

Modulo 1 – Química Orgânica

2. Grupos funcionais e características das moléculas orgânicas

Função e grupos funcionais

Isomeria, isómeros de constituição, Isomeria cis-trans. Carbono assimétrico. Estereoisomeria.

Polarização das ligações covalentes, cargas parciais, momento dipolar das moléculas.

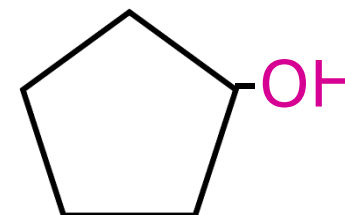
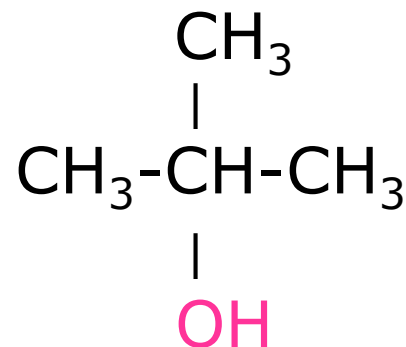
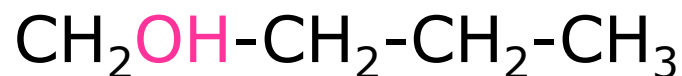
Interações intermoleculares: pontes de hidrogénio, ligação dipolo-dipolo, forças de van der Waals, ligações iónicas.

Influência nas propriedades físicas. Solubilidade.

Função e grupos funcionais

Compostos do mesmo grupo funcional são compostos orgânicos que têm elementos de estrutura química semelhante que lhes confere comportamento químico e propriedades também semelhantes.

Em compostos da mesma função são encontrados arranjos iguais entre determinados elementos:



Função e grupos funcionais

TABLE 11.4 Compounds Containing a Carbon–Heteroatom Single Bond

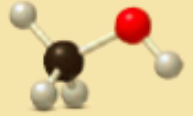
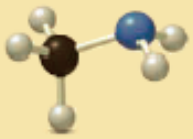
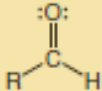
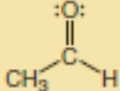
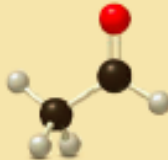
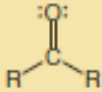
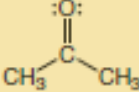
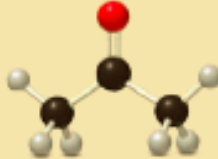
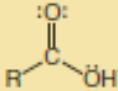
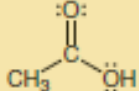
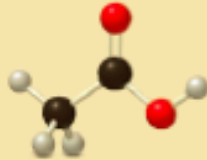
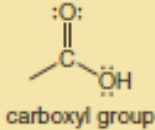
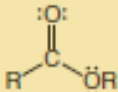
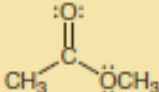
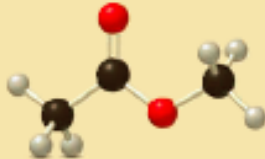
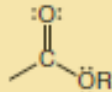
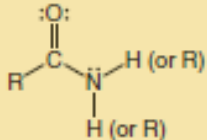
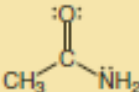
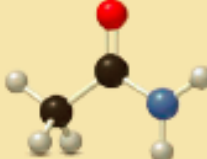
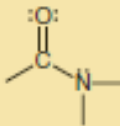
Type of Compound	General Structure	Example	3-D Structure	Functional Group
Derivados Halogenados	$\text{R}-\ddot{\text{X}}:$ (X = F, Cl, Br, I)	$\text{CH}_3-\ddot{\text{Br}}:$		-X
Alcoois	$\text{R}-\ddot{\text{O}}\text{H}$	$\text{CH}_3-\ddot{\text{O}}\text{H}$		-OH hydroxyl group
Éteres	$\text{R}-\ddot{\text{O}}-\text{R}$	$\text{CH}_3-\ddot{\text{O}}-\text{CH}_3$		-OR
Aminas	$\text{R}-\ddot{\text{N}}\text{H}_2 \text{ or } \text{R}_2\ddot{\text{N}}\text{H} \text{ or } \text{R}_3\ddot{\text{N}}$	$\text{CH}_3-\ddot{\text{N}}\text{H}_2$		-NH ₂ amino group

