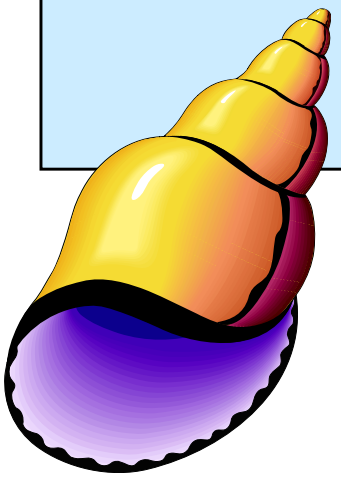
CHIRALITY, SYMMETRY PLANES AND ENANTIOMERS



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October 17th, 2008
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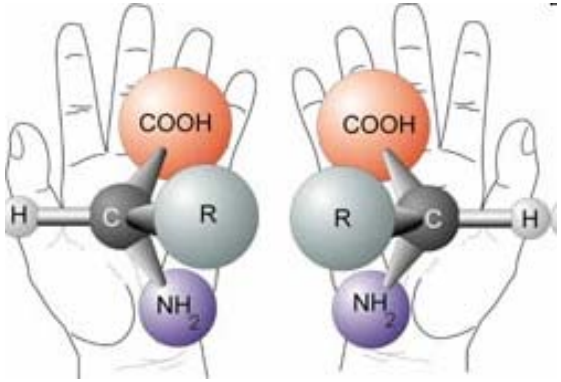
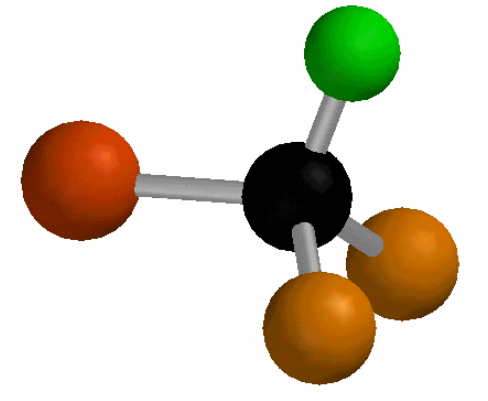
http://www.metabolomics.se/

(copies of slides can be downloaded from my homepage)

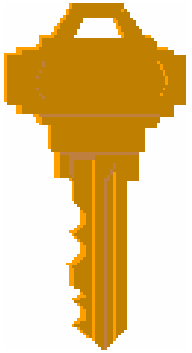




WHICH OBJECTS ARE SYMMETRIC ?

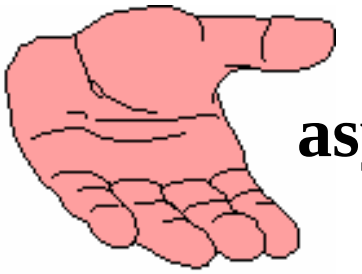
(mirror image is identical)

sym

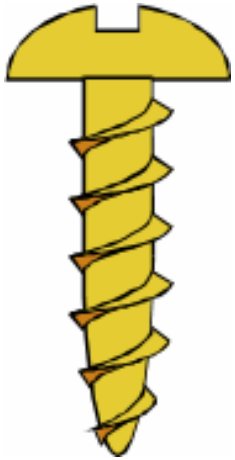


asym

sym (outside)

