draw and interpret reaction coordinate diagrams.
6. Predict the products of reactions.
7. Be able to count the number of σ- and π-bonds.
8. Be able to differentiate between *cis* and *trans* Isomers and use the E, Z dezignations.
9. Differentiate between compounds in which resonance is important.
10. Predict the effect of resonance on the stability of compounds and reactive intermediates.
11. Draw or represent resonance structures.
12. Identify conjugated π-systems and explain the effect of conjugation on molecular structure and reactivity.

Provided during Exam

IUPAC Naming

1. Name the parent hydrocarbon. Find the longest hydrocarbon chain that contains the double or triple bond. Triple bonds take precedence over double bonds.
2. Number the carbon atoms in the chain. Begin numbering the parent hydrocarbon at the end nearer the double or triple bond. (Again triple bonds recieve precedence.) The numbering should be such that the double/triple bonds recieve the lowest number possible. If there is a tie, then use the numbering that gives other substituents the lowest numbers possible.
3. Write the full name. Number the substituents using the carbon atom that the substituent is attached to. Note the first alkene/yne carbon and place it before the -ene suffix. For an example, hex-2-ene.

Memorize

1. IUPAC Naming Rules for alkanes.
   (a) Find the parent hydrocarbon.
   (b) Number the atoms in the main chain.
   (c) Identify and number the substitutents.
   (d) Write the name as a single word.
2. Names, structures of the common alkanes: methane, ethane, propane, butane, pentane, hexane.
3. Names, endings and structures of the common alkyl groups: methane, ethane, propane, butane.
4. Names, structures and endings of common functional groups: halide, alkene, alkyne, aldehyde, ketone, carboxylic acid, amine.
5. For the common reactions of alkanes, know their reactants, products, and conditions, if any.

Skills Needed

1. Be able to draw chemical structures given a name.
2. Be able to determine the IUPAC name given the chemical structure.
3. Be able to determine whether a carbon atom is primary, secondary, or tertiary.
4. Be able to draw Newman diagrams for conformers, classify the conformers as staggered or eclipsed and be able to draw a potential energy diagram showing the conformations.
5. Be able to identify steric interactions between functional groups.
6. Be able to draw Fischer Projections for stereoisomers and determine the configuration of the isomers using the rules below.
7. Be able to predict the products of reactions between alkanes: chlorination, bromination, and oxidation.
8. Be able to draw mechanisms for reactions of alkanes: chlorination and bromination.
9. Be able to draw and interpret reaction coordinate diagrams.

Provided during Exam

Assigning Abs. Config. to Wedge/Dashed 3D Structures

1. Prioritize the four groups around a chiral center according to atomic number. The highest atomic number is assigned priority #1, and the lowest atomic number is assigned priority #4.[1]
2. Orient the chiral centre such that the #4 priority substituent is pointing away from the viewer.
3. Trace the path of priorities #1, #2 and #3. (For this part you ignore #4).
4. If the path traced from 1-2-3 is clockwise, the chiral center is assigned (R) (from Latin, rectus)
5. If the path traced is counter clockwise, the chiral center is assigned (S) (from the Latin sinister)

Assigning Abs. Cong. to Fischer Proj.

1. Prioritize the four groups around a chiral center according to atomic number. The highest atomic number is assigned priority #1, and the lowest atomic number is assigned priority #4.[1]
2. Perform the two allowed manipulations of the Fischer projection to place the lowest priority group on one of the vertical positions (either top or bottom).
3. If the priorities of the other three groups (1-2-3) proceed clockwise, the stereogenic center is assigned as R. If the priorities of the other three groups (1-2-3) proceed counter clockwise, the stereogenic center is assigned as S.

Lab Exam

1. Be aware of safety rules for the organic lab and why they are important.
2. Know what to do in the case of an accident.
3. Be able to read information out of the CRC Handbook and Aldrich Catalog.
4. Know how to keep a high-quality lab notebook.
5. Know the difference between colorless, cloudy, and clear.

[1] If two adjacent atoms are tied then you go to the next atom away from the center until the tie is broken.

Memorize

Reaction Patterns

1. Addition Reactions: Two reactants add together to give a single new product. The reactions also follow Markovnikov's Rule.

   Markovnikov's Rule In the addition of HX to an alkene, the H attaches to the carbon with fewer alkyl substituents and the X attaches to the carbon with more alkyl substituents.

   $H_2C=CH_2 + H-X \xrightarrow{\text{ether}} CH_3CH_2X$

   where X=Cl, Br, or I.

   $H_2C\equiv CH_2 + H-X \xrightarrow{\text{ether}} CH_2=C(X)(H)$

   $HC\equiv CH + 2H-X \xrightarrow{\text{ether}} CH_2X-CH_2X$

   where X=Cl or Br.

2. Elimination Reaction: One reactant splits into two products. Typically one product is a small molecule such as H_2O or HCl.