TABLE 11.5 Compounds Containing a C=O Group

Type of Compound	General Structure	Example	3-D Structure	Functional Group
Aldeídos				
Cetonas				
Ácidos carboxílicos				
Estéres				
Amidas				

Função e grupos funcionais

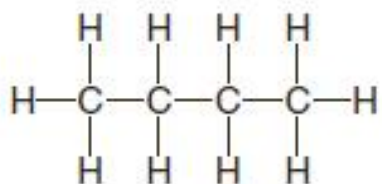
TABLE 10.2 Common Functional Groups

Type of compound	Structural formula	Condensed formula	Structural formula	Example I.U.P.A.C. name	Common name
Alcohol	$\text{R}-\text{O}-\text{H}$	ROH	$\text{CH}_3\text{CH}_2-\text{O}-\text{H}$	Ethanol	Ethyl alcohol
Aldehyde	$\text{R}-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{H}$	RCHO	$\text{CH}_3-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{H}$	Ethanal	Acetaldehyde
Amide	$\text{R}-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\overset{\text{H}}{\underset{ }{\text{N}}}-\text{H}$	RCONH_2	$\text{CH}_3-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\overset{\text{H}}{\underset{ }{\text{N}}}-\text{H}$	Ethanamide	Acetamide
Amine	$\text{R}-\overset{\text{H}}{\underset{ }{\text{N}}}-\text{H}$	RNH_2	$\text{CH}_3\text{CH}_2-\overset{\text{H}}{\underset{ }{\text{N}}}-\text{H}$	Aminoethane	Ethyl amine
Carboxylic acid	$\text{R}-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{O}-\text{H}$	RCOOH	$\text{CH}_3-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{O}-\text{H}$	Ethanoic acid	Acetic acid
Ester	$\text{R}-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{O}-\text{R}'$	RCOOR'	$\text{CH}_3-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{OCH}_3$	Methyl ethanoate	Methyl acetate
Ether	$\text{R}-\text{O}-\text{R}'$	ROR'	CH_3OCH_3	Methoxymethane	Dimethyl ether
Halide	$\text{R}-\text{Cl}$ (or $-\text{Br}$, $-\text{F}$, $-\text{I}$)	RCl	$\text{CH}_3\text{CH}_2\text{Cl}$	Chloroethane	Ethyl chloride
Ketone	$\text{R}-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{R}'$	RCOR'	$\text{CH}_3-\overset{\text{O}}{\underset{\text{ }}{\text{C}}}-\text{CH}_3$	Propanone	Acetone
Alkene	$\begin{array}{c} \text{R} \quad \quad \text{R} \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{H} \quad \quad \text{H} \end{array}$	RCHCHR	$\text{CH}_3\text{CH}=\text{CH}_2$	Propene	Propylene
Alkyne	$\text{R}-\text{C}\equiv\text{C}-\text{R}$	RCCR	$\text{CH}_3\text{C}\equiv\text{CH}$	Propyne	Methyl acetylene

Isomeria, isómeros de constituição

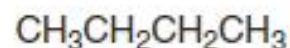
Compostos diferentes com a mesma fórmula molecular

Isómeros de constituição diferem na forma como os átomos se ligam entre si



butane

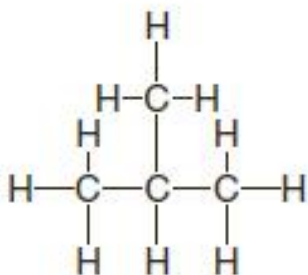
=



4 C's in a row

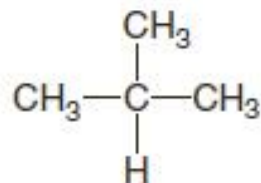


straight-chain alkane



isobutane

=



3 C's with a one-carbon branch



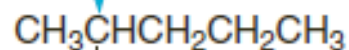
branched-chain alkane

Isómeros de constituição:

A

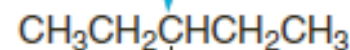
Constitutional isomers with the same functional group

CH₃ group at C2



2-methylpentane
C₆H₁₄

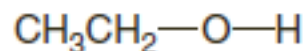
and



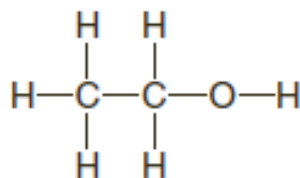
3-methylpentane
C₆H₁₄

B

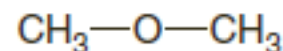
Constitutional isomers with different functional groups



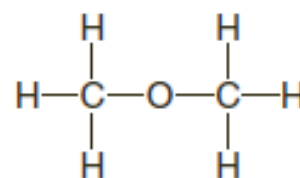
ethanol
C₂H₆O



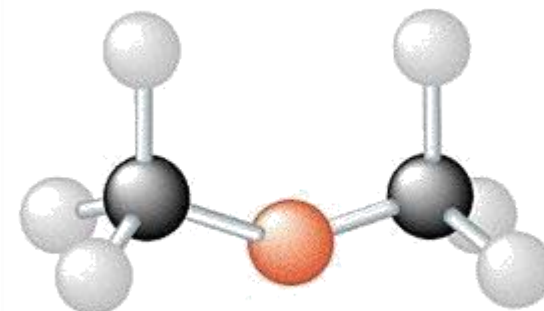
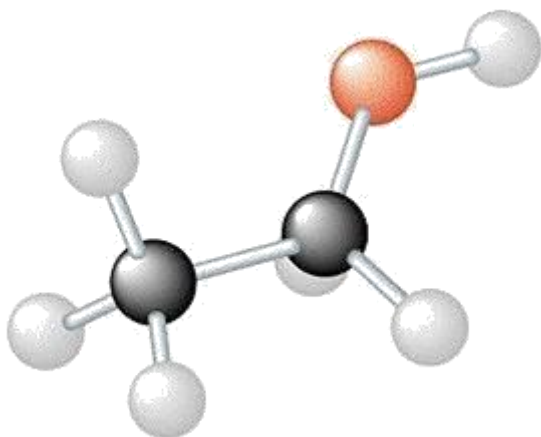
CH₃CH₂OH
ethanol



dimethyl ether
C₂H₆O



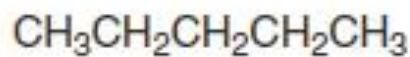
CH₃OCH₃
dimethyl ether



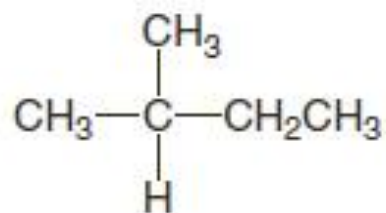
Isómeros de constituição:

-diferem na posição de elementos, grupos substituintes, grupos funcionais

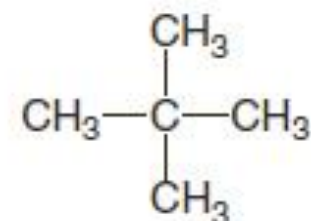
-diferem na posição de grupos substituintes:



pentane



isopentane
(2-methylbutane)



neopentane
(2,2-dimethylpropane)



- diferem na posição de grupos funcionais:



São alcoóis: -Reactividade química semelhante;
-Características físicas diferentes (por exemplo, temperatura de fusão e de ebulição)

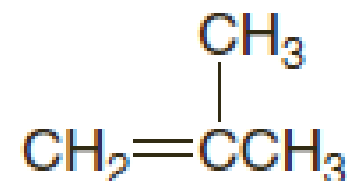
- diferem na posição da insaturação:



1-butene



2-butene



2-methylpropene

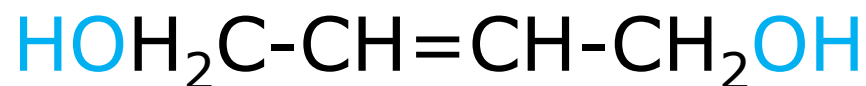
difere na posição
da insaturação e
dos substituintes

Exemplo:

Formula molecular: $C_4H_8O_2$



ácido



di-álcool

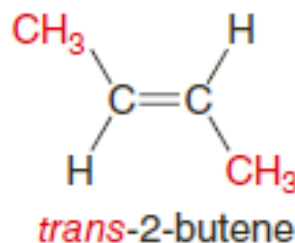
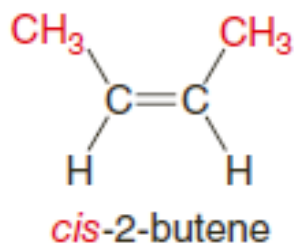


aldeído-álcool

Isomeria cis-trans (geométrica): -isomeria de especifica de alcenos e alguns ciclos

C

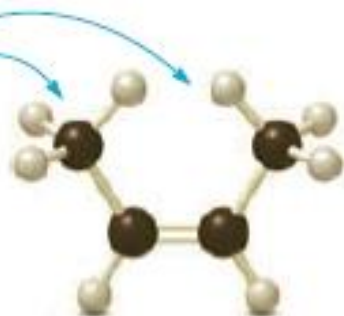
One example of stereoisomers—Isomers at a double bond



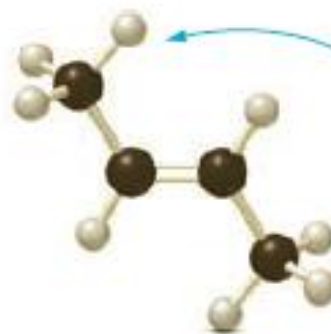
2-butenos
 $\text{CH}_3\text{CH}=\text{CHCH}_3$

