ORGANIC CHEMISTRY 1 LECTURE GUIDE 2019

BY RHETT C. SMITH

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Executive Editor: Rhett C. Smith, Ph.D. You can reach him through our office at: IQ@protonguru.com

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Organic Chemistry 1
Lecture Guide 2019

By Rhett C. Smith, Ph.D.

Companion Books from the Proton Guru:

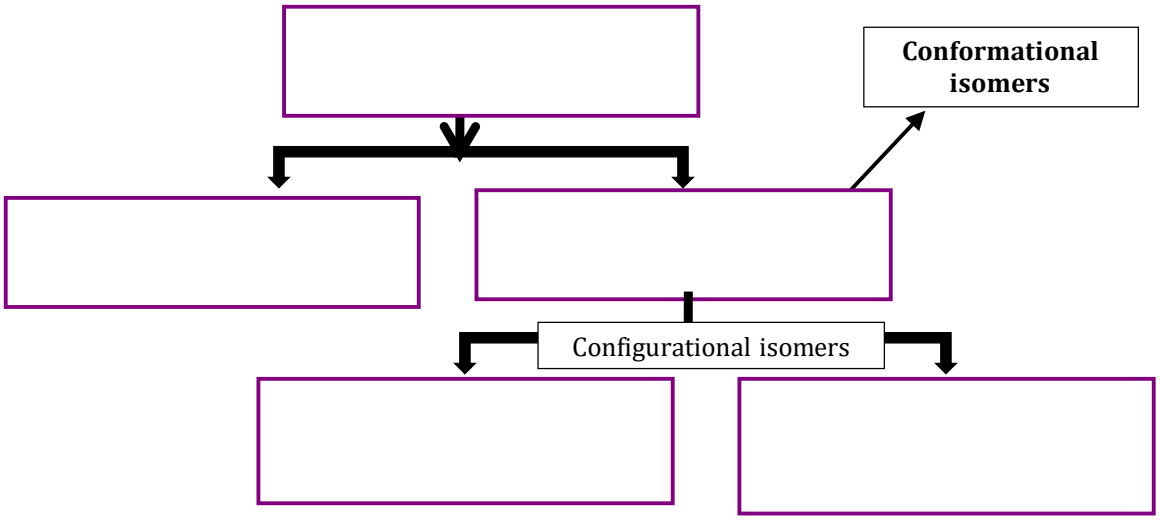
Organic Chemistry 1 Reactions and Practice Problems 2019

by Rhett C. Smith

Organic Chemistry 1 Primer 2019,

by Rhett C. Smith, Andrew G. Tennyson, and Tania Houjeiry

Lecture Topic I.17-20: Stereochemistry
Types of Isomerism



Notes

Lecture Topic I.17-20: Stereochemistry
Definitions

Stereoisomers:

A

Conformational stereoisomers:

B

- staggered and eclipsed conformers
- *gauche* and *anti* conformers
- Chair or boat chair conformers of cyclohexane

Configurational stereoisomers:

C

NOW:

enantiomers:

D

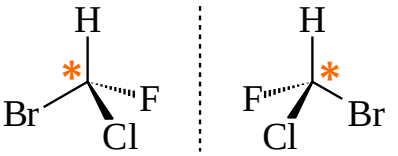
diastereomers:

E

Notes

Molecules with "handedness" possess (A)

and are (B)



These are nonsuperimposable mirror images; using definitions on the previous slide, this is a pair of **enantiomers** ("left- and right-handed" isomers). The molecule is chiral and possesses a **chiral** (**stereogenic**) **center** (also called a **stereocenter**). These centers can be labeled with asterisks for clarity.

(C)

Notes

A For a carbon atom to be a stereocenter it must:

B

A molecule WITHOUT a stereocenter is

C

If the molecule has a **plane of symmetry** it is

D

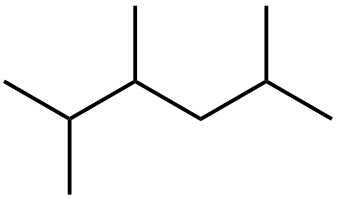
A molecule with a stereocenter **and** a plane of symmetry is achiral.

