Organic Molecular Modeling

Last revised: 2025/02/06

Prelab Preparation

- Lab coat and goggle are not necessary
- Self-prepared digital camera, smartphone, laptop
- Complete the data sheet in your pre-lab report, each one shall include
  - Hand-draw structural formula
- Download Avogadro and Chemsketch free software beforehand (**optional**)

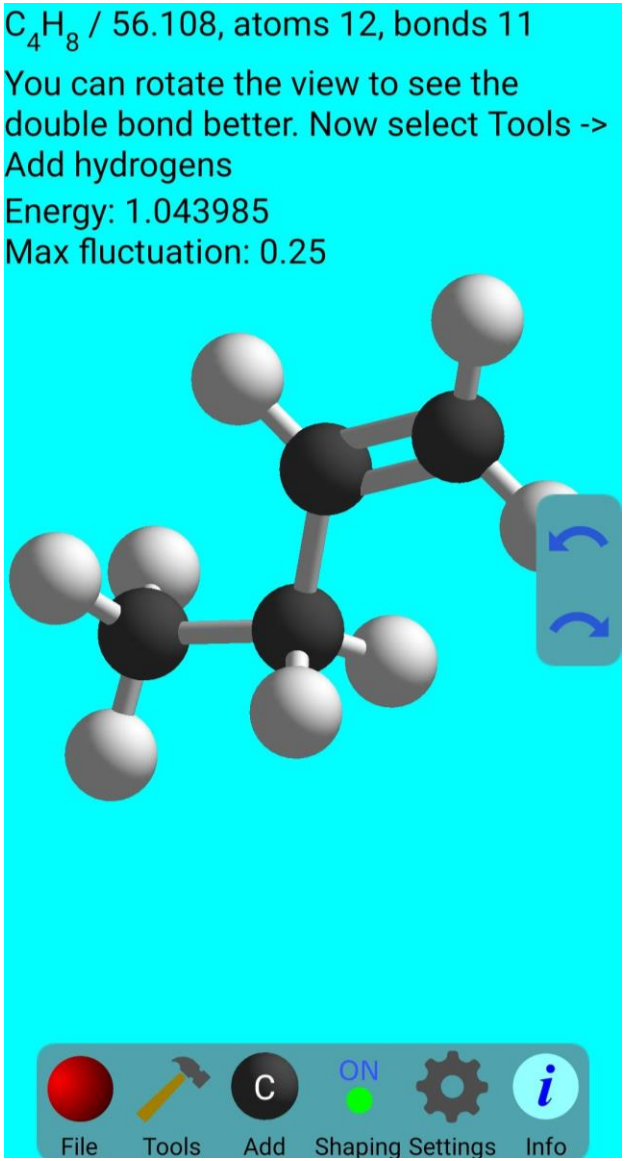
✓ Tutorial for Chemsketch: http://www.youtube.com/watch?v=5kaU5iEqifQ

✓ Tutorial for Avogadro: http://www.youtube.com/watch?v=ohdMhGaaP68

Calculate bond-angle, bond-length, and bond energy

Smartphone App (Optional)

1. Add main atoms
2. Add bonds
3. Add hydrogen
4. Shaping



Preparation

Collect and check MOLYMOD organic set contents

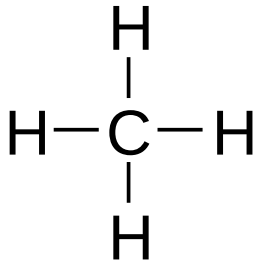
- White ball: 20
- Black ball: 12
- Red ball: 6
- Blue ball: 4
- Green ball: 4
- Yellow ball: 2
- Grey ball: 1
- Purple ball: 1
- Short white link: 26 / 10.13 g
- Medium grey link: 26 / 23.11 g
- Long grey link: 12 / 9.95 g
- Link remover: 1

Objective

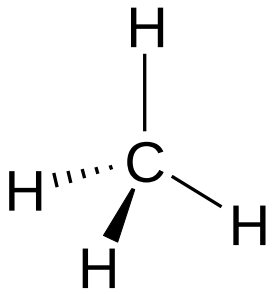
- Construct and learn spatial arrangements of organic molecules
- Use MOLYMOD® organic set to build ball-and-stick model and observe the conformers and isomers
- Use free software Chemsketch and Avogadro to sketch the structural formulas (optional)

