CH 105 – Reading Assignements

CIP Rules

Naming Enantiomers (Absolute Configuration)

- A self consistent and unambiguous system of configurational nomenclature based on 3-D structure
- Introduced by Cahn-Ingold-Prelog (hence CIP rules!)
- R (rectus – right) and S (sinister – left) describe topography and have no correlation with the sign of rotation
- Two rules are used to assign configuration

  (i) The sequence Rule

  (ii) Chirality rule

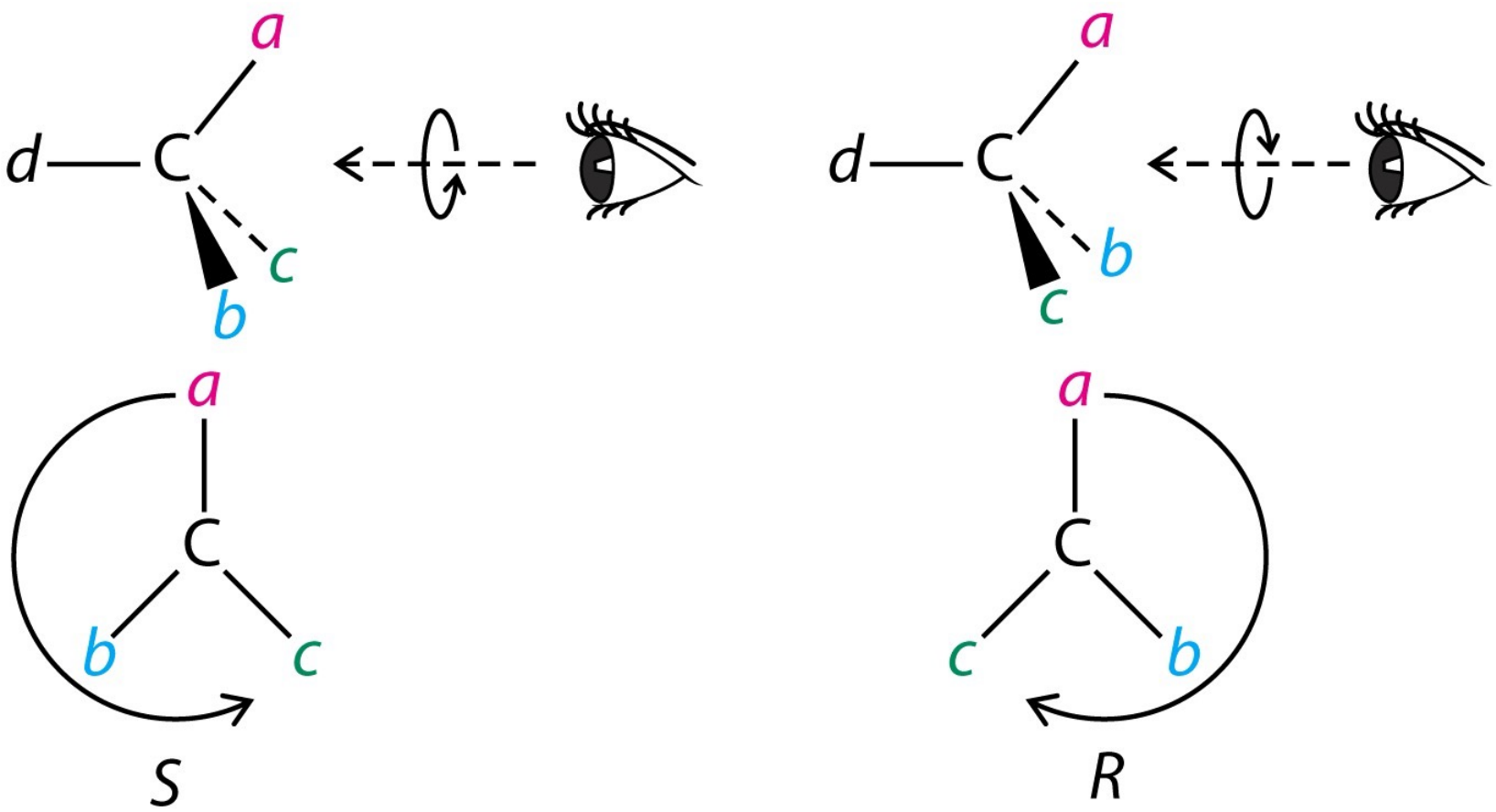
CIP rule

- Arrange the four ligands of a chiral centre (Cabcd) in a priority sequence e.g. a>b>c>d or the ligands are numbered 1>2>3>4. (Sequence rule)

- The chiral centre is then viewed from the side remote from the lowest ranking group (d or 4).

- If from this point of view, the arrangement a → b → c (or 1 → 2 → 3) appears in the clockwise direction, the configuration is R and if the arrangement appears in the anticlockwise direction, the configuration is S (Chirality Rule)

