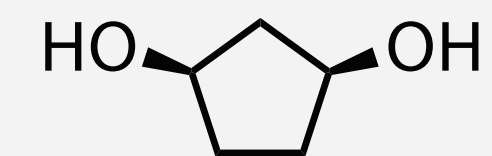
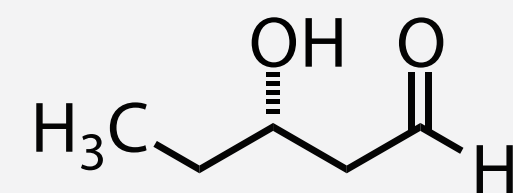
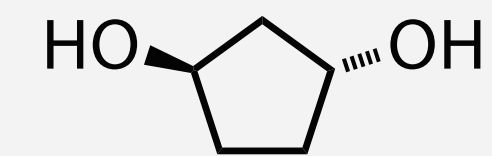
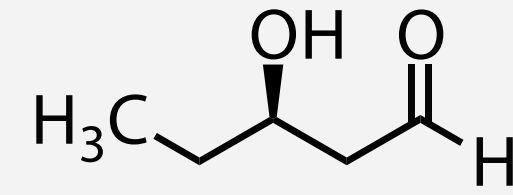
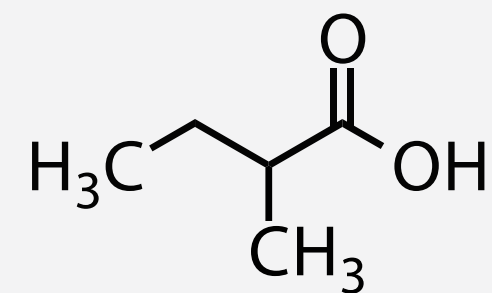
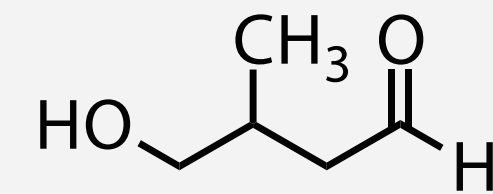
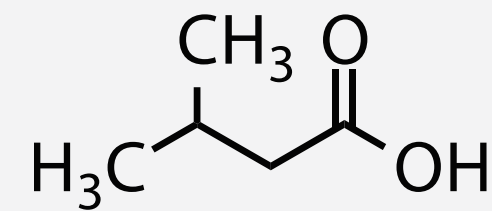
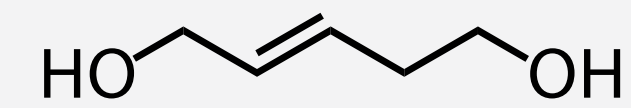
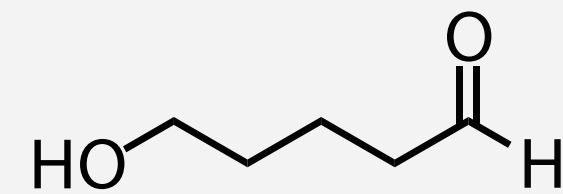
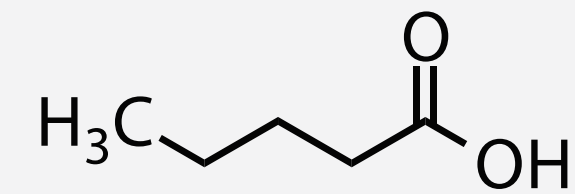