two CH₃ groups
on the same side

Dois grupos
CH₃ no
mesmo lado



cis-2-butene



trans-2-butene

two CH₃ groups
on opposite sides

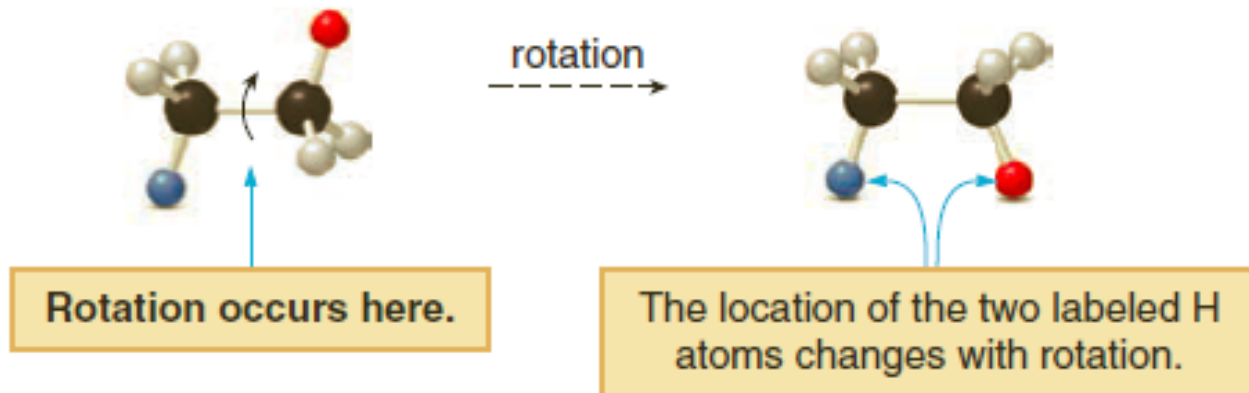
Dois grupos
CH₃ em lados
opostos

different compounds

Isomeria cis-trans

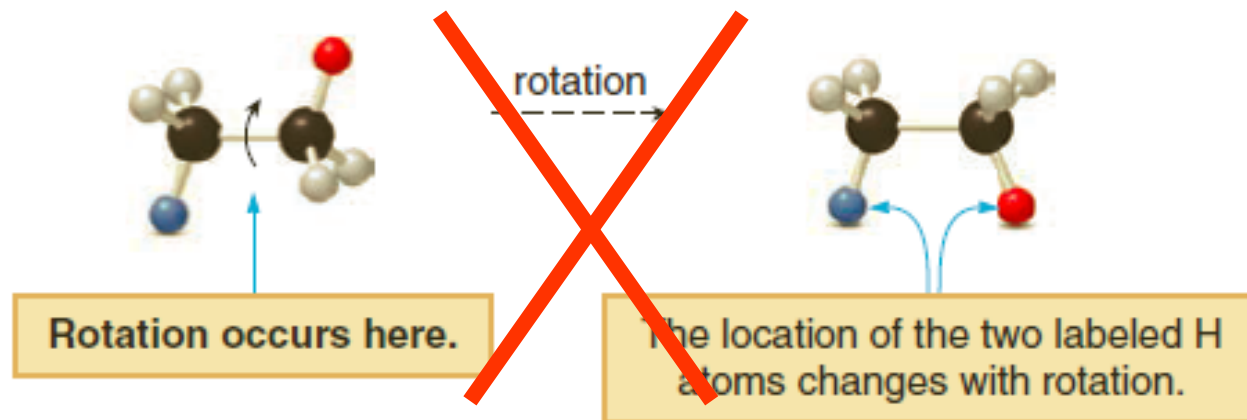
Força da ligação $\sigma = 3-6 \text{ kcal mol}^{-1}$

Alcanos, ligação C-C
covalente simples
(orbital molecular sigma)



Força da ligação $\pi = 63 \text{ kcal mol}^{-1}$

Alcenos, ligação C=C
covalente dupla
(orbital molecular σ , orbital molecular π)

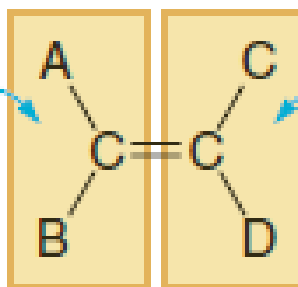


Há restrições à rotação

Isomeria cis-trans

é gerada por restrição à rotação da ligação C=C que origina isómeros quando há substituintes diferentes nos átomos de C envolvidos na ligação

These two groups
must be **different**
from each other...

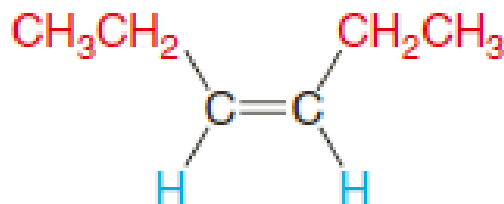


...and these two groups
must also be **different**
from each other.

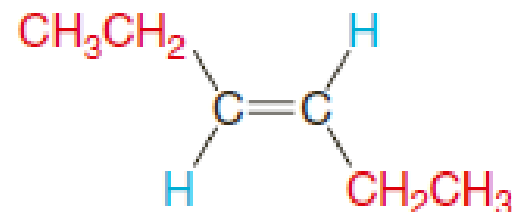


1 2 3 4 5 6

3-hexene



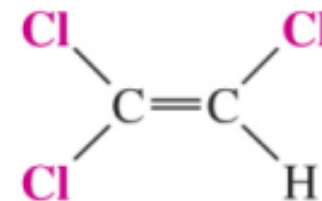
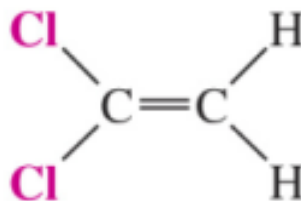
cis-3-hexene



trans-3-hexene

No caso da dupla ligação os dois átomos de carbono e os quatro átomos (ou grupos de átomos) a eles diretamente ligados são mantidos **num mesmo plano pela dupla ligação**

