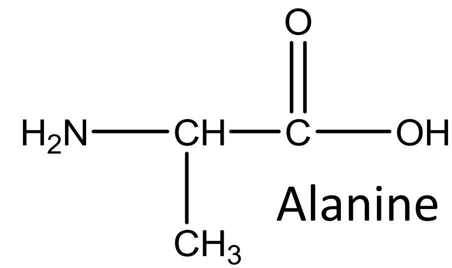
Isomerism of Organic Molecules

Organic Molecules
molecules containing carbon, hydrogen, oxygen, nitrogen and other atoms except any metal atom

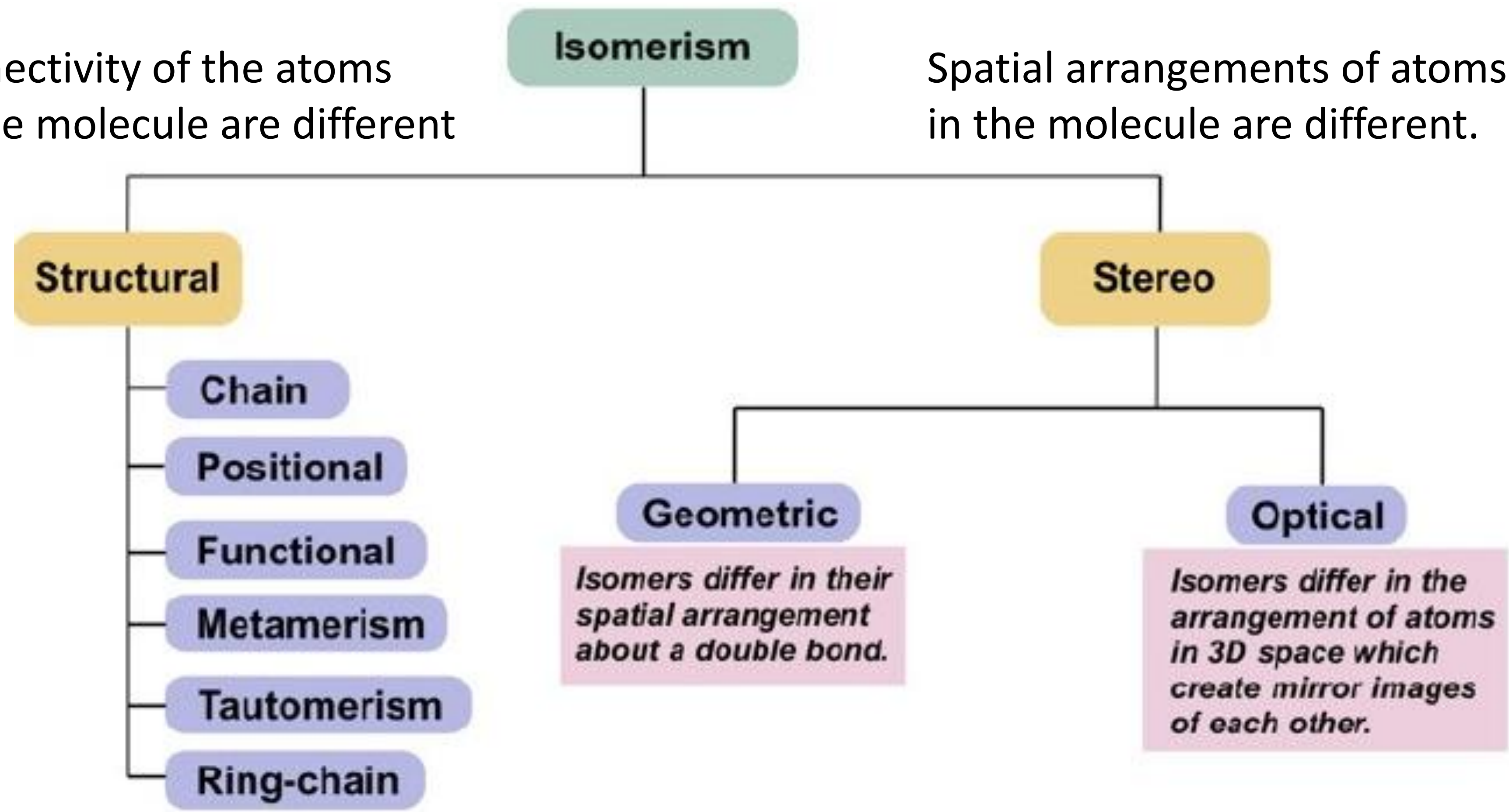


Alanine

Isomers
Compounds that have the same molecular formula but are not identical

Connectivity of the atoms in the molecule are different

Spatial arrangements of atoms in the molecule are different.