3.2. Isomerism

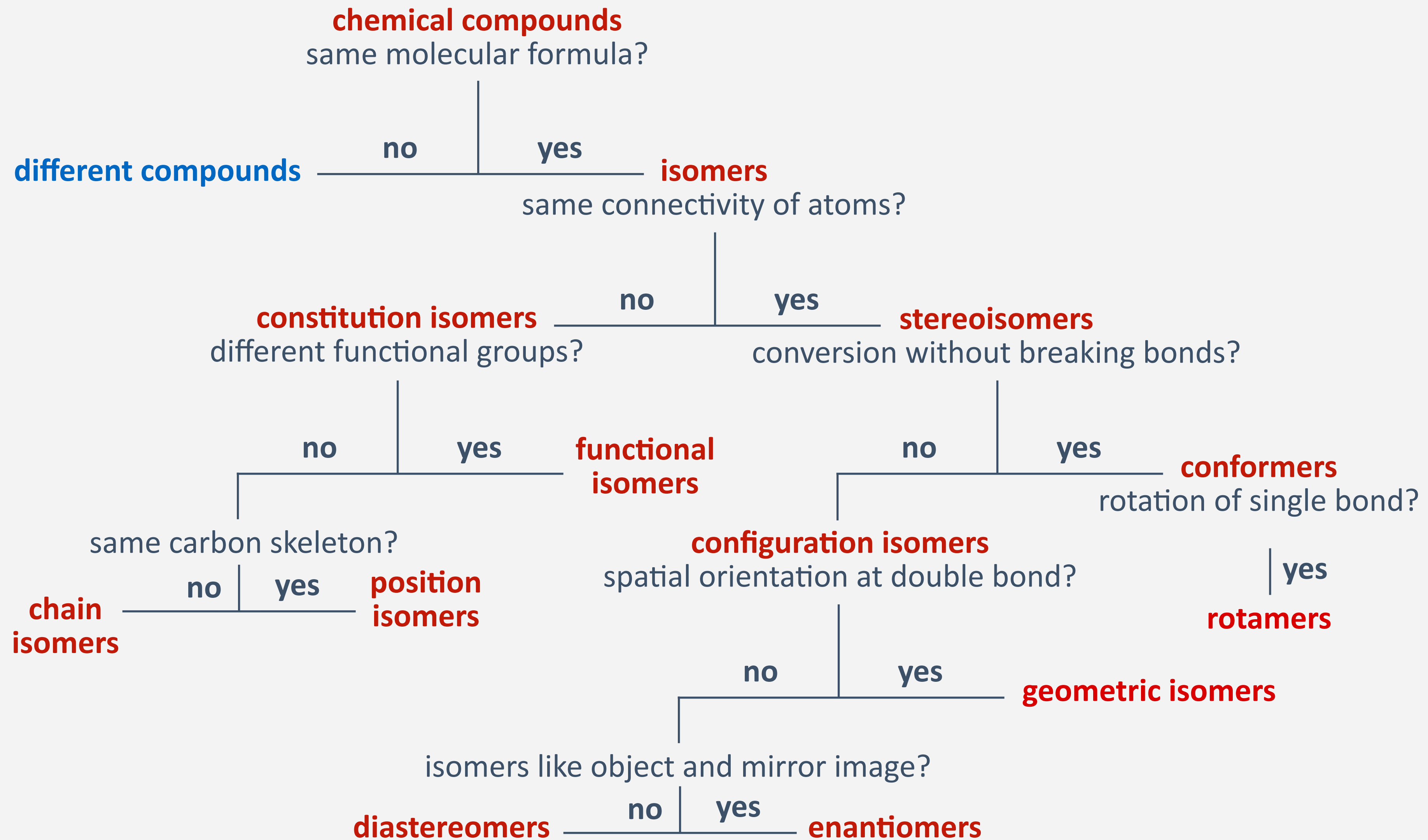
Isomers

- examples of a few isomers, that is, molecules with the molecular formula $C_5H_{10}O_2$

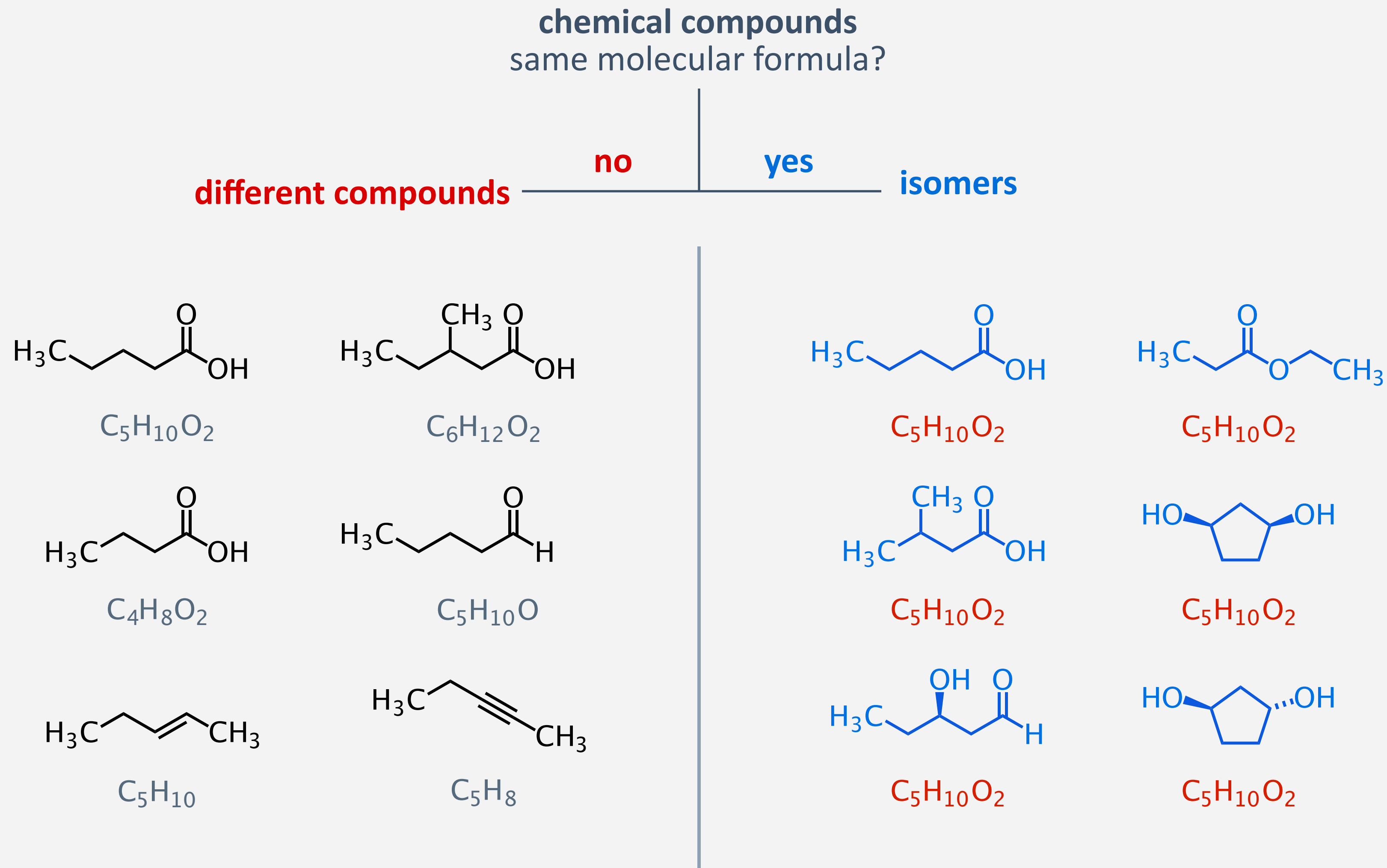


- isomers have the **same molecular formula** but **different structural formula**