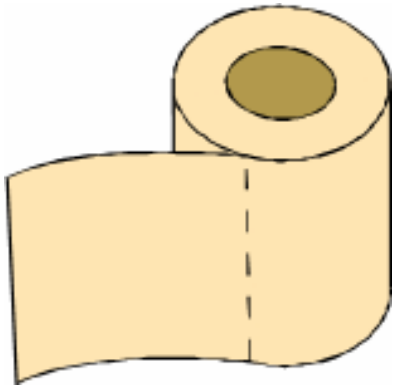


asym



asym

asym

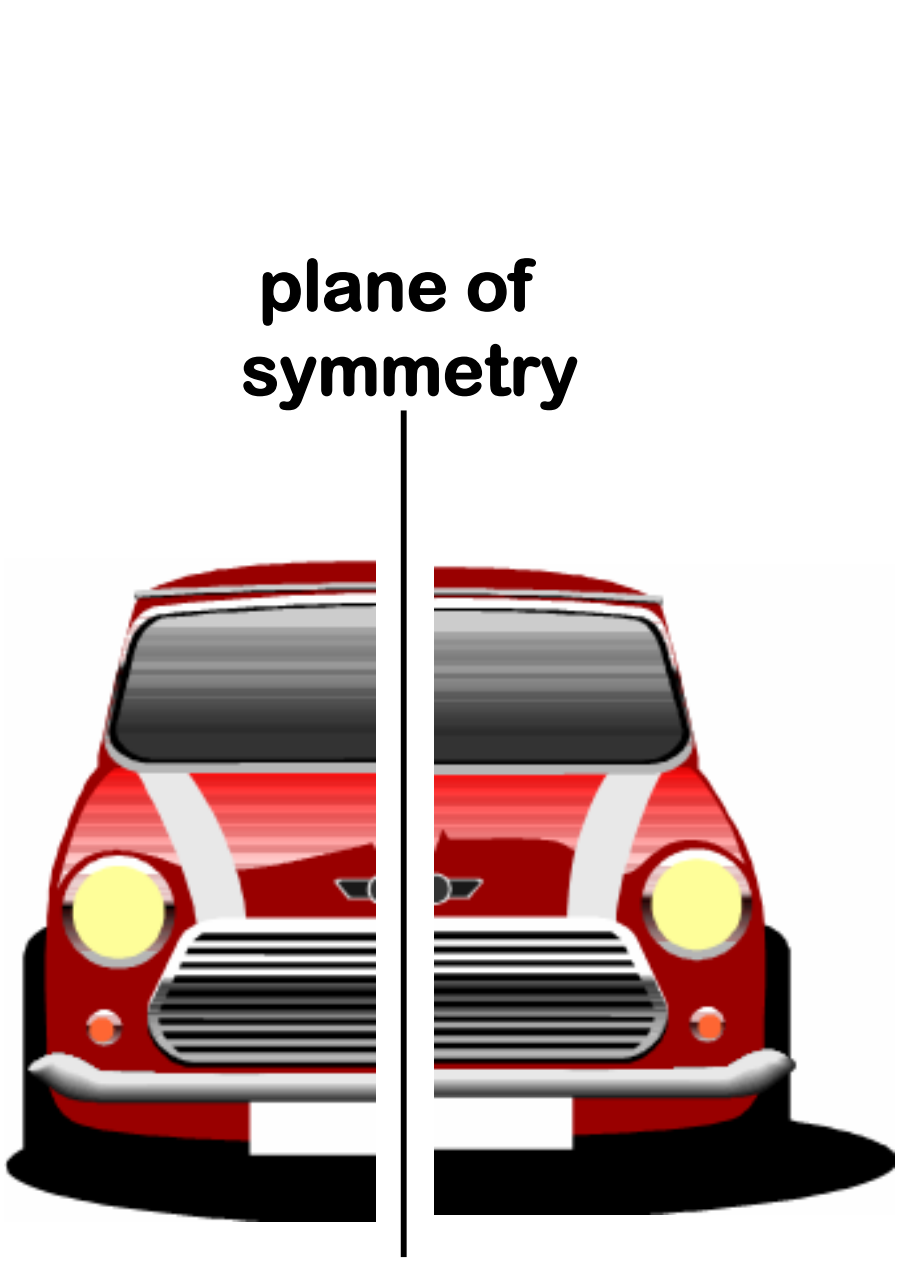


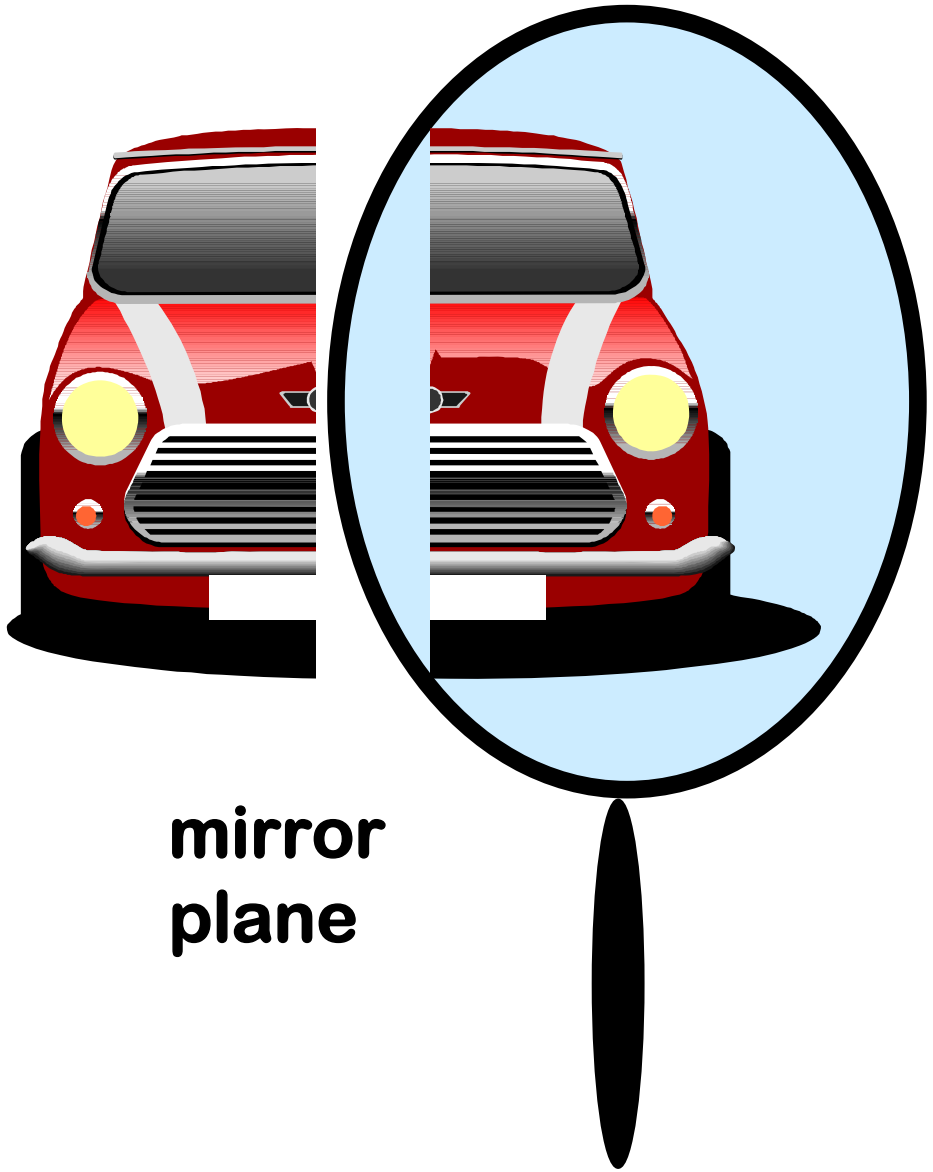
sym

sym

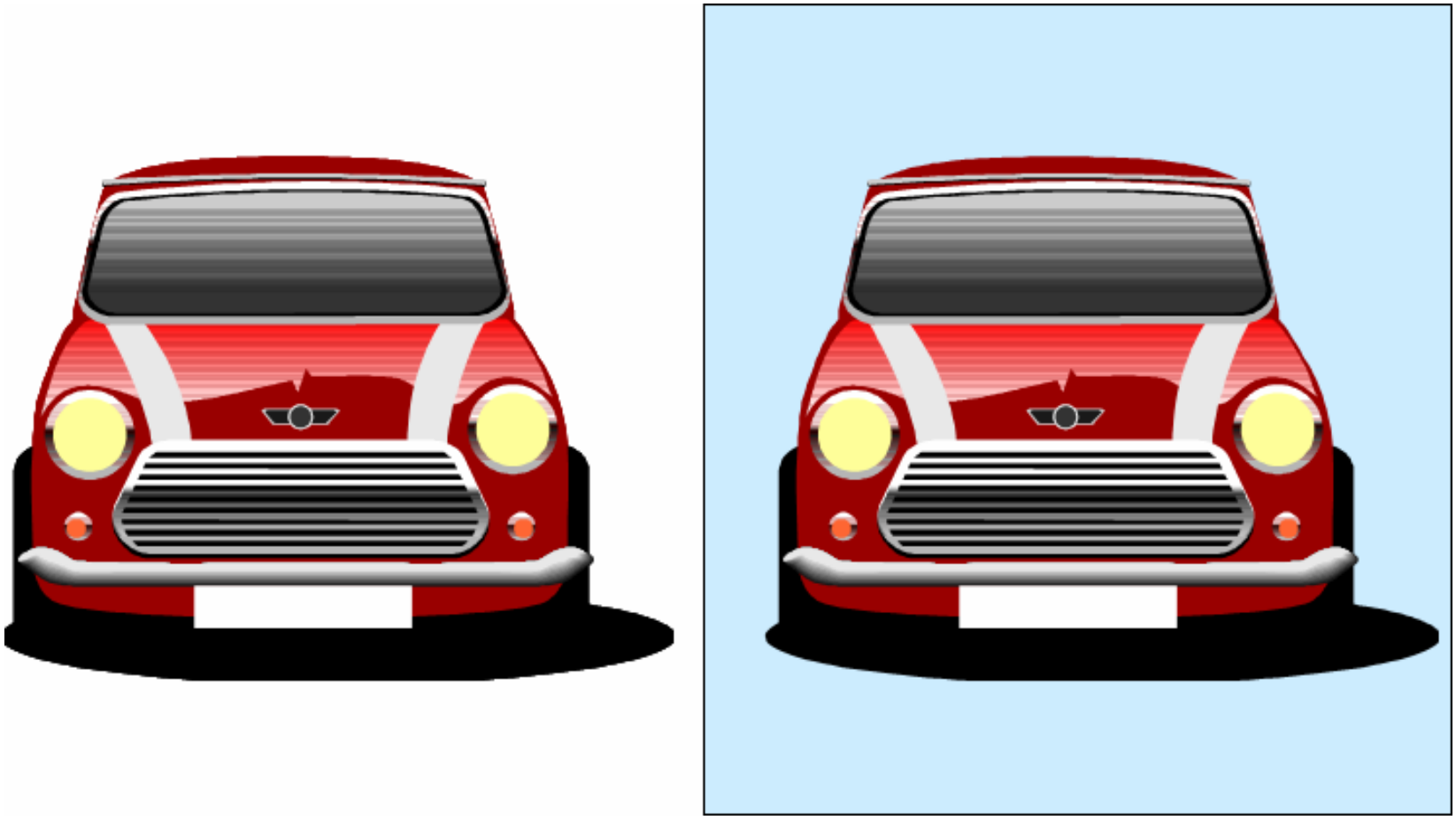
PLANES OF SYMMETRY

A SYMMETRIC OBJECT HAS A PLANE OF SYMMETRY
- ALSO CALLED A MIRROR PLANE





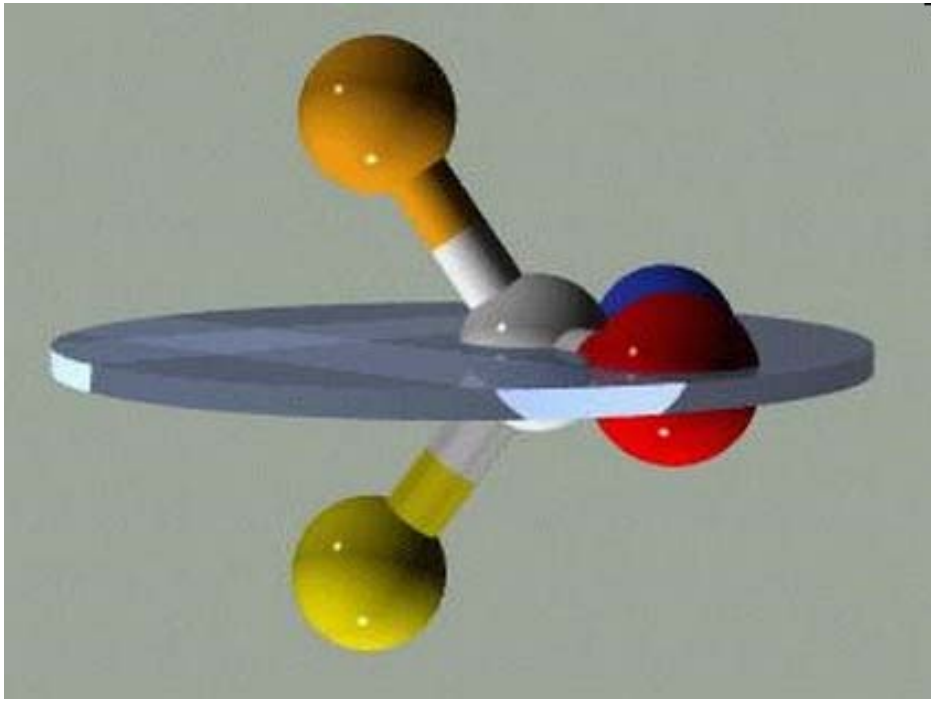
IF AN OBJECT HAS A PLANE OF SYMMETRY, ITS MIRROR IMAGE WILL BE IDENTICAL



IDENTICAL MIRROR IMAGES WILL SUPERIMPOSE

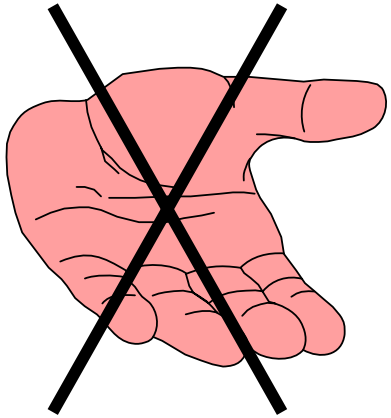
(MATCH EXACTLY WHEN PLACED ON TOP OF EACH OTHER)