Procedure for Assignment of *R*, *S*



The sequence rule for deciding priority

(0) Near end of an axis or a plane precedes the farther end (proximity rule)
(1) Higher atomic number precedes lower e.g. S > F > O > N > C > H
(2) Higher atomic mass no. precedes lower e.g. T > D > H
(3) Like pair R,R or S,S precedes unlike pair R,S or S,R
(4) R precedes S; M precedes P

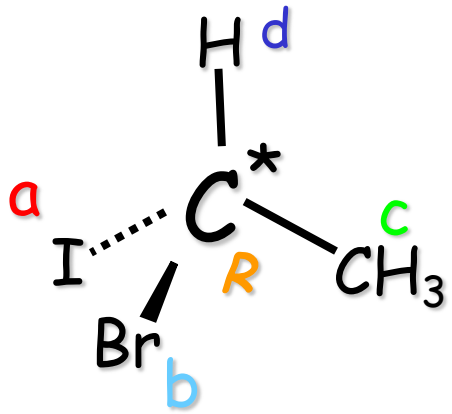
NOTE: For most cases only rule (1) and (2) are important

Subrule (0) is applicable to axial and planar chirality

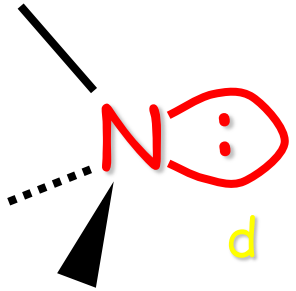
There are subrules of rule (1) and use rule (2) after exhausting rule (1)!

Sequence Rules

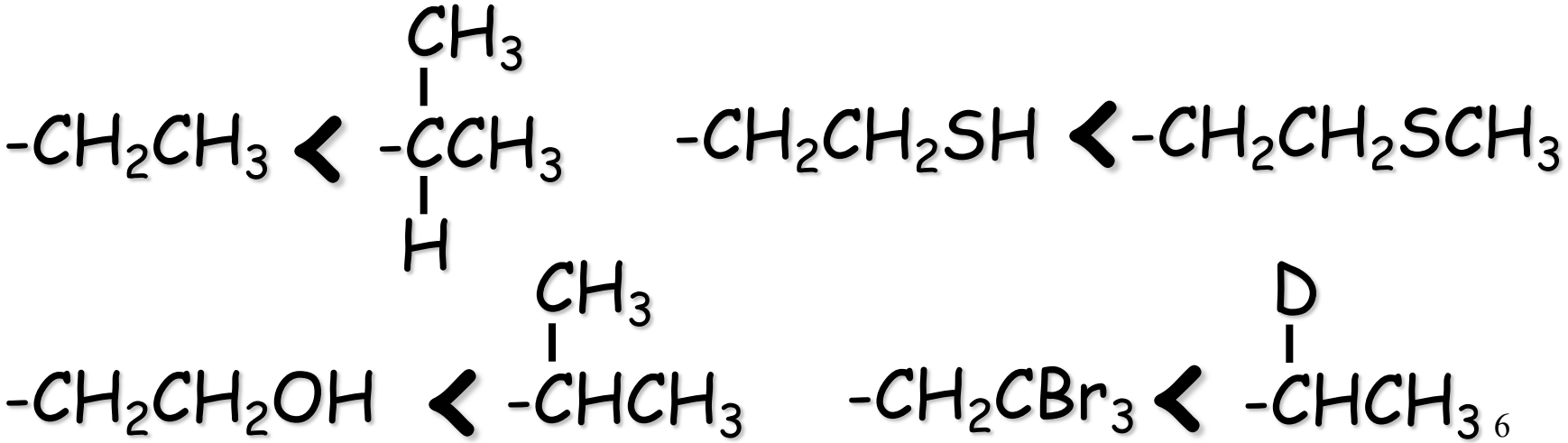
1. Order by atomic number, i.e. H = 1, lowest.



