Stereochemistry
and
Molecular Models
Lab

1013-435

Part II: Exploration

During the exploration portion of the lab you will work with handheld models. You will need to make notes and answer the questions in this section in your laboratory notebook. A glossary of terms has been provided for you, simply click any word in blue to go there and click the word again to return.

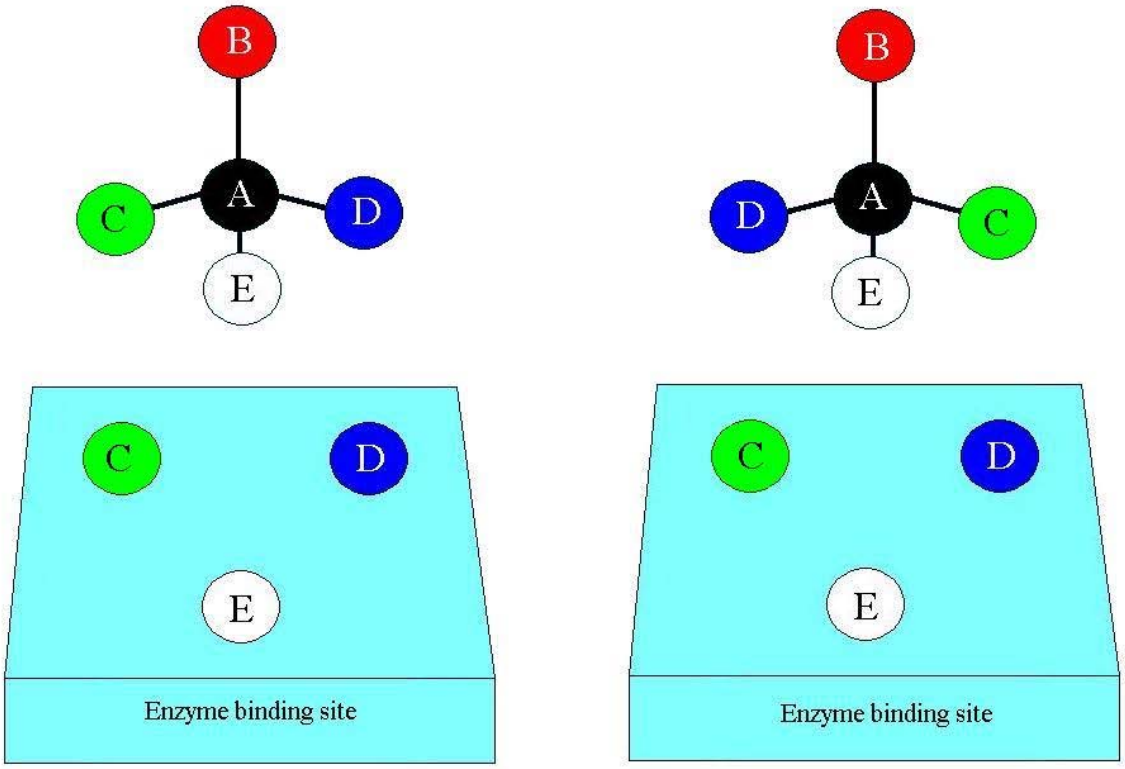
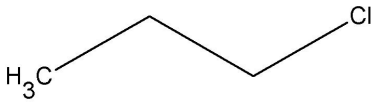


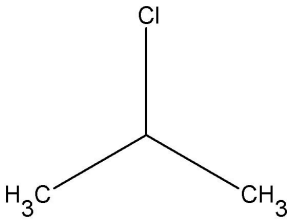
Figure 1. The two molecules are enantiomers, that is, non-super-imposable mirror images. The molecule on the left fits tightly into the binding site while its enantiomer on the right doesn't fit so it cannot bind.

A. Constitutional Isomers

1. One of the first types of isomers you learned about were constitutional isomers. The molecules 1-chloropropane and 2-chloropropane are constitutional isomers.



1-chloropropane



2-chloropropane

Prepare handheld models of 1-chloropropane and 2-chloropropane (Ask your lab instructor for assistance if needed). Notice that the connectivity for the two isomers is different, but the number of atoms needed to make either isomer is the same (isomers have identical molecular formulas).

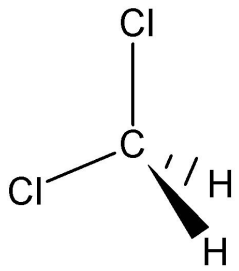
2. Prepare a handheld model of ethanol. Draw ethanol in your lab notebook. Compare your handheld model of ethanol to the answer by clicking the button on the right.

Answer

3. Using your handheld model kit construct a constitutional isomer of ethanol. Draw this isomer in your lab notebook. Compare your drawing to the correct answer by clicking the answer button on the right.

Answer

4. Below is a perspective drawing of dichloromethane.



Make a handheld model of the above molecule. Draw an accurate representation of this molecule in your lab notebook using a perspective drawing with wedges and dashed lines. Using the handheld model, find the two planes of symmetry. In your lab notebook draw the two planes of symmetry of dichloromethane by redrawing and rotating the molecule as appropriate. Did you draw the correct planes of symmetry?

Answer

B. Geometric Isomers

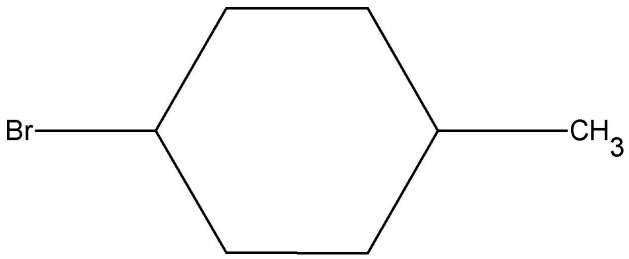
1. Assemble two models of 1,2-dichloroethene. One model should have the Cl atoms on the same side and the second model should have the Cl atoms on opposite sides. To represent a double bond use two of the longer flexible bonds (seek assistance from the lab instructor if needed). Draw the two molecules in your lab notebook as skeletal structures. Designate the geometric isomer that has a dipole?