   $CH_3-CH_2OH \xrightarrow[\text{heat}]{H_3O^+} H_2C=CH_2 + H_2O$

   $CH_4-CH_2X \xrightarrow{KOH} H_2C=CH_2 + KX + H_2O$

   $CH_3-CHX_2 \xrightarrow{2KOH} HC\equiv CH + 2KX + 2H_2O$

   $CH(H)(X)-CH(H)(X) \xrightarrow{2KOH} HC\equiv CH + 2KX + 2H_2O$

   where X=Cl, Br, or I.

3. Substitution Reaction: Two reactants exhange parts to give two new products. (X=Cl, Br, or I)

   $CH_4 + X_2 \xrightarrow{h\nu} CH_3X + HCl$

4. Rearrangement Reaction: One reactant undergoes a reorganiziation to yield a single isomeric product.

   $Br(H)C=C(H)Br \xrightarrow{\text{catalyst}} Br(Br)C=C(H)H$

Mechanisms

1. Addition Mechanism:

   $H_2C=CH_2 + H-X \xrightarrow{\text{ether}} CH_3-CH_2(X)$

   where X=Cl, Br, or I.

2. Elimination Mechanism:

   $CH_3CH_2OH \xrightarrow[\text{heat}]{H_3O^+} H_2C=CH_2 + H_2O$

Skills Needed

1. Write the mechanisms for the addition and elimination reactions of alkenes.
2. Predict the products of alkene reactions.
3. Compare the bonding and reactions of alkynes to alkenes.
4. Be able to count the number of σ- and π-bonds.
5. Be able to differentiate between Cis and Trans Isomers and use the *E*, *Z* dezignations.

Lab Exam

1. Synthesis Lab Notebook - Be able to list the elements of a good Synthesis Experiment lab notebook section.
2. Perform a theoretical and experimental yield calculation given the mass of reactants, products, and the chemical equation.
3. Melting Point Lab Exp. - Be able to outline the steps involved in performing a measurement of the melting point, and be able to discuss sample results of a melting point measurement.

Provided during Exam

Naming Alkenes/Alkynes

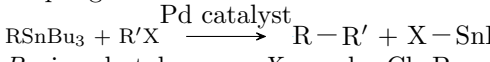
1. Name the parent hydrocarbon. Find the longest hydrocarbon chain that contains the double or triple bond. Triple bonds take precedence over double bonds.
2. Number the carbon atoms in the chain. Begin numbering the parent hydrocarbon at the end nearer the double or triple bond. (Again triple bonds recieve precedence.) The numbering should be such that the double/triple bonds recieve the lowest number possible. If there is a tie, then use the numbering that gives other substituents the lowest numbers possible.
3. Write the full name. Number the substituents using the carbon atom that the substituent is attached to. Note the first alkene/yne carbon and place it before the -ene suffix. For an example, hex-2-ene.

Memorize

Mechanisms and Reaction Patterns You should know the mechanisms and reaction patterns for all of the below.

Dienes

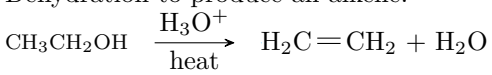
- Dienes can be made through a number of different reactions. We will focus on using Stille coupling.



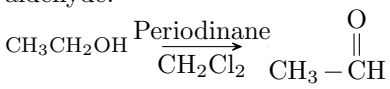
Bu is a butyl group, *X* can be Cl, Br, or I. *R* and *R'* can be aryl or vinyl groups. If two vinyl groups are used, then a conjugated diene is produced.

Alcohols

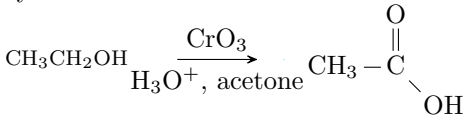
- Dehydration to produce an alkene.



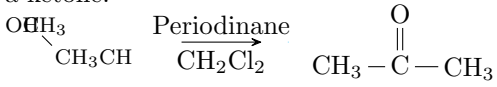
- Primary alcohols with periodinane to produce an aldehyde.



- Primary alcohols with CrO_3 to produce a carbocylic acid.

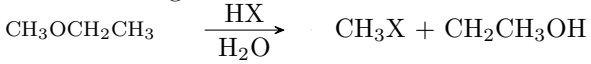


- Secondary alcohols with periodinane to produce a ketone.

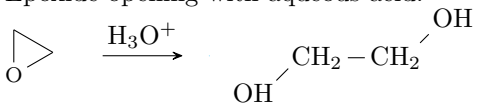


Ethers and Epoxides

- Acidic cleaveage of an ether with HBr or HI

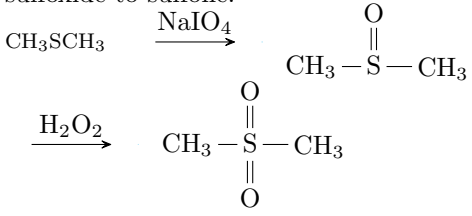


- Epoxide opening with aqueous acid.



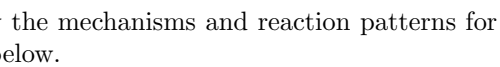
Sulfur compounds

- Oxidation of sulfur compounds from sulfide to sulfoxide to sulfone.