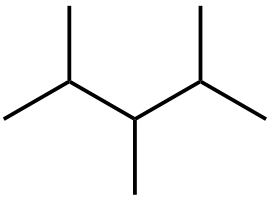
E example:

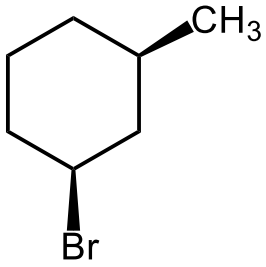
Such compounds are called **meso** compounds.

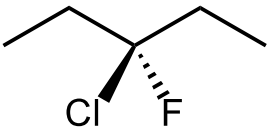
Notes

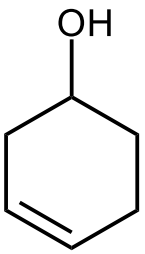
Mark the stereocenters with asterisks.

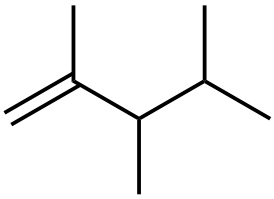












Notes

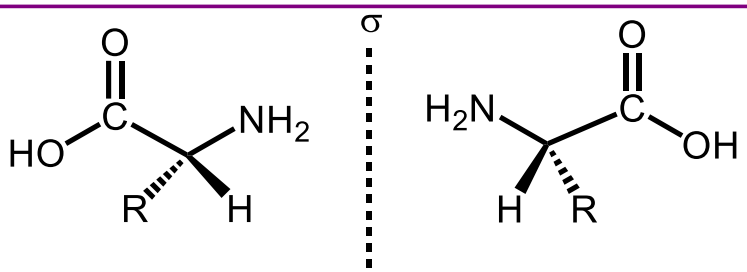
Many physical properties of enantiomers are **IDENTICAL**

A

Two Enantiomers can interact very differently with other chiral molecules. **This is especially important in biological systems!**

1. Amino acids

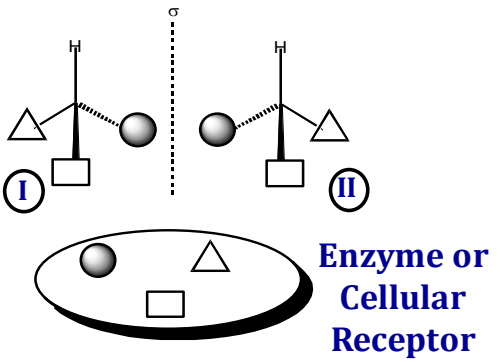
B



Notes

2. Enzymes/cellular signaling

A



3. Drugs

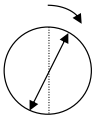
B

Notes

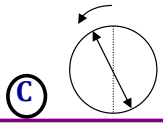
If many physical properties are identical, we use to distinguish two enantiomers?

A

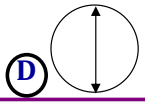
B



C



D



Notes

Optically inactive:

(A)

Optically pure:

(C)

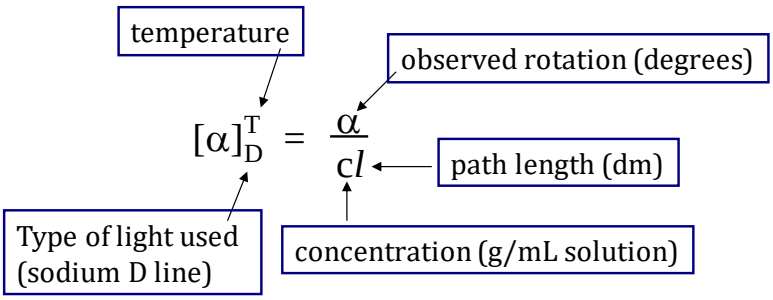
Optical purity:

(B)

(a sample with 80% enantiomer '**X**' and 20% enantiomer '**Y**' has 60% e.e. or 60% optical purity)

Notes

Enantiomers of different compounds rotate light by different amounts, so an optically pure compound has a characteristic **specific rotation [α]**. Two enantiomers of the same compound have **specific rotations** with the same magnitude but in opposite directions. The equation used to calculate the specific rotation is:

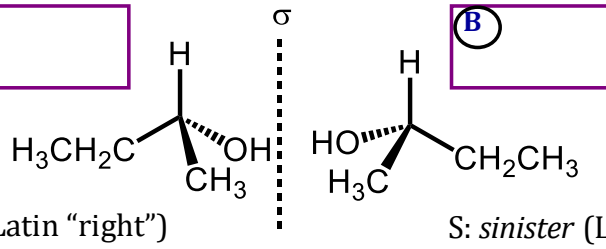


(+)-2-butanol $[\alpha]_D^{27}$ = + 13.5°
(–)-2-butanol – 13.5°

Notes

We obviously need a convention to designate the **absolute configuration** of a given molecule.