Answer

2. Assemble two models of 1,2-dibromocyclopropane. The carbon-carbon bonds in the cyclopropane ring are often called "banana bonds". In constructing your carbon-carbon bonds in the cyclopropane ring use the larger and more flexible bonds you used for the double bonds above (see instructor for assistance if needed). One of the models should have the bromine substituents on the same side of the ring and the second should have the bromine substituents on opposite sides. Draw the two isomers in your notebook and label them as *cis* or *trans*-1,2-dibromocyclopropane as appropriate. The button on the right can be used to check your answer. Did you assign *cis* and *trans* correctly?

Answer

3. Below is a skeletal drawing of a molecule



Make a handheld model of *trans*-1-bromo-4-methylcylohexane (above molecule). Draw an accurate representation of the molecule in your lab notebook using a perspective drawing and a chair drawing (chair conformation).
Using the handheld model, determine if the molecule has a plane of symmetry. If the molecule has a plane of symmetry draw it in your lab notebook. Use the button on the right to check your drawings. Did you identify the correct plane of symmetry if there is one?

Answer

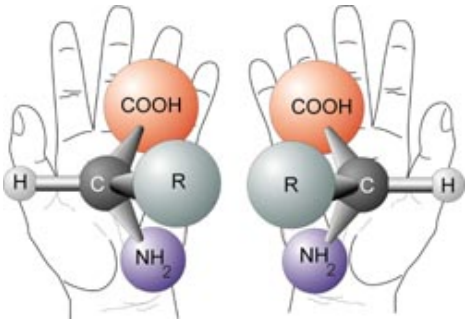
C. Enantiomers

1. Build a bromochlorofluromethane molecule using the handheld models. Draw this molecule in your lab notebook using a perspective drawing. Modify your handheld model by exchanging bromine and chlorine atoms. Make a perspective drawing in your notebook of this new molecule beside your old drawing. Remake a handheld model of your original drawing by starting over with a new carbon atom so that you now have a handheld model of both your drawings.

Answer

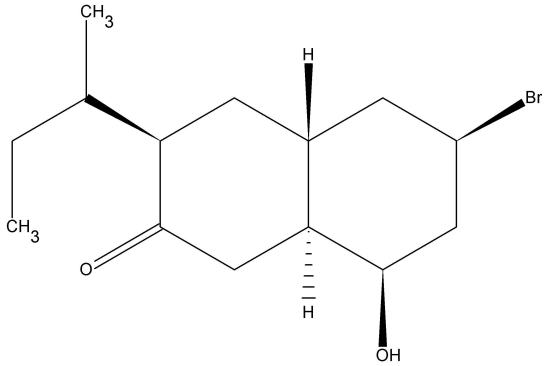
2. How are your images in step 1 related to each other? Are they the same molecule? The molecules representing bromochlorofluromethane are related to each other the same way your left and right hands are related to each other. They are mirror images that are non-superimposable. Take your handheld models and try to superimpose them. Non-superimposable mirror images are enantiomers of each other. Do either of the molecules have a plane of symmetry? Use the button on the right to check the symmetry of the molecule.

Answer

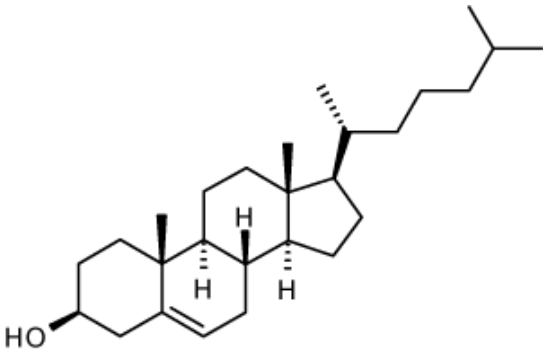


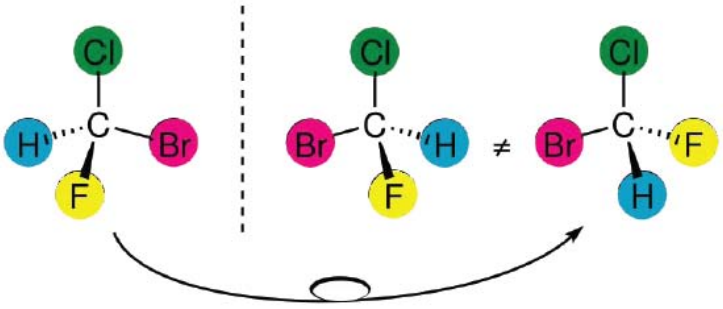
3. A sp^3 hybridized carbon that has four different groups attached to it, like bromochlorofluromethane, is an asymmetric center, or a chiral center. The following image contains a molecule with more than one asymmetric center (chiral carbon). Draw the perspective drawing of the molecule in your lab notebook and determine how many asymmetric carbons (sp^3 hybridized with four different groups attached) are present in the molecule by placing an asterisk on each asymmetric carbon. Use the button on the right to check your answer.

Answer

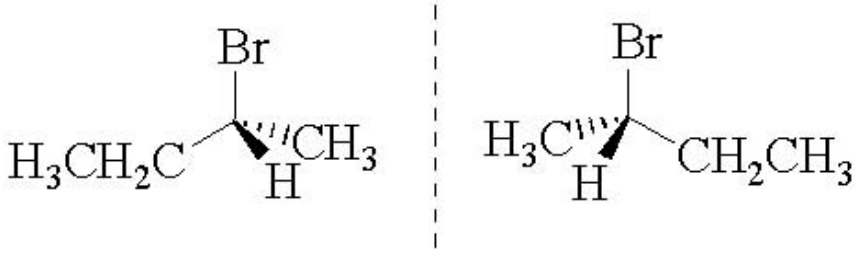


4. Cholesterol (image below) has eight asymmetric centers. Therefore, it can have a maximum of $2^8 = 256$ stereoisomers. The general formula for determining the **maximum** number of stereoisomers for a given number of asymmetric carbons is 2^n where n = number of asymmetric centers.