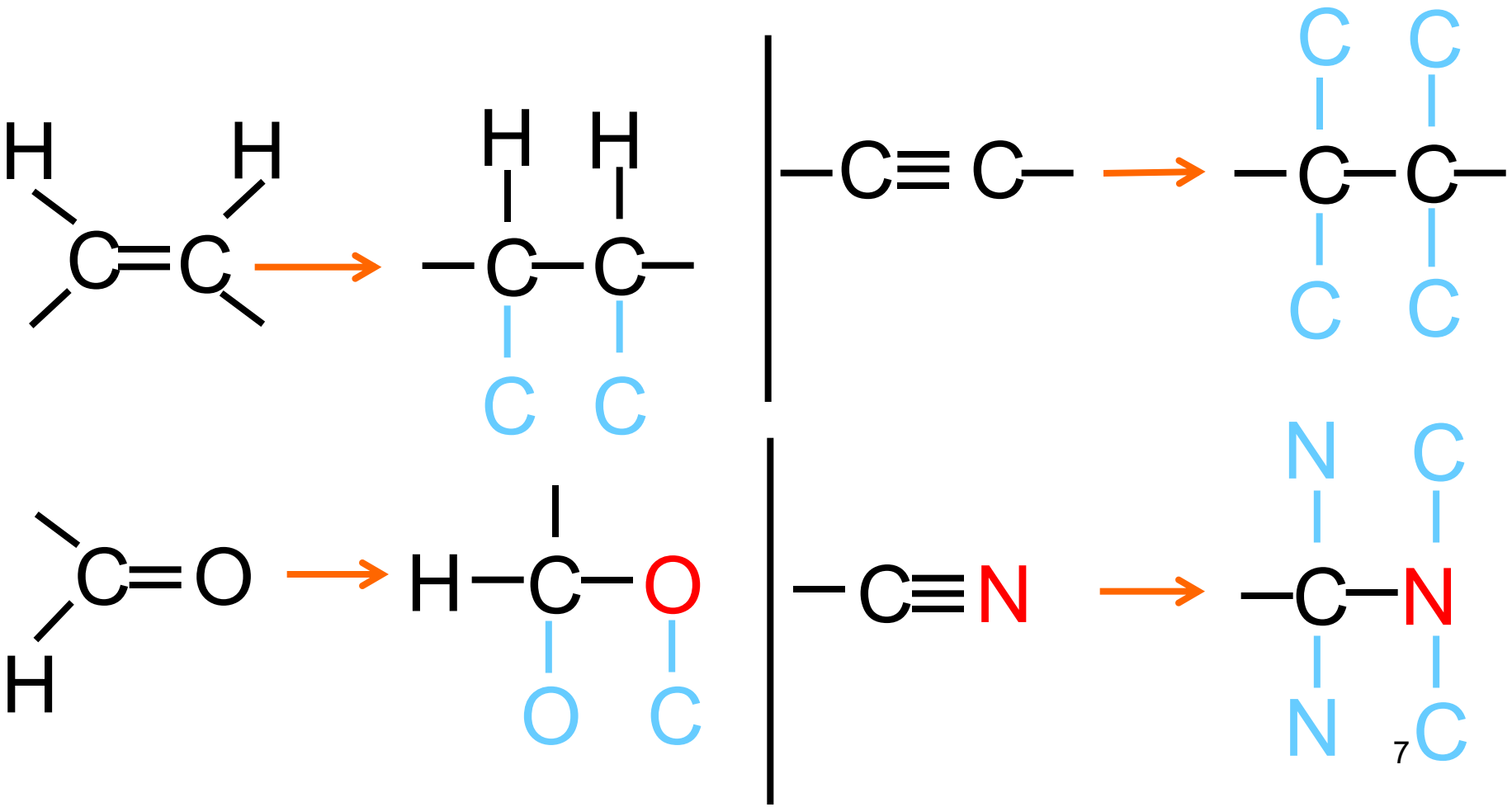
Exception: lone pair, # "zero". E.g., amines:



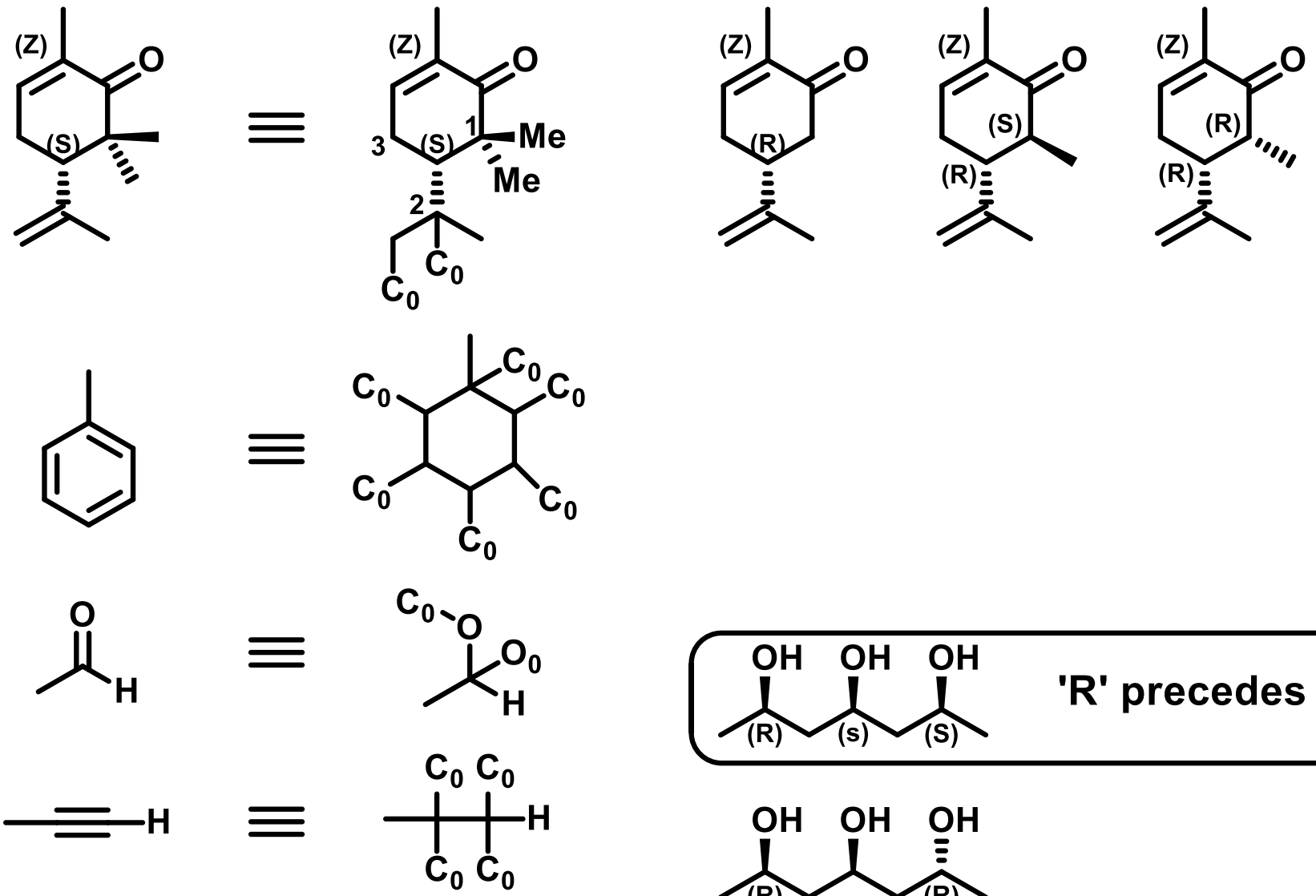
2. If same priority at first atom: Go to first point of difference.