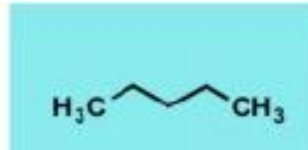


Isomerism of Organic Molecules: Structural Isomerism

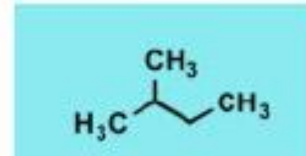
Chain Isomerism

carbon atoms are linked to the main chain in different ways

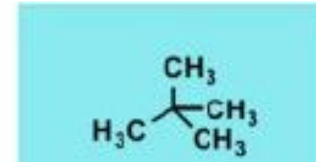
C_5H_{12}



pentane



isopentane

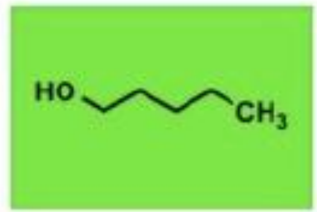


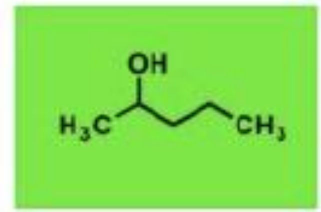
neopentane

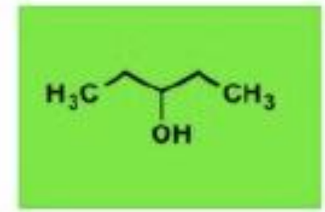
Position Isomerism

functional groups are attached on different positions on a carbon chain

$C_5H_{11}OH$



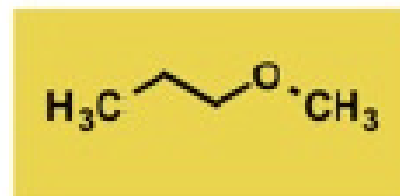


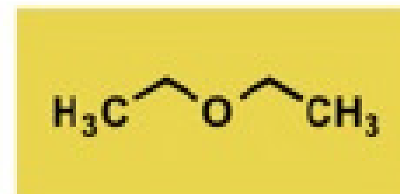


Metamerism

limited to molecules having a divalent atom like O or S and alkyl groups around it

$C_4H_{10}O$

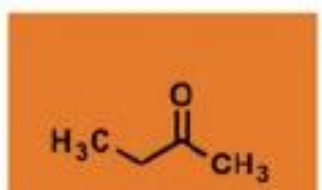




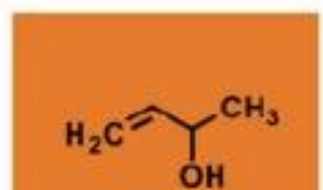
Functional Isomerism

compounds are different due to different arrangements of atoms leading to different functional groups.