Se um dos carbonos da dupla ligação tem 2 substituintes iguais **não há isomeria *cis-trans***

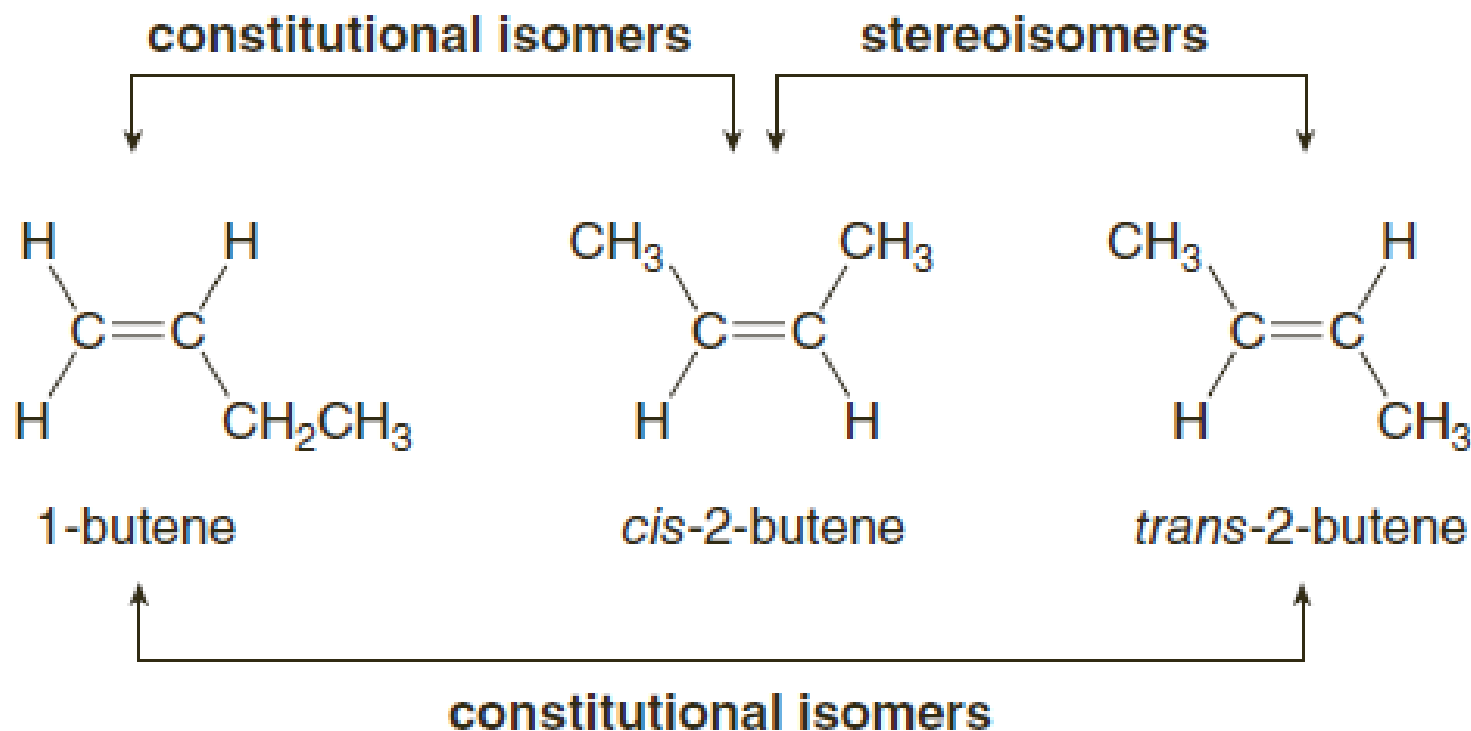


- **CIS**, os dois substituintes idênticos estão “**acima**” da dupla ligação ou do mesmo lado do plano da dupla ligação.
- **TRANS**, os dois substituintes idênticos estão “**em lados opostos**” do plano da dupla da ligação.