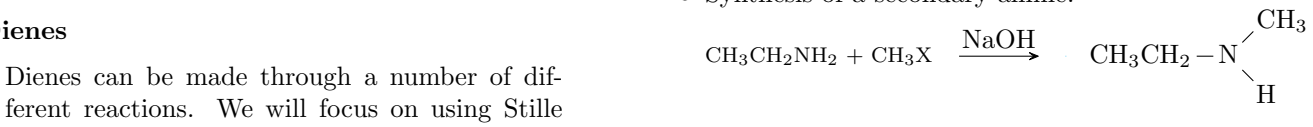


Amines

- Synthesis of a primary amine.



- Synthesis of a secondary amine.



Skills

1. Differentiate between compounds in which resonance is important.
2. Predict the effect of resonance on the stability of compounds and reactive intermediates.
3. Draw or represent resonance structures.
4. Identify conjugated π-systems and explain the effect of conjugation on molecular structure and reactivity.
5. Compare and contrast the mechanisms for substitution and elimination reactions; and predict the effect of nucleophile; leaving group; and solvent on the relative rates of SN1 versus SN2; and E1 versus E2 reactions; as well as on the relative rates of substitution versus elimination.

Lab Exam

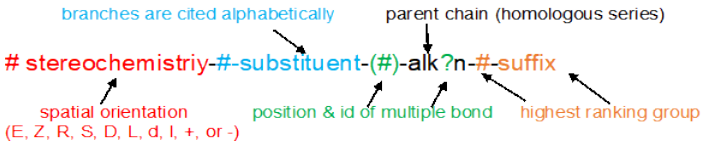
1. Be able to draw diagrams and describe the gravity filtration setup and vacuum filtration setup with Buchner flask.
2. Understand and be able to describe the recrystalization technique.

Provided during Exam

IUPAC Naming Be able to name alcohols, amines, ethers, epoxides, and sulfur compounds.

1. Recognize and prioritize the functional group(s) present.
2. Identify and number the longest continuous carbon chain to give the highest ranking group the lowest possible number.
3. Cite the substituents (branches) alphabetically using the numbering determined above.
4. Recognize an classify any stereochemistry (E/Z, R/S, cis/trans, etc).

With these four pieces of information, the IUPAC name is written using the format below. This same format applies to ALL the organic compounds.



Memorize

Mechanisms You will need to be able to write mechanisms for reactions that follow the patterns shown below.

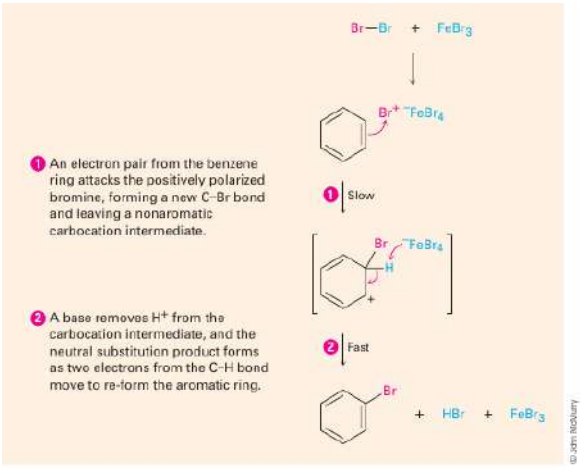


Figure 1: The mechanism of the electrophilic bromination of benzene. The reaction occurs in two steps and involves a resonance-stabilized carbocation intermediate.

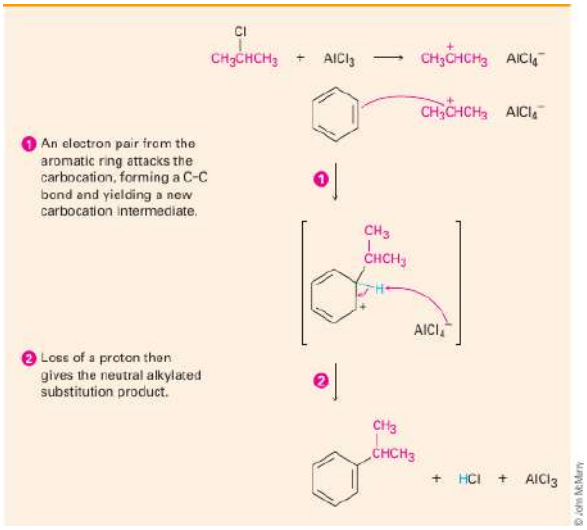
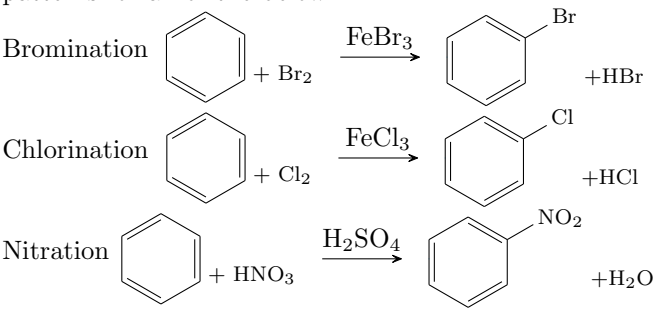
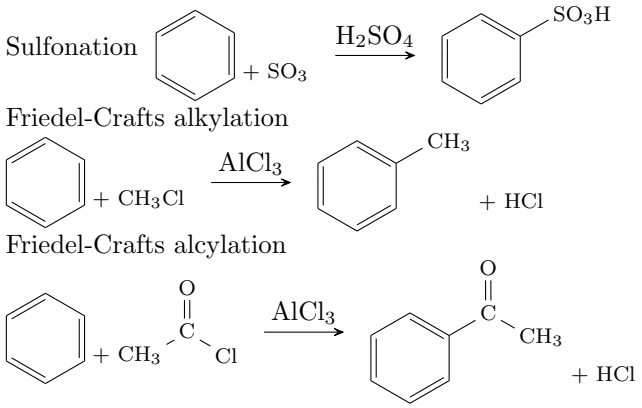