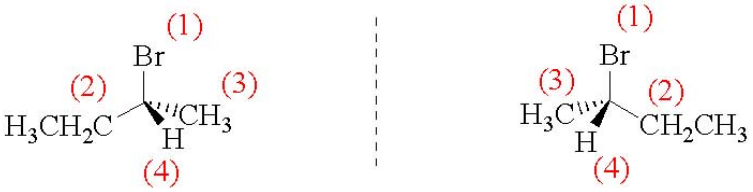




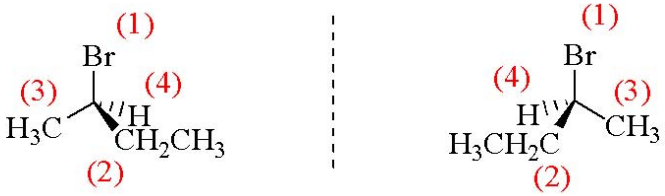
Looking at the two models of bromochlorofluromethane that you prepared, you determined that your two molecules were enantiomers and therefore not the same molecule. How do we differentiate the two molecules in the name? The Cahn-Ingold-Prelog Rule of naming is used to assign each enantiomer as either *S* or *R*.



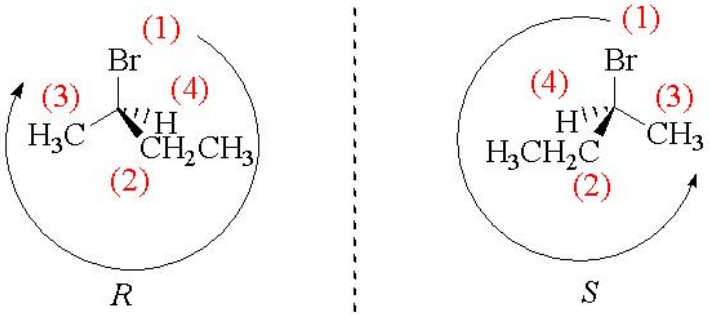
Using 2-bromobutane, lets review how to assign which is the *R* or *S* enantiomer. First, assign priority to the groups attached to the chiral center (the greater the atomic number of the atom attached the higher the priority - same rule as assigning *E* and *Z* isomers).



Rotate the molecule so that the lowest priority group is directly away from your eye.



Trace a path from highest priority to the second highest to the third (from 1 to 2 to 3). If the path traced goes in the clockwise motion the asymmetric center is designate *R* (rectus - Latin for right). If the path traced goes in the counterclockwise motion the asymmetric center is designated *S* (sinister - Latin for left).



5. In your notebook define the absolute stereochemistry (R or S) of your models of bromochlorofluromethane from step one and compare your answers by clicking the answer button on the right.

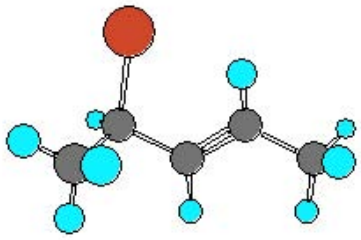
Answer

6. Using your handheld models prepare (*R*)-2-butanol. Draw this molecule in your lab notebook using dashes and wedges. Build (*S*)-2-butanol using your handheld models and draw this molecule in your notebook using dashes and wedges so that the stereochemistry is clear. Compare your structures to the perspective drawing by selecting the button on the right.

Answer

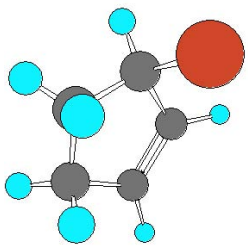
7. Given the 3-D image below draw the molecule in perspective (using dashes and wedges) in your lab notebook and determine whether it is R or S.

Answer



8. Using the 3-D image (below) draw the molecule using a perspective drawing in your lab notebook and assign the absolute stereochemistry as *R* or *S*.

Answer



D. Diastereomers

1. Build a handheld model of 3-bromo-2-butanol and draw this model in your lab notebook with stereochemistry (build any of the four stereoisomers).
Draw the enantiomer (non-super-imposable mirror image) and label both structure's stereocenters with *R* or *S* as appropriate.
Notice the absolute stereochemistry (*R* and *S* assignments) is reversed in the enantiomer- what was *R* is now *S* and vice versa. To change the absolute stereochemistry of an asymmetric carbon just switch out two of the groups attached to that carbon. Convert your handheld model to its enantiomer. Do your drawing and model agree?

2. So we have learned when you have two or more stereocenters, switching all the stereocenters to the opposite absolute stereochemistry gives the enantiomer of the original molecule. If we switch the absolute stereochemistry of just one stereocenter the relationship between the original molecule and the new molecule will be diastereomers. To prepare the diastereomer of your handheld model of 2-bromo-3 butanol simply switch only one stereocenter. After switching only one stereocenter of your model draw the new molecule and then draw its enantiomer. Label both structures stereocenters with *R* or *S* as appropriate. The four molecules of 2-bromo-3-butanol are all stereoisomers of each other. Since there are two stereocenters in 2-bromo-3-butanol the maximum number of stereoisomers is four (2^2), which means you have drawn all possible stereoisomers. To check if your drawings are correct click button to the right to compare.

Answer

3a. Construct a handheld model of (2S,3S)-2,3-butadiol. Draw the molecule you built in your lab notebook and compare your drawing to the answer by clicking the button to the right.

Answer

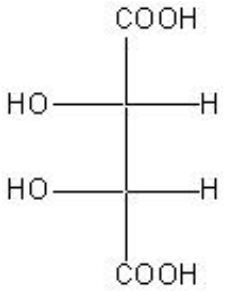
3b. Now draw all possible stereoisomers for 2,3-butadiol in your lab notebook.
How many stereoisomers are possible? Two of the four possible isomers are actually identical. They are called meso compounds and are easily identified because they have a plane of symmetry. Use the button on the right to check your stereoisomers.

Answer

3c. To visualize the plane of symmetry of acyclic molecules rotate the central sigma bonds so that the substituents are eclipsed. Draw all four stereoisomers in the eclipsed conformation. Check answers by clicking the answer button to the right.

Answer

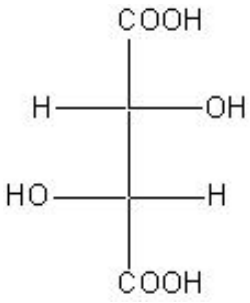
4a. In 1849 Louis Pasteur was working with tartaric acid and noticed that the naturally occurring form of the compound rotated plane polarized light, whereas a sample prepared in the lab did not. This discrepancy was due to the fact that the prepared form of tartaric acid was a racemic mixture. Often stereoisomers are drawn as Fisher projections. Fischer projections are two-dimensional drawings that represent three-dimensional molecules. By definition, the horizontal bonds are out (wedge) and the vertical bonds are back (dotted). Build a model for tartaric acid shown here.