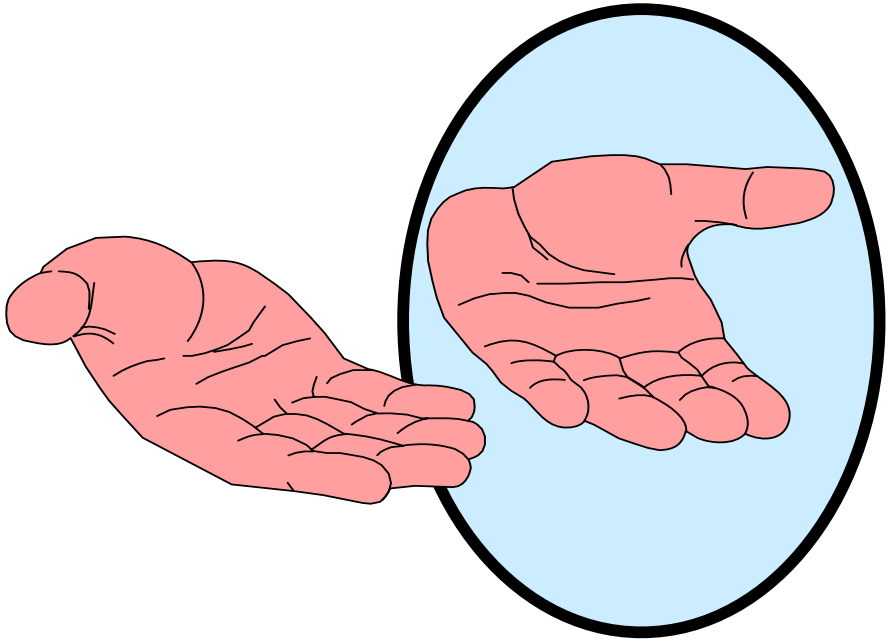
CHIRALITY



An object without symmetry is CHIRAL

no symmetry



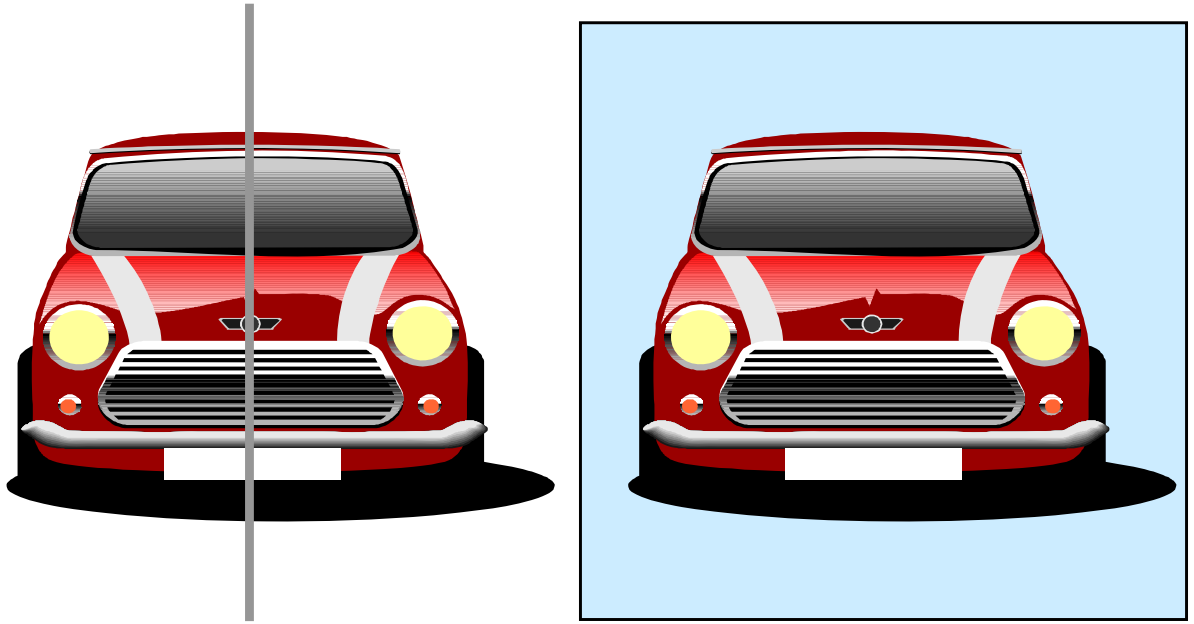


The mirror image of a chiral object is different and will not superimpose on the original object.

OBJECTS WHICH ARE CHIRAL HAVE A SENSE OF "HANDEDNESS" AND EXIST IN TWO FORMS

An object with symmetry is ACHIRAL (not chiral)

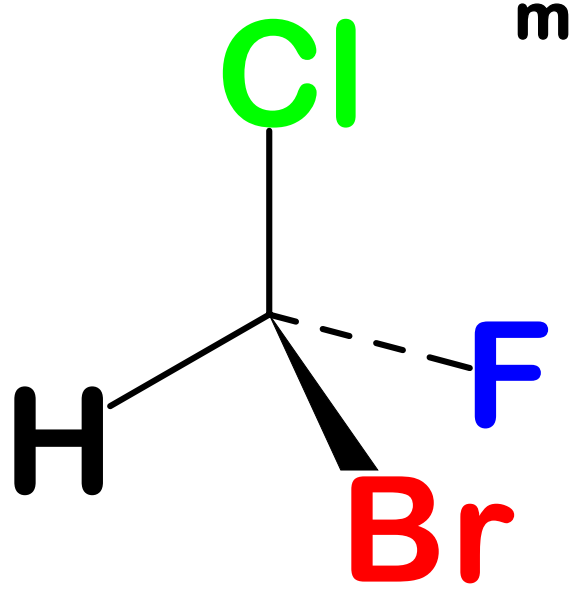
The mirror image of an achiral object is identical and will superimpose on the original object.