Figure 2: Mechanism of the Friedel Crafts alkylation reaction. The electrophile is a carbocation, generate by $AlCl_3$-assisted ionization of an alkyl chloride.

Reaction Patterns You should know the reaction patterns for all of the below.





Huckel's Rule The strict version of Huckel's Rule only applies to monocyclic molecules. It is often true for polycyclic molecules as well though. There are 4 parts to the rule:

1. The molecule must be planar.
2. The molecule must consist of one ring.
3. The molcule must have conjugated π-bonds to allow electrons to flow around the ring as demonstrated by drawing resonance structures.
4. The number of π-electrons for an aromatic structure is $4n + 2$ and for an anti-aromatic structure it is $4n$, where n is a whole number.

If parts 1-3 are violated, then it is non-aromatic. If parts 1-3 are followed, then part 4 determines whether the molecule is aromatic or anti-aromatic.

Substituent Effects Disubstituted benzene rings are given the following designations to describe the relationship about substituents.

ortho- (o-) 1,2- (next to each other in a benzene ring)

meta- (m) 1,3- (separated by one carbon in a benzene ring)

para- (p) 1,4- (across from each other in a benzene ring)

Different substituents can activate the ring making it more reactive. Or, deactivate it making it less reactive. Notice that all meta-directing substituents are deactivators. And, all ortho/para-directing substituents are activators except for the halogens.

Meta-directing deactivators Nitro ($-NO_2$), Sulfonate($-SO_3H$), Carbocyclic acid ($-CO_2H$)

Ortho/Para-directing deactivators Halogens ($-F$, $-Cl$, $-Br$, $-I$)

Ortho/Para-directing activators Alkyl (e.g. $-CH_3$, $-CH_2CH_3$), Alcohol ($-OH$), Amine ($-NH_2$)

Skills

1. Identify aromatic and antiaromatic compounds. (Huckel's Rule)
2. Appreciate the chemical consequences of aromaticity.
3. Write the mechanisms for electrophilic aromatic substitution reactions.
4. Predict the products of electrophilic aromatic substitution reactions.
5. Relate the effects of substituents on the reactivity and regiochemistry of electrophilic aromatic substitution reactions.

Lab Exam

1. Be able to differentiate between simple, vacuum, fractional and steam distillation.
2. Be able to describe how to setup a simple and fractional distillation.
3. Be able to draw the apparatus involved with simple and fractional distillations.
4. Be able to describe azeotropes.

Provided during Exam

IUPAC Naming for Aromatic Compounds

Monosubstituted Aromatic Rings Monosubstituted benzenes are systematically named in the same manner as other hydrocarbons, with -benzene as the parent name. Also, many monosubstituted benzene rings go by their common names. If the benzene ring is considered to be a substituent, then the name phenyl sometimes abbreviated as Ph.

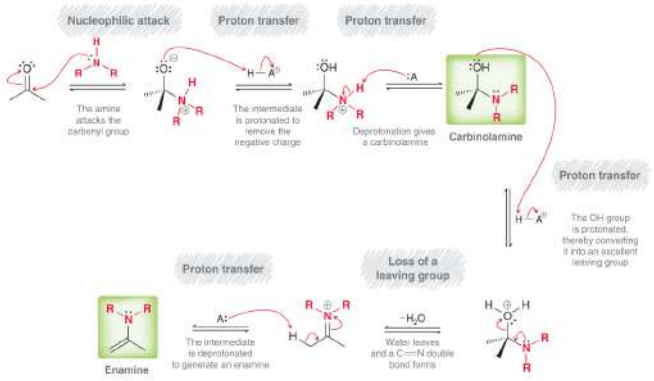
Disubstituted Aromatic Rings Use ortho, meta, or para to describe the relative positions of substituents around the ring.

Trisubstituted Aromatic Rings benzenes with more than two substituents are named by choosing a point of attachment as carbon 1 and numbering the substituents on the ring so that the second substituent has as low a number as possible. The substituents are listed alphabetically when writing the name.