3. **Multiple bonds:** Add double or triple representations of atoms at the respective other end of the multiple bond.



Some examples

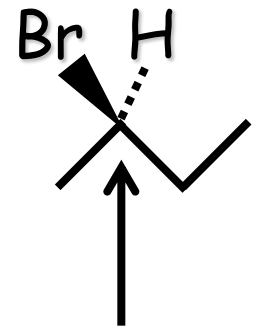


C_0 = 'Phantom' atom

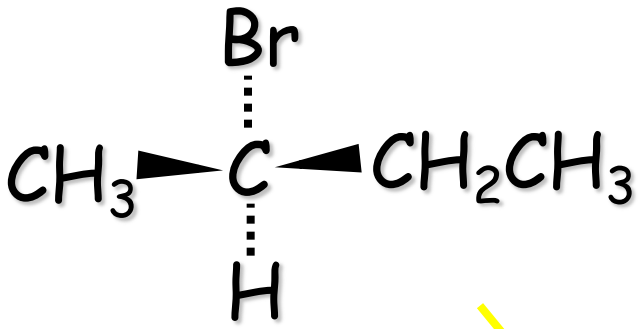
HINT

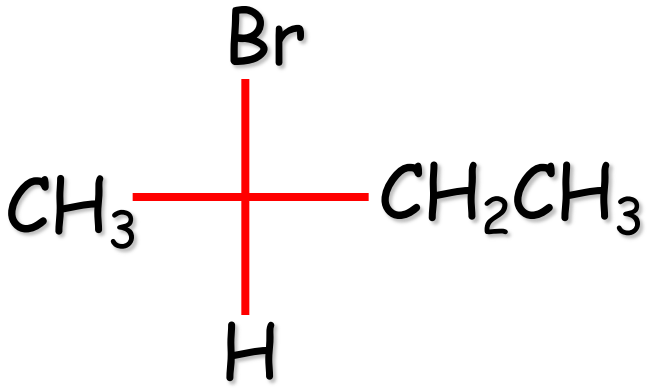
If the lowest-priority atom (usually H) is oriented toward you, you don't need to turn the structure around. You can leave it as it is with the H toward you and apply the *R/S rule backward*.