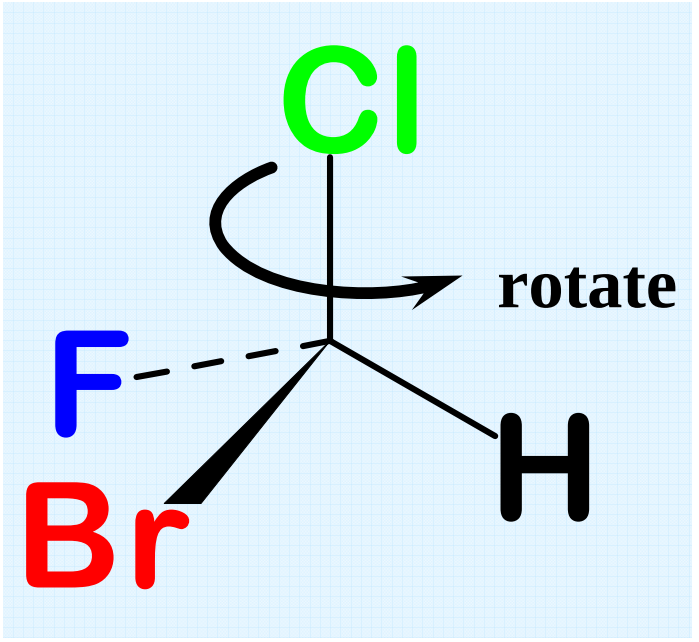


plane of symmetry

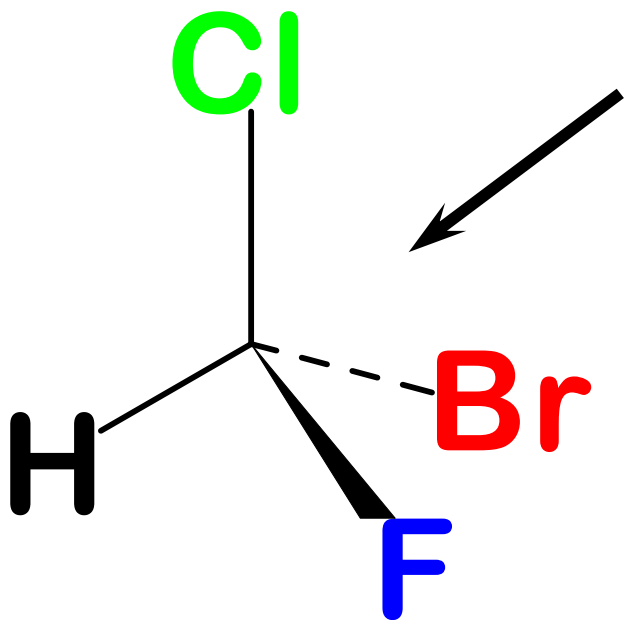
ENANTIOMERS

non-superimposable
mirror images

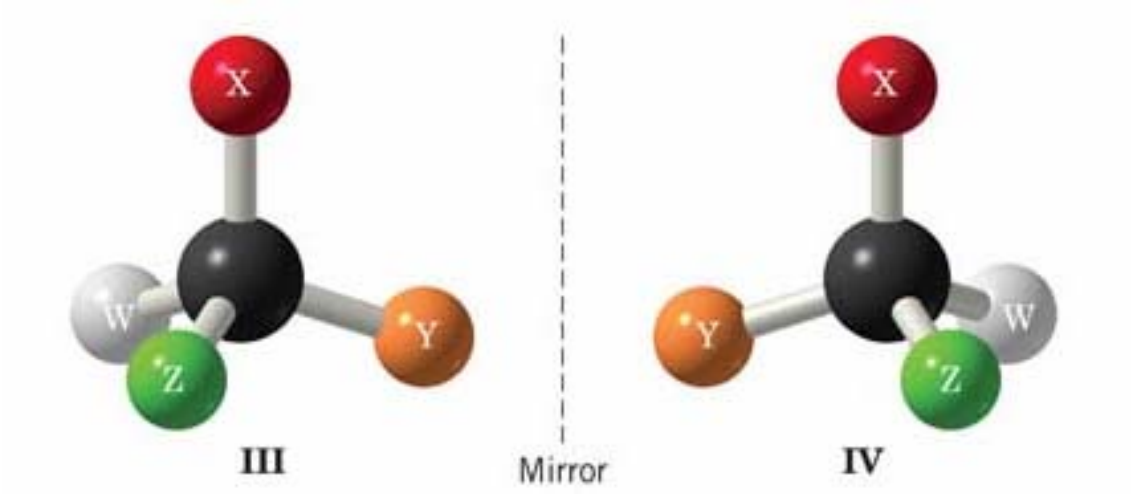


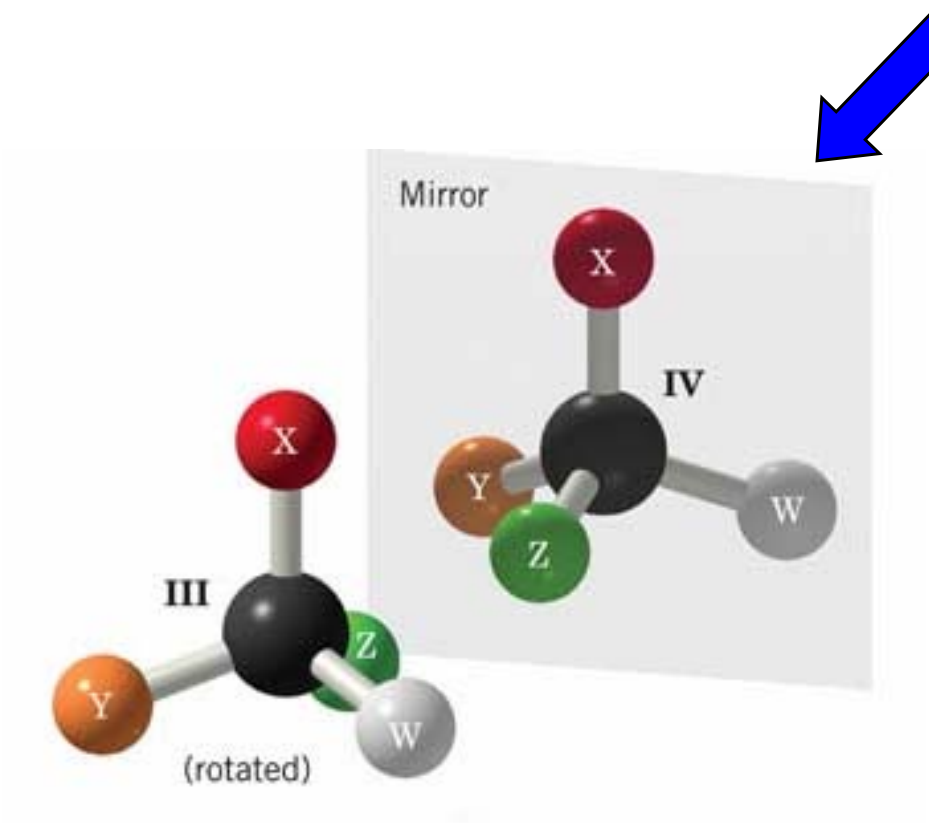


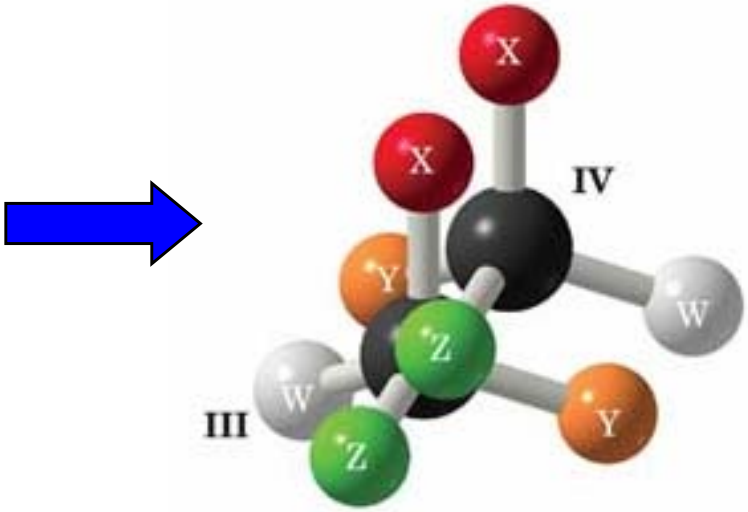
this molecule
is chiral



note that the fluorine and bromine have been interchanged in the enantiomer





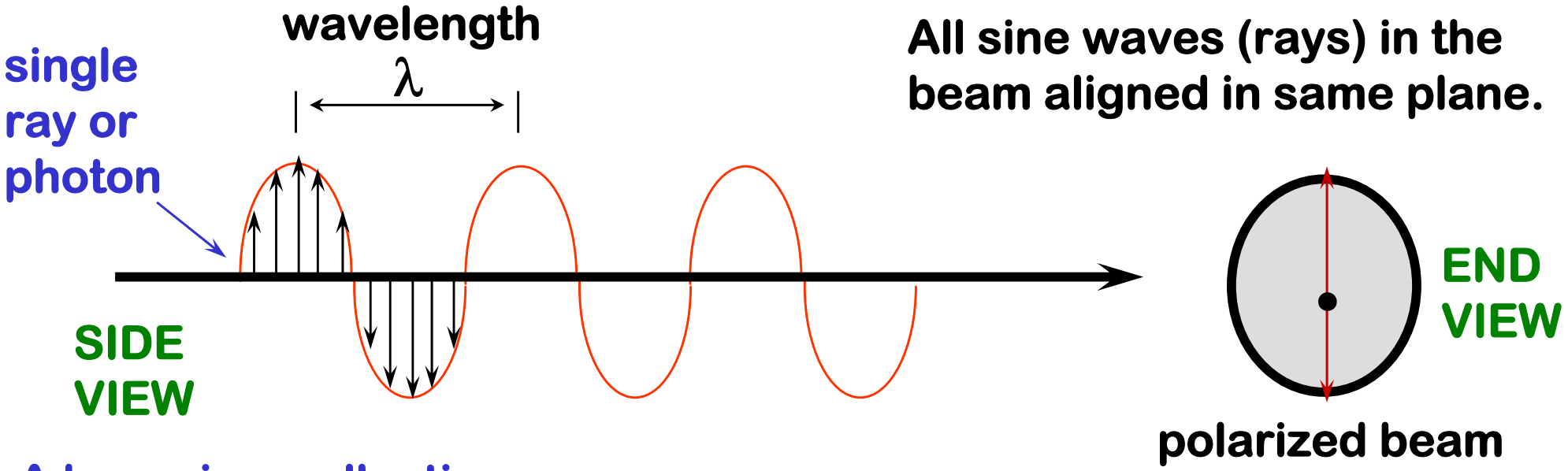


non-superimposable

OPTICAL ACTIVITY

PLANE-POLARIZED LIGHT

PLANE-POLARIZED LIGHT BEAM



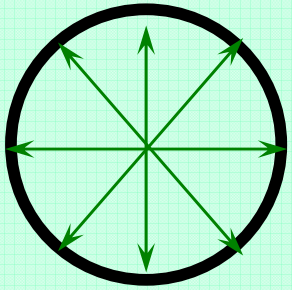
A beam is a collection of these rays.