A Decision Tree to Assign Types of Isomers

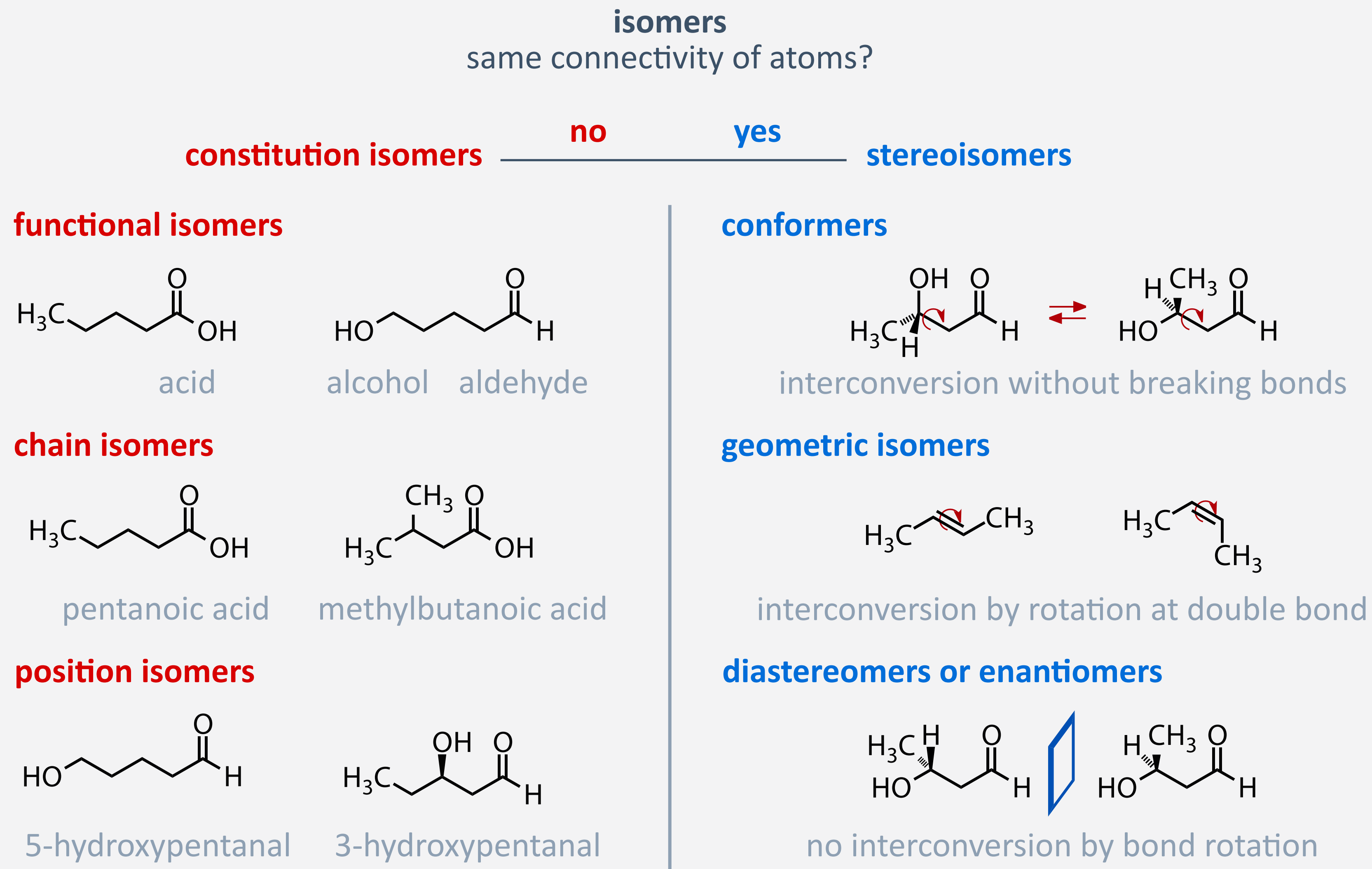


Different Compounds versus Isomers



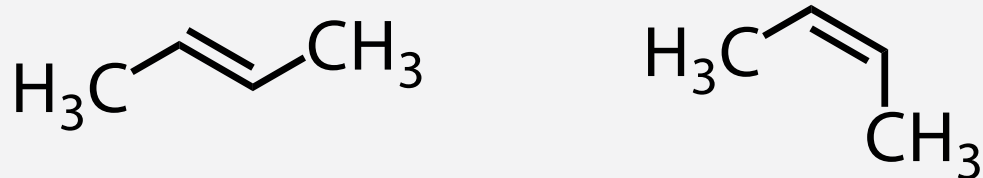
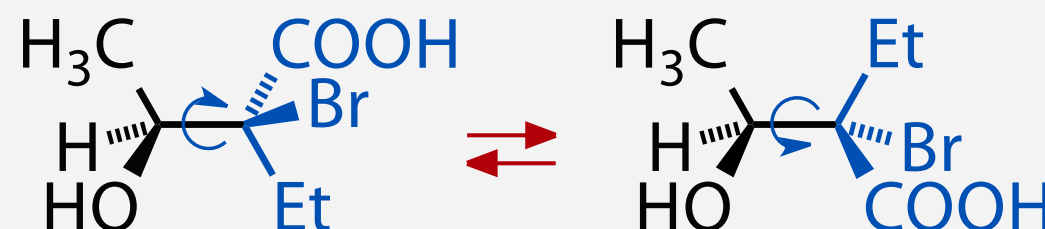
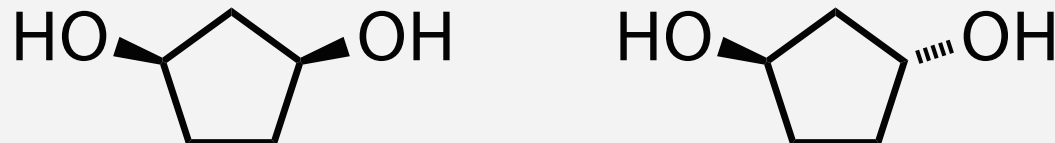
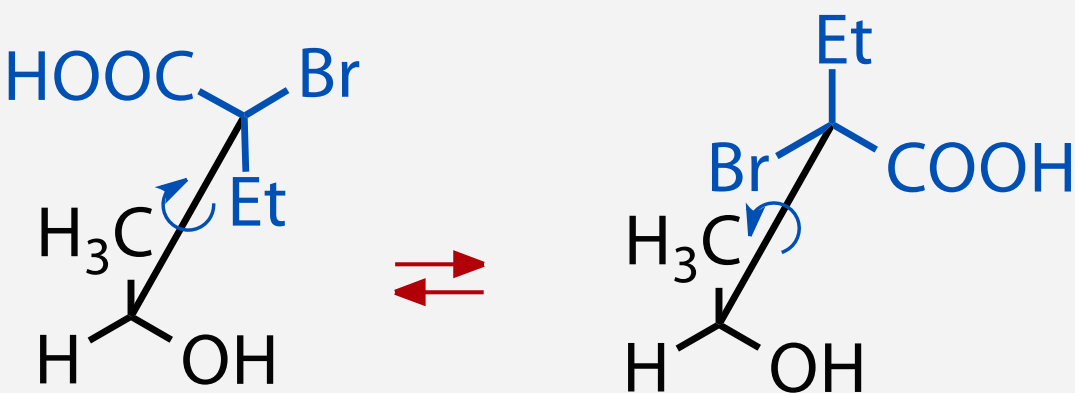
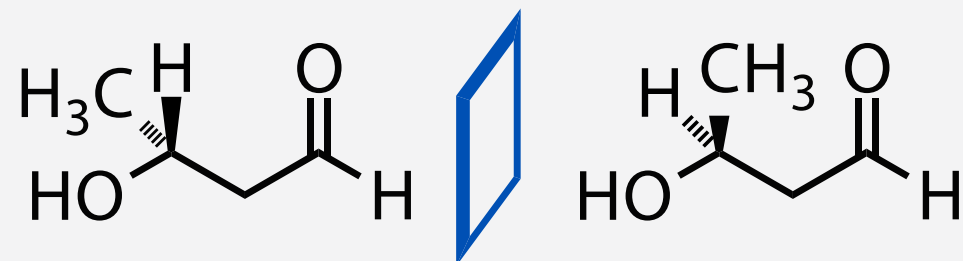