Fischer Projection: A flat stencil



Eyes in the plane of the board

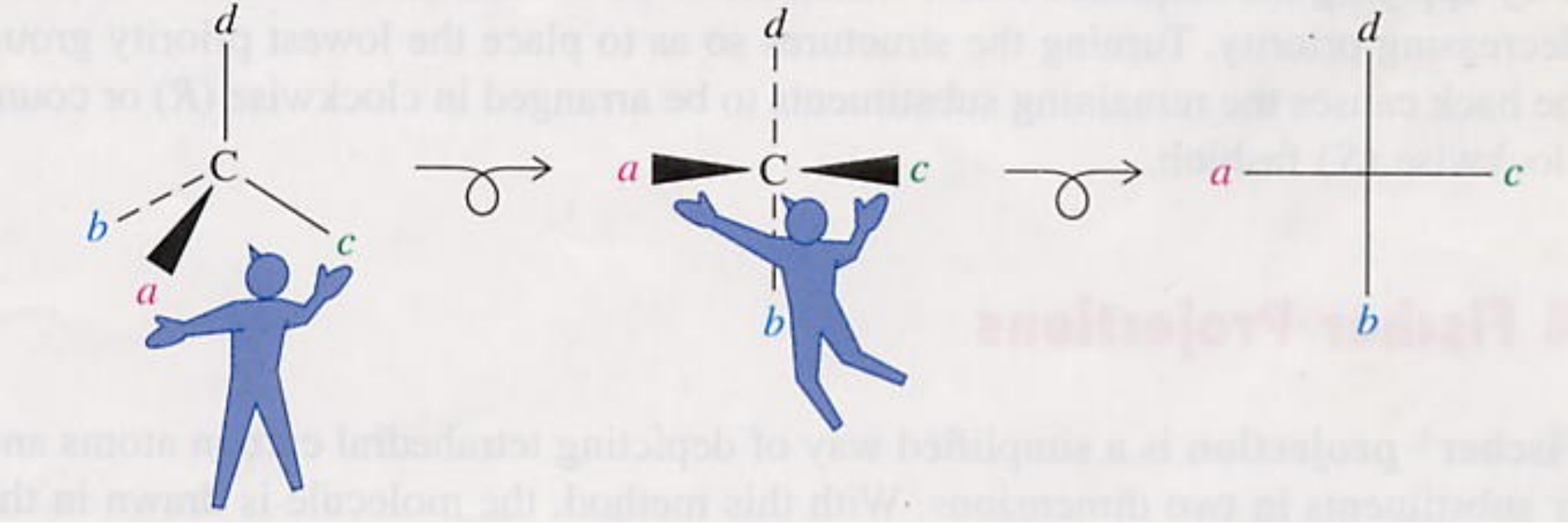




Depending on your starting dashed-wedged line structure, several Fischer projections are possible for the same molecule.

Fischer Projections

A Simple Mental Exercise:
Conversion of Dashed-Wedge Line Structures into Fischer Projections

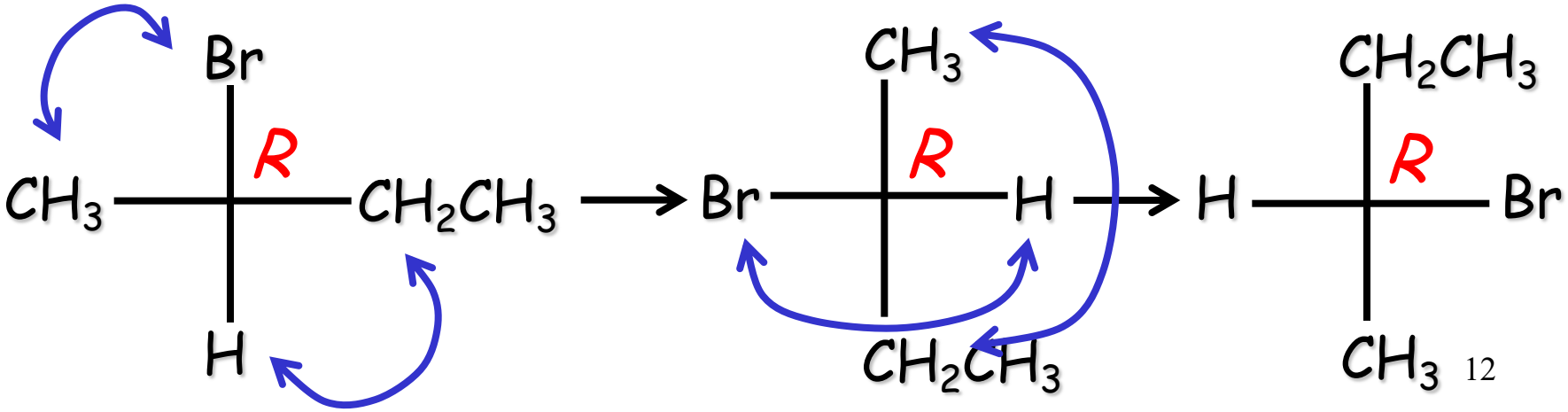


Rules for handling Fischer projections:

1. Don't rotate.

2. The mutual exchange of any pair gives the other enantiomer

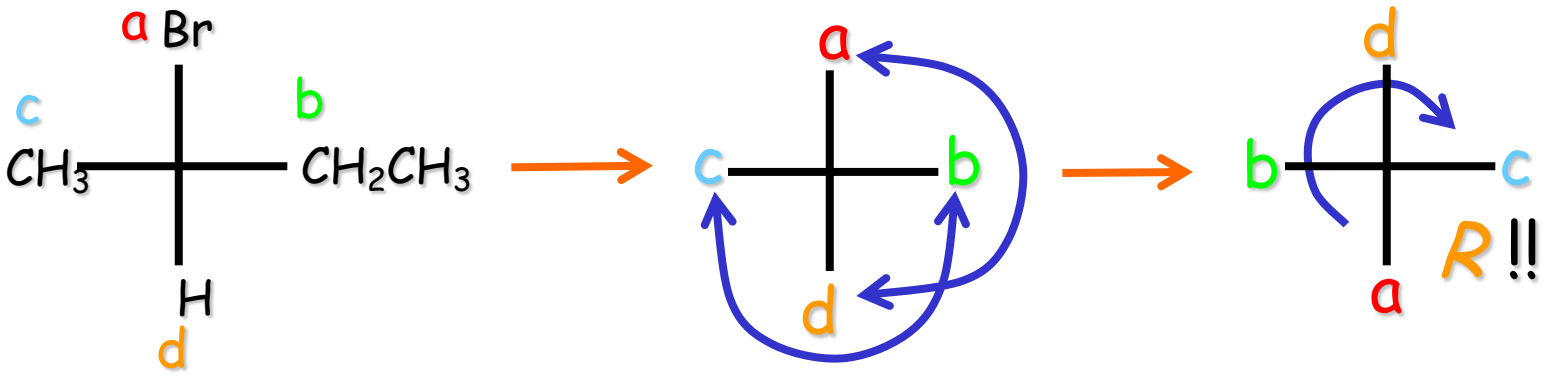
Therefore: Two exchanges leave absolute configuration. Example: (2*R*)-Bromobutane



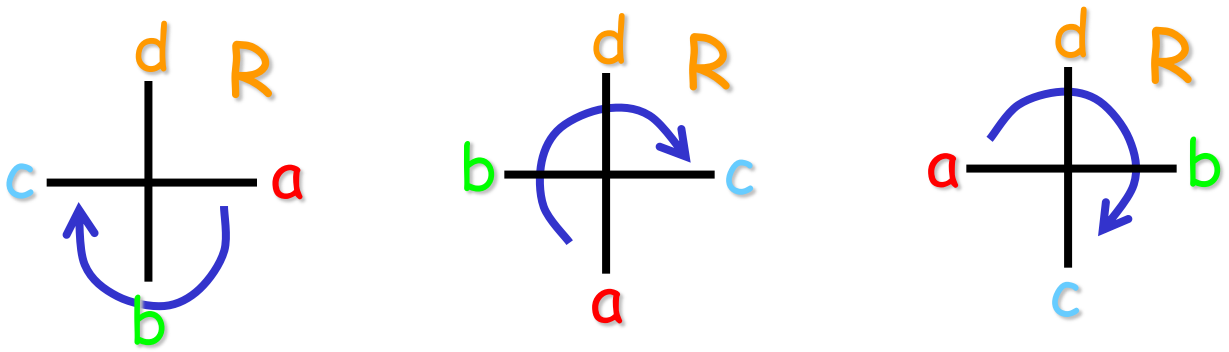
This procedure can be used to readily assign *R*,*S* :

Do double exchanges to place d on top.