A



B

R: *rectus* (Latin "right")

S: *sinister* (Latin "left")

Whether the configuration of a chiral center is *R* or *S* depends only on

C

and is **NOT** determined by

D

So, we need a convention for assigning "priority" to the units that are attached to a chiral atom …

Notes

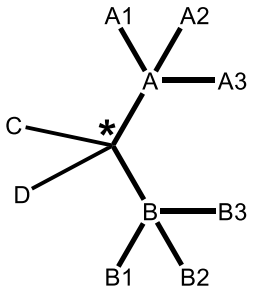
Priority Rules:

1. First look at atom directly attached to the stereogenic atom

A

2. If same atomic number, higher mass = higher priority (D > H, $^{13}C > ^{12}C$, etc.)

3. If atoms A and B are identical, move to highest priority atom attached to A and B until a break in the tie is found (first compare A1 to B1 priority. If tie, compare A2 to B2. If tie, compare A3 to B3, etc.)

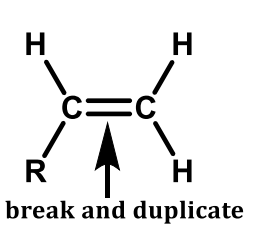


4. For Example:

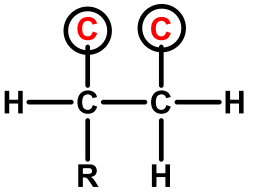
B

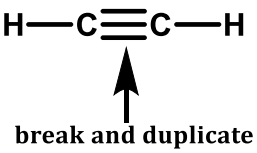
Notes

4. If a substituent is doubly or triply bonded to another atom, use the 'break and duplicate' strategy to create 'false atoms' as a visual aid to prioritize:



Becomes

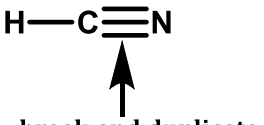




Becomes

A

B

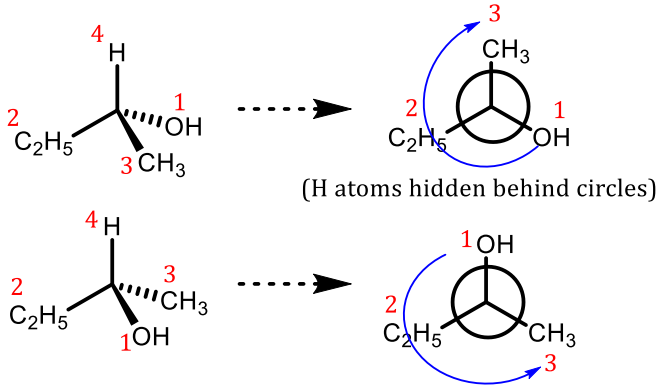


Becomes

Notes

1. (A)
   (using CIP rules)
2. Point the **lowest** priority group away from you

3. Determine the direction of procession from **1-2-3** priorities:



Clockwise 1-2-3:

(B)

Counterclockwise 1-2-3:

(C)