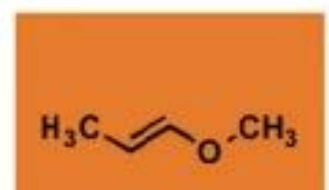
C_4H_8O



Ketone



Alcohol



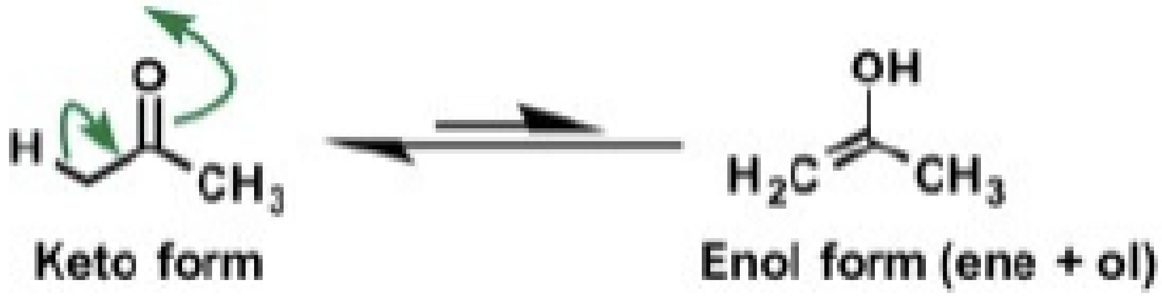
Ether

Isomerism of Organic Molecules: Structural Isomerism

Tautomerism

isomerism is due to spontaneous inter-conversion of two isomeric forms with different functional groups

C_4H_6O



Ring-Chain isomerism

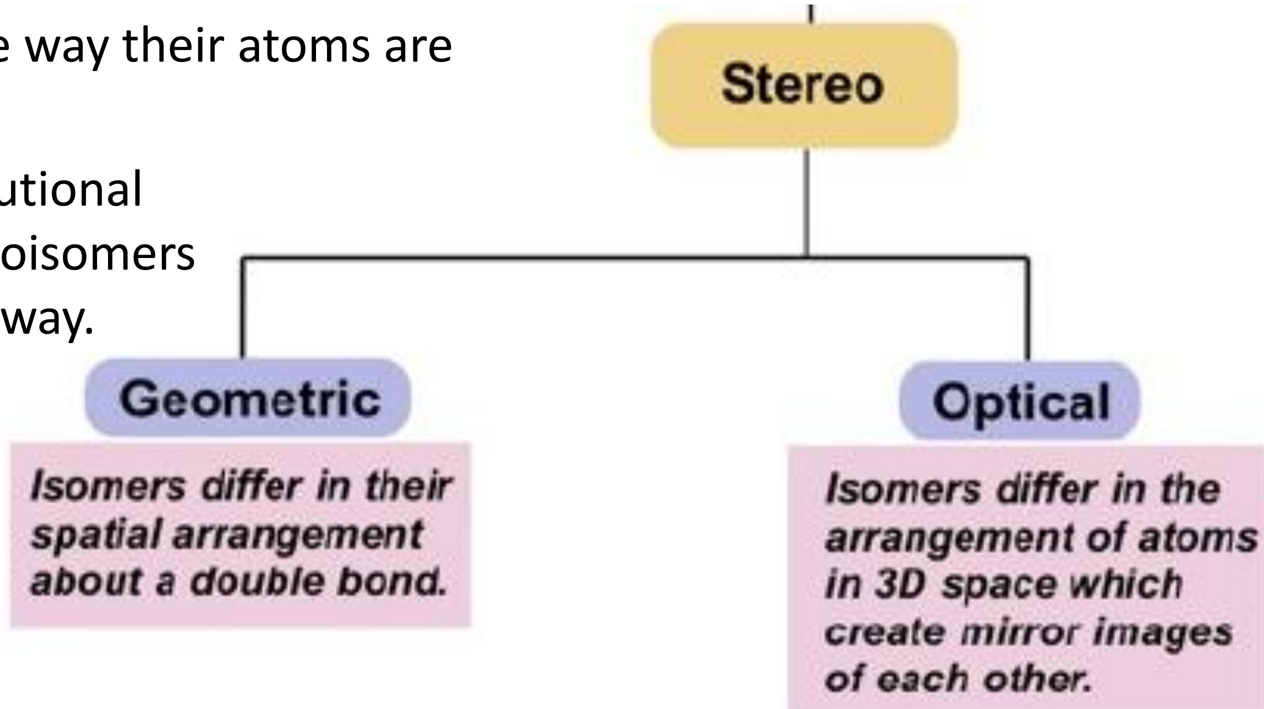
one isomer is an open chain molecule and the other a cyclic molecule

C_3H_6

Isomerism of Organic Molecules: Stereoisomer

Stereoisomers differ in the way their atoms are arranged in **space**.

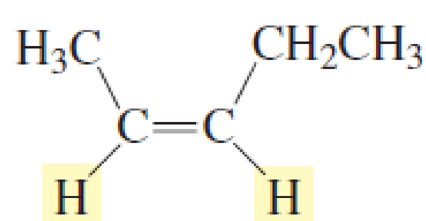
Unlike the atoms in constitutional isomers, the atoms in stereoisomers are connected in the same way.