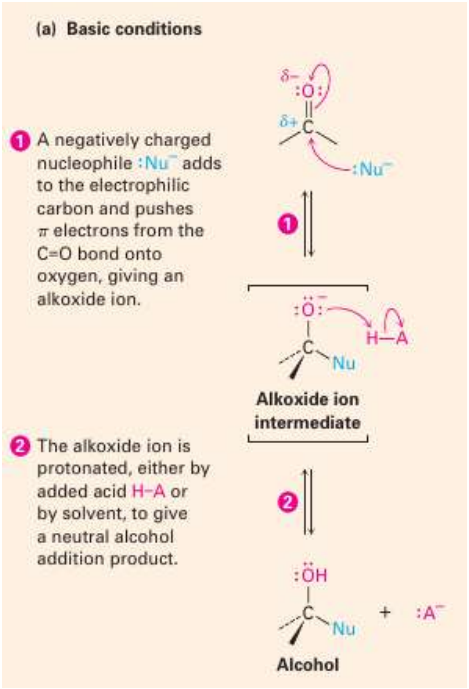
Memorize

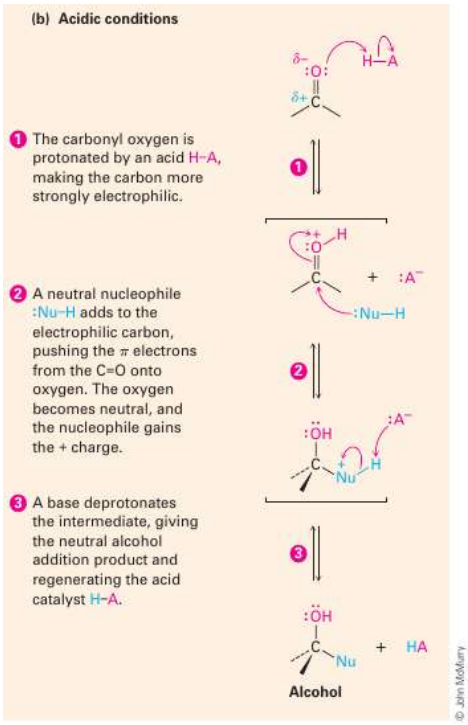
Mechanisms

Addition-elimination reaction of aldehydes/ketones The mechanism for enamine formation occurs under acidic conditions with aldehyde or ketone reacts with a secondary amine. (Klein)

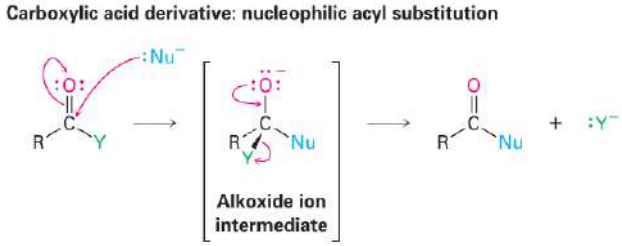


Nucleophilic addition reaction of aldehydes/ketones "General mechanism of a nucleophilic addition reaction of aldehydes and ketones under both basic and acidic conditions. (a) Under basic conditions, a negatively charged nucleophile adds to the carbonyl group to give an alkoxide ion intermediate, which is subsequently protonated. (b) Under acidic conditions, protonation of the carbonyl group occurs first, followed by addition of a neutral nucleophile and subsequent deprotonation." (McMurry)

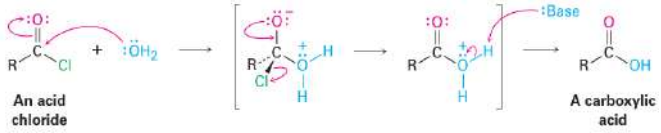




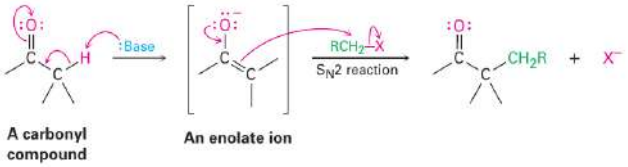
Nucleophilic substitution of a carboxylic acid derivative "The general mechanisms of nucleophilic addition and nucleophilic acyl substitution reactions. Both reactions begin with the addition of a nucleophile to a polar C=O bond to give a tetrahedral, alkoxide ion intermediate. The intermediate formed from an aldehyde or ketone is protonated to give an alcohol, but the intermediate formed from a carboxylic acid derivative expels a leaving group to give a new carbonyl compound." (McMurry)



Acid chlorides react with water to yield carboxylic acid–the substitution of −Cl by −OH. This hydrolysis reaction is a typical nucleophilic acyl substitution process and is initiated by attack of the nucleophile water on the acid chloride carbonyl group. The initially formed tetrahedral intermediate undergoes loss of HCl to yield the product. (McMurry)

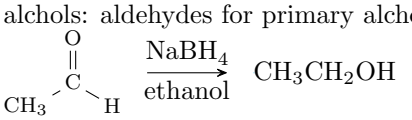


A reaction utilizing the enolate anion "Perhaps the most useful reaction of enolate ions is their alkylation by treatment with an alkyl halide, thereby forming a new C−C bond and joining two smaller pieces into one larger molecule. Alkylation occurs when the nucleophilic enolate ion reacts with an electrophilic alkyl halide in an S_N2 reaction, displacing the halide ion in the usual way." (McMurry)