Molecular Geometry

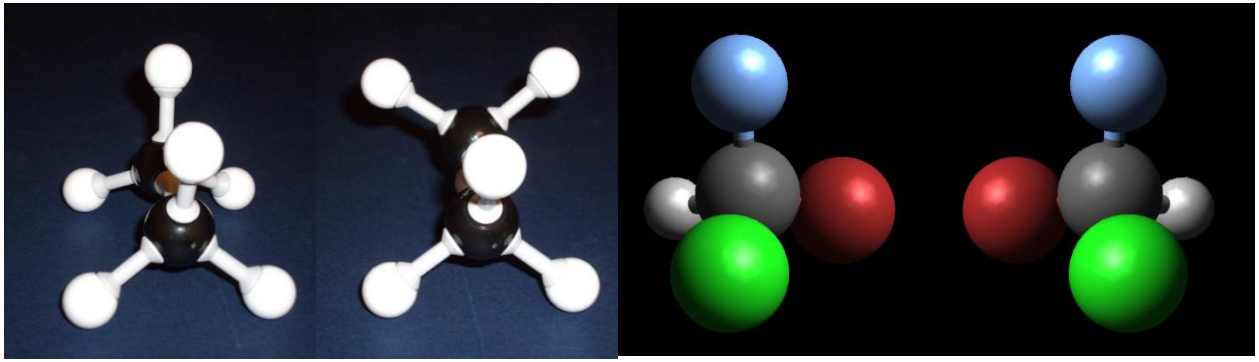
- Lewis structure



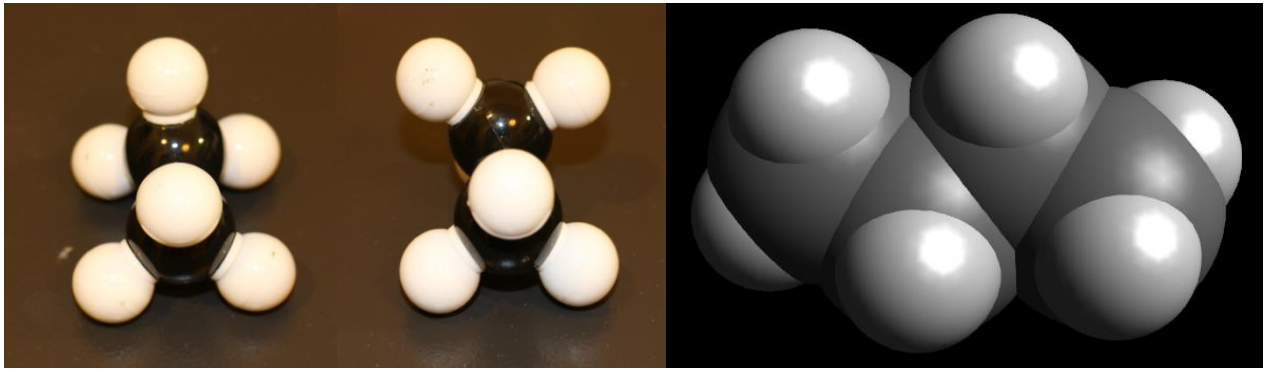
Wedge-and-dash



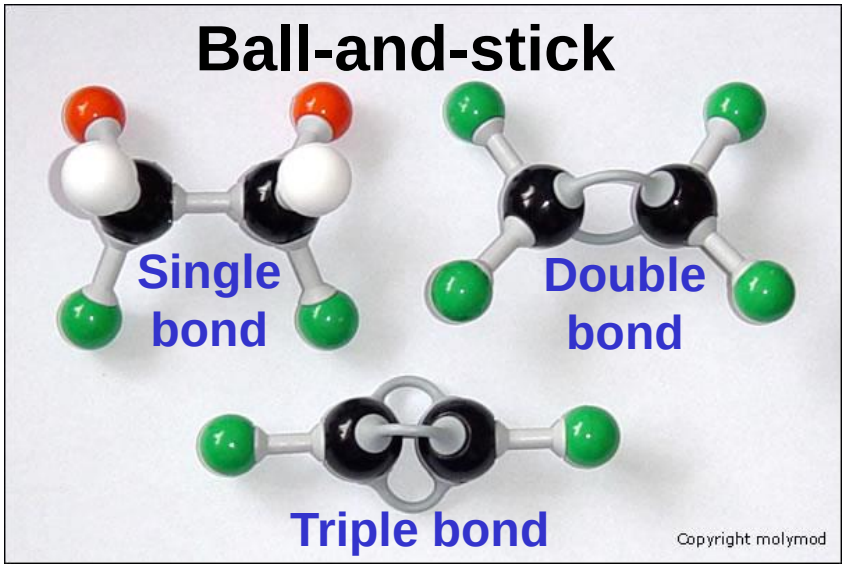
- Ball-and-stick