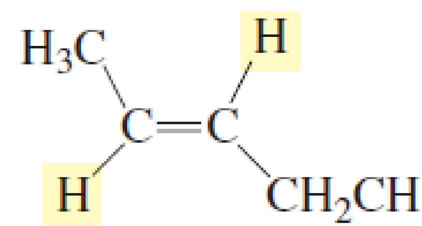
Geometric isomers

also called cis–trans isomers **result from restricted rotation** caused either by a double bond or by a cyclic structure

cis isomer has the hydrogens (less priority group) on the *same side of the double bond*



cis-2-pentene



trans-2-pentene

***trans* isomer has the** hydrogens **(less priority group)** on *opposite sides of the double bond*

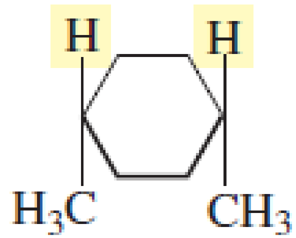
restricted rotation caused by a double bond

Isomerism of Organic Molecules: **Geometric isomers**

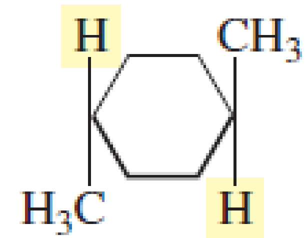
Cis- isomer has the hydrogens on the same side of the ring

trans -isomer has the hydrogens on opposite sides of the ring.

restricted rotation
caused by a cyclic structure

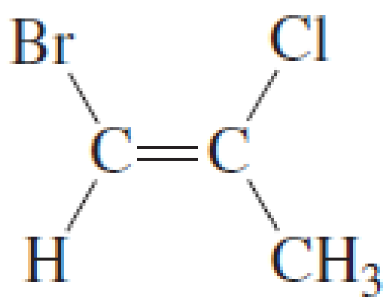


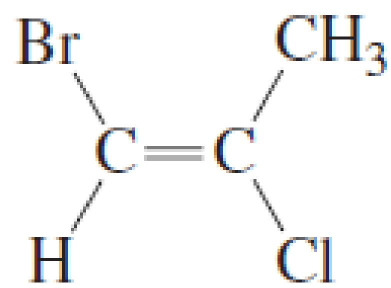
cis-1,4-dimethylcyclohexane



trans-1,4-dimethylcyclohexane

The cis–trans system of nomenclature cannot be used because there are four different substituents on the two vinylic carbons.





Which isomer is cis and which is trans?

The *E,Z system of nomenclature was devised for these kinds of situations.*

Isomerism of Organic Molecules: ***E,Z*- Nomenclature**

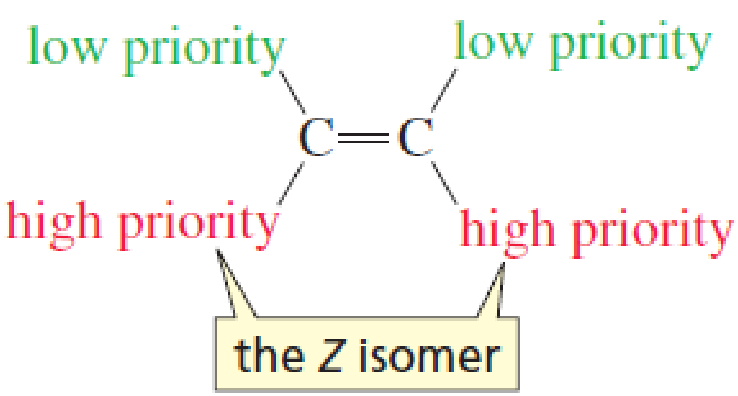
First determine the relative priorities of the two groups bonded to one of the sp^2 carbon then the relative priorities of the two groups bonded to the other sp^2 carbon.