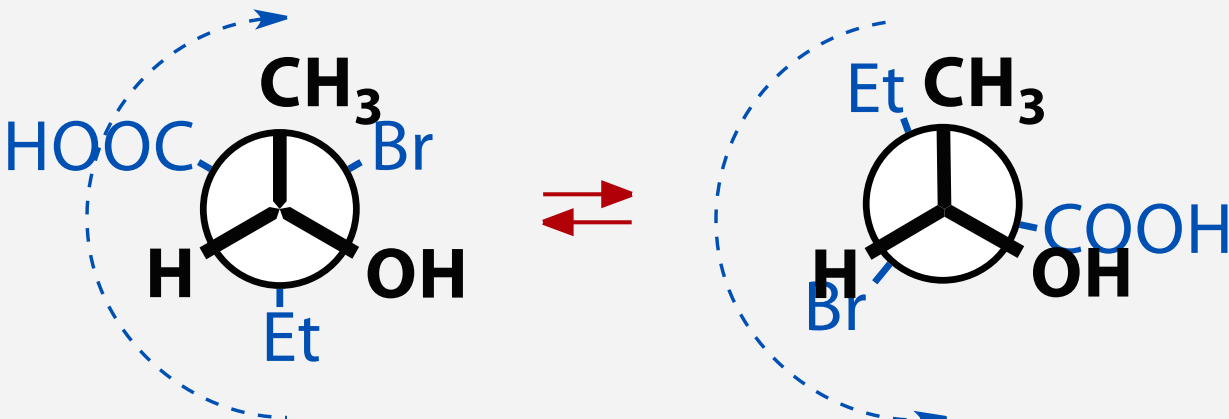
- all types of **isomers** have the **same molecular formula** but **different structural formula**

Constitution Isomers versus Stereoisomers



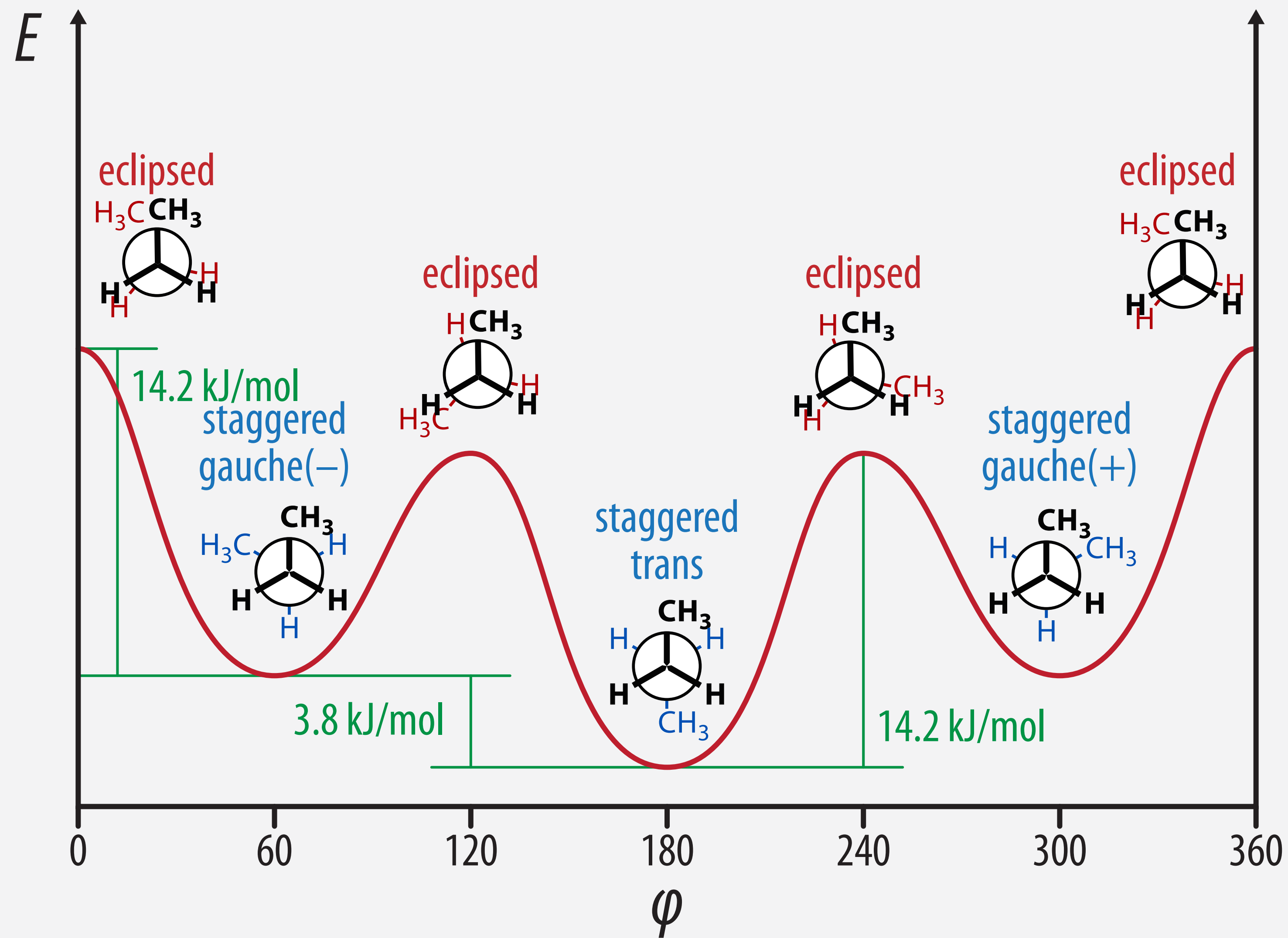
- **constitution** refers to the **connectivity** of atoms, **stereoisomers have the same constitution**