Does the above stereoisomer have a plane of symmetry and is it therefore, a meso compound? Build the mirror image of the molecule to your right, is it super-imposable?

Answer

4b. Build a model for L-tartaric acid shown here. Does it have a plane of symmetry? Notice that the Fisher projection drawings are in the eclipsed form. Therefore, the determination whether the molecule has a plane of symmetry is obvious.



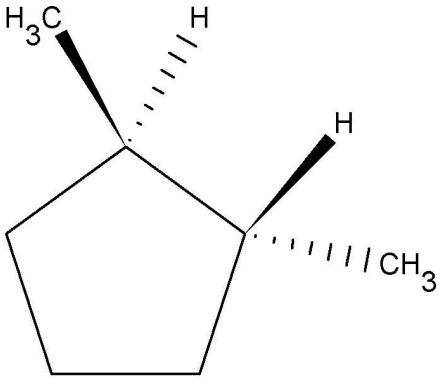
4c. Using the four conformations of tartaric acid, two of which are shown above assign which structures are the meso compounds and which structures correspond with the 2-D images above. Write your answers in your lab notebook and then compare to the given answer using the button below.

Answer

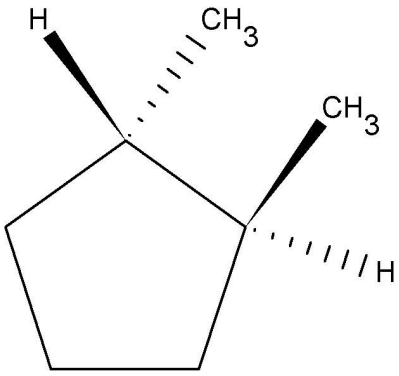
5. Now if given two stereoisomers you should be able to determine what their relationship is (either identical, enantiomers, or diastereomers). Compare the two sets of stereoisomers below and determine how they are related (identical, enantiomers, or diastereomers)? Feel free to assemble handheld models if needed. Click button to see answers.

Answer

1a.

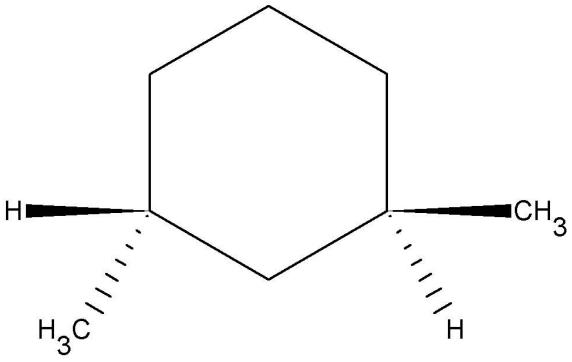


1b.

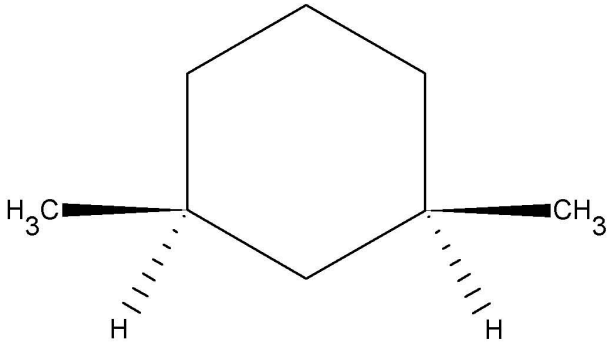


Answer

2a.



2b.



This is the end of the lab. The rest of the document contains answers and glossary you have already seen.

Glossary

To go back, simply click on the word in question

Absolute Configuration: The configuration of each stereocenter in a molecule in terms of R and S.

Absolute Stereochemistry: See Absolute Configuration.

Asymmetric Carbon: A carbon atom directly bonded to four different substituent groups.

Banana Bonds: Refers to the bonds inside the three membered ring cyclopropane, they are bent to resemble bananas due to the large amount of steric strain on the ring.

Bond Angle: Is the three-dimensional arrangement of the atoms that constitute a molecule, inferred from the spectroscopic studies of the compound. It determines several properties of a substance including its reactivity, polarity, phase of matter, color, magnetism, and biological activity.

Cahn-Ingold-Prelog Rule: CIP system or CIP conventions are a set of rules used in organic chemistry to name the stereoisomers of a molecule. A molecule may contain any number of stereocenters and any number of double bonds, and each gives rise to two possible configurations. The purpose of the CIP system is to assign an R or S descriptor to each stereocenter and an E or Z descriptor to each double bond so that the configuration of the entire molecule can be specified uniquely by including the descriptors in its systematic name.

Chair Drawing: A method of drawing six membered rings, specifically cyclohexane so that it is in the lowest possible energy conformation.

Chiral Center: See Asymmetric Center.

Cis: Characterized by having certain atoms or groups of atoms on the same side of the longitudinal axis of a double bond or of the plane of a ring in a molecule.

Constitutional Isomer: Constitutional Isomers are compounds that have the same Molecular Formula (that is the same number of atoms of each element represented in the molecule) but these compounds differ in the way the atoms are connected in three dimensional space. Constitutional isomers often vary dramatically in their physical and chemical properties. This is a testament to the way that structure determines the properties of matter.

Diastereomer: Are stereoisomers that are not enantiomers (non-super-imposable mirror images of each other).

E: cis and trans cannot be applied when there are 3 or more different substituents bonded to the double bond carbons, therefore the E/Z system is applied separately to the 2 groups on each double bonded carbon. When the 2 groups of higher priority are on opposite sides the molecule is in the E configuration. (E coming from the German word entgegen, meaning opposite)

Enantiomers: One of two stereoisomers that are non-super-imposable complete mirror images of each other, much as one's left and right hands are "the same" but opposite.

Hybridization: The concept of mixing atomic orbitals to form new *hybrid orbitals* suitable for the qualitative description of atomic bonding properties. Hybridized orbitals are very useful in the explanation of the shape of molecular orbitals for molecules.

Isomer: Any of two or more compounds, such as lactose and sucrose, composed of the same elements in the same proportions but differing in structure and other properties. There are two types of isomers, structural isomers and stereoisomers.

