Properties of Stereoisomers

UCI Chem 51A
Dr. Link

Goals

- After this lesson you should be able to:
  - Calculate specific rotation
  - Identify a racemic mixture
  - Calculate enantiomeric excess
  - Calculate ratios of enantiomers in a mixture
  - Explain differences in chemical properties of enantiomers

Stereoisomer Review

* Enantiomers: mirror images, not superimposable, all stereocenters inverted
* Diastereomers: not mirror images, not superimposable, some (but not all) stereocenters inverted

Physical Properties

Diastereomers

different MPs

different BPs

different polarities*

Can be separated by various physical means.

Enantiomers

same MPs

same BPs

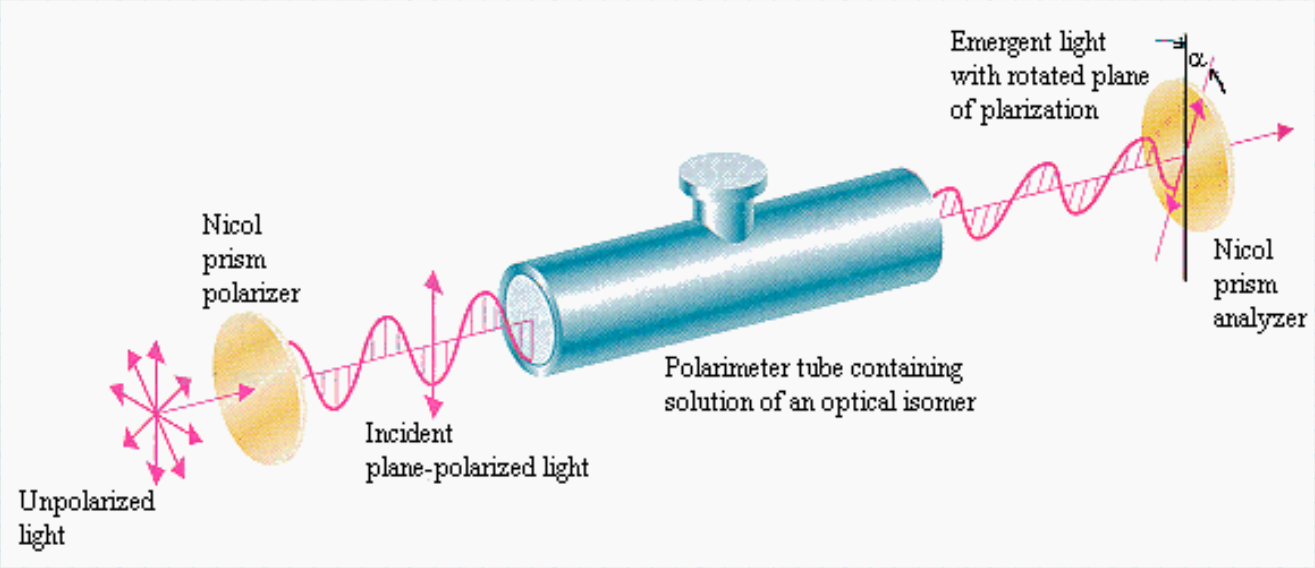
same polarities

different optical rotation!

Can only be separated by special techniques.

Optical Rotation

* Rotation of plane-polarized light



http://chemed.chem.purdue.edu/genchem/topicreview/bp/1organic/chirality.html

Enantiomeric Excess

* Enantiomers rotate plane-polarized light in opposite directions (+ & -).
* racemic mixture: equal amounts of both enantiomers, no optical rotation observed
* What if the quantities are not equal?

Specific Rotation

* specific rotation: optical rotation observed under specific conditions
  * 1.0 dm tube length
  * 1 g/mL concentration
  * 589 nm light wavelength (rarely changes)

Calculating specific rotation

$$[\alpha] = \frac{\alpha}{l \times c}$$

R/S vs (+)/(-)

Calculating %EE

$$\%ee = \frac{[\alpha]_{obs}}{[\alpha]_{std}} \times 100$$

Also...

%ee = %enantiomer A - %enantiomer B

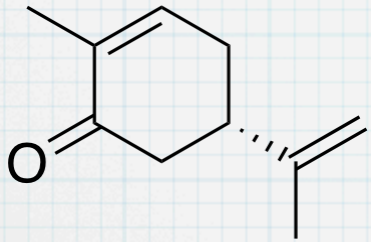
How much of each enantiomer do we have?

Totals

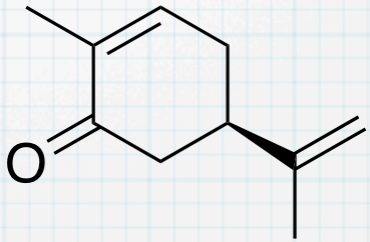
(-) (+)

Why Do Enantiomers Matter?

* Smell!

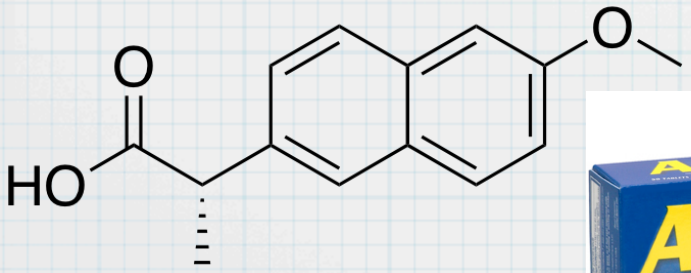


(S)-carvone

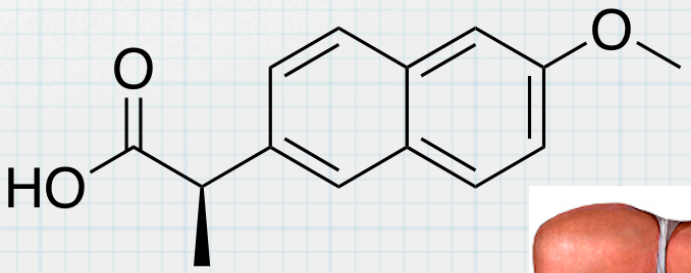


(R)-carvone

* Biological systems!



naproxen



liver toxin!

Some Optical Rotation Resources

* How molecule rotate plane-polarized light: http://physics.unl.edu/~tgay/content/OA2.html
* Visuals of polarized light and rotation: http://dl.clackamas.cc.or.us/ch106-07/optical.htm
* Video of optical rotation: http://www.youtube.com/watch?v=HuHphmJw-fA

Wrapping Up

* Practice working with specific rotation equation
* Practice calculating %ee
* Practice determining quantities of each enantiomer present