frequency (ν)

$$\nu = \frac{c}{\lambda}$$

c = speed of light

NOT PLANE-POLARIZED



Sine waves are not aligned in the same plane.

unpolarized beam

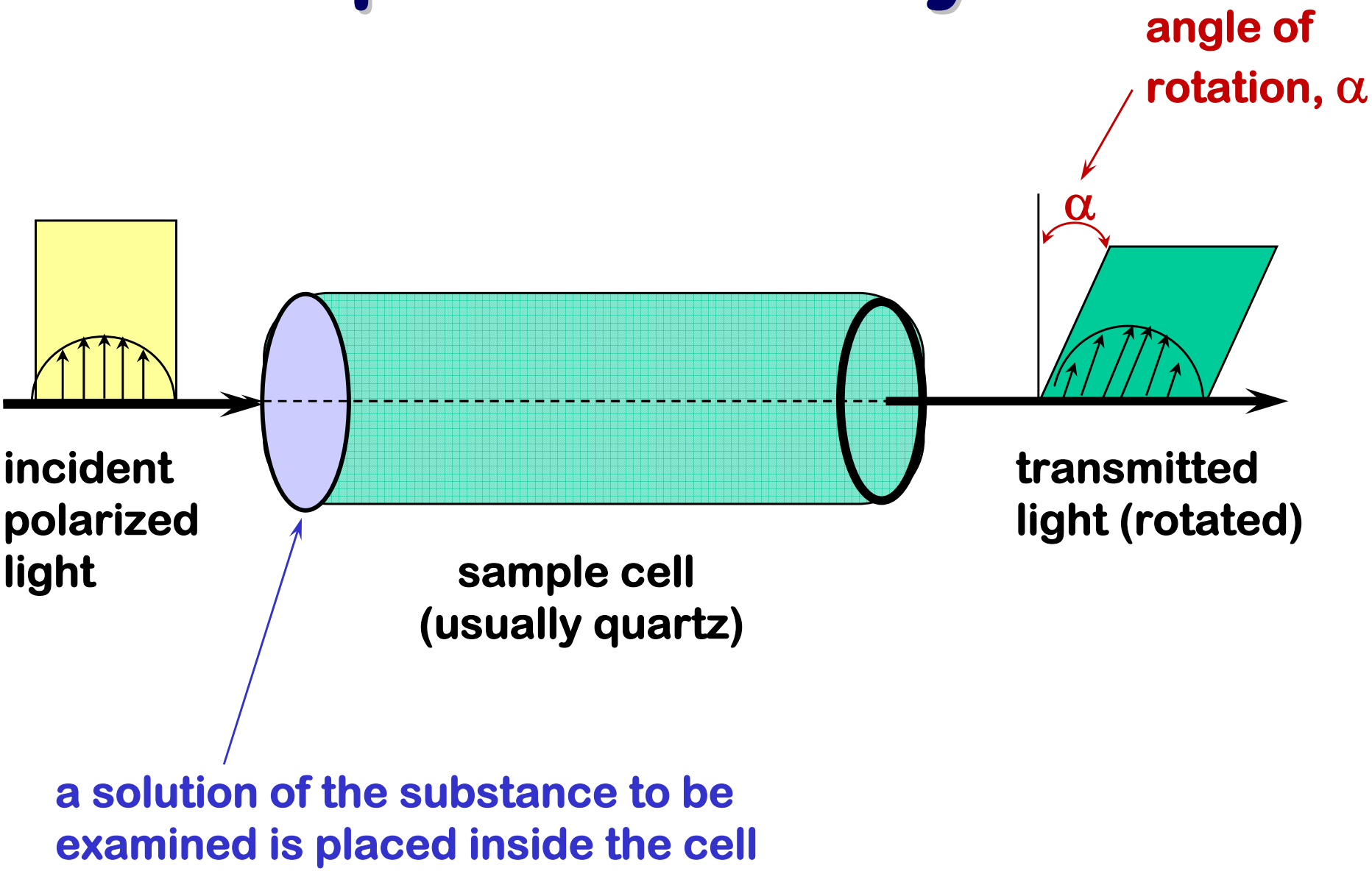
Optically Active

- **Refers to molecules that interact with plane-polarized light**

Jean Baptiste Biot
French Physicist - 1815

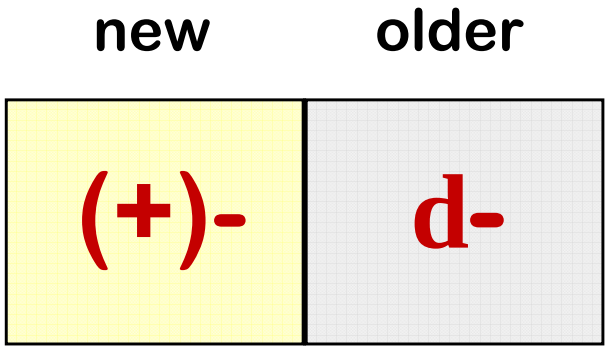
He discovered that some natural substances (glucose, nicotine, sucrose) rotate the plane of plane-polarized light and that others did not.

Optical Activity



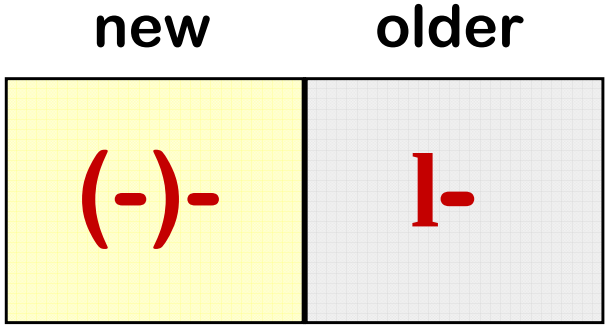
TYPES OF OPTICAL ACTIVITY

Dextrorotatory



Rotates the plane of plane-polarized light to the right.

Levorotatory

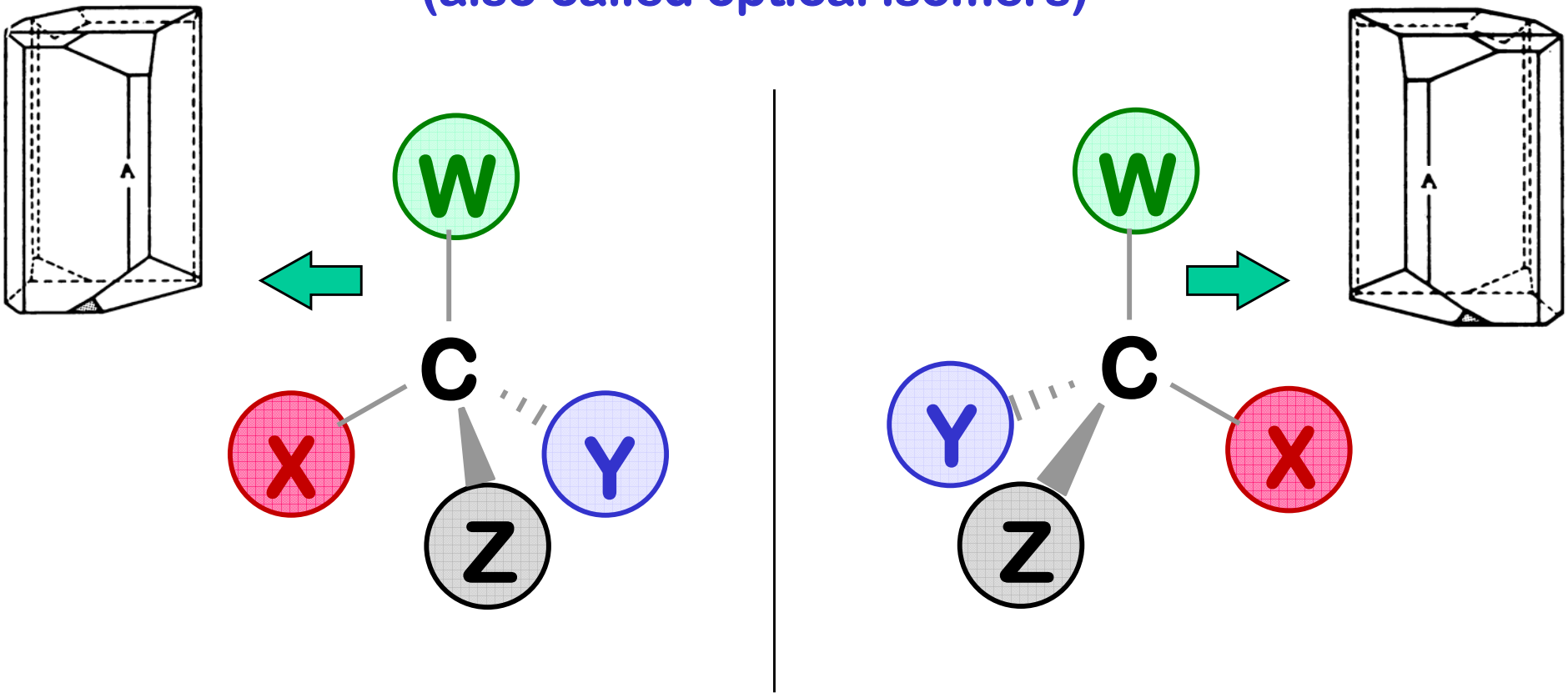


Rotates the plane of plane-polarized light to the left.