Meso Compound: Is a chemical compound whose molecules contain 2 or more asymmetric atoms (stereocenters) but is optically inactive (or achiral) due to the molecule containing a plane of symmetry.

Mirror Images: Two molecules that, side by side, appear to be only one molecule and its image as though through a mirror.

Non-super-imposable: To be unable to lay or place (something) on or over something else.

Perspective Drawing: Method of drawing three dimensional molecules on a two dimensional medium (paper), used dashed lines and wedges to show bonds not in the plane of the page.

Planes of Symmetry: In two dimensions there is an axis of symmetry, in three dimensions there is a plane of symmetry. An object that is indistinguishable from its other half when folded over this plane is said to have symmetry.

R/S: Designations devised by Cahn, Ingold and Prelog used to determine the absolute configuration or each stereocenter in a given molecule.

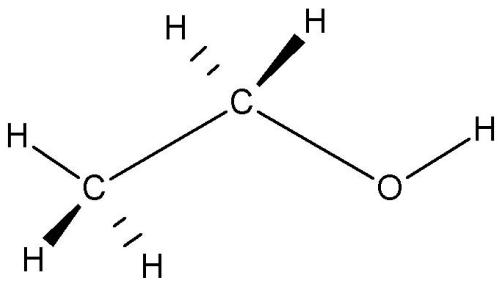
Skeletal Structures: An organic compound shorthand representation of molecular structure. Skeletal formulae are ubiquitous in organic chemistry because they show complicated structures clearly and they are quick and simple to draw.

Stereocenters: Is any atom in a molecule bearing groups such that an interchanging of any two groups leads to a stereoisomer.

Super-imposable: To lay or place (something) on or over something else.

Trans: Characterized by having certain atoms or groups of atoms on the opposite sides of the longitudinal axis or a double bond or of the plane of a ring in a molecule.

Z: cis and trans cannot be applied when there are 3 or more different substituents bonded to the double bond carbons, therefore the E/Z system is applied separately to the 2 groups on each double bonded carbon. When the 2 groups of higher priority are on the same side the molecule is in the Z configuration. (Z coming from the German word zusammen, meaning together)



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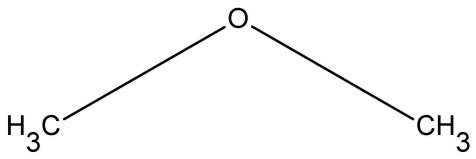

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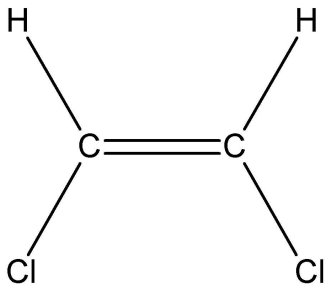
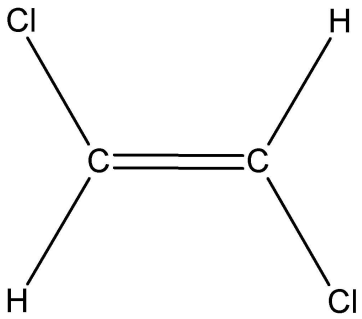
two planes of symmetry

Back



(*Z*)-1,2-dichloroethene



(*E*)-1,2-dichloroethene

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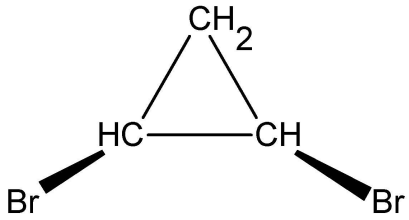
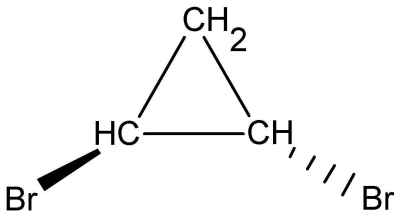


cis-1,2-dibromocyclopropane



trans-1,2-dibromocyclopropane

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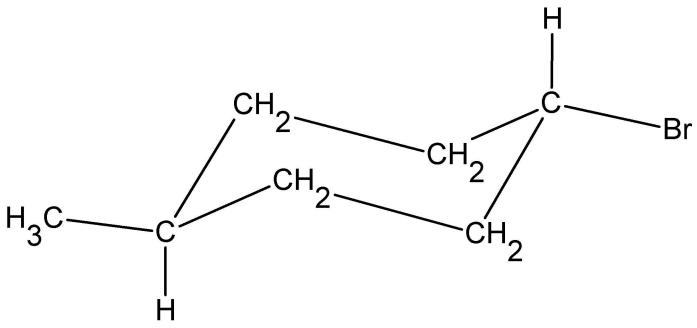

Chair Drawing

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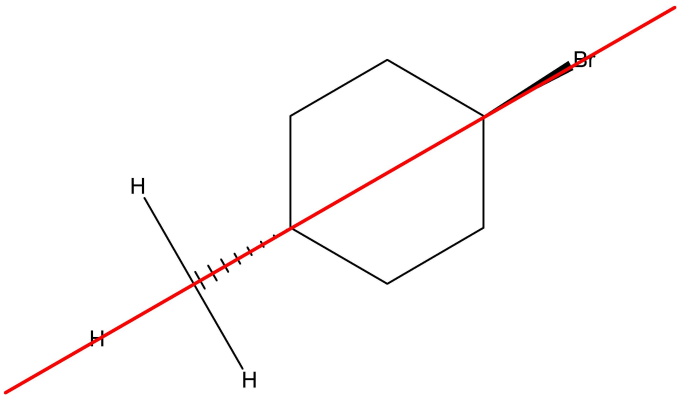
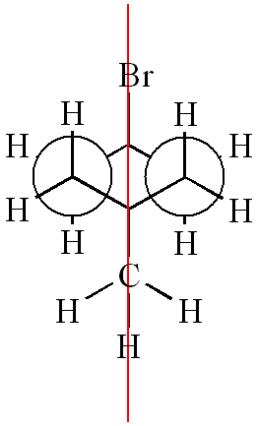
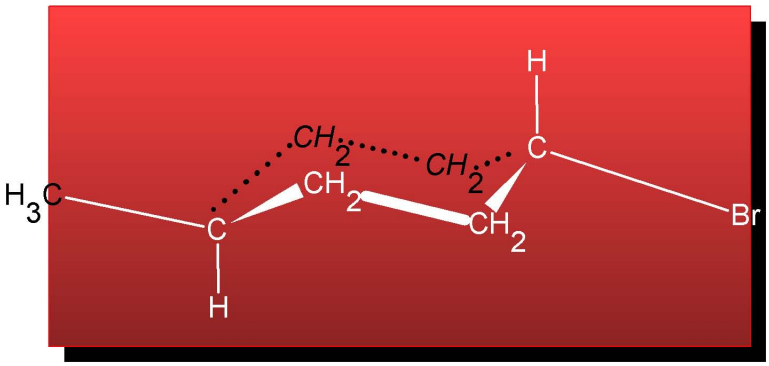
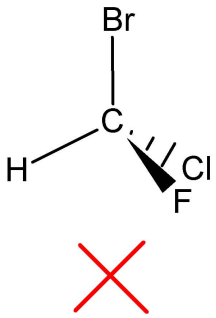
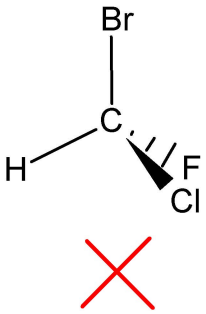