Configuration Isomers versus Conformers

stereoisomers			
interconversion without breaking bonds?			
configuration isomers	no	yes	conformers
geometric isomers	Natta projection		
			
diastereomers	Sawhorse projection		
			
enantiomers	Newman projection		
			

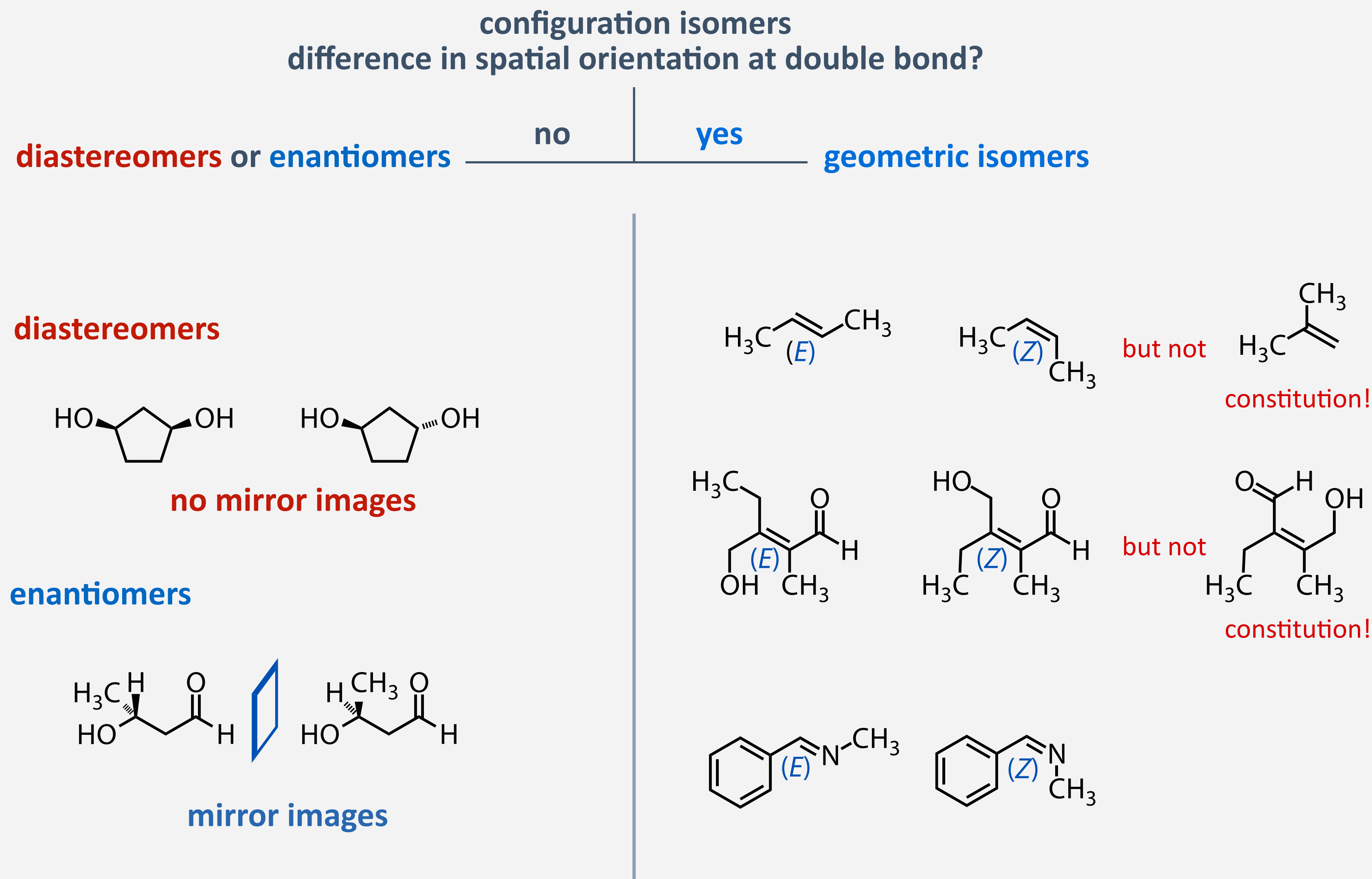
- **configuration** refers to **fixed shape in space**, **conformers** have the the same configuration