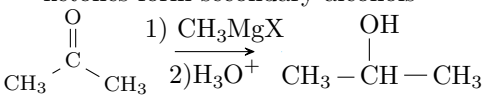


Reaction Patterns

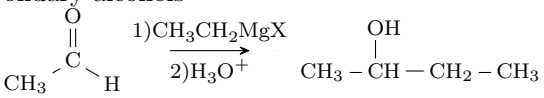
Nucleophilic addition reactions Reduction to alchols: aldehydes for primary alchols



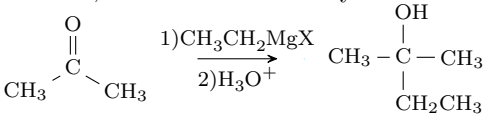
ketones form secondary alcohols



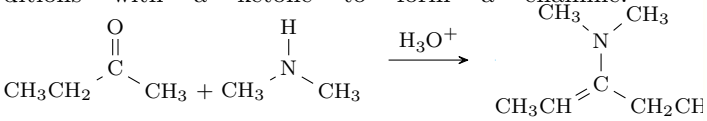
Grignard Reagents are similar to the above except they can also link in other alkyl groups. The X can be chloride, bromide, or iodide. Aldehydes form secondary alcohols



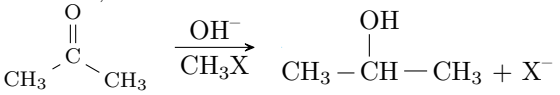
And, ketones form tertiary alcohols.



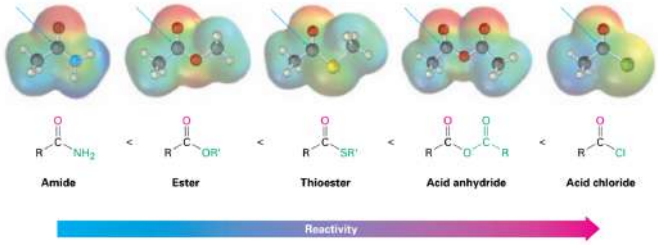
Addition-elimination reactions A secondary amine can react under acidic conditions with a ketone to form a enamine.



Enolate anions Note that X can be chloride, bromide, or iodide.



Carboxylic acid derivative "As a general rule, the more electron-poor the C=O carbon, the more readily the compound reacts with nucleophiles. Thus, acid chlorides are the most reactive compounds because the electronegative chlorine atom strongly withdraws electrons from the carbonyl carbon, whereas amides are the least reactive compounds. ... A consequence of these reactivity differences is that it's usually possible to convert a more reactive acid derivative into a less reactive one. Acid chlorides, for example, can be converted into esters and amides, but amides and esters can't be converted into acid chlorides."



Acidity of alpha protons This table "lists the approximate pKa values of some different types of carbonyl compounds and shows how these values compare with other common acids. Note that nitriles, too, are acidic and can be converted into enolate-like anions." A lower pKa value indicates a more acidic proton.

Table 11.1 Acidity Constants for Some Carbonyl Compounds

Functional group	Example	pK_a
Carboxylic acid	CH_3COH	5
1,3-Diketone	$CH_3CCH_2CCH_3$	9
3-Keto ester	$CH_3CCH_2COCH_3$	11
1,3-Diester	$CH_3OCCH_2COCH_3$	13
[Alcohol	CH_3OH	16]
Acid chloride	CH_3CCl	16
Aldehyde	CH_3CH	17
Ketone	CH_3CCH_3	19
Thioester	CH_3CSCH_3	21
Ester	CH_3COCH_3	25
Nitrile	$CH_3C{\equiv}N$	25
N,N-Dialkylamide	$CH_3CN(CH_3)_2$	30

Skills

1. Identify the structures and chemical properties of carboxylic acid derivatives
2. Describe and analyze the consequences of the

acidity of protons alpha to carbonyl groups

3. Write mechanisms for the reactions of enolate anions and predict the products of such reactions.

4. Write the mechanisms for nucleophilic substitution and hydrolysis reactions of carboxylic acid derivatives.

5. Write mechanisms for nucleophilic addition reactions and for addition-elimination reactions of aldehydes and ketones; and predict the products of such reactions.

Lab Exam

1. Be able to draw diagrams and describe the reflux setup.

2. Be able to list the steps involved in performing a reflux reaction.

Provided during Exam

IUPAC Naming for Ketones, Aldehydes, and Carboxylic acids Be able to name aldehydes (-al), ketones (-one), and carboxylic acids (-ic acid). These ending take precendence over the others that we've learned.

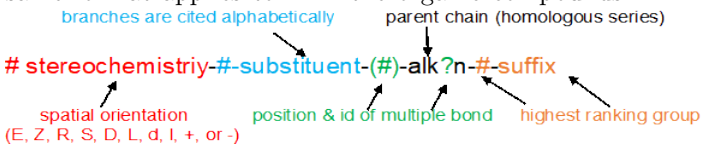
1. Recognize and prioritize the functional group(s) present.

2. Identify and number the longest continuous carbon chain to give the highest ranking group the lowest possible number.

3. Cite the substituents (branches) alphabetically using the numbering determined above.

4. Recognize an classify any stereochemistry (E/Z, R/S, cis/trans, etc).

With these four pieces of information, the IUPAC name is written using the format below. This same format applies to ALL the organic compounds.