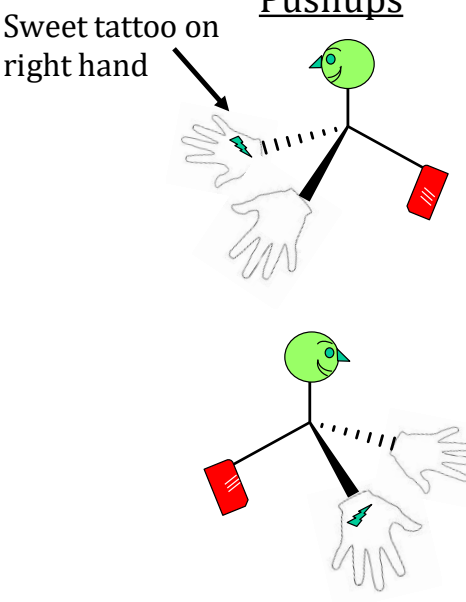
Notes

Lecture Topic I.17-20: Stereochemistry

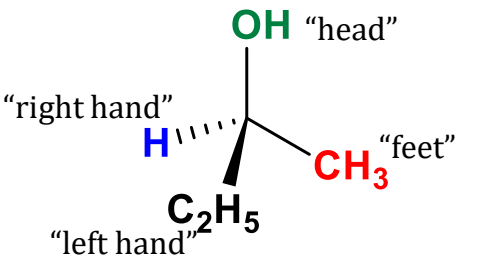
There are Many Ways to Draw a Chiral Object

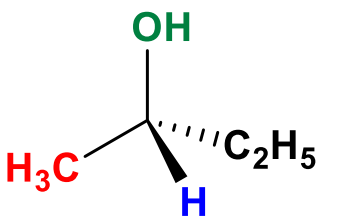
Introducing the Creepy Chiral Stickman!

Chiral Athlete Doing Pushups



Chiral Molecule … Doing Pushups (?)

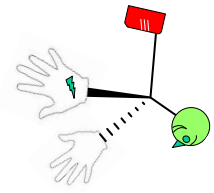


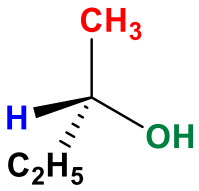


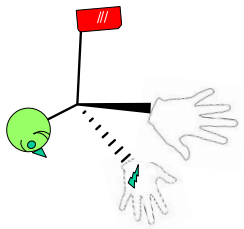
We need a way to visualize rotation of a chiral molecule without losing stereochemical information

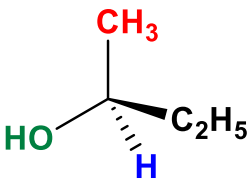
Notes

Hand-Stand

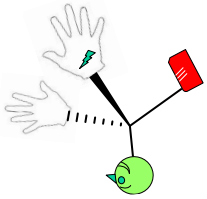


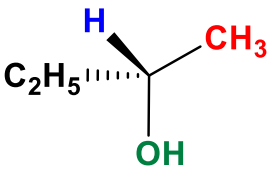


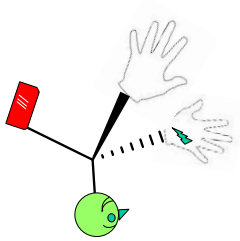


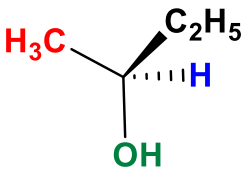


Ceiling Pushup!





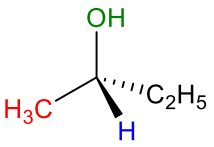


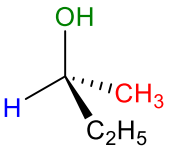


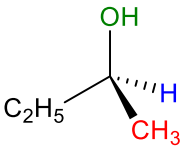
Notes

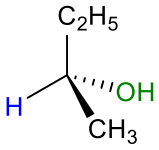
Lecture Topic I.17-20: Stereochemistry

Many Ways to Draw (S)-2-butanol

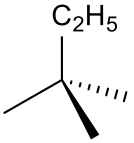


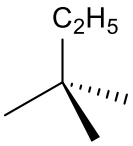


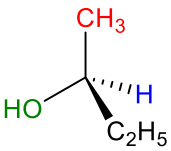


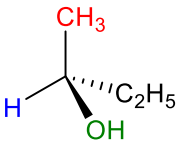


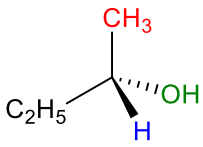
A Two other ways:



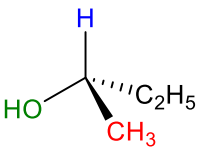


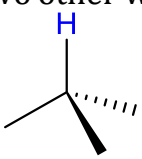


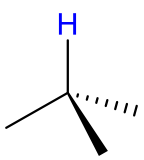




B Two other ways:







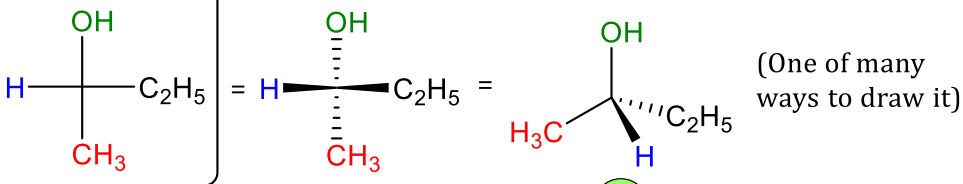
Notes

In addition to standard dash-wedge notation, a **Fischer projection** can show 3D shape.

In a Fischer projection, horizontal lines: (A)

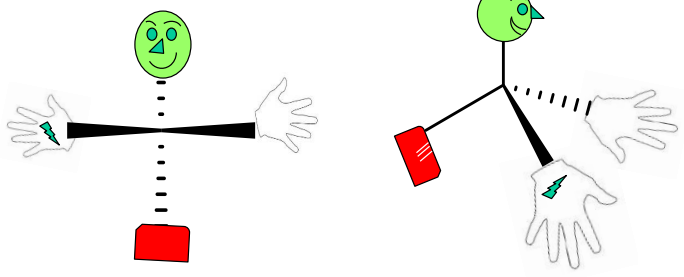
Vertical lines: (B)

Fischer Projection

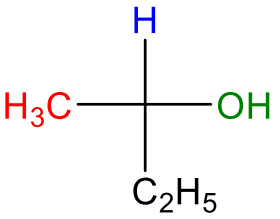


(One of many ways to draw it)

Coming in for a hug but leaning away
(tattoo on palm as well apparently)



Notes



A Name:

Convert to wedge and dash structure (several correct representations):

B

Fischer Projection and Wedge/Hashed Lines for (*R*)-3-methylheptane:

C

Notes

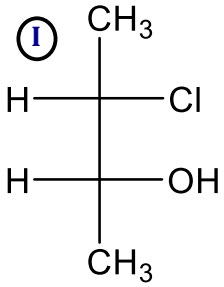
Diastereomers:

A

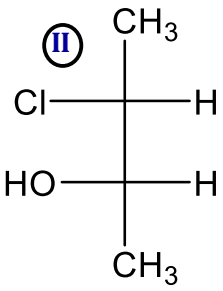
A compound with 'n' chiral centers can have up to 2^n stereoisomers.

Consider 3-chloro-2-butanol, which has Stereocenters at C2 and C3:

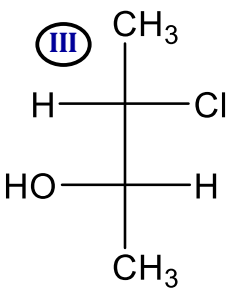
I



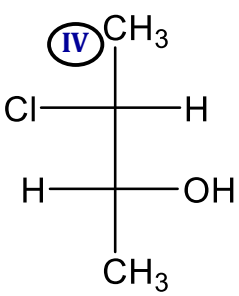
II



III



IV



I and II = **B**

Any other pair = **D**

III and IV = **C**

Notes

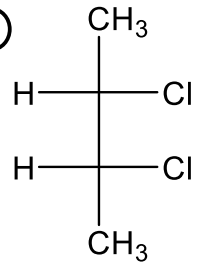
Meso Compounds:

A

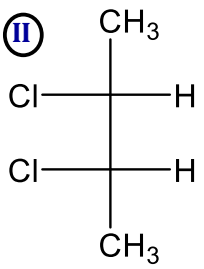
So compounds I and II are ACHIRAL!

Consider 2,3-dichlorobutanol, which has Stereocenters at C2 and C3:

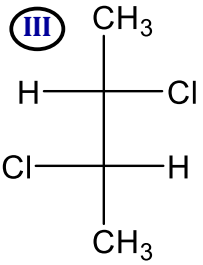
I



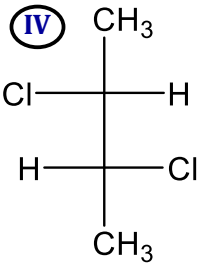
II



III



IV



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Notes