Conformations of Alkanes



- fast rotation around single bonds at room temperature, conformers are identical compounds

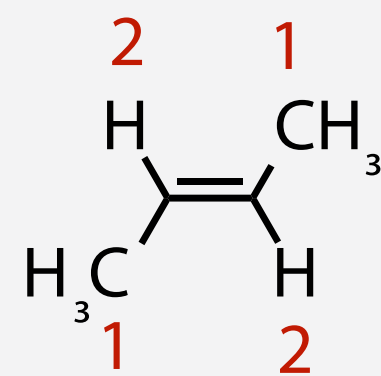
Stereoisomers versus Diastereomers and Enantiomers



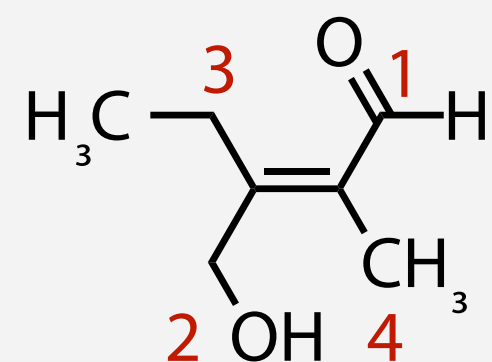
- geometric isomers exist due to lack of rotation around double bond (at room temperature)

Cahn-Ingold-Prelog Nomenclature of Geometric Isomers

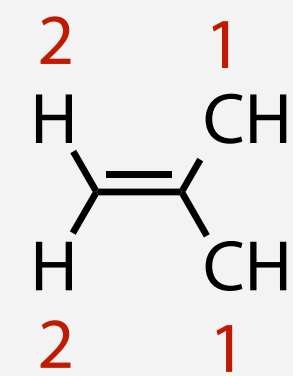
- an additional label is necessary to distinguish geometric isomers



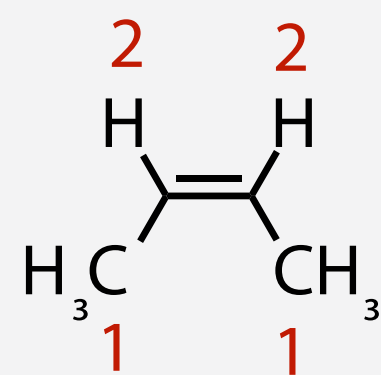
(*E*)-2-butene



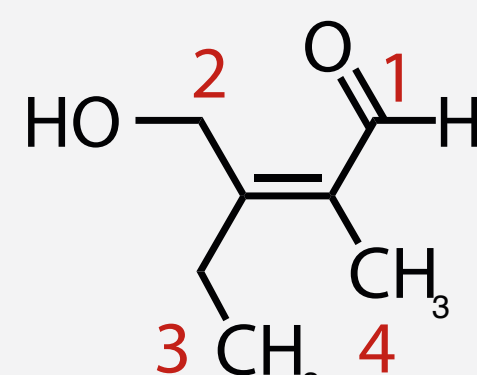
3-ethyl-4-hydroxy-2-methylbut-2*E*-enal



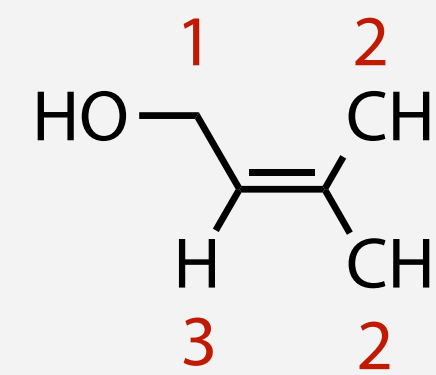
2-methylprop-1-ene
(no isomers)