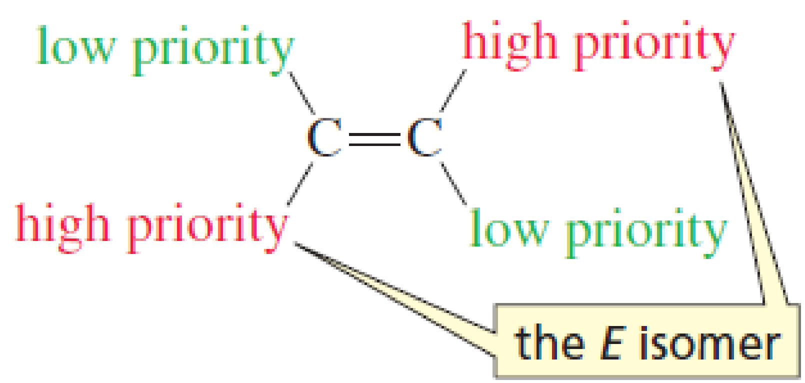
If the high-priority groups are on the same side of the double bond, the isomer has the ***Z*** *configuration*

(Z is for zusammen, German for "together")

If the high-priority groups are on opposite sides of the double bond, the isomer has the ***E*** *configuration*

(E is for entgegen, German for "opposite")

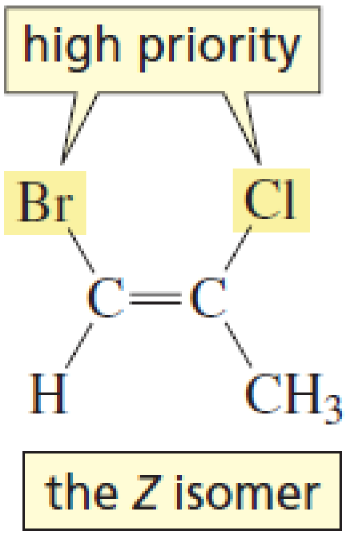




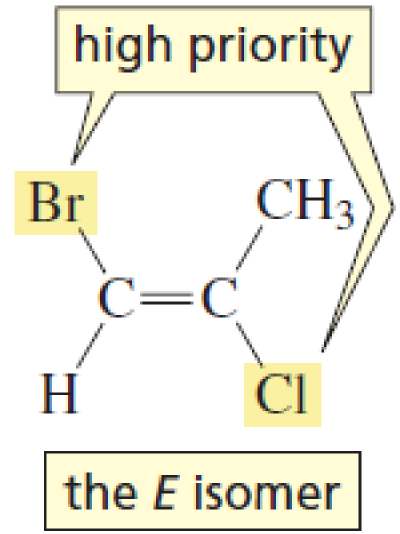
Isomerism of Organic Molecules: ***E,Z*- Nomenclature**

Rules to determine the relative priorities of the two groups bonded to an carbon are

Rule 1. The relative priorities of the two groups depend on the atomic numbers of the atoms that are bonded directly to the sp^2 carbon.
The greater the atomic number, the higher is the priority.



Atomic number
Br: 35
Cl: 17
C: 6
H: 1



Br has a greater atomic number than H, so **Br has a higher priority than H.**

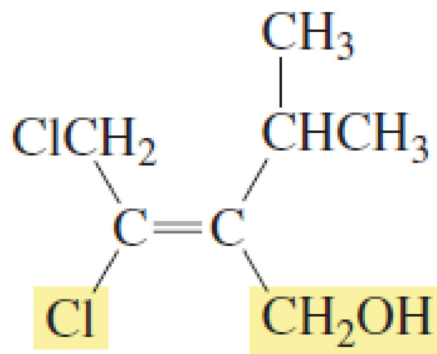
Cl has the greater atomic number, so **Cl has a higher priority than C.**

Notice that you use the atomic number of C, not the mass of the group, because the priorities are based on the atomic numbers of atoms, *not on the masses of groups.*

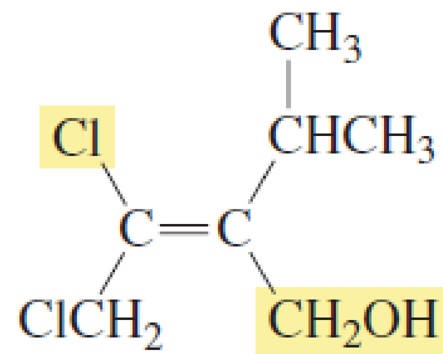
Isomerism of Organic Molecules: ***E,Z*- Nomenclature**

Rule 2: If the atoms attached to sp^2 carbons are the same, the atoms attached to the "tied" atoms are compared; the one with the greatest atomic number belongs to the group with the higher priority.