- Space-filling



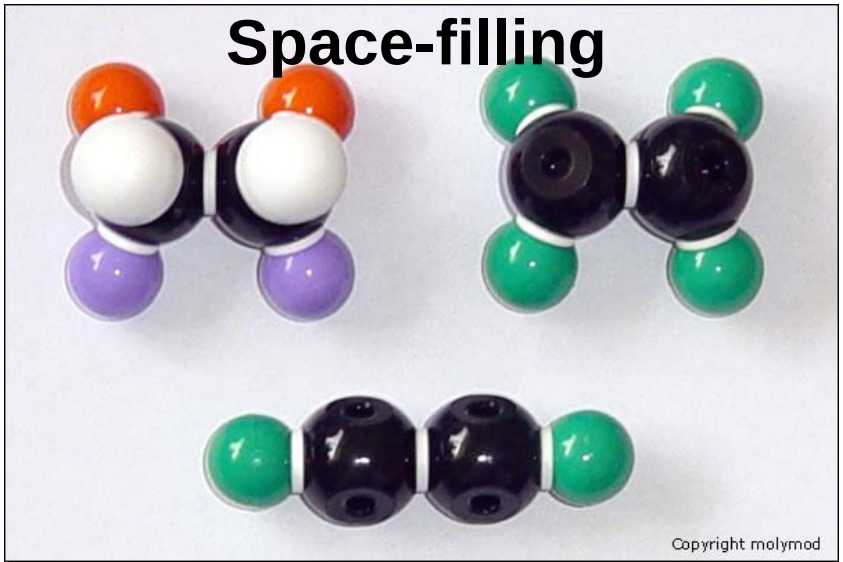
MOLYMOD® Organic Set



Single bond Multiple bond

CPK coloring

C	
H	
O	
N	
Cl/F	

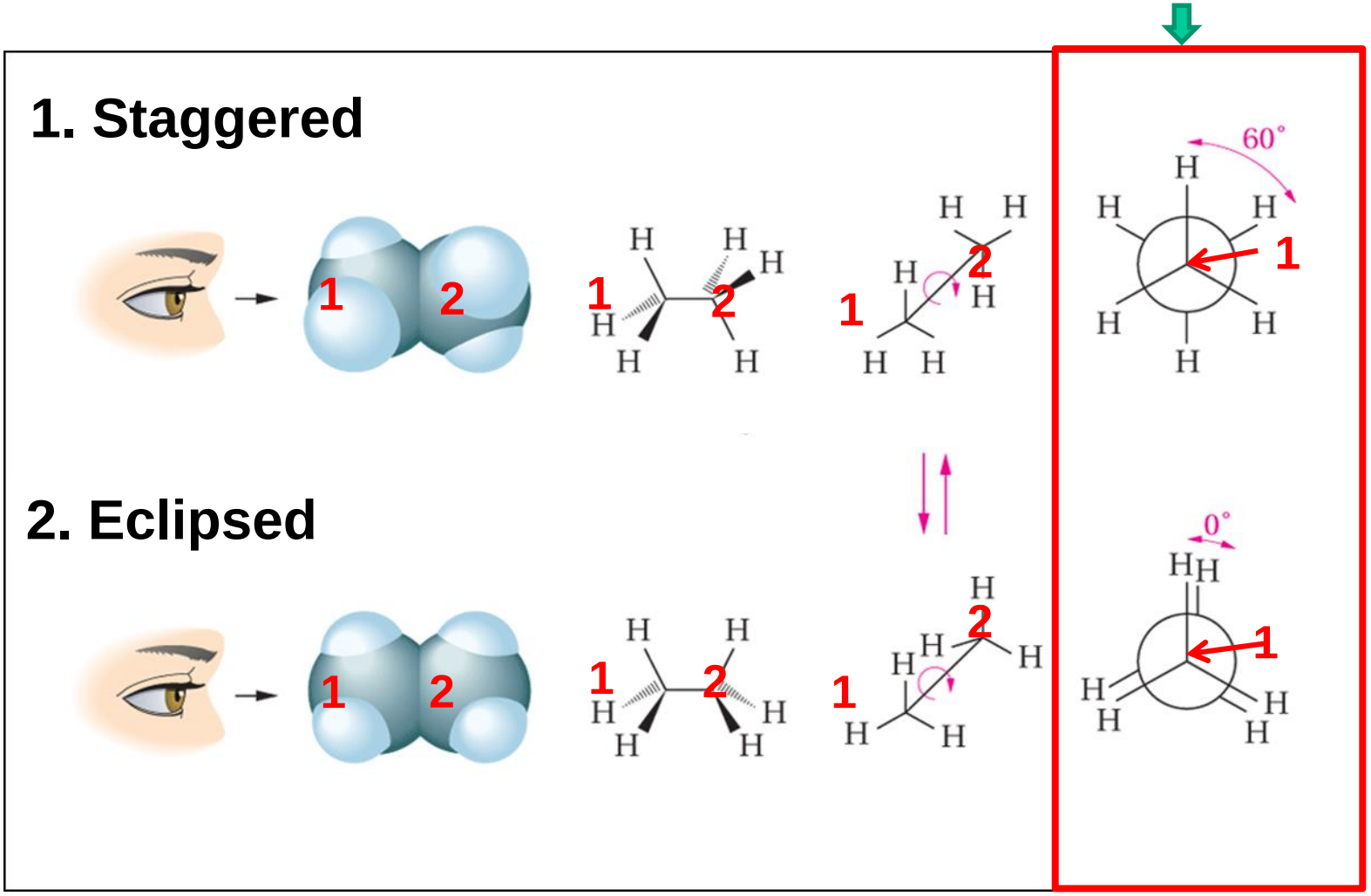


Link remover

Newman Projection

