

Assigning R & S Configuration

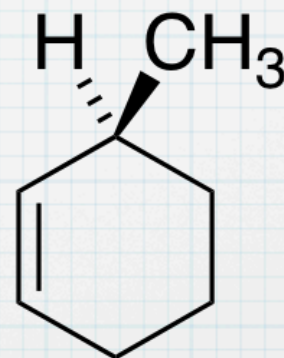
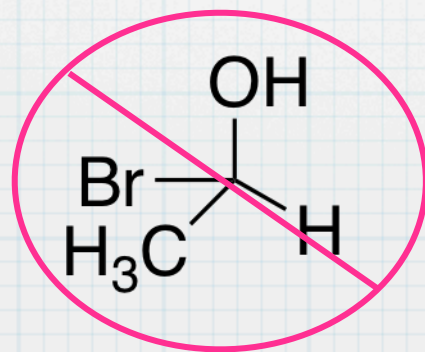
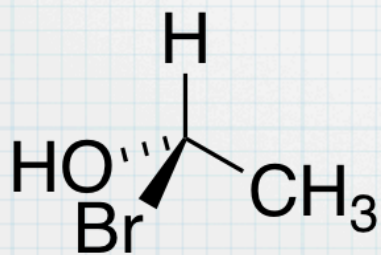
UCI Chem 51A
Dr. Link

Goals

- * After this lesson you should be able to:
 - * Assign priority to groups attached to a stereocenter
 - * Assign R or S designation to a stereocenter
 - * Rotate molecules in space to facilitate the assignment of R & S
 - * Invert the configuration of a stereocenter

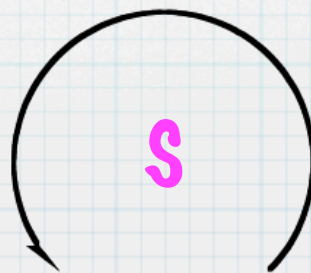
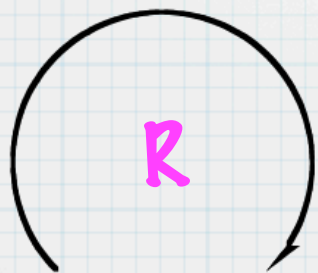
Quick Stereocenter Review

- * 4 different groups attached to C
- * MUST USE WEDGE & DASH!!!



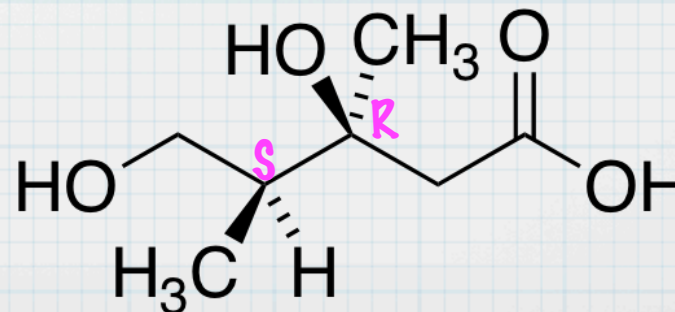
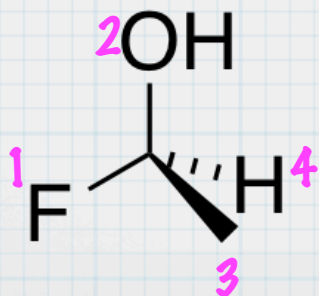
R & S Configurations

- * How can we include spatial arrangement in name?
- * absolute configuration
 - * R = clockwise arrangement
 - * S = counterclockwise arrangement



How to Assign R & S

- * 1. Assign priorities to the groups, 1-4.
- * 2. Arrange so that group 4 is pointing back.
- * 3. Determine whether 1-3 goes clockwise or counterclockwise
 - * Clockwise = R
 - * Counterclockwise = S
- * (Each stereocenter gets its own assignment.)