(*Z*)-2-butene



3-ethyl-4-hydroxy-2-methylbut-2*Z*-enal

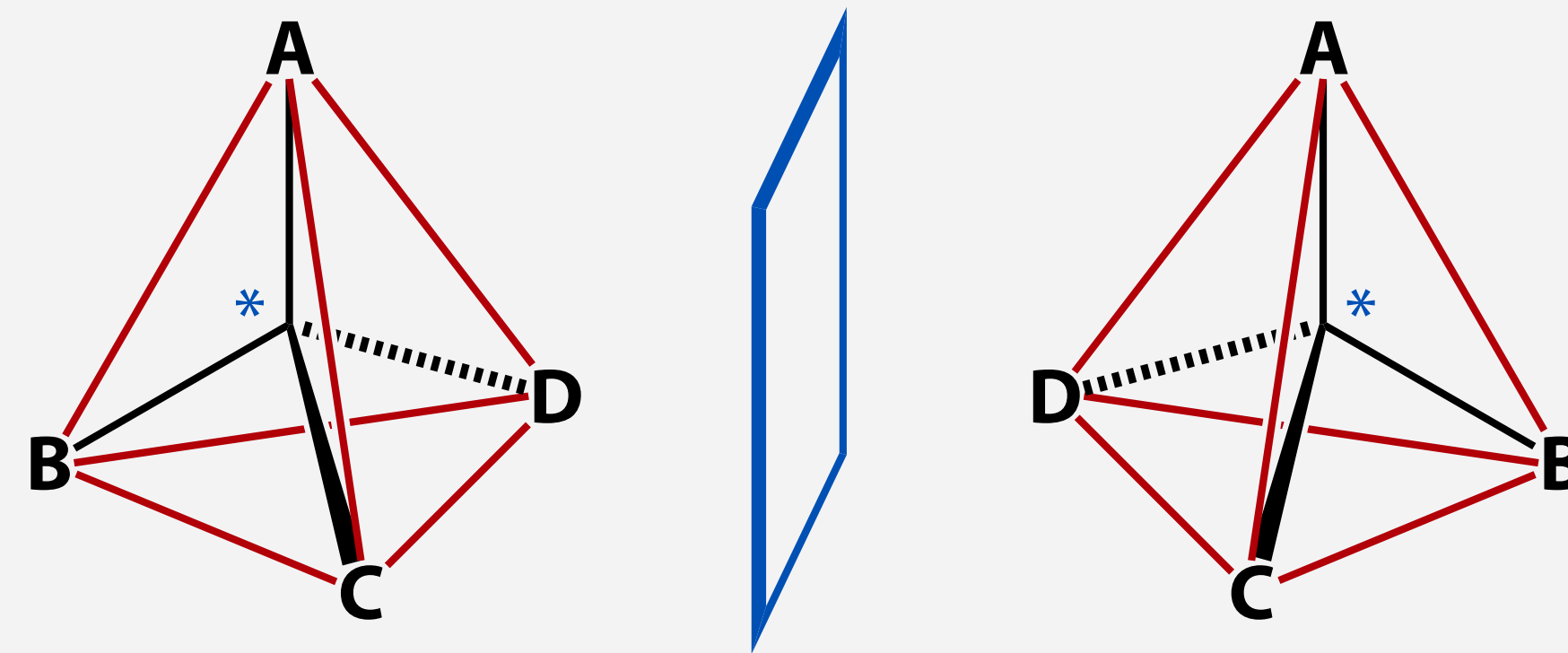


3-methylbut-2-en-1-ol
(no isomers)

- IUPAC nomenclature, following the “Cahn-Ingold-Prelog” rules**
 - assign priorities to substituents according to increasing atomic weight of connecting atom
 - if the first connecting atom is the same, proceed to next connected atoms (highest wins)
 - (*Z*) if the two higher priority substituents on each carbon are on same side of double bond
 - (*E*) if the two higher priority substituents on each carbon are on opposite sides
 - labels used as prefix or added to the number prefixes in the compound names

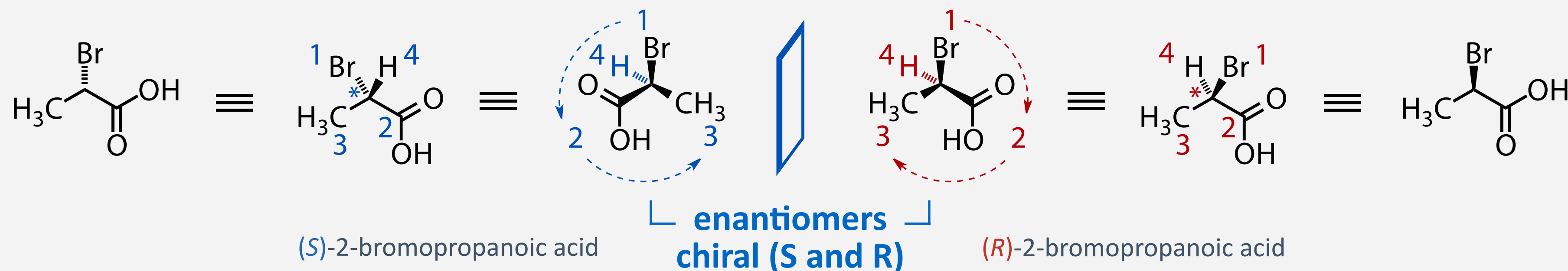
Stereocenters and Chirality

- tetrahedral carbon atoms with four different residues are called “stereocenters”



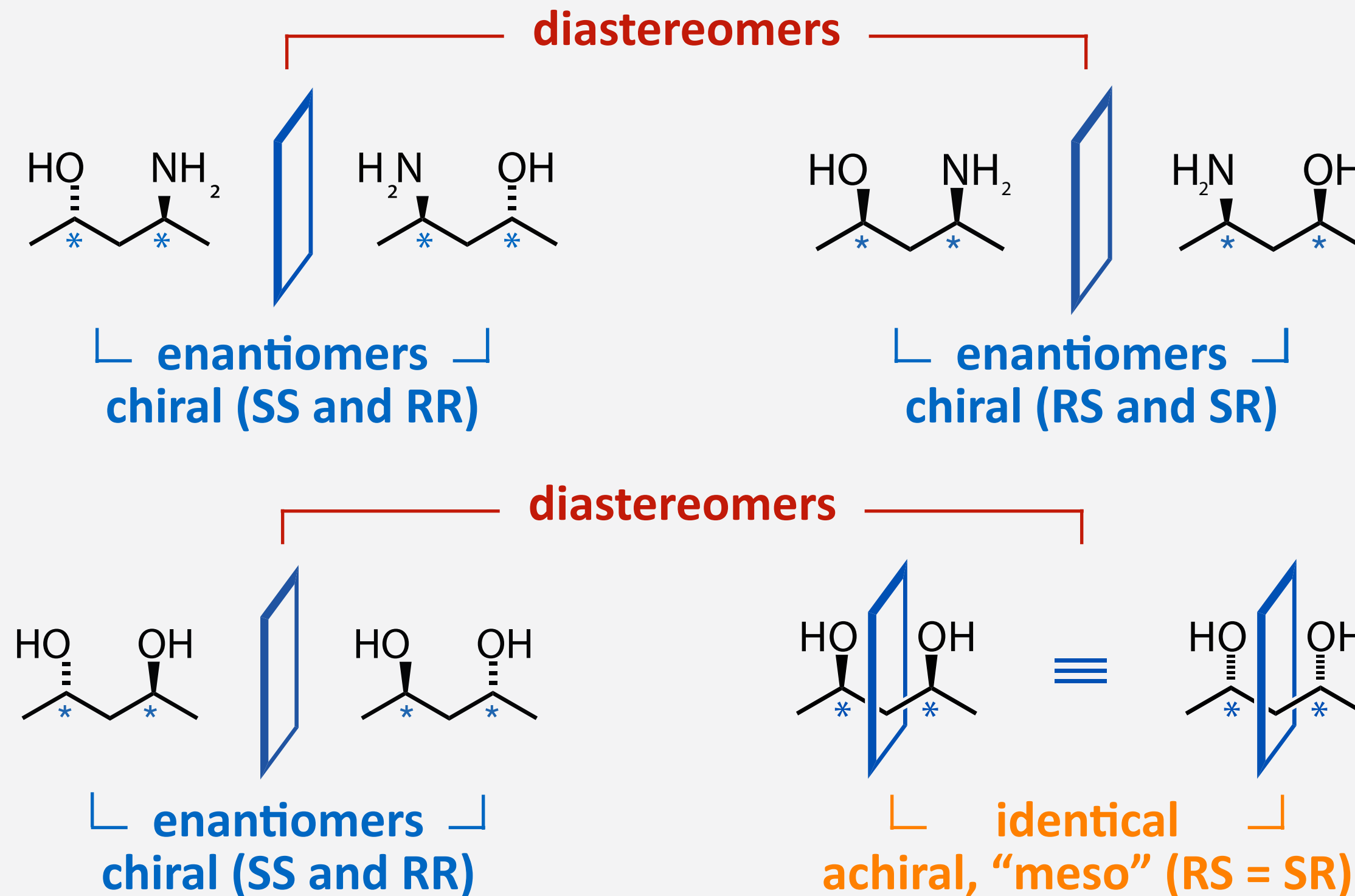
- the presence of **stereocenters** implies the **possibility** to observe **chirality** (“handedness”)
 - chirality requires absence of intramolecular mirror plane / inversion center
 - chiral molecules exist as two enantiomers (non-superimposable mirror images)
 - molecules with a single stereocenter **must** be chiral
 - molecules with more than one stereocenter **can** be chiral (see next slide)