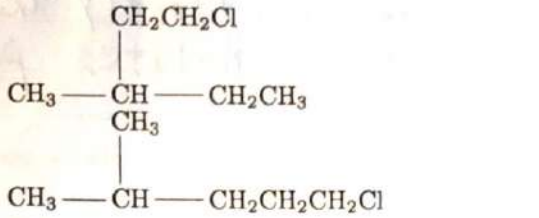


Show all work leading up to **all** responses. You may attach additional pages if needed.

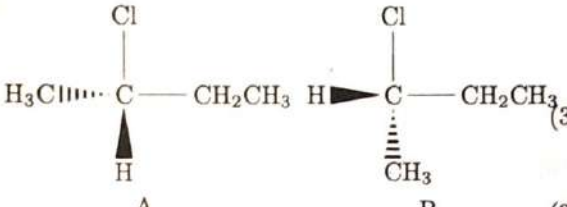
1. Identify and explain the isomeric relationship between the following pairs of compounds.

(3) (a) 2,2-Dibromopentane and 2,3-Dibromopentane

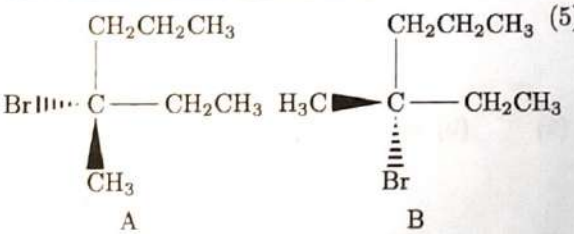
Constitutional isomers

(3) (b) 

Constitutional isomers

(3) (c) 

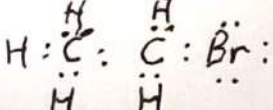
Identical

(3) (d) 

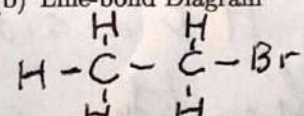
Identical

2. Represent bromomethane using the following kinds of diagrams:

(3) (a) Lewis-Dot Diagram



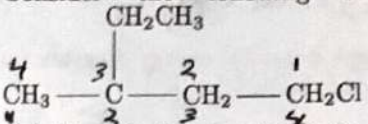
(3) (b) Line-bond Diagram



(3) (c) Condensed structural formula

CH_3-CH_2Br

3. Consider the following structural formula:



(3) (a) Identify the parent alkane.

butane

(3) (b) Identify all functional groups in the compound.

3-ethyl

~~bromo~~ 1-chloro

(5) (c) Write the IUPAC name of the compound.

1-chloro-3-ethylbutane

4. Consider 2-bromo-4-ethylhexane:

(3) (a) Identify the parent alkane.

hexane

(3) (b) Identify all functional groups in the compound.

2-bromo

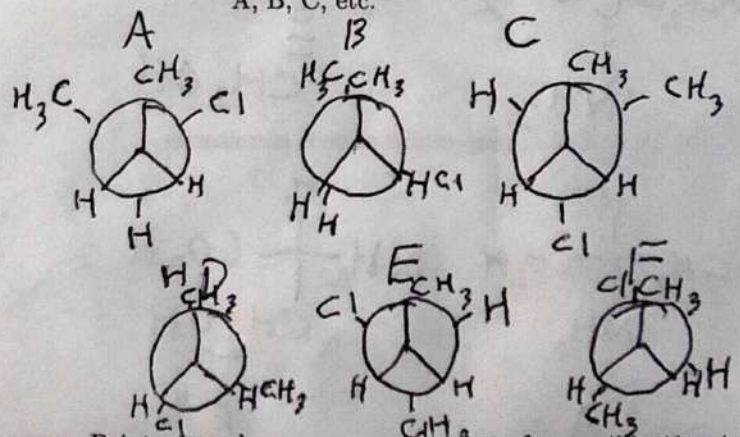
4-ethyl

(5) (c) Draw the chemical structure of the compound.

2-bromo-4-ethylhexane

5. Consider the bond between the 2nd and 3rd carbon of 2-chlorobutane. $CH_3-CH_2-CHCl-CH_3$

(5) (a) Draw the Newman projections for all possible conformations. Label them with letters such as A, B, C, etc.

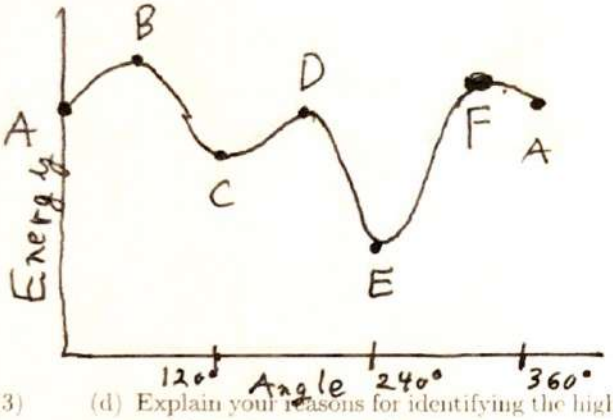


Points earned: _____ out of a possible 48 points

(3) (b) Which conformers are eclipsed? Which are staggered?

