

8B. Racemic Forms and Enantiomeric Excess

- ❖ A sample of an optically active substance that consists of a single enantiomer is said to be **enantiomerically pure** or to have an **enantiomeric excess** of 100%

- ❖ An enantiomerically pure sample of (*S*)-(+)-2-butanol shows a specific rotation of +13.52

$$[\alpha]_{\text{D}}^{25} = +13.52$$

- ❖ A sample of (*S*)-(+)-2-butanol that contains less than an **equimolar** amount of (*R*)-(–)-2-butanol will show a specific rotation that is less **than 13.52 but greater than zero**
- ❖ Such a sample is said to have an *enantiomeric excess* less than 100%

❖ Enantiomeric excess (ee)

- Also known as the optical purity

$$\% \text{ enantiomeric excess} = \frac{\left(\text{mole of one enantiomer} \right) - \left(\text{moles of other enantiomer} \right)}{\text{total moles of both enantiomers}} \times 100$$

- Can be calculated from optical rotations

$$\% \text{ enantiomeric excess}^* = \frac{\text{observed specific rotation}}{\text{specific rotation of the pure enantiomers}} \times 100$$

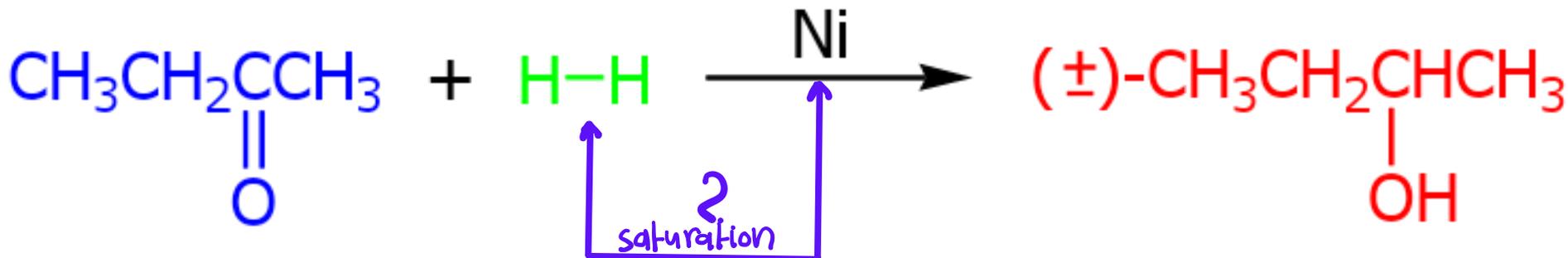
❖ Example مثبت عطلوبن طريره اكل

- A mixture of the 2-butanol enantiomers showed a specific rotation of +6.76. The enantiomeric excess of the (S)-(+)-2-butanol is 50%

$$\% \text{ enantiomeric excess}^* = \frac{+6.76}{+13.52} \times 100 = 50\%$$

9. The Synthesis of Chiral Molecules

9A. Racemic Forms



ketone?
Butanone
(achiral
molecules)

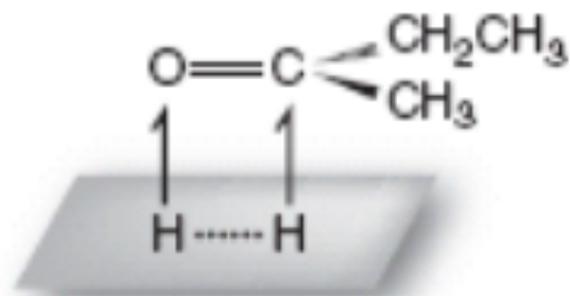
Hydrogen
(achiral
molecules)

(±)-2-Butanol
(chiral
molecules; but
50:50 mixture
(R) & (S))

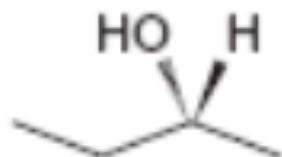
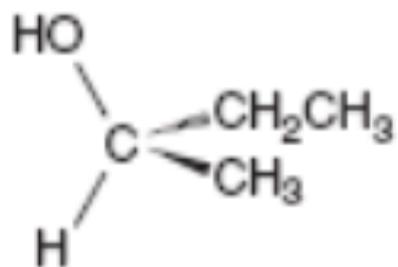
وحدة رج اعمل
فيها التفاعل ووحدة لا

or

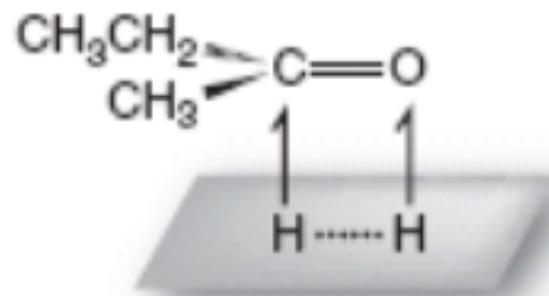
اذا كان وحدة منهم safe
والثانية toxic لانهم افضل بينهم