- For ethane, C_2H_6

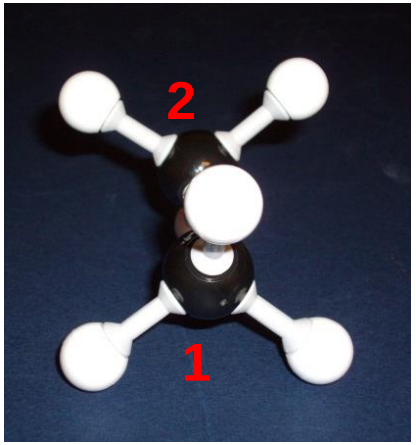
Newman Projection



Conformation

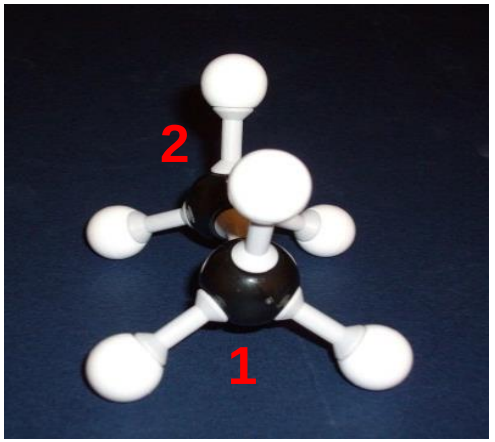
- **Conformation**
  - Differs by rotations about single bonds