Atomic number
Cl: 17
O: 8
C: 6
H: 1



the *Z* isomer



the *E* isomer

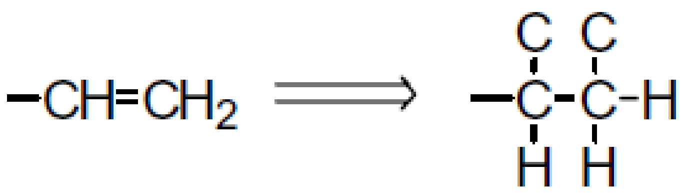
Cl has a greater atomic number than C, so the Cl group has the higher priority CH_2Cl.

Both atoms bonded to the other sp^2 carbon are Carbon atoms , so there is a tie at this point. The C of the group CH_2OH is bonded to **O, H, and H, and the C of the $CH(CH_3)_2$ group is bonded to C, C, and H. Of these six atoms, O has the greatest atomic number, so** CH_2OH **has a higher** priority than $\mathbf{CH(CH_3)_2}$

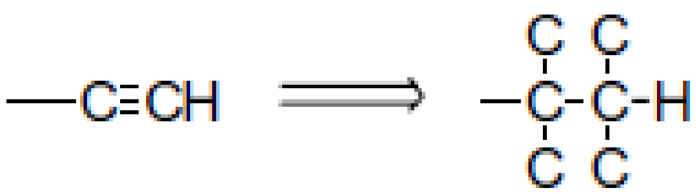
Note that you **do not add** the atomic numbers; you take the single atom with the greatest atomic number.

Isomerism of Organic Molecules: ***E,Z*- Nomenclature**

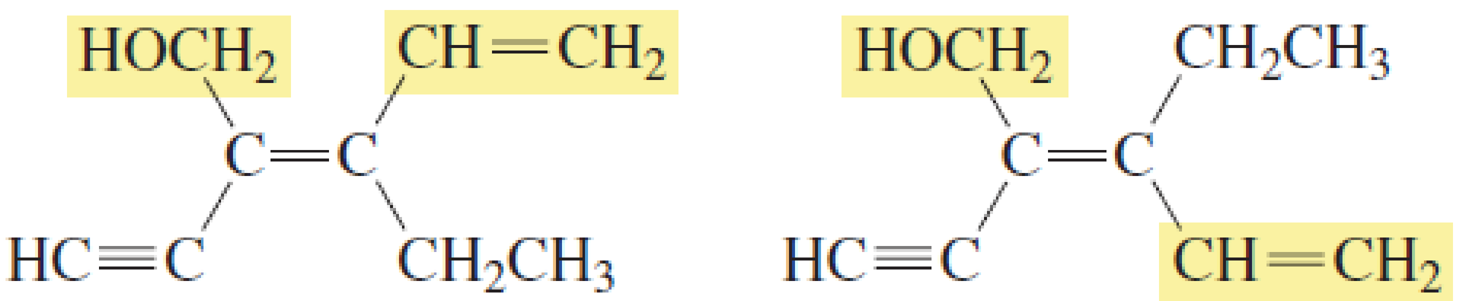
Rule 3: If an atom is doubly bonded to another atom, treat it as if it were singly bonded to two of those atoms.



If an atom is triply bonded to another atom, treat it as if it were singly bonded to three of those atoms.



Cancel atoms that are identical in the two groups; use the remaining atoms to determine the group with the higher priority.