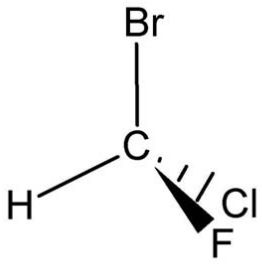
= 1 plane of symmetry

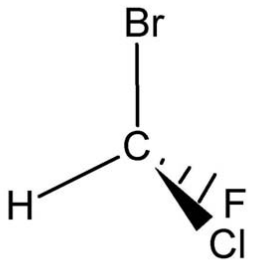




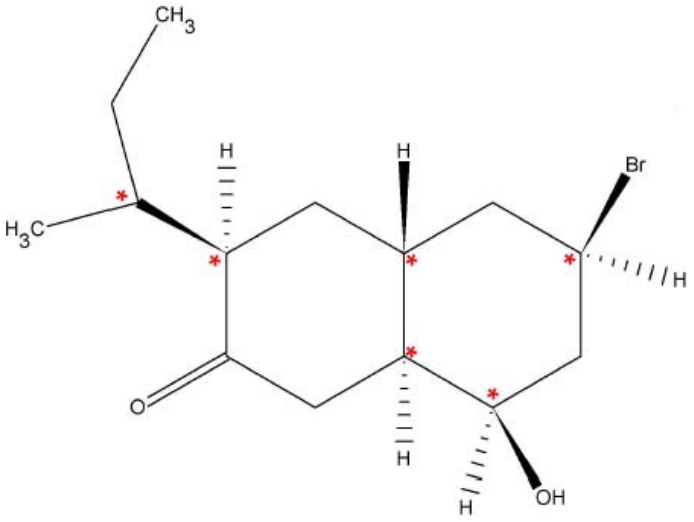
= no symmetry

Back



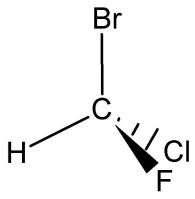


Back

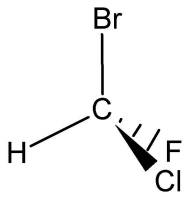


6 Chiral Centers

Back

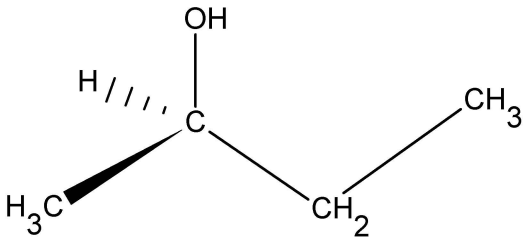


(R)-bromochlorofluromethane

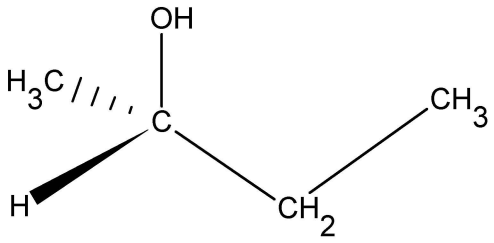


(S)-bromochlorofluromethane

Back

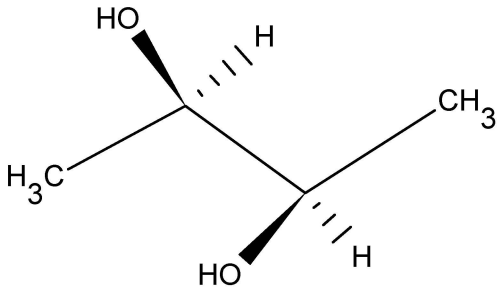


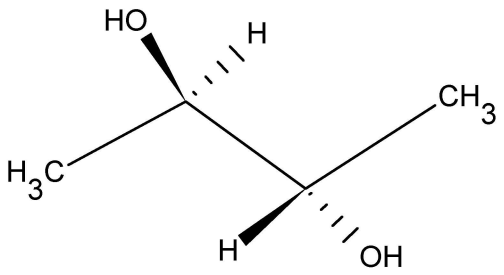
(*R*)-2-butanol

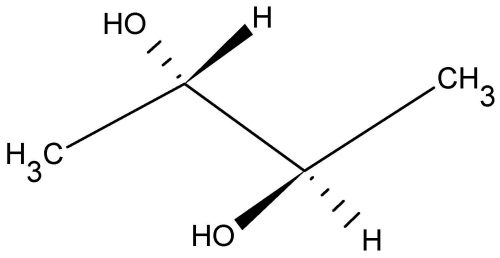


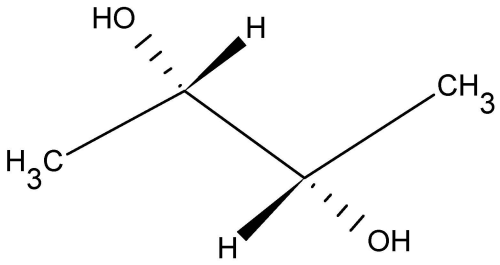
(*S*)-2-butanol

Back









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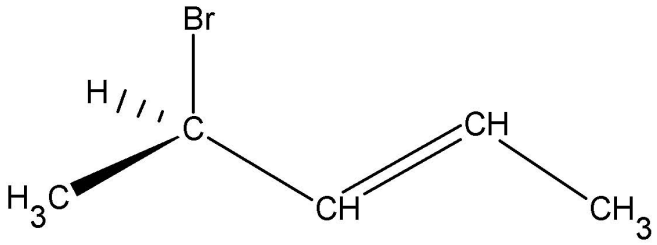