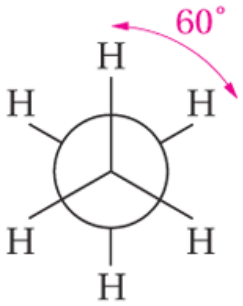
Staggered, lower energy

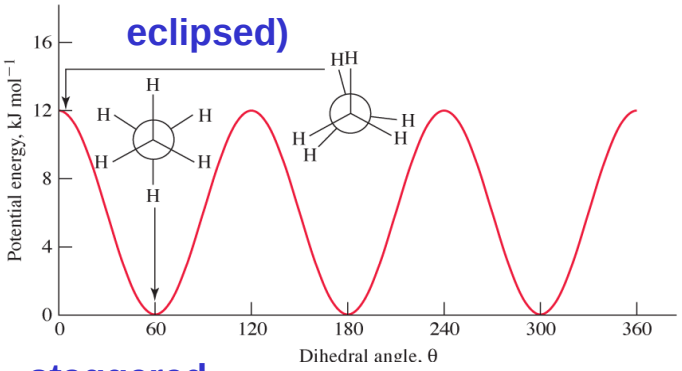


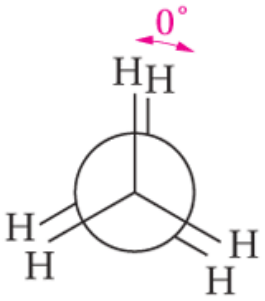
More stable

Eclipsed, higher energy





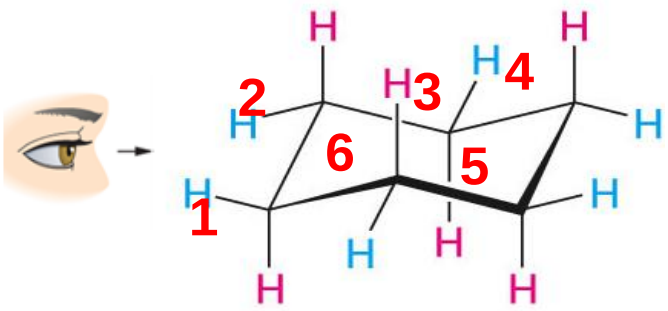


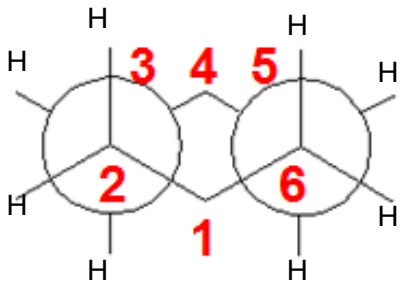


Conformation

- **Chair form and boat form of cyclohexane, C_6H_{12}**

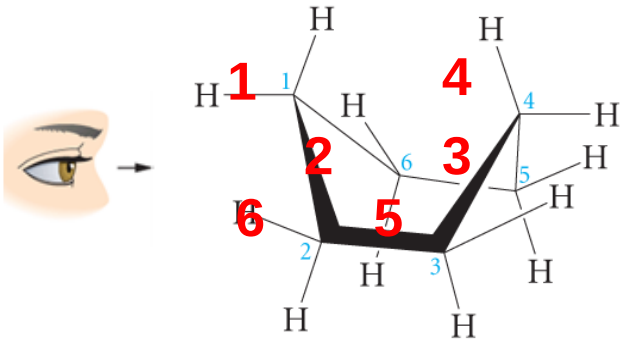
Chair form

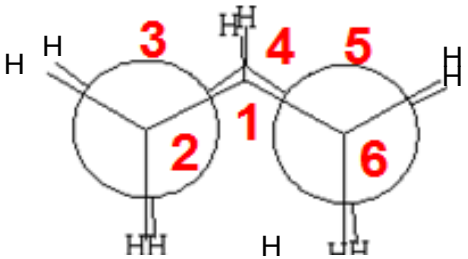




More stable

Boat form





Isomers

Isomers

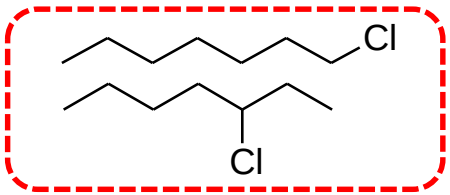
✓ Same formula, but different structure

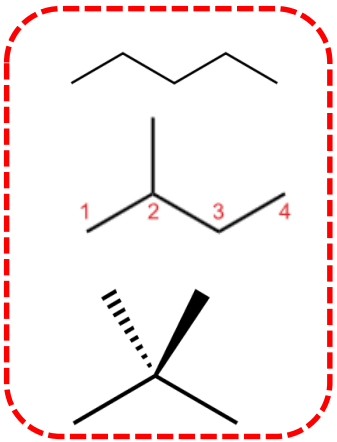
✓ Different skeleton

✓ Same skeleton, but different spatial arrangement

Structural isomers

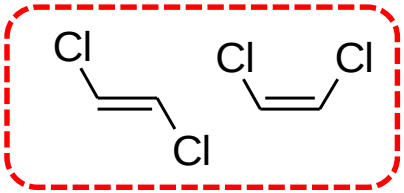
Stereoisomers

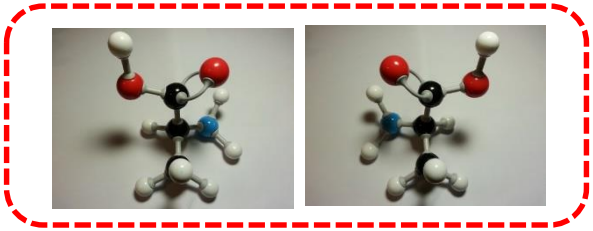




CH_3OCH_3

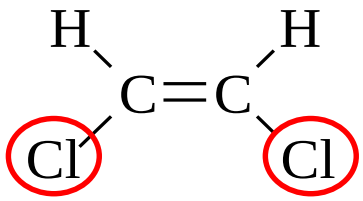
CH_3CH_2OH



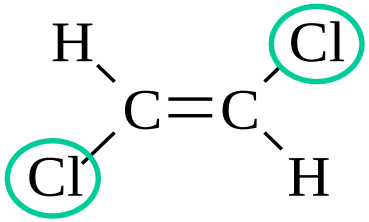


Diastereomers

- ***cis*, *trans*-isomers**
  - C=C double bond cannot rotate
  - Molecule with C=C double bond or ring structure
    - *cis*: on the same side
    - *trans*: on the other side