Nomenclature of Stereocenters



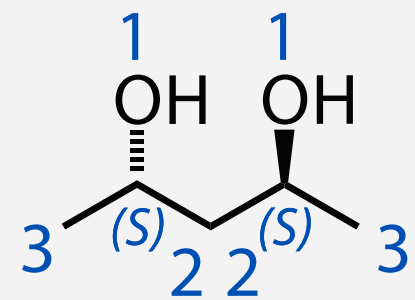
- IUPAC nomenclature, following the “Cahn-Ingold-Prelog” rules
 - assign priorities to substituents according to increasing atomic weight of connecting atom
 - if the first connecting atom is the same, proceed to the next connected atoms (highest priority wins)
 - turn the molecule such that the lowest priority substituent is pointing away from you
 - if substituents 1 → 2 → 3 are arranged clockwise, the configuration is *R* (for rectus/right)
 - if substituents 1 → 2 → 3 are arranged counter-clockwise, the configuration is *S* (for sinister/left)
- stereochemical notation is used as prefix or added to the number prefixes

Molecules with Multiple Stereocenters

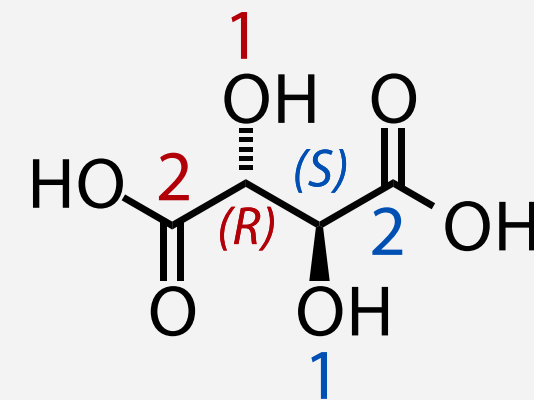


- molecules with multiple stereocenters can be chiral or achiral, depending on symmetry
 - chirality requires absence of an intramolecular mirror plane or inversion center
 - chiral molecules with n stereocenters exist as 2^{n-1} pairs of enantiomers (2^n stereoisomers)
 - stereoisomers with multiple stereocenters that are not enantiomers are diastereomers
 - molecules with multiple stereocenters but internal mirror plane are achiral

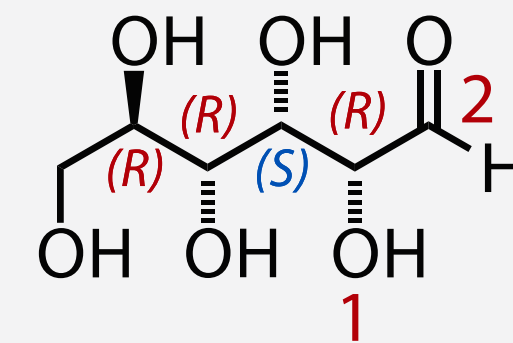
Examples of Molecules with Single and Multiple Stereocenters



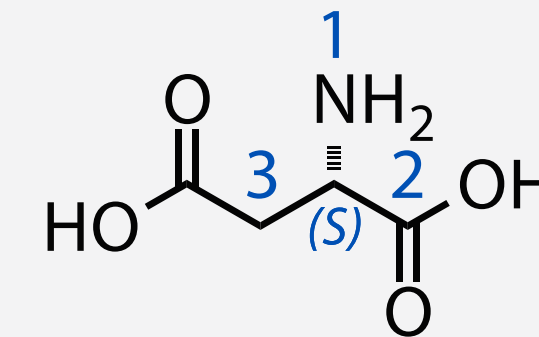
2S,4S-pentandiol



2S,3R-dihydropentandioic acid
D,L-tartric acid



2R,3S,4R,5R,6-pentahydroxyhexanal
D-glucose



2S-aminobutandioic acid
L-glutamic acid

Learning Outcomes

- differentiate different compounds, isomers, and identical compounds
- assign the type of isomer relationship between two molecules
- understand stereochemical notation in structure formulae
- name different conformers (using different stereochemical projections)
- assign stereochemistry of geometric isomers (E/Z, Cahn-Ingold-Prelog)
- find stereocenters and identify chirality
- differentiate enantiomers / diastereomers
- assign stereoconfiguration (R/S, Cahn-Ingold-Prelog)