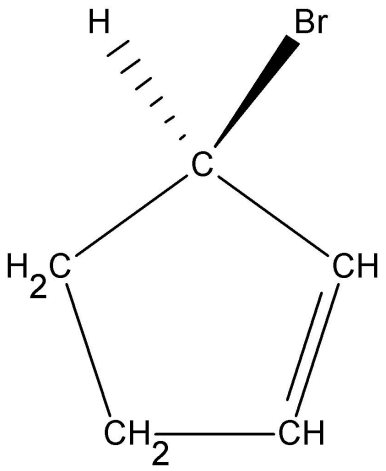


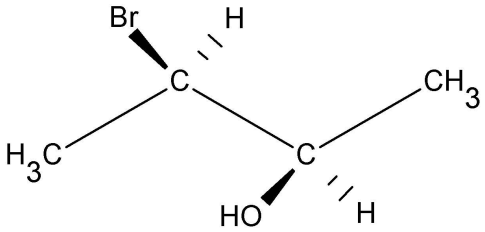
(*R*)-4-bromo-2-pentene

Back

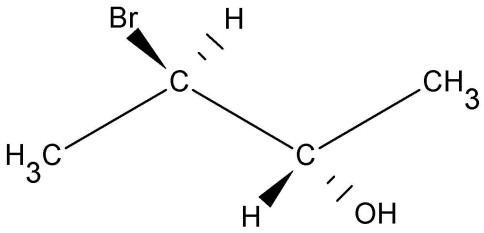


(*R*)-3-bromo-1-cyclopentene

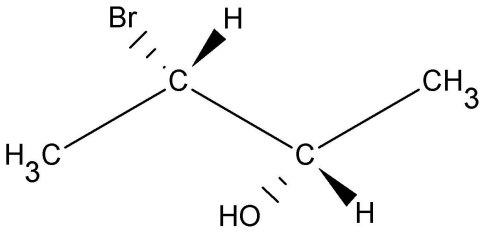
Back



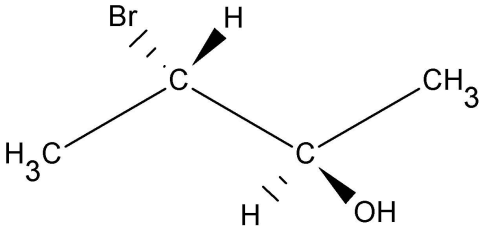
(2R,3R)-2-bromo-3-butanol



(2S,3R)-2-bromo-3-butanol

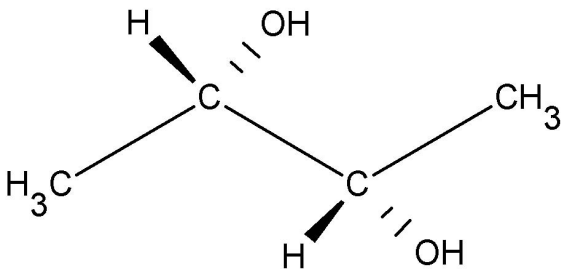


(2S,3S)-2-bromo-3-butanol



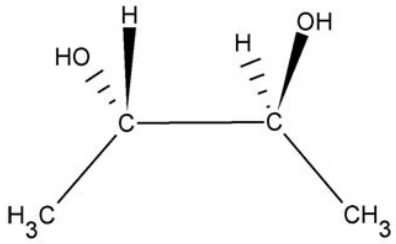
(2R,3S)-2-bromo-3-butanol

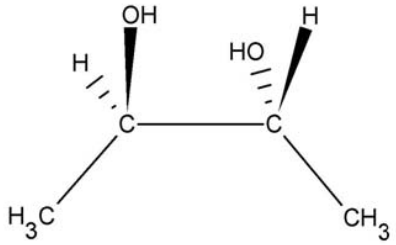
Back



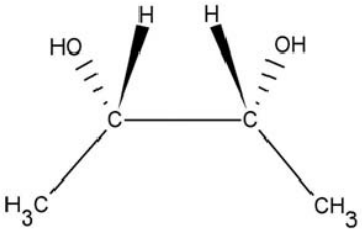
(2S,3S)-2,3-butadiol

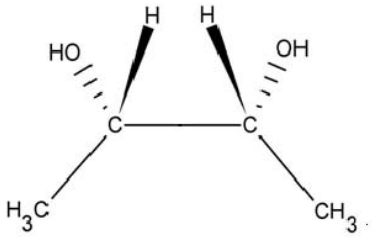
Back





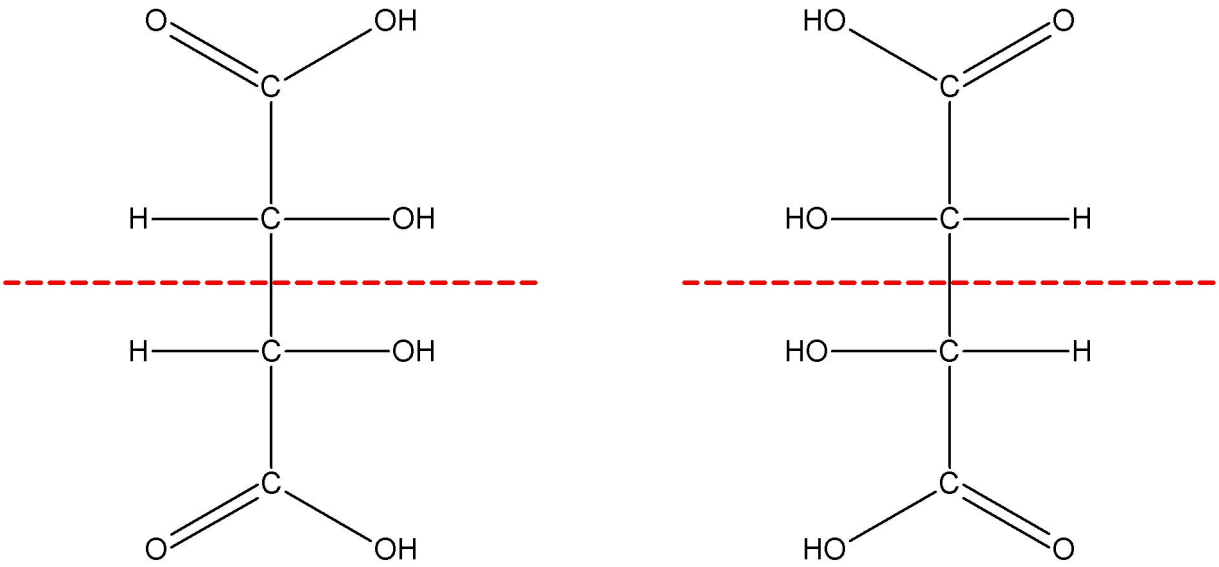
As you can clearly see these two molecules do not contain a plane of symmetry





