polarimeter

منْ أين جاءت فكرته ؟!

- دواء Thalidomide يوصف للمرأة الحامل لتخفيف غثيان الصباح فأدى هذا الدواء إلى حدوث birth difict (missing limb).

- chiral drug (s)

* 25%. of drugs racemic (R and S).

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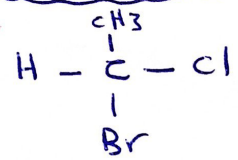
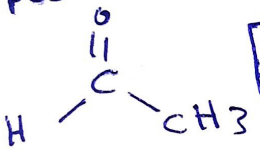
chirality

- asymmetric center



- nonsuperimposable on its mirror image. → غير متطابق

- 4 groups



a chiral

- enantiomers → rotate light by same amount
  → opposite direction (L, D)
  يسار ← → يمين

- optical activity → ability to rotate light.

- degree of rotate
  - identity unknown compound
  - identity it's concentration.
  - enantiomeric purity (R,S)

عن طريق حساب
specific rotation (D)
$[\alpha]$

(+) يمين → clockwise مع عقارب الساعة

(L) (−) يسار → counterclockwise عكس عقارب الساعة

polarimetry

- for analysis.
- measure rotation of the polarized light as it pass through optical active (chiral) compound.

* لا يجب أن يكون light polarized ؟!

light source → ordinary light → in all direction.

↓

- يجب تحويله إلى Polarized light

. عن طريق تمريره بـ → polarizer

. Nicol prism

* polarized light → in one direction.

↳ vector sum of two component ⟨ left. / right.

Dextro = D = (+) = clockwise

Levo = L = (-) = counterclockwise.

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*polarimeter → detected and measured optical activity of molecule in solution.

light source (ordinary) → polarizer → polarized light (in one direction) → polarimeter tube (compound) → Analyzer ↳ rotatable polarizer. → detector

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- Analyzer (lens) :-
  - measure rotation angle (α)
  - Nicol prism.
- light source → sodium vapor lamp.
- polarizer → quartz prism.

$[\alpha]$ Spicific rotation

$$[\alpha]_{\lambda}^{T} = \frac{\alpha}{l \times c}$$

α : observed rotation of light in degree. (زاوية الدوران)

c : concentration in gram per milliliter (g/ml) w/v.

l : cell length (dm)

T : tempreture of solution.

λ : Wavelength of light.

$[\alpha]$ → fixed physical properities of material

* يعني حتى لو غيرت التركيز أو ~~[illegible]~~ ال length & يتغير.

* الـ enantiomers لها نفس $[\alpha]$ ولكن بعكس الاتجاه.

* هدف التجربة :- قياس ال angle لل unKnown sugar واستخدامها في حساب ال specific rotation له.

Enantiomiric excess

↓

How mush of excess one enantiomer in mixture

$$e.e = \frac{\text{observed specific rotation}}{\text{specific rotation of pure enantiomers}} \times 100\%$$

مثلاً : % e.e = 40%

↓ excess enantiomers

two enantiomer الـ 1 على تقسم 60% المحلول من الباقي

30% 30%

excess enatiomer = 70%

another enantiomer = 30%

> 100%

racemic : equal amount of enantiomers. ; غلط

What is the specific rotation of a compound 'X' when the concentration is 0.5% w/v, angle of rotation is 1.3 and tube length is 25 cm?

- 10.4°
- 52.0°
- **104.0°**
- 5.2°

Angle of rotation (α) = 1.3° , Tube length = 25 cm = 2.5 dm

Concentration = 0.5% w/v

Formula $$[\alpha]^{T}_{\lambda} = \frac{100 \times \alpha}{l \times c}$$

$$[\alpha]^{T}_{\lambda} = \frac{100 \times 1.3}{2.5 \times 0.5}$$

$$[\alpha]^{T}_{\lambda} = 104.0°$$

optical purity = % enantiomeric excess
= % of one enantiomer - % of other enantiomer

2. Calculate the % ee for the following

100% 0%

a) a solution containing a single enantiomer

% ee = 100 − 0 = 100%

b) a solution containing equal amounts of both enantiomers (racemic mixture)

% ee = 50% − 50% = 0

c) a solution containing 75% of one enantiomer and 25% of the other enantiomer

% ee = 75 − 25 = 50%

So we have 50% excess of this enantiomer,

$$\%\ ee = \frac{\text{observed } [\alpha]}{[\alpha] \text{ of pure enantiomer}} \times 100$$

% α = 13% − 7% = 86%

3. A mixture of natural cholesterol and its enantiomer has a specific rotation (at 20°C) of -27. Calculate the % ee of this mixture. What % of the mixture is natural cholesterol?

13%

$$\%\ ee = \frac{-27}{-315} \times 100$$

86% nat cholesterol

14%

7% nat 7% enantiomer

So that's just a nice
little check to make sure

Example 1: If a mixture of this R and S has an observed rotation (α_{obs}) of +3.97, then the percent composition is calculated as follows.

- The overall rotation is positive so there is an excess of the S enationmer.
- We know from the above equation that ee $=\alpha_{obs}$ /[c‹] x 100%,
- therefore ee =3.97/16.7 * 100 = 23.8%.
- This means that the rest of the material (100.0 — 23.8 = 76.2%) is equally divided between the R and S (100 % - % e.e. = % of balanced material).
- Therefore, there is 76.2/2 or 38.1% R material,
- and 38.1% +23.8 % = 61.9% S material.
- To check, 61.9% + 38.1% = 100 %,
- the difference between the two is 23.8%.

- **Example 2:** If a pure R material has a specific rotation of -16.70
- a mixture of 40% R and 60% S will result in a 20% enantiomeric excess (The 40%R cancels 40% of the S, and leaves 20% excess S).
- The 20%e.e. is then divided by 100 =0.20,
- and multiplied by the absolute value of [u] of |-16.70| or 16.70 to show this mixture will rotate light by =|3.35|.
- Knowing that the R material rotates in the negative direction,
- and knowing that this mixture has an excess of the S enantiomer, means that this material will rotate light in the positive or clockwise direction by 3.35 degrees.

e.e. = |R-S| / (R+S) * 100%= |60-40|/(60 +40) *100% = 20%
20% of |-16.70| = |3.35|, and an excess of S means +3.35.