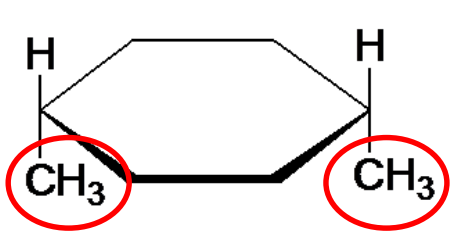


Cis-form

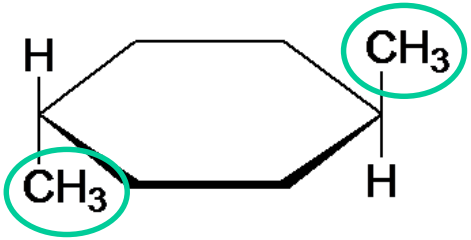


Trans-form

1,2-dichloroethene



Cis-form

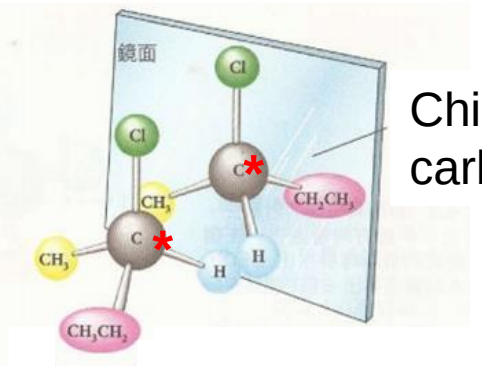


Trans-form

1,4-dimethylcyclohexane

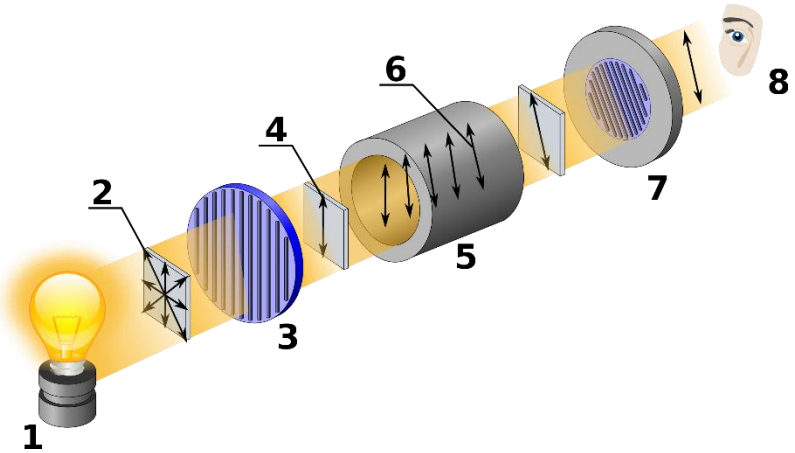
Enantiomers

- **Chiral carbon**: Carbon with four different substituents, labeled as C*
- **Enantiomers**: One of a pair of molecular entities which are mirror images of each other and non-superposable (IUPAC)



Chiral carbon

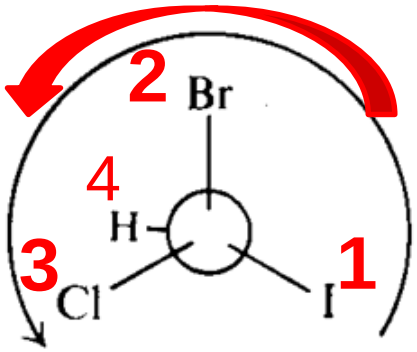
- **Enantiomers** could rotate plane-polarized light with same angle but different direction
  - Rotate **clockwise**, i.e. **dextrorotatory**, denoted as (**+**) or ***d-***
  - Rotate **counterclockwise**, i.e. **levorotatory**, denoted as (**−**) or ***l-***