Back

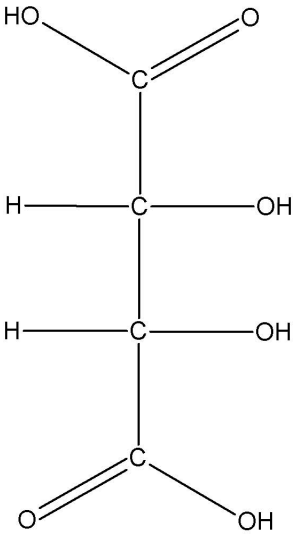
These molecules on the other hand are identical, and being meso compounds clearly contain a plane of symmetry.



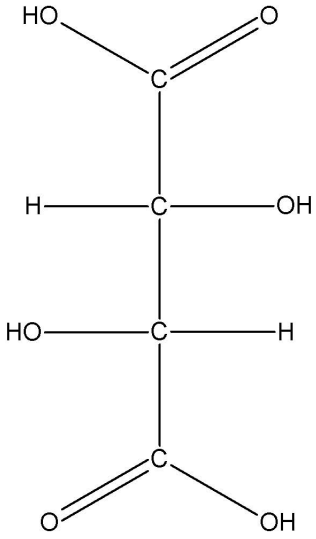
Back

This molecule and its mirror image clearly have a plane of symmetry so yes, it is a meso compound.

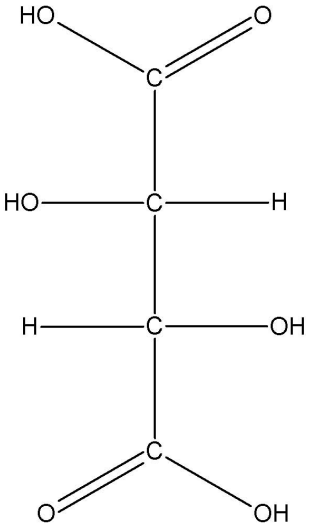
Structure A =



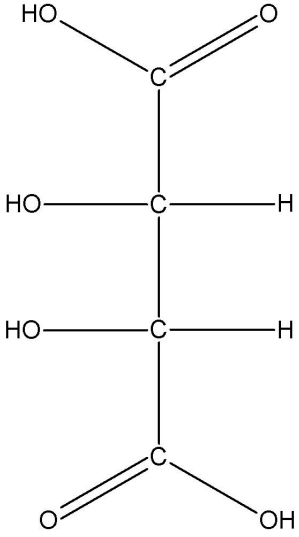
Structure C =



Structure B =

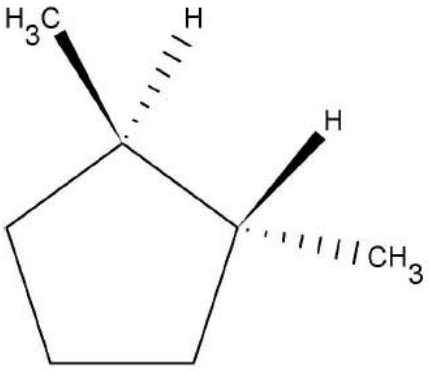


Structure D =

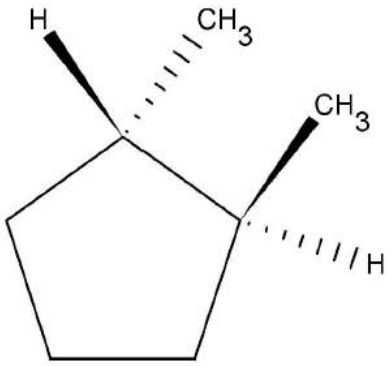


Back

1a.



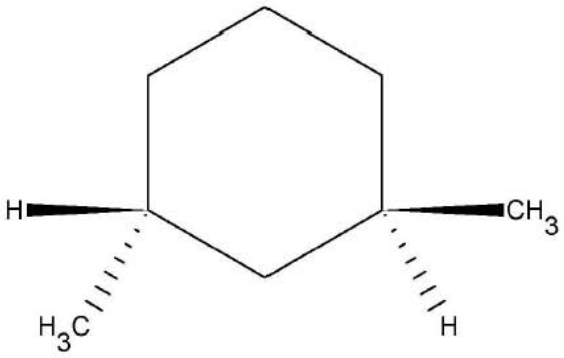
1b.



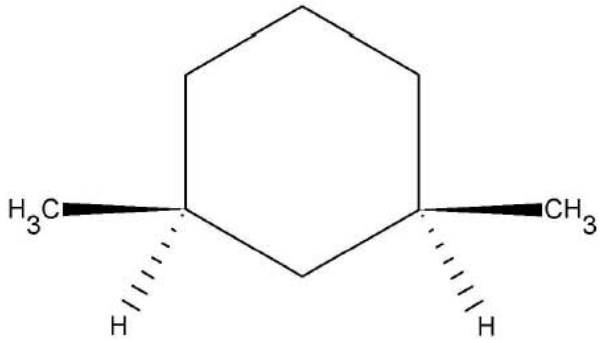
Enantiomers

Back

2a.



2b.



Diastereomers

Back