Example:



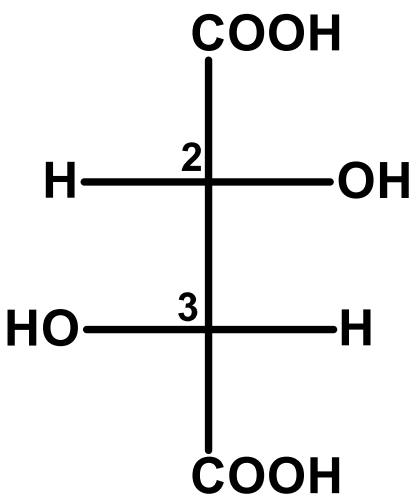
Note: There are three possible arrangements for each, *R* or *S*, e.g., *R* :



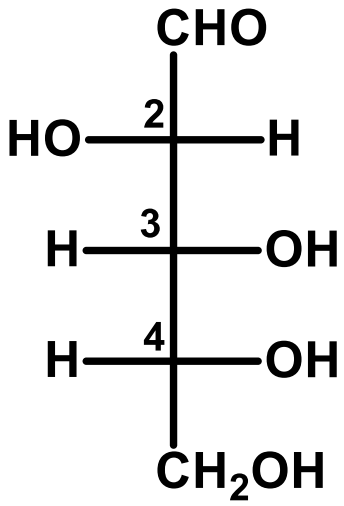
R/S in Fischer Projection

- Remember “Very Good” = “Vertical is Good”!
- Assign priority 1-4.
- Don’t worry about no. 4
- Find direction from 1-3
- If substituent 4 is on vertical line, it’s correct R/S nomenclature
- If no. 4 substituent is not on vertical line, the answer is wrong and you write opposite!

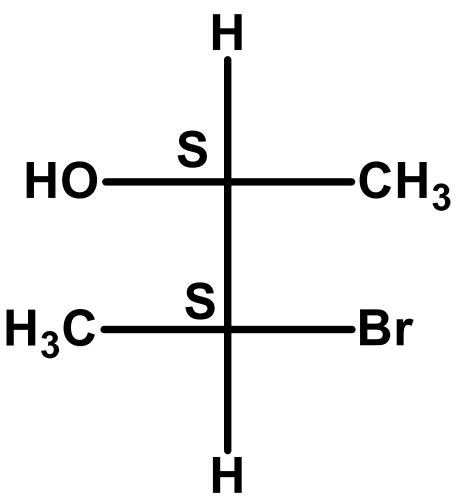
Some examples



2R, 3R



2S, 3R, 4R

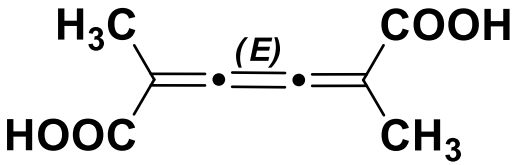


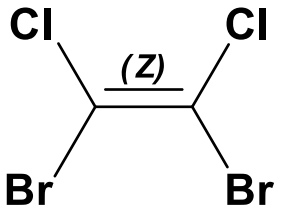
Assign absolute configuration for all stereocentres of

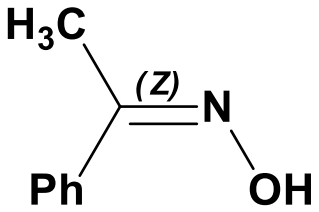
1. (D)-glucose
2. All natural amino acids

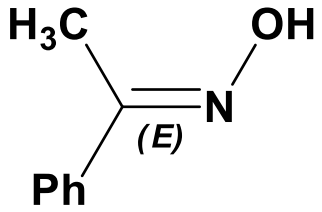
E,Z nomenclature

- Use CIP rule and assign priority for substituents on each atom of double bond
- If top priority substituents are on same side of olefin its ‘Z’ else ‘E’.









•Note: lone pair gets low priority