1. Light resource
2. Unpolarized light
3. Linear polarizer
4. Linear polarized light
5. Sample (enantiomer)
6. Rotated polarized light
7. Rotatable linear polarizer
8. Detector

Naming Stereocenters by *R*, *S* System

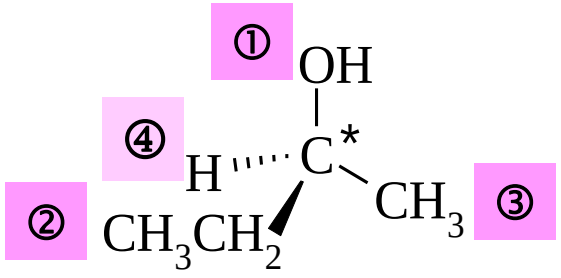
- **Priority rules:**
  - Higher atomic number with higher priority (assign 1)



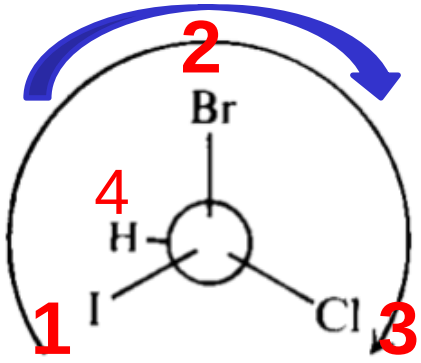
S

Counter-clockwise

S-



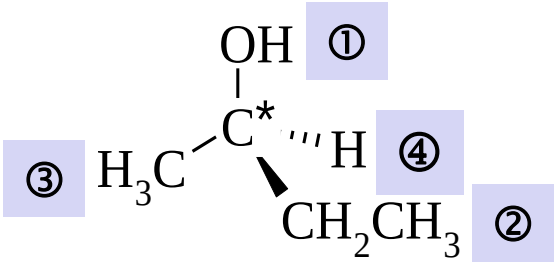
$[\alpha]_D^{25}$ +13.52



R

Clockwise

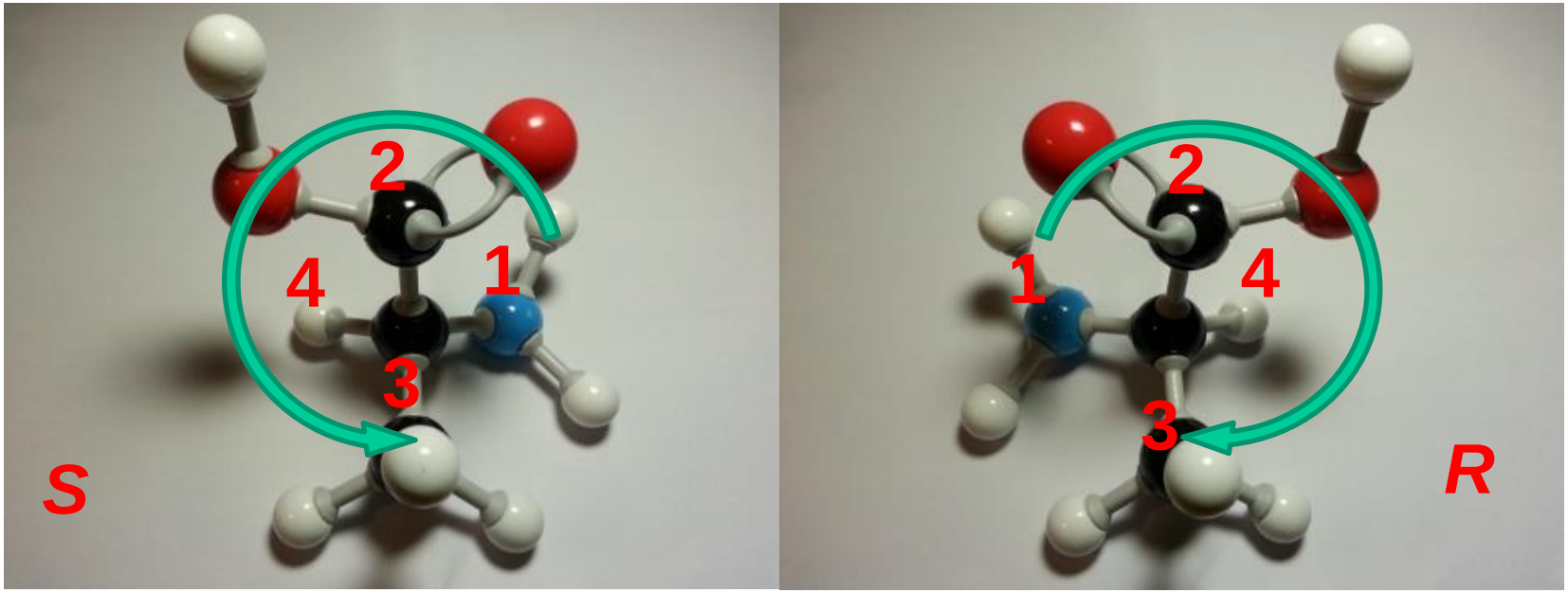
R-



$[\alpha]_D^{25}$ -13.52

IUPAC name (*S*)-(+)-2-Butanol (*R*)-(−)-2-Butanol

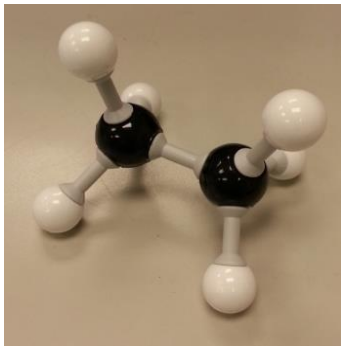
Compare the Enantiomers



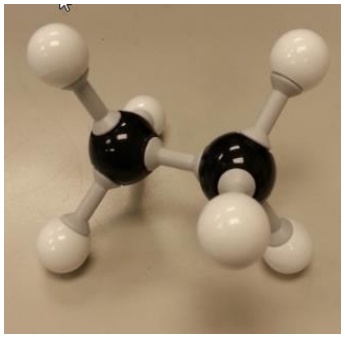
1. Assemble the molecules
2. Determine the *R*- or *S*- configurations
3. Compare and take picture

Experiment Tasks

MOLYMOD organic set



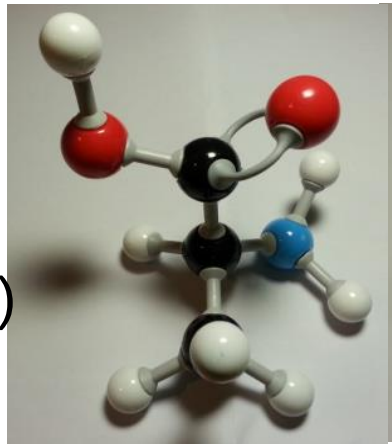
Eclipsed



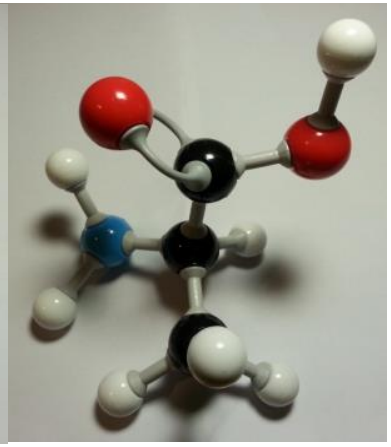
Staggered

MOLYMOD ball-and-stick model

- Draw structural formulas (pre-lab report)
- Check the contents in the box
- Construct ball-and-stick model
- Compare and take picture
- After lab, recheck the contents in the box



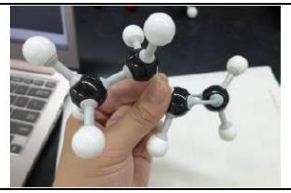
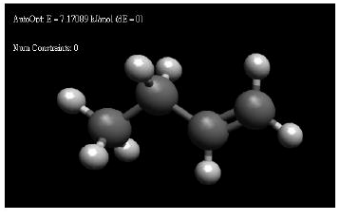
S



R

Additional Notes

- Using a selfie camera will get you a mirror image
- Before uploading your e-report to NTUCOOL, check the followings:
  - **Systematic name in Chinese and English (IUPAC)**
  - **The pictures (in the most stable form)**
  - Avogadro (for correction)
  - Save as pdf format

中文系統命名 (化學命名原則)	1-丁烯
英文系統命名 (IUPAC 命名法則)	1-butene
MOLYMOD®球-棍模型	
Avogadro 模型	

✓ https://teaching.ch.ntu.edu.tw/gclab/en/announcements.html

Clean-Up and Check-Out

- Use link remover to disassemble the white short link to prevent damaging the links
- Clean up the lab bench and check the contents of MOLYMOD set (have an associate TA sign the check list)

- This is a **Full Report** experiment:
  - Results checked by the TA, and upload e-table

- Groups on duty shall stay and help clean up the lab

Link remover