Enantiomers

non-superimposable mirror images

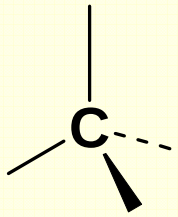
(also called optical isomers)



Pasteur decided that the molecules that made the crystals, just as the crystals themselves, must be mirror images. Each crystal must contain a single type of enantiomer.

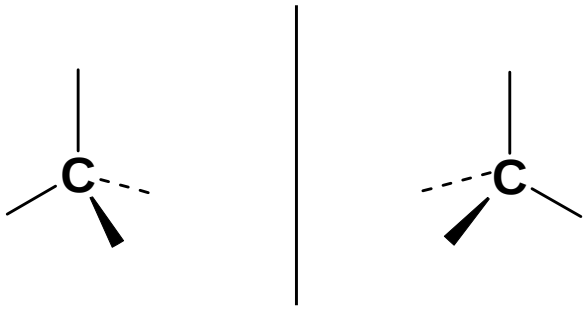
Pasteur's hypothesis eventually led to the discovery that tetravalent carbon atoms are tetrahedral.

Van't Hoff and LeBel (1874)

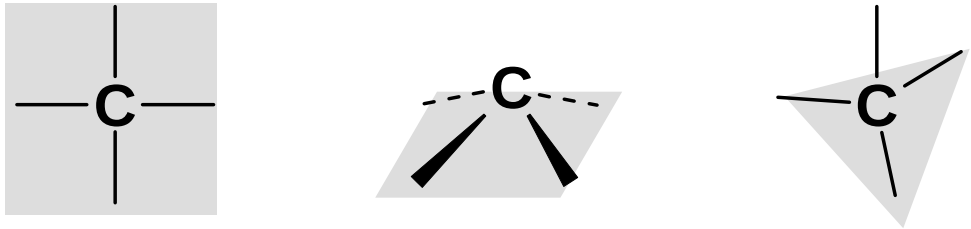


tetrahedral carbon

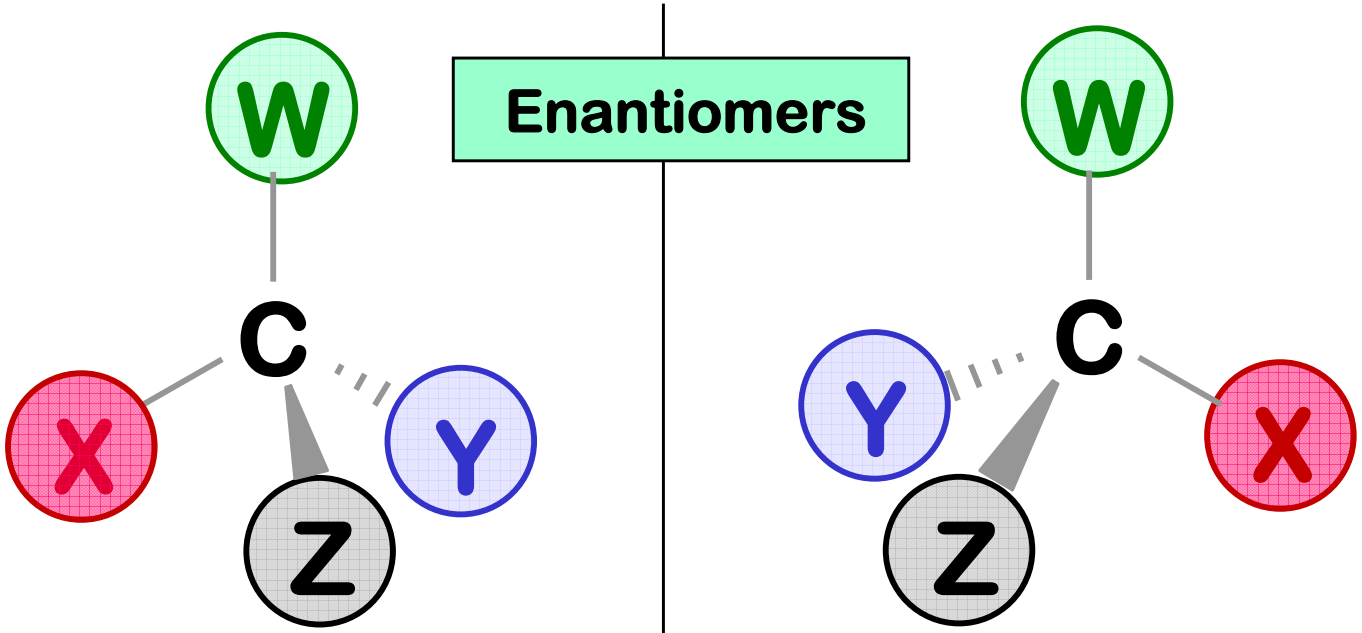
Only tetrahedral geometry can lead to mirror image molecules:



Square planar, square pyrimidal or trigonal pyramid will not work:



ENANTIOMERS HAVE EQUAL AND OPPOSITE ROTATIONS



(+)-nn°

(-)-nn°

dextrorotatory

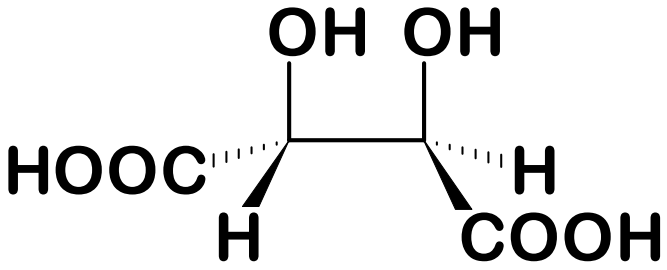
levorotatory

ALL OTHER PHYSICAL PROPERTIES ARE THE SAME

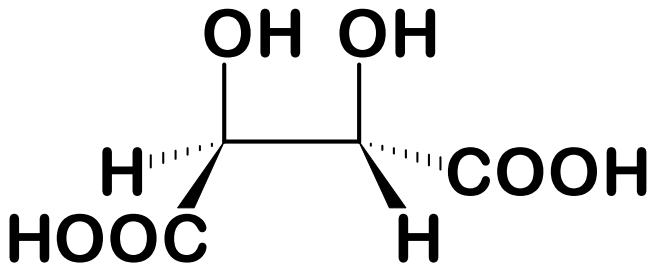
TARTARIC ACID

from fermentation of wine

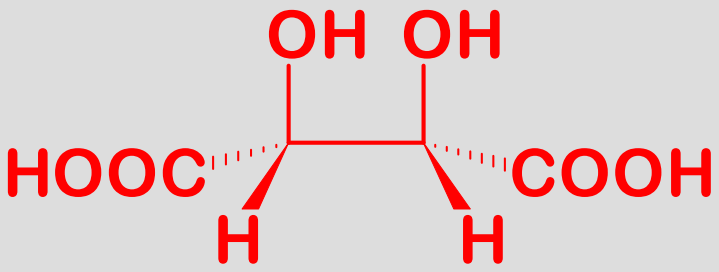
Enantiomers



(+)-tartaric acid



(-)-tartaric acid



***meso*-tartaric acid**

ALSO FOUND
(as a minor component)

$[\alpha]_D = 0$

more about this compound later

TARTARIC ACID

(-) - tartaric acid

$[\alpha]_D = -12.0^o$

mp 168 - 170°
solubility of 1 g
0.75 mL H_2O
1.7 mL methanol
250 mL ether
insoluble $CHCl_3$
d = 1.758 g/mL

(+) - tartaric acid

$[\alpha]_D = +12.0^o$

mp 168 - 170°
solubility of 1 g
0.75 mL H_2O
1.7 mL methanol
250 mL ether
insoluble $CHCl_3$
d = 1.758 g/mL

meso - tartaric acid

$[\alpha]_D = 0^o$

mp 140°
d = 1.666 g/mL

solubility of 1 g
0.94 mL H_2O
insoluble $CHCl_3$

RACEMIC MIXTURE

an equimolar (50/50) mixture of enantiomers

$$[\alpha]_D = 0^o$$

the effect of each molecule is cancelled out by its enantiomer

STEREOISOMERS

ENANTIOMERS are a type of STEREOISOMER

Stereoisomers are the same constitutional isomer, but differ in the way they are arranged in 3-D space at one or more of their atoms.