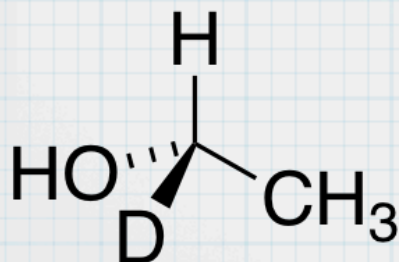
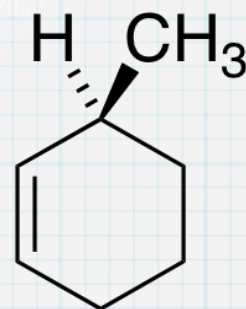
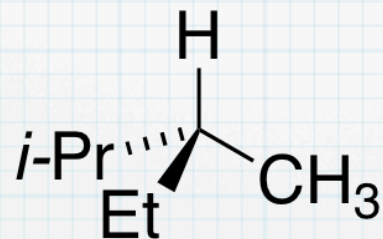
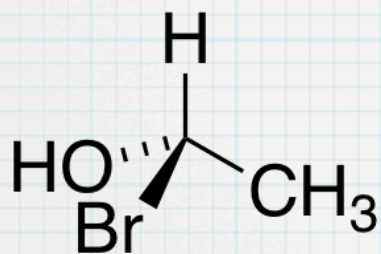


Assigning Priorities to Groups

- * Priority goes by **atomic number** (then mass for isotopes)
- * Look out from stereocenter **1 atom at a time!**
- * If the first atom out is the same, keep going until you find the **first** difference.
- * Multiple bonds count as equal number of single bonds.

Priority Examples

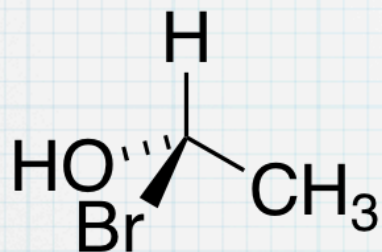
* Assign priority to the groups on each stereocenter.



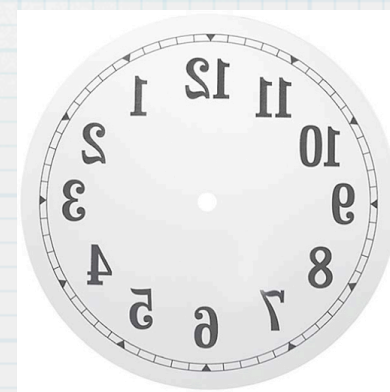
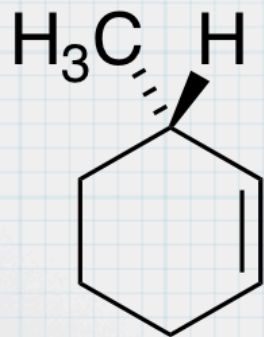
What If H Is Not in Back?

- * Group 4 (usually H) must be either on wedge or dash!
 - * If not, rotate until it is!
- * On dash? Continue as usual.
- * On wedge?
 - * 1. Rotate until it's on dash. OR...
 - * 2. Assign as is, then reverse assignment.

Some Rotations

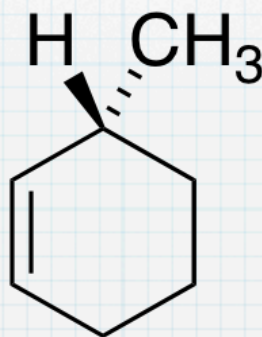
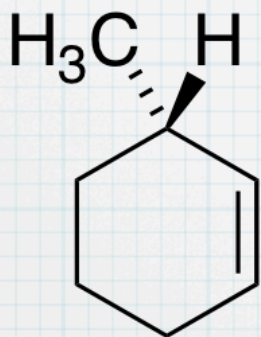


Why reverse? Looking at it backward!



Relationship Between R & S Configurations

* What is the relationship?



How to invert stereocenters (R \leftrightarrow S)?

Switch two groups

OR

Draw mirror image.

Wrapping Up

- * Practice identifying stereocenters (again)
- * Practice assigning priority to groups on stereocenters
- * Practice assigning R & S configurations
- * Practice rotating drawings of molecules