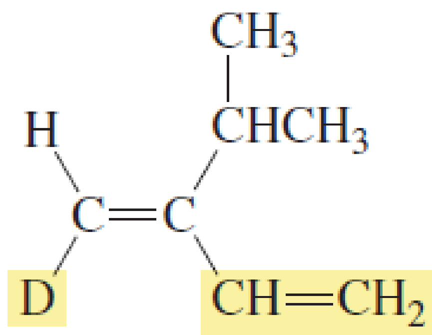


the *Z* isomer

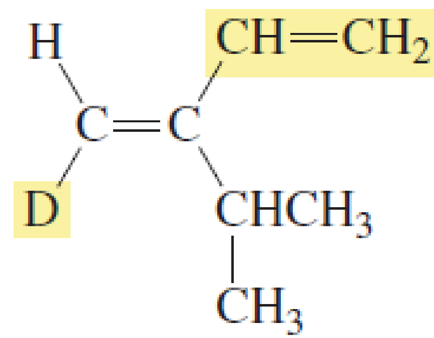
the *E* isomer

Isomerism of Organic Molecules: ***E,Z-* Nomenclature**

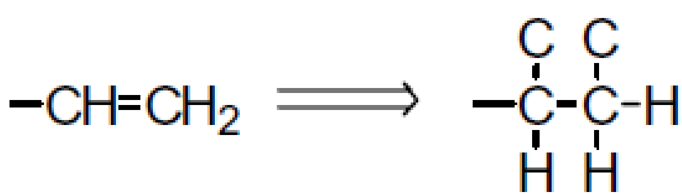
Rule 4. In the case of isotopes (atoms with the same atomic number, but different mass numbers), the mass number is used to determine the relative priorities.



the *Z* isomer

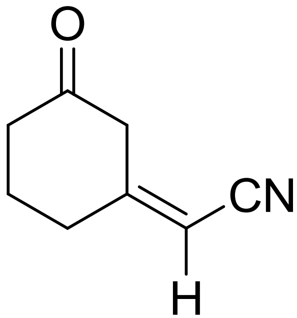


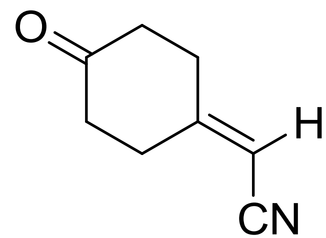
the *E* isomer

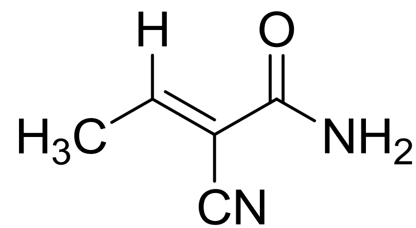


D and H have the same atomic number, but D has a greater mass number, so **D** has a higher priority than **H.**

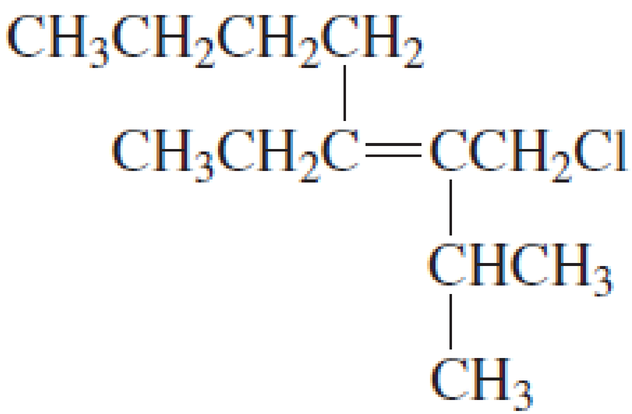
Isomerism of Organic Molecules: ***E,Z*- Nomenclature**

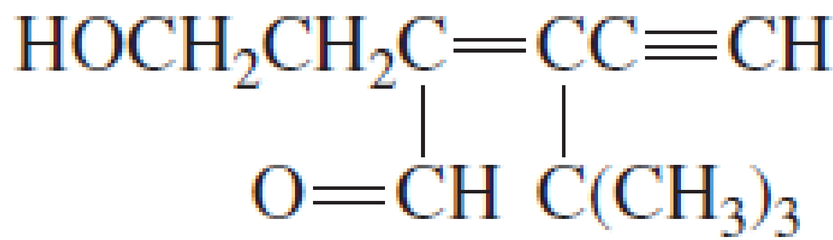






Draw and label the *E and Z isomers for each of the following compounds:*





Looking forward

Optical Isomerism:

Optical activity

Chiral and achiral compounds

R/S- Nomenclature

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