STEREOCENTERS

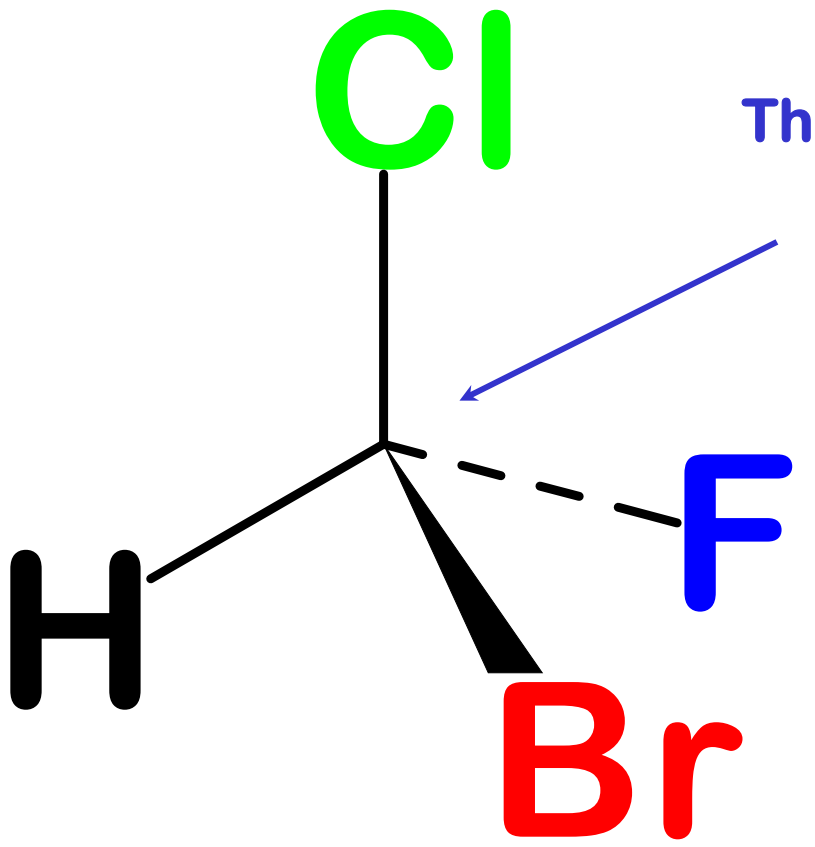
One of the ways a molecule can be chiral is to have a stereocenter

A stereocenter is an atom, or a group of atoms, that can potentially cause a molecule to be chiral

stereocenters - can give rise to chirality

STEREOGENIC CARBONS

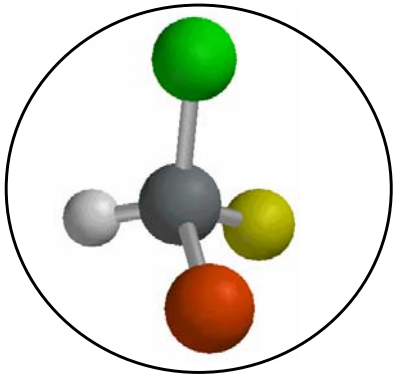
(called “chiral carbons” in older literature)



This is one type of ….

stereocenter

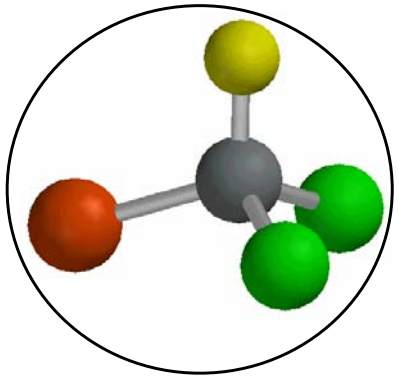
…. others are possible



A **stereogenic carbon** is tetrahedral and has four different groups attached.

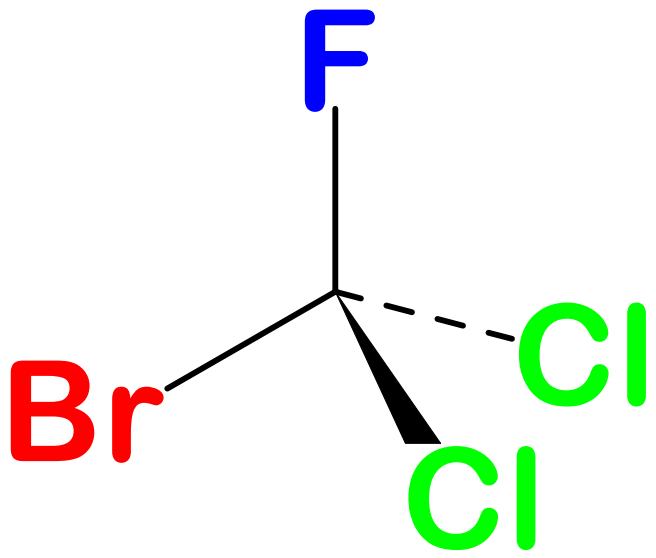
H
F
Cl
Br

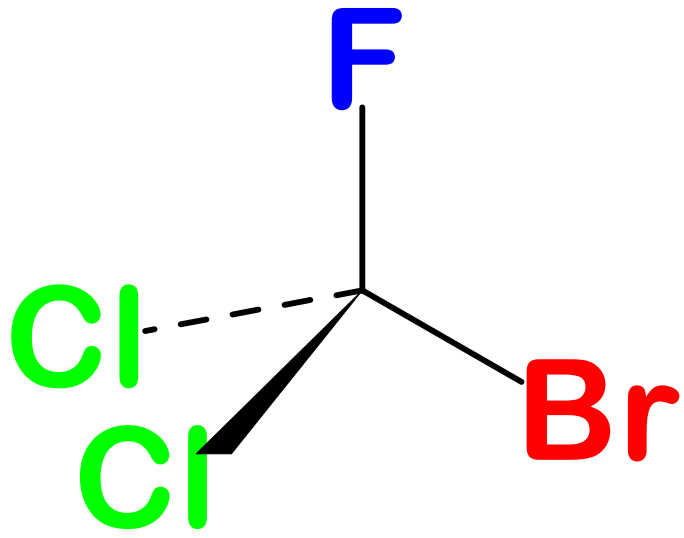
F
Cl
Br



ACHIRAL

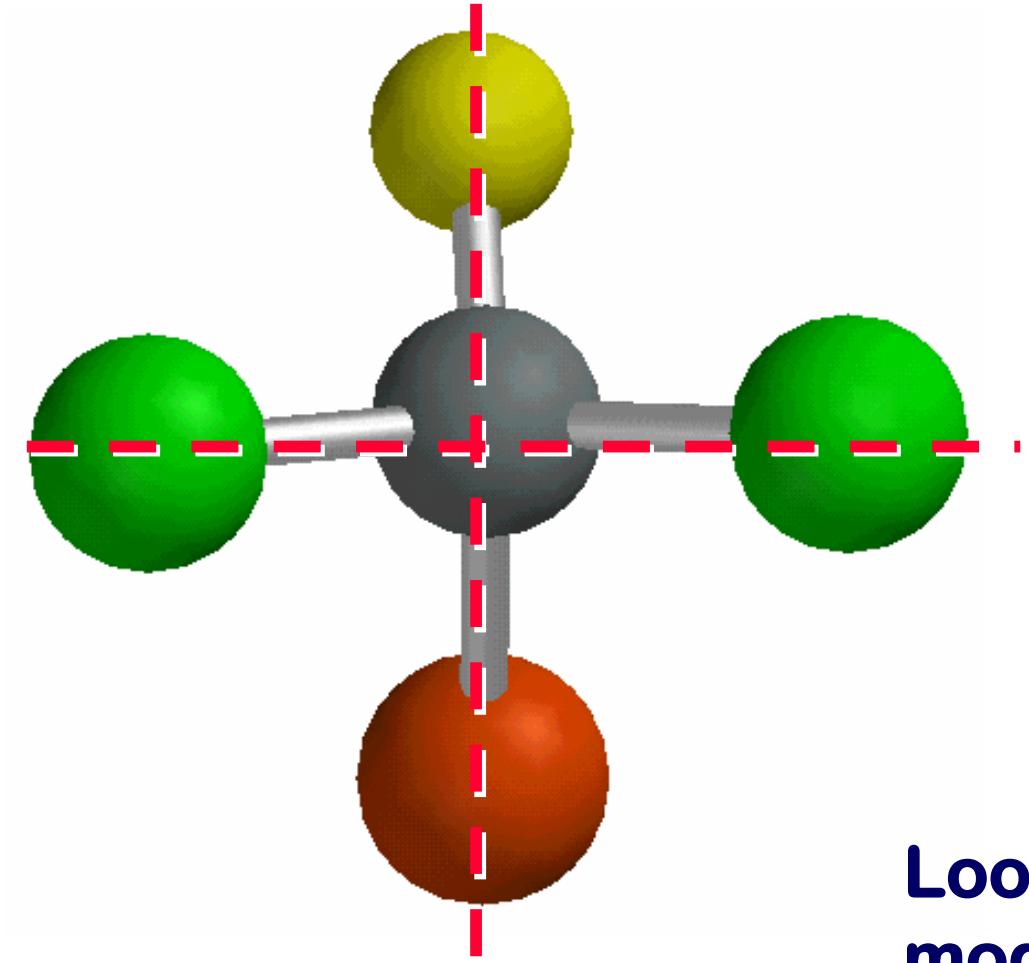
The plane of the paper is a plane of symmetry