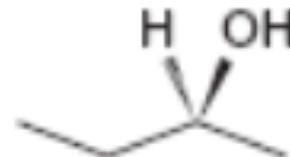
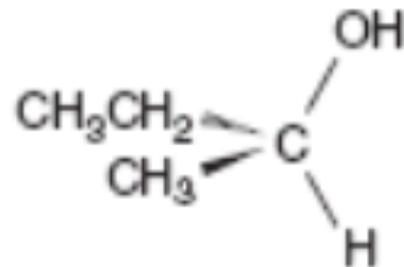
(a)



(R)-(-)-2-Butanol (50%)



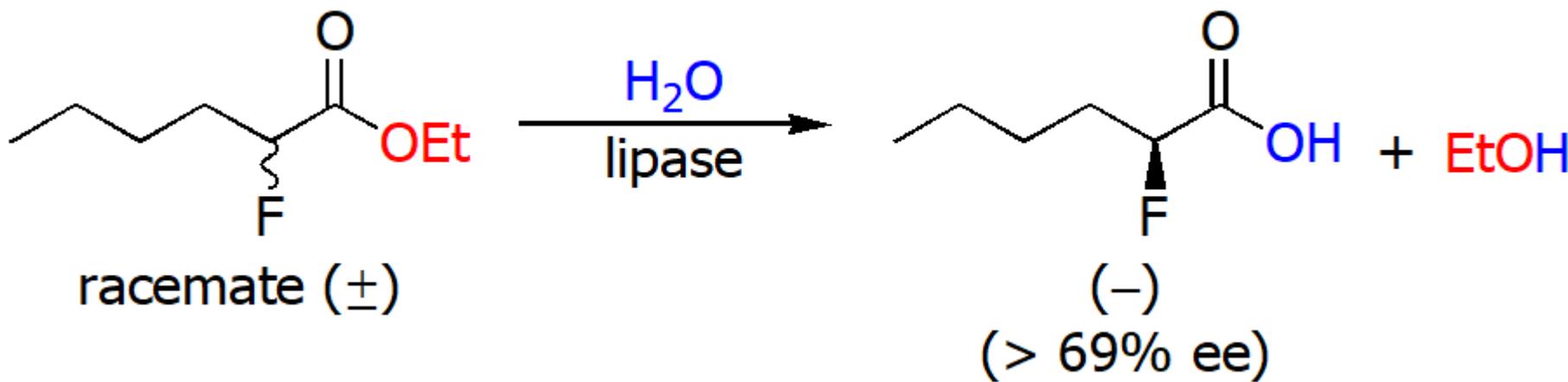
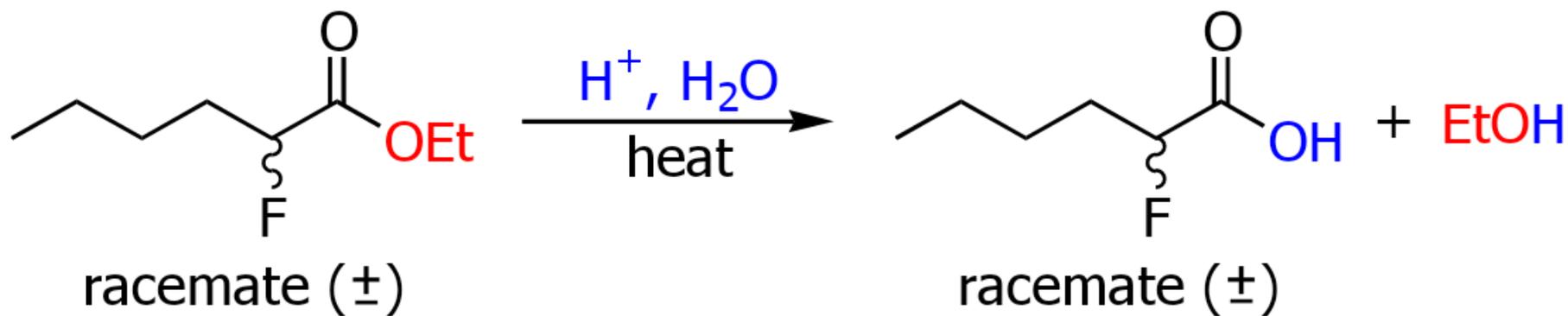
(b)