Eclipsed: B, D, F
staggered: A, C, E

(4) (c) Draw a rough potential energy diagram for rotating around the bond.



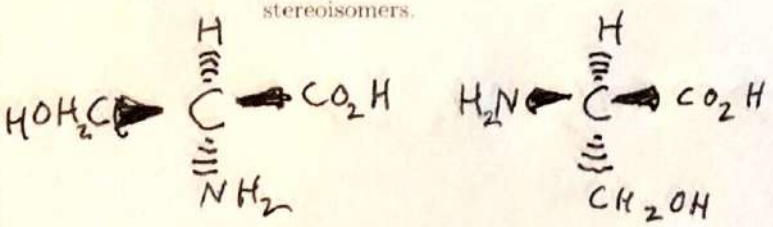
(3) (d) Explain your reasons for identifying the highest and lowest energy conformers.

E is the lowest b/c the largest side groups are far away from one another, B is the highest b/c the largest groups are eclipsing each other.

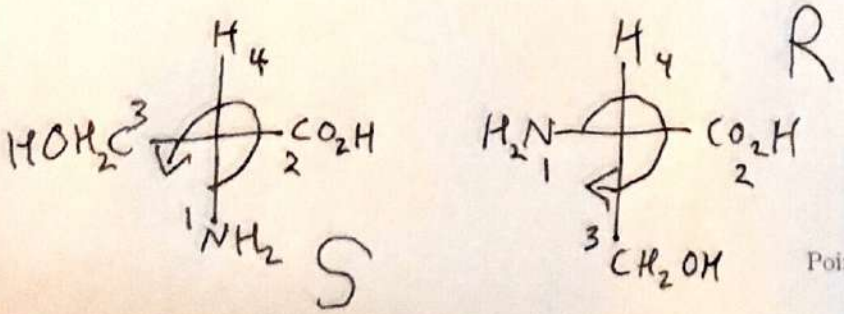
6. HO—CH_2—CH(NH_2)—CO_2H

Serine

(2) (a) Draw a 3D line-bond diagrams of both stereoisomers.



(2) (b) Draw Fisher projections of each steroisomer.



(3) (c) Use the Cahn-Ingold-Prelog Rules to determine the configuration of each steroisomer (R or S).

#1: NH_2
#2: CO_2H
#3: CH_2O
#4: H

(1) (d) Compare and constrast the stereoisomers physical properties.

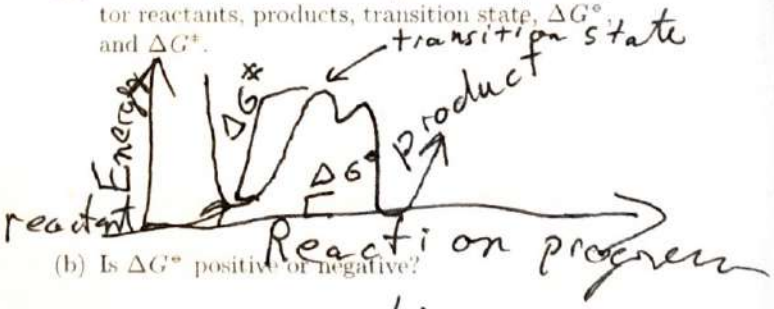
Mostly the same but the pure solution and crystal rotate polarized light.

(1) (e) Compare and constrast the stereoisomers chemical activity.

Mostly the same, except when reacting with other pure stereoisomers

7. Draw a reaction energy diagram for a two-step reaction with $K_{eq} > 1$, whose second step is faster than the first step of the reaction.

(5) (a) Label the parts of the diagram corresponding tor reactants, products, transition state, $\Delta G°$, and $\Delta G^{\ddagger}$.



(2) (b) Is $\Delta G°$ positive or negative?

negative

(2) (c) Why is the second step as you have drawn it faster than the first step?

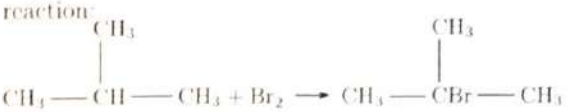
The second step has a lower activation energy.

Points earned: _____ out of a possible 28 points

(8) 8. Predict the products of the following reaction and balance the resulting equation:

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

(6) 10. Explain the lack of side reactions for the following reaction:

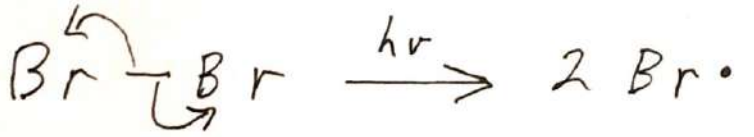


Br_2 is less reactive than Cl_2 or F_2. A tertiary carbocation is more stable than a primary carbocation.

(10) 9. Predict the products and draw the mechanism for the following reaction:

$CH_3CH_3 + Br_2 \rightarrow CH_3CH_2Br + HBr$

Step 1: Initiation



Step 2: Propagation

Step 3: Termination

Points earned: _____ out of a possible 24 points