TWO IDENTICAL GROUPS RENDERS A TETRAHEDRAL CARBON ACHIRAL

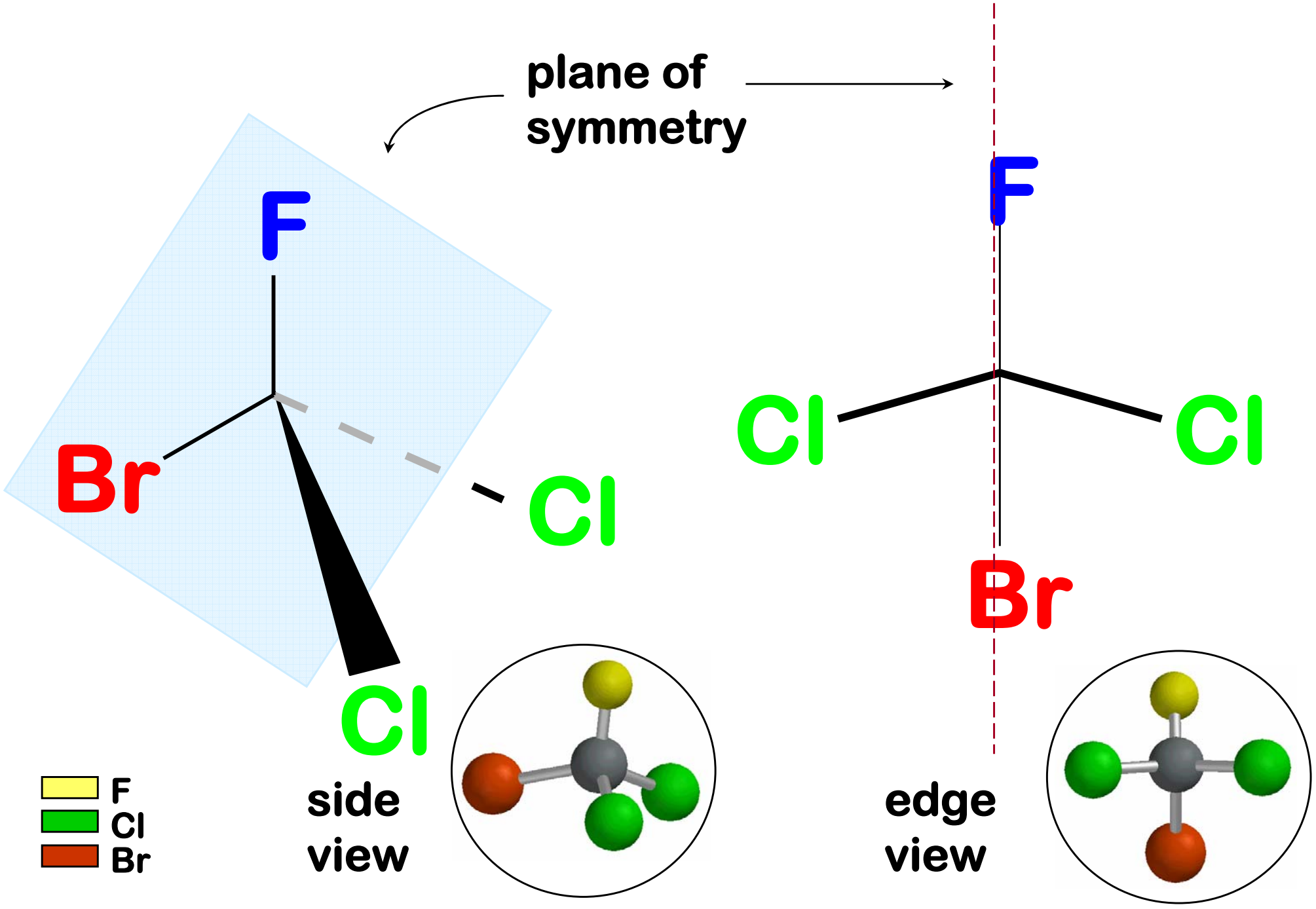
ONE PAIR OF ATOMS ATTACHED TO A TETRAHEDRAL CARBON IS IN A PLANE PERPENDICULAR TO THE OTHER PAIR



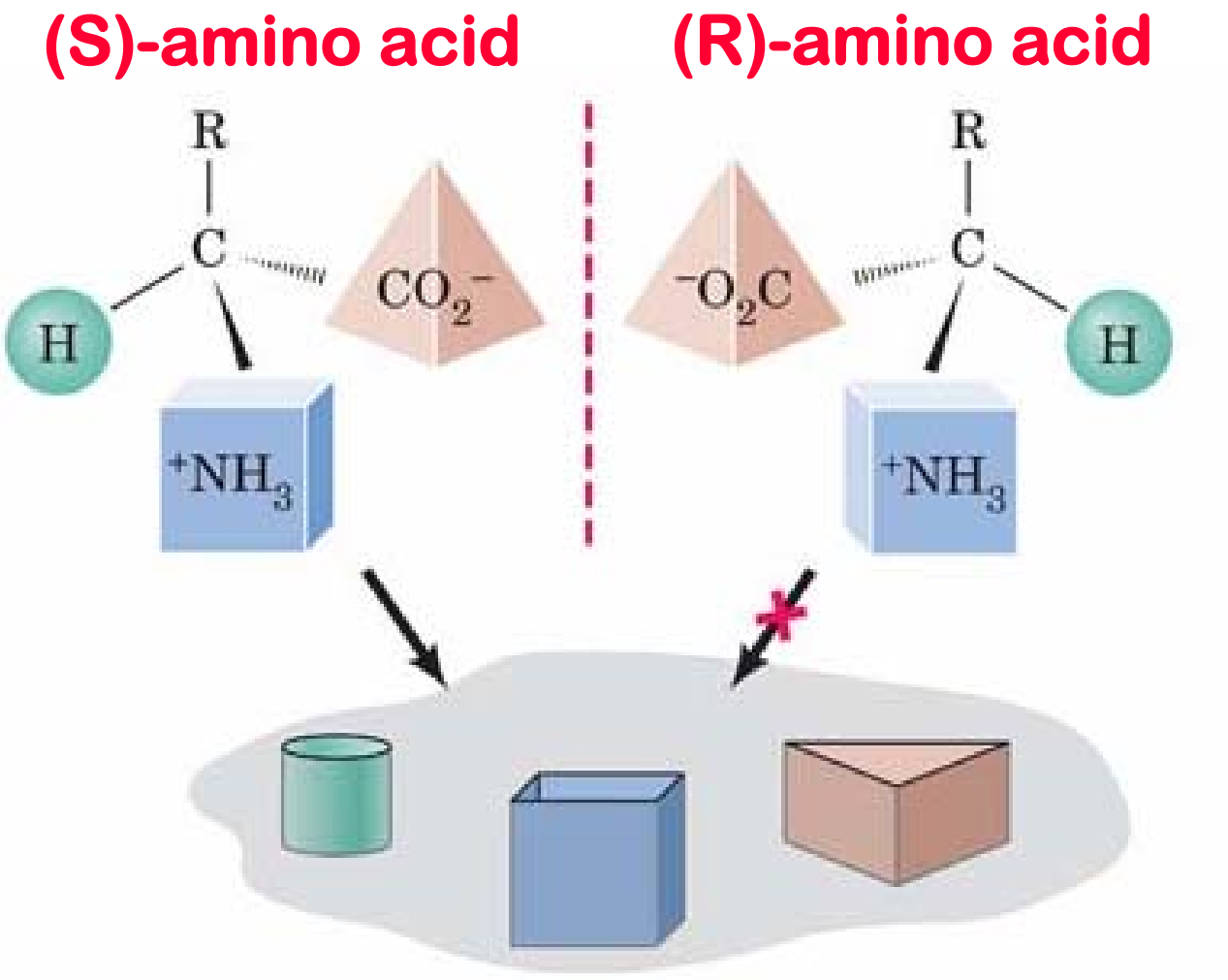
F
Cl
Br

Look at your model set !!!!

TWO VIEWS OF THE PLANE OF SYMMETRY



Biological role of stereochemistry



Only one of the 2 amino acid enantiomers can achieve 3-point binding with the enzyme binding site