(S)-(+)-2-Butanol (50%)

9B. Stereoselective Syntheses → لاجاد D كاله او L كاله

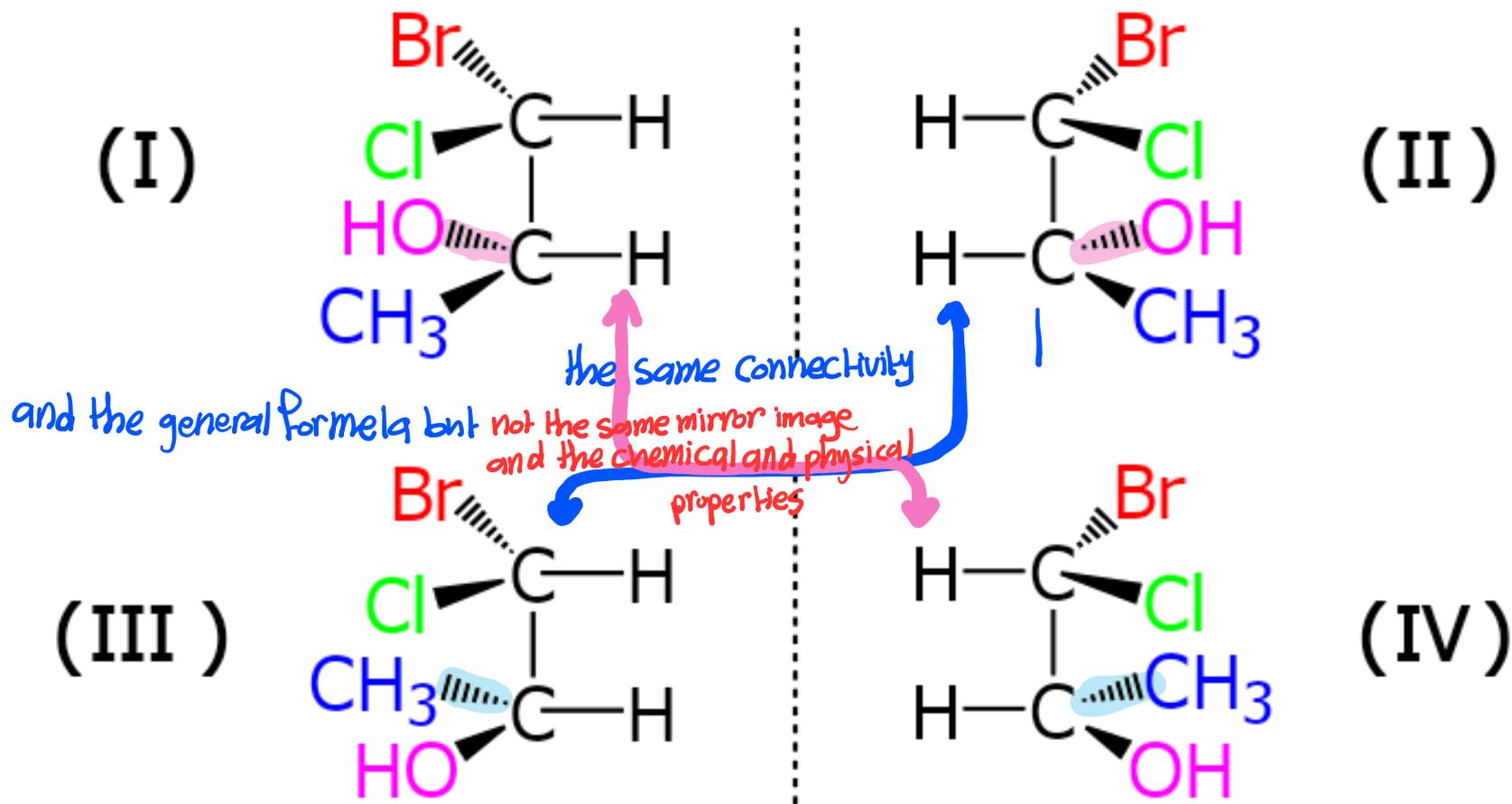
- ❖ **Stereoselective reactions** are reactions that lead to a preferential formation of one stereoisomer over other stereoisomers that could possibly be formed (*it need higher cost*)
 - **enantioselective** – if a reaction produces preferentially one enantiomer over its mirror image
 - **diastereoselective** – if a reaction leads preferentially to one diastereomer over others that are possible