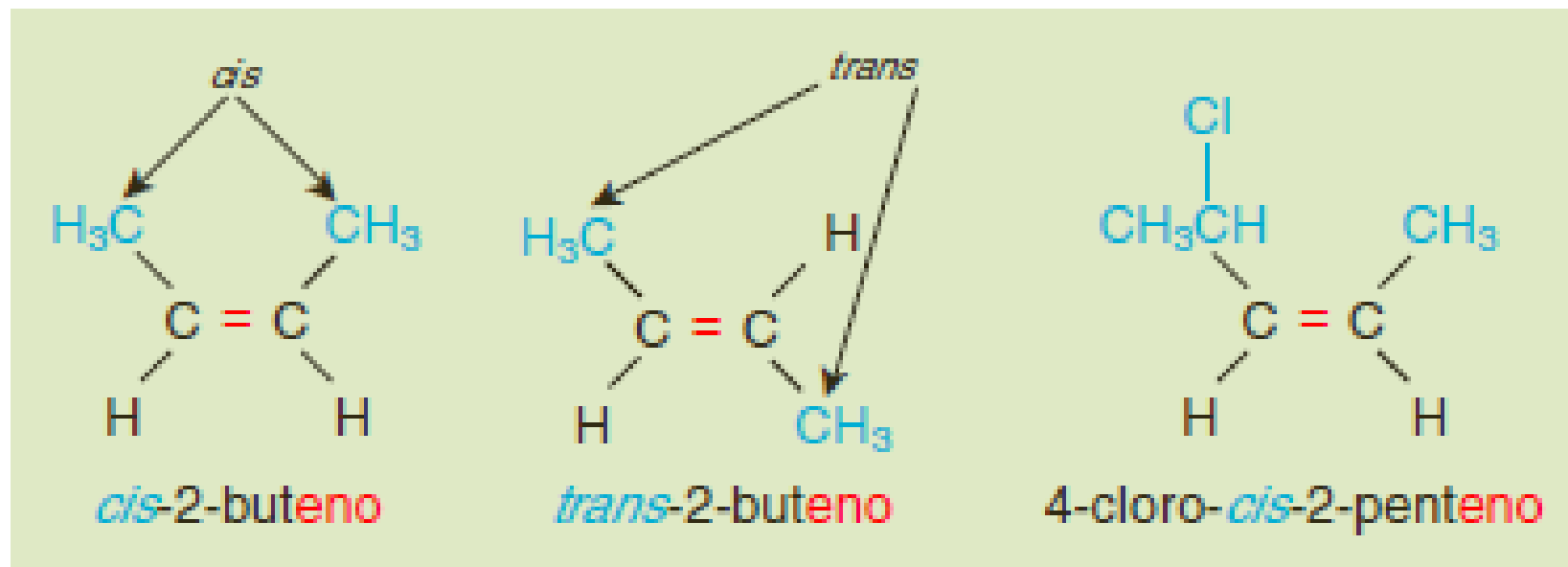
As formas **CIS** e **TRANS** diferem nas propriedades físicas e químicas

Que tipo de isómeros são:

1-buteno *cis*-2-buteno *trans*-2-buteno



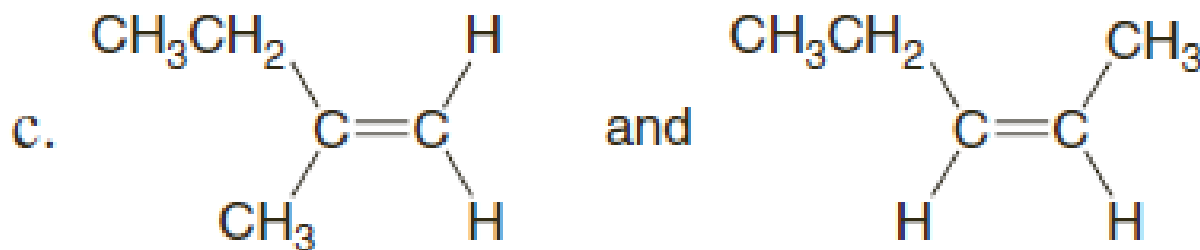
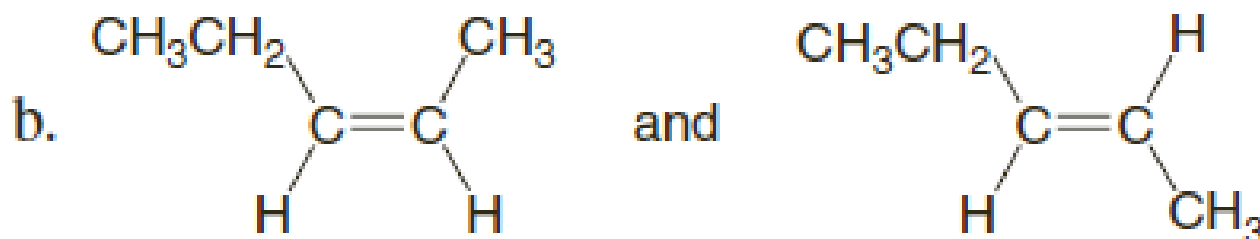
Exemplo de isomeros *Cis* e *Trans*:



Exercicio: Identificar o tipo de isomeria

i) isomeria de constituição

ii) isomeria cis-trans



Moléculas orgânicas no nosso dia-a-dia

Os ácidos gordos insaturados isomeria *cis-trans*

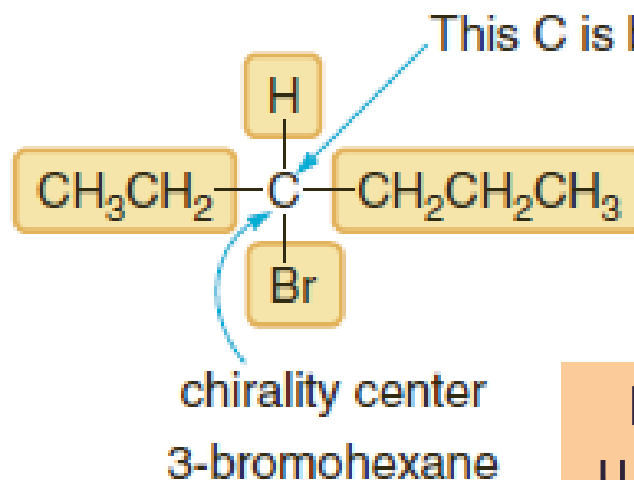
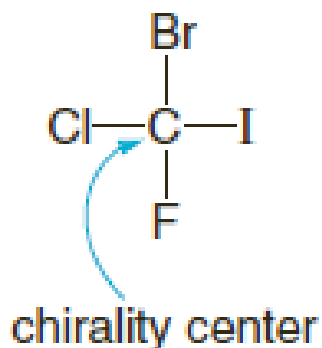
Nas gorduras naturais todas as ligações duplas são *CIS*

TABLE 13.1 Common Saturated and Unsaturated Fatty Acids

Name	Structure
Stearic acid (0 C=C)	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{COOH}$
Oleic acid (1 C=C)	$ \begin{array}{c} \text{H} \quad \text{H} \\ \diagdown \quad \diagup \\ \text{C} = \text{C} \\ \diagup \quad \diagdown \\ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 \quad \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{COOH} \end{array} $ <i>cis</i>
Linoleic acid (2 C=C)	$ \begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \\ \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \text{C} = \text{C} \quad \text{C} = \text{C} \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \\ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 \quad \text{CH}_2 \quad \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{COOH} \end{array} $ <i>cis</i>
Linolenic acid (3 C=C)	$ \begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \\ \diagdown \quad \diagup \quad \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \text{C} = \text{C} \quad \text{C} = \text{C} \quad \text{C} = \text{C} \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \quad \diagup \quad \diagdown \\ \text{CH}_3\text{CH}_2 \quad \text{CH}_2 \quad \text{CH}_2 \quad \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{COOH} \end{array} $ <i>cis</i>

Estereoisomeria (isomeria ótica)

Molécula quiral:
não se sobrepõe com
imagem no espelho



two different alkyl groups

