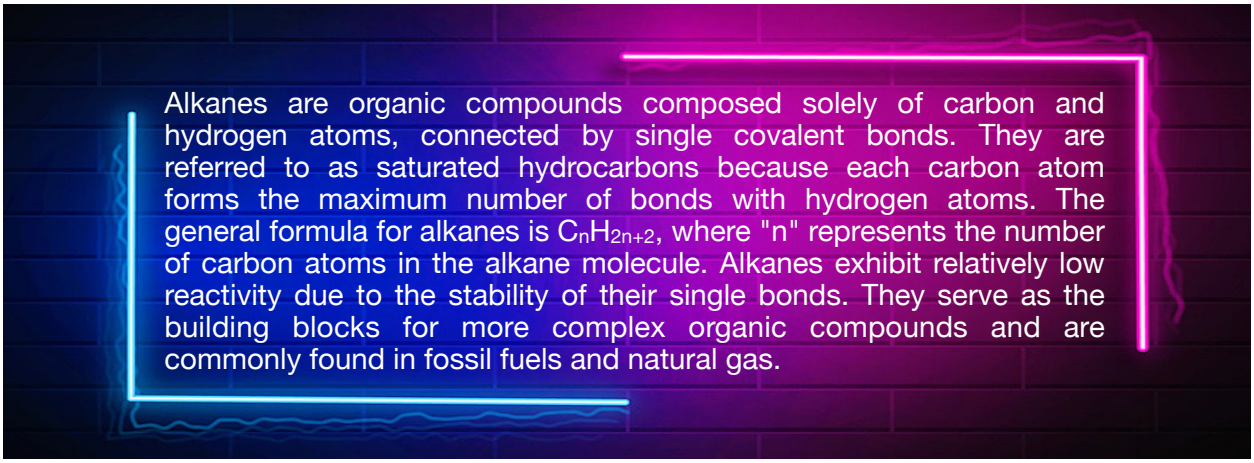
MEGA MOLECULES

Name _____

Lesson 3: Alkanes, cycloalkanes, and functional groups

Lesson three explores the fundamental concepts of alkanes, cycloalkanes, and functional groups. Students practice naming and building models of alkanes, straight-chain saturated hydrocarbons, and cycloalkanes which are closed-ring structures. The process of forming alkyl groups by replacing one hydrogen atom at the end of the chain and naming the resulting substituents is investigated. Students delve into common branched substituents, such as isopropyl, sec-butyl, tert-butyl, and isobutyl, understanding both their common and systematic names. Lastly, lesson three investigates combustion reactions, isomers, conformational analysis of alkanes and cycloalkanes using Newman projections, and different functional groups such as alcohols, carboxylic acids, aldehydes, ketones, ethers, and amines. By the end of this lesson, a solid foundation in understanding the nomenclature and structures of various organic compounds is established.

THINK! What are the characteristics of alkanes?



Go to https://www.khanacademy.org/science/organic-chemistry
Watch the videos on Naming alkanes

1. The names of the straight chain saturated hydrocarbons for up to a 12 carbon chains are shown in the table below. Build models of methane (CH_4), ethane (C_2H_6), and propane (C_3H_8).

Carbon atoms	Name	Carbon atoms	Name	Carbon atoms	Name
1	methane	5	pentane	9	nonane
2	ethane	6	hexane	10	decane
3	propane	7	heptane	11	undecane
4	butane	8	octane	12	dodecane

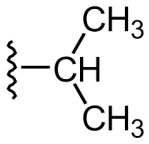
THINK! What are alkyl groups and how are they named?

Alkyl groups are formed by removing one hydrogen atom from an alkane molecule. To name an alkyl group, the suffix "-ane" of the corresponding alkane is replaced with "-yl." The name of the alkyl group is based on the number of carbon atoms it contains. For example, removing one hydrogen atom from methane (CH_4) forms the alkyl group called methyl (CH_3). The naming of larger alkyl groups follows the same pattern. It's important to note that alkyl groups can be attached to other compounds, forming substituents or side chains, which are named separately from the main compound.

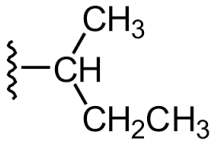
2. Change the molecules built in question #1 to alkyl groups. Name the three alkyl groups.

Disassemble the structures!

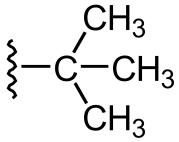
3. There are a few common branched substituents which you should memorize. These are shown below. Build a model of isopropyl, the branched substituent with three carbon atoms. Modify the isopropyl group to form a sec-butyl group. Now build tert-butyl and isobutyl groups. Study and memorize both the common name and systematic name for each branched substituent.



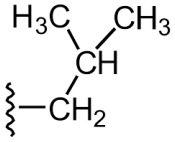
Common name: isopropyl
Systematic name: (1-methyl ethyl)



Common name: sec-butyl
Systematic name: (1-methyl propyl)



Common name: tert-butyl
Systematic name: (1,1-dimethyl ethyl)

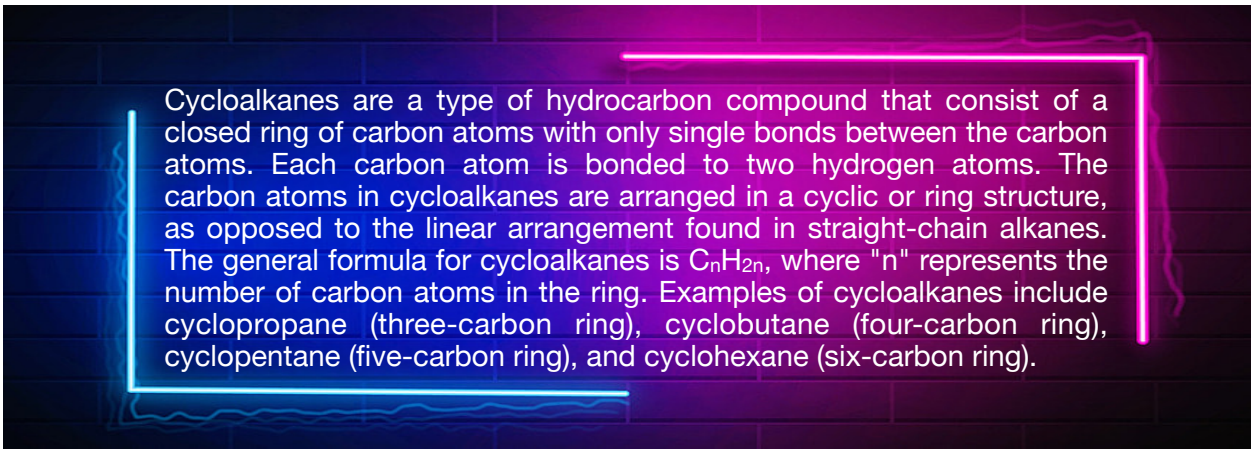


Common name: isobutyl
Systematic name: (2-methyl propyl)

Disassemble the structures!

4. After watching the video, Naming alkanes with alkyl groups, build a model of 4-ethyl-2-methylhexane. Draw the structural formula.

THINK! What are cycloalkanes?



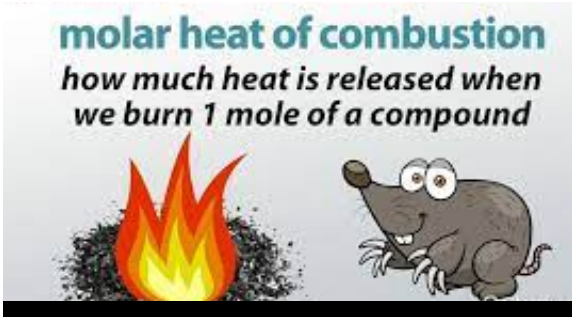
5. Cycloalkanes are alkanes formed into a closed ring. Modify the structure in question #4 to form isobutylcyclopentane. Draw the structural formula.

By the time you get to five carbons in a ring, you might have some pent up frustration! Keep practicing with the Kahn Academy videos and Mega Molecules models.

Disassemble the molecules!

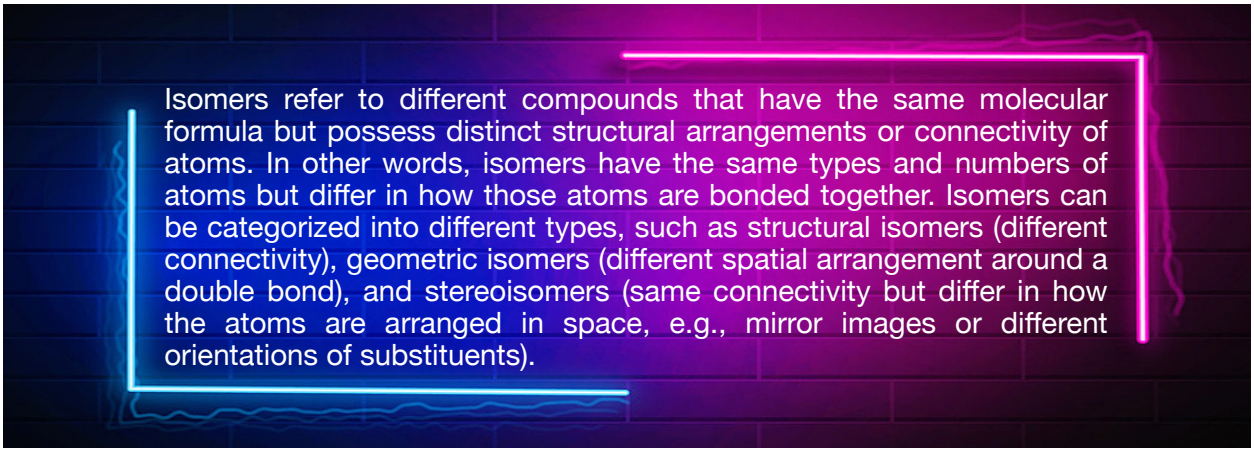
6.

Alkane	Combustion Reaction	Molar heat of combustion (kJ/mole)
Hexane	$2C_6H_{18} + 21O_2 \rightarrow 12CO_2 + 18H_2O$	-4163
Heptane	$C_7H_{16} + 11O_2 \rightarrow 7CO_2 + 8H_2O$	-4817
Octane	$2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O$	-5471



State the trend in the molar heats of combustion for hexane, heptane, and octane. Offer an explanation for the trend in the heats of combustion.

THINK! What are isomers?



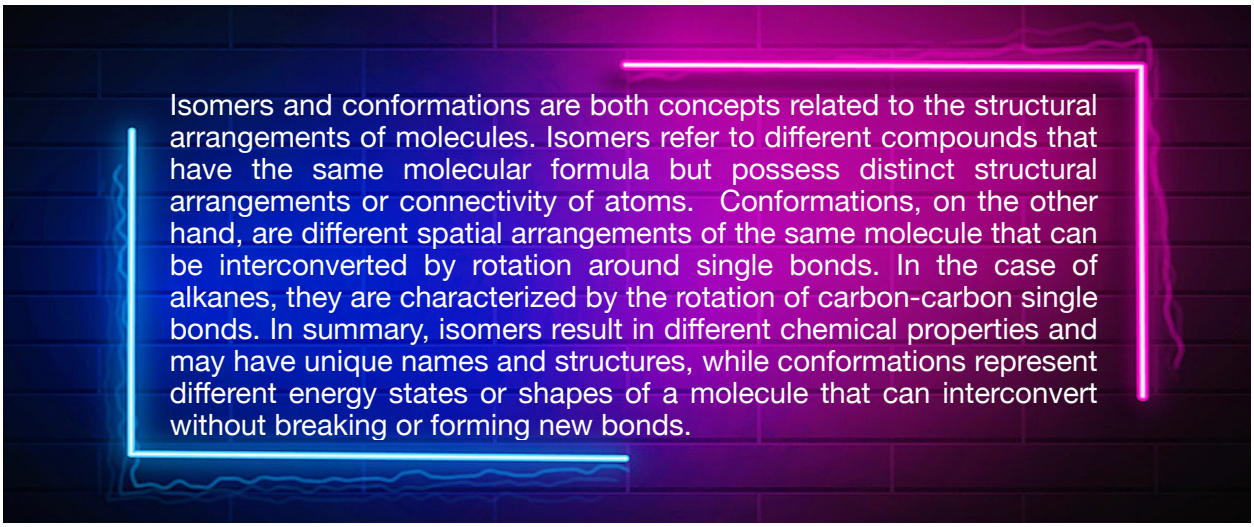
7. Octane, 2-methylheptane, 2,2-dimethylhexane, and 2,2,3,3-tetramethylbutane are isomers. They all have the molecular formula, C_8H_{18}, and the same combustion reaction.

Isomer	Molar Heat of Combustion (kJ/mole)
Octane	-5471
2-methylheptane	-5466
2,2-dimethylhexane	-5458
2,2,3,3-tetramethylbutane	-5452

Build a model of straight-chain octane. Move the atoms to build each of the isomers. State the relationship between branching within the compound and molar heat of combustion. Based on the molar heat of combustion, which isomer of octane is most stable?

Disassemble the molecule.

THINK! Explain the difference between isomers and conformations for alkanes?

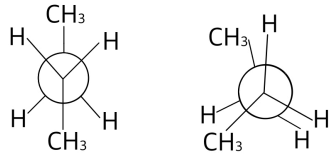


Go to https://www.khanacademy.org/science/organic-chemistry
Watch the videos on Conformations of alkanes and cycloalkanes.

8. A halogen is treated as a substituent on an alkane chain and is listed in alphabetical order in the name. Build a model of 1,2-dichloroethane. Draw the structural formula for the molecule.

In organic chemistry, a Newman projection is a way to visualize the conformation of a molecule around a specific bond. It provides a simplified 2D representation of the molecule by looking directly down the axis of a chosen carbon-carbon (C-C) bond. The Newman projection consists of two intersecting lines. The front line represents the carbon atom from which we are looking, and the back line represents the carbon atom to which it is bonded. By rotating the back carbon atom in the Newman projection, different conformations of the molecule can be observed. The most common conformations studied are the staggered and eclipsed conformations.

Staggered and Eclipsed Conformations of Butane

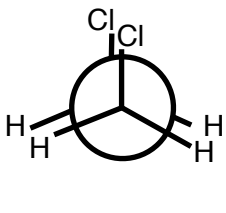


Staggered Eclipsed

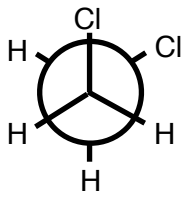
In a staggered conformation, the atoms or groups on the two carbon atoms are as far apart as possible, resulting in lower steric hindrance or strain. This conformation is more stable than the eclipsed conformation. In an eclipsed conformation, the atoms or groups on the two carbon atoms are in line with each other, causing increased steric hindrance and higher energy. Newman projections are used to analyze and understand the spatial arrangement of atoms in a molecule. They provide a clear perspective of the molecule's torsional strain and help predict stability and reactivity based on molecular geometry.

9. Turn the molecule, 1,2-dichloroethane, so that you can sight down the carbon-carbon bond. Rotate the back carbon until it matches the Newman projection shown in the first box below. Continue rotating the back carbon 60°. Label each Newman projection as an eclipsed or staggered conformation.

1. _____
2. _____
3. _____
4. _____
5. _____
6. _____



1



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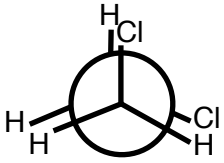

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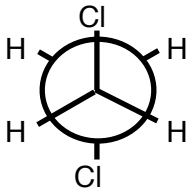

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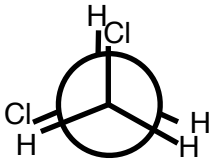

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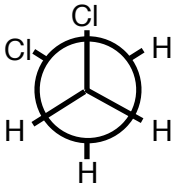

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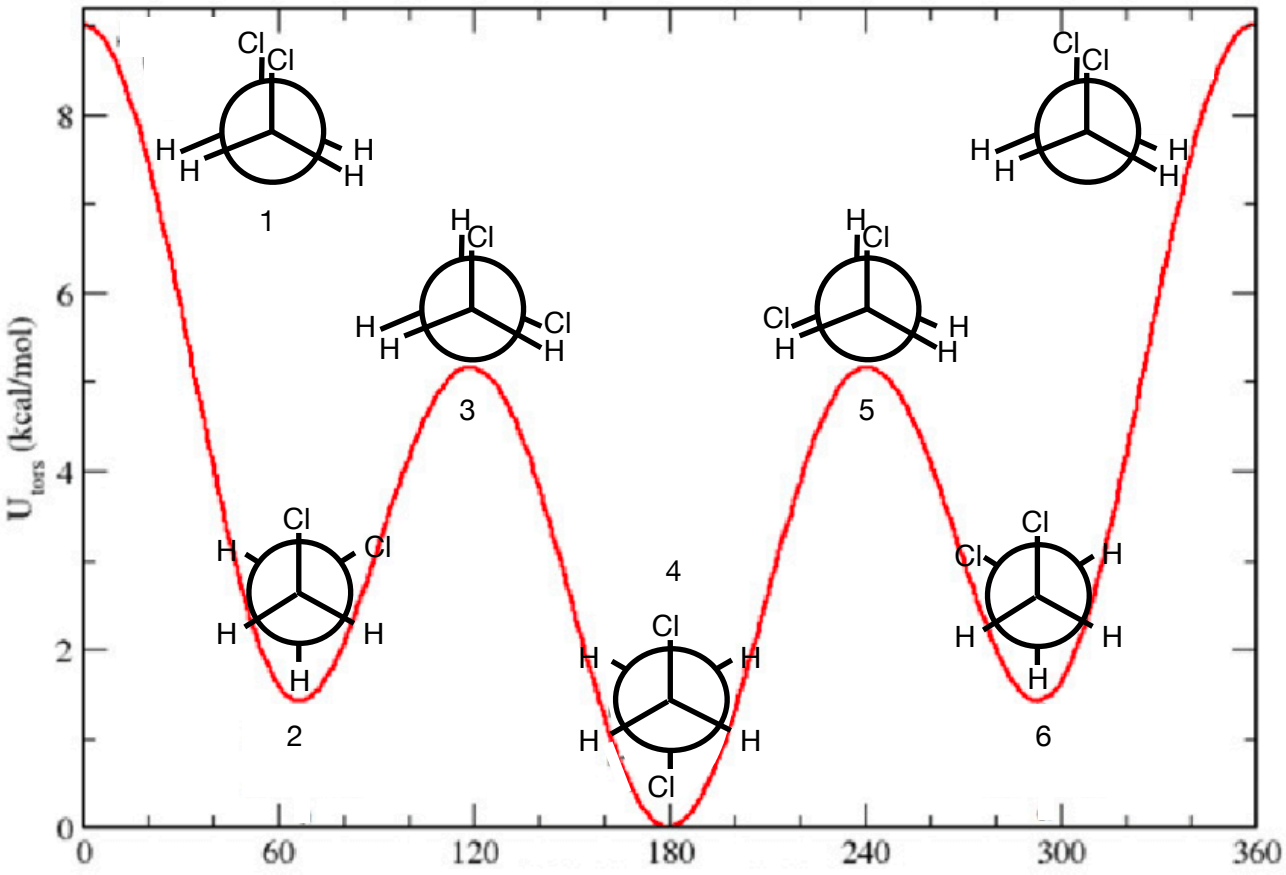
10. Torsional strain refers to the strain or deformation experienced by a molecule due to the rotation of groups around a single bond. Torsional potential energy, on the other hand, is a measure of the potential energy associated with the rotation of groups around a single bond. Typically, the potential energy exhibits a periodic variation, with minima corresponding to energetically favorable conformations and maxima corresponding to high-energy, strained conformations. The torsional potential energy is affected by various factors, including the nature of the groups involved, the bond strength, and the steric interactions between atoms. Torsional strain can contribute to the overall torsional potential energy of a molecule. Below is a graph of potential energies of the conformations vs. dihedral angle.

    Select the Newman projection of 1,2-dichloroethane with the highest potential energy. _____

    The staggered conformation, in which the dihedral angle between the halides is 180°, is called the anti conformation. Select the Newman projection of the anti conformation of 1,2-dichloroethane. _____
    Describe the energy of the anti conformation.

Torsional potential energy (kcal/mole) vs Cl-C-C-Cl dihedral angle (degrees)

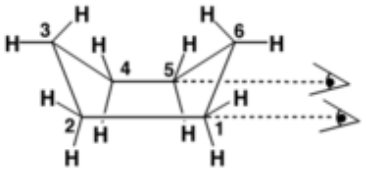


Cl-C-C-Cl dihedral angle (degrees)

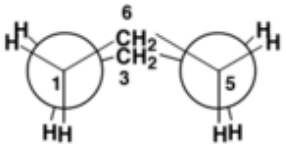
The most common example of conformational analysis of cycloalkanes is the conformational analysis of cyclohexane, which can adopt chair, boat, or twist-boat conformations due to the rotation around its carbon-carbon bonds.

11. Build the boat conformation for cyclohexane. Use black bonds between the carbon atoms. Is the boat conformation an eclipsed or staggered arrangement?

perspective line diagram



Newman projection

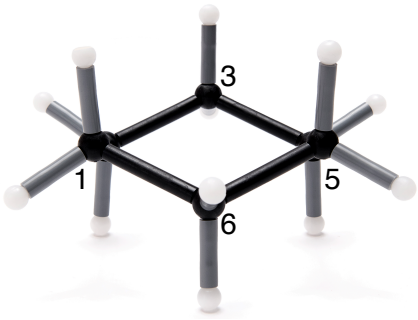


carbon atoms 2 and 4 are obscured

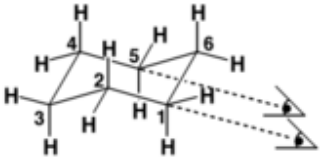
12. Flip the boat conformation to form the chair conformation for cyclohexane.

    Is the chair conformation an eclipsed or staggered arrangement?

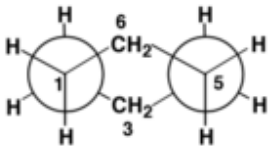
    Predict which conformation is more stable.



perspective line diagram

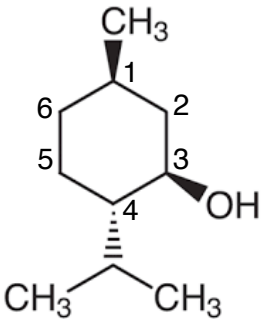


Newman projection



carbon atoms 2 and 4 are obscured

13. Menthol is an organic compound found naturally in peppermint. Build a model of menthol by substituting methyl, hydroxyl, and isopropyl groups on cyclohexane. The structure of menthol is numbered the same as it is in the Kahn Academy video. The chair conformation is more stable than the boat conformation. There are two possible chair conformations as shown below. Axial (A) and equatorial (E) are types of bonds found in the chair conformation of cyclohexane. Axial bonds point up or down. The equatorial bonds lie about the "equator" of the cyclohexane ring, or in the "plane" of the ring. Flip the molecule to form both chair conformations. Determine which of the chair conformations would give menthol the most stable configuration. Defend your selection.



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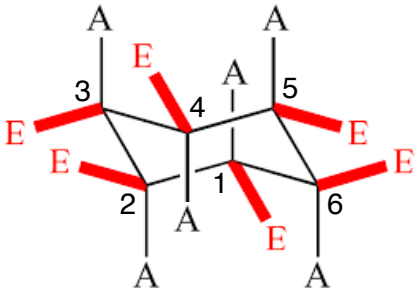
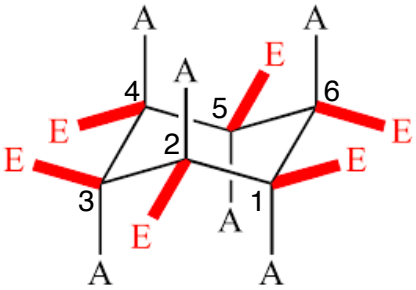


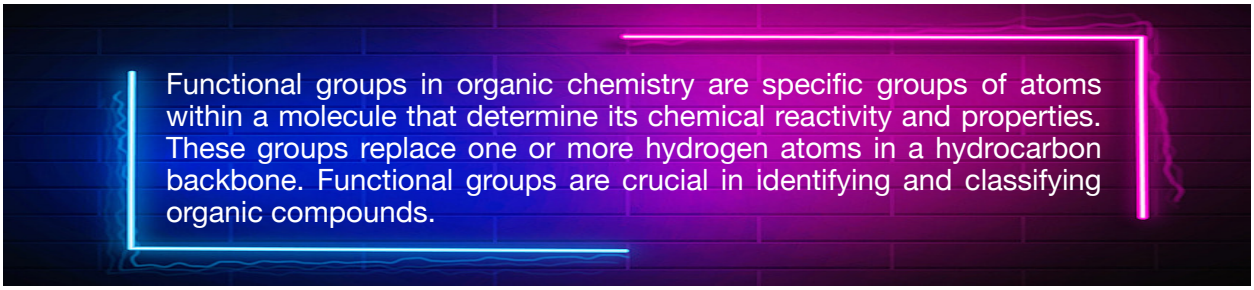
chair conformation 1



chair conformation 2

Disassemble the molecule.

THINK! What are functional groups in organic chemistry?

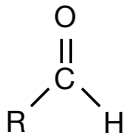


Go to https://www.khanacademy.org/science/organic-chemistry
Watch the videos on Functional groups.

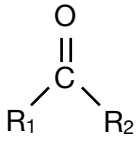
Functional Groups

Hydroxyl (-OH): Found in alcohols, phenols, and carboxylic acids, the hydroxyl group imparts polarity, hydrogen bonding capability, and increased acidity to the molecule.

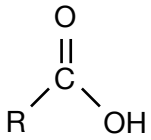
Carbonyl (C=O): Present in aldehydes, ketones, carboxylic acids, esters, and amides. The carbonyl group is highly reactive and responsible for various chemical reactions, such as nucleophilic addition or condensation reactions.



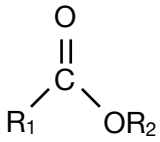
Aldehyde: The carbonyl group is located at the terminal end of the chain. R - represents the hydrocarbon chain.



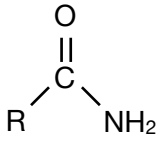
Ketone: The carbonyl group is located within the carbon chain of the ketone. Both ketones and aldehydes exhibit similar reactivity due to the electrophilic nature of the carbon atom in the carbonyl group.



Carboxyl: The carboxyl group combines the characteristics of a carbonyl group and a hydroxyl group. It is responsible for the acidity of carboxylic acids.



Ester: The ester group results from the condensation of a carboxylic acid and an alcohol. It plays a role in esterification and hydrolysis reactions.



Amide: The amide group consists of a carbonyl group attached to a nitrogen atom. It is found in proteins and plays a crucial role in peptide bond formation.

Amino ($-NH_2$): Present in amines and amino acids, the amino group is basic and can accept protons to form a positive charge.

Ether (-O-): The ether group is formed by the linkage of two alkyl or aryl groups to an oxygen atom. Ethers are characterized by their low reactivity and use as solvents.

Halogen (-X, where X=F, Cl, Br, I): The halogen group includes elements such as fluorine, chlorine, bromine, and iodine. Halogens, when attached to an organic molecule, can impact reactivity and polarity.

Functional groups greatly influence the chemical behavior, physical properties, and functional characteristics of organic compounds. They allow for a diverse range of compounds with unique reactivity and functionality.

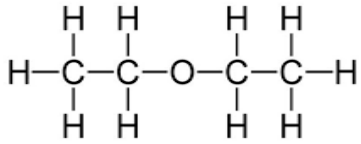
14. Build models of butanol and butanoic acid. Describe the similarities and differences between an alcohol and a carboxylic acid functional group.

15. Change the functional group on butanol to form butanal. Describe the similarities and differences between an aldehyde and a carboxylic acid functional group.

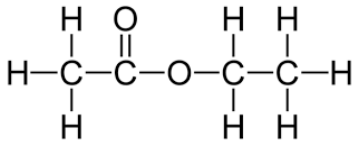
16. Build a model of butanone. The functional group of a ketone is between R-groups. Name another functional group that is within the molecule (between R-groups).

Disassemble the molecules.

17. Build a model of diethyl ether and a model of ethyl acetate (also known as ethyl ethanoate). Identify and label the functional group in each of the molecules. Research the uses of diethyl ether and ethyl acetate. Although the molecules look similar, the functional groups give the molecules unique properties.



diethyl ether



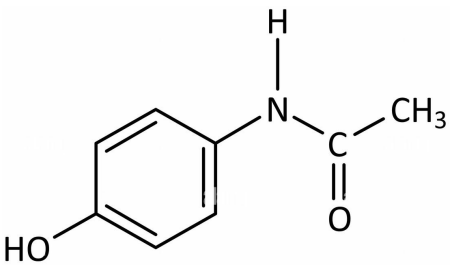
ethyl acetate

Disassemble the molecules

18. Research and draw the structural formulas for diethyl amine and butanamide. Build a models of diethyl amine and butanamide. Identify and label the functional group in each of the drawings. Describe the similarities and differences between these two molecules.

Circle and label the functional groups in each of the molecules below.

19. Tylenol (acetaminophen)



20. Artificial sweetener (aspartame)