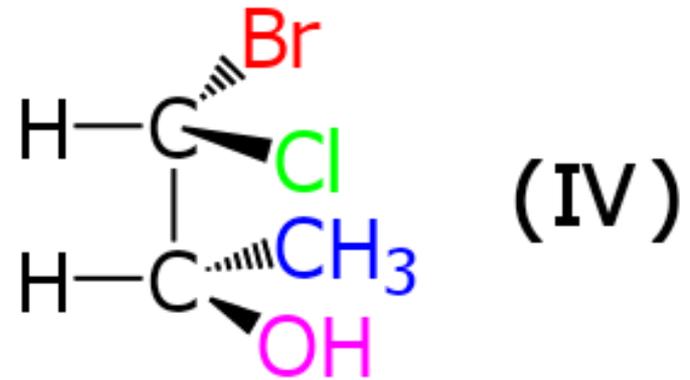
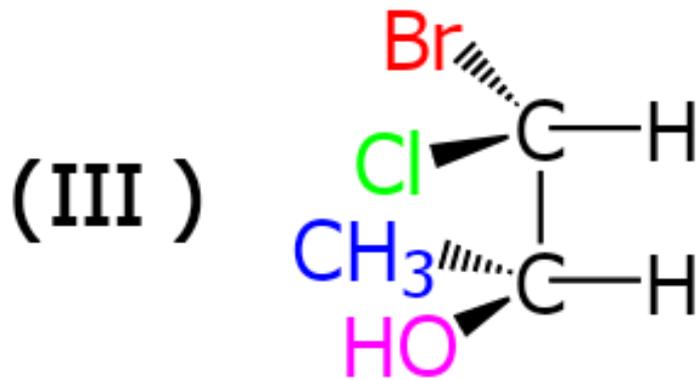
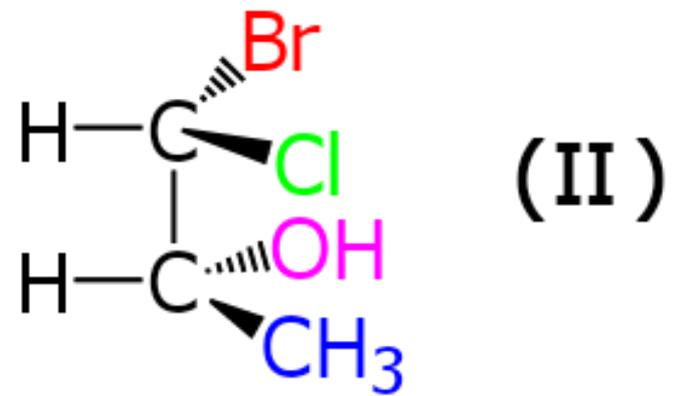
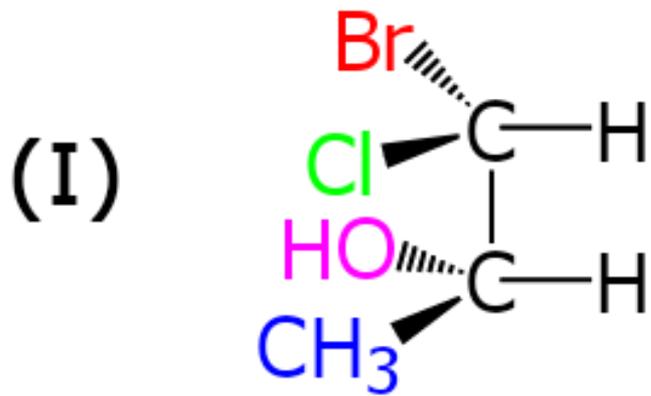
10. Molecules with More than One Chirality Center

❖ Diastereomers

- Stereoisomers that are not enantiomers
- Unlike enantiomers, diastereomers usually have substantially different chemical and physical properties



Note: In compounds with n tetrahedral stereocenters, the maximum number of stereoisomers is 2^n .



- ❖ (I) & (II) are enantiomers to each other
- ❖ (III) & (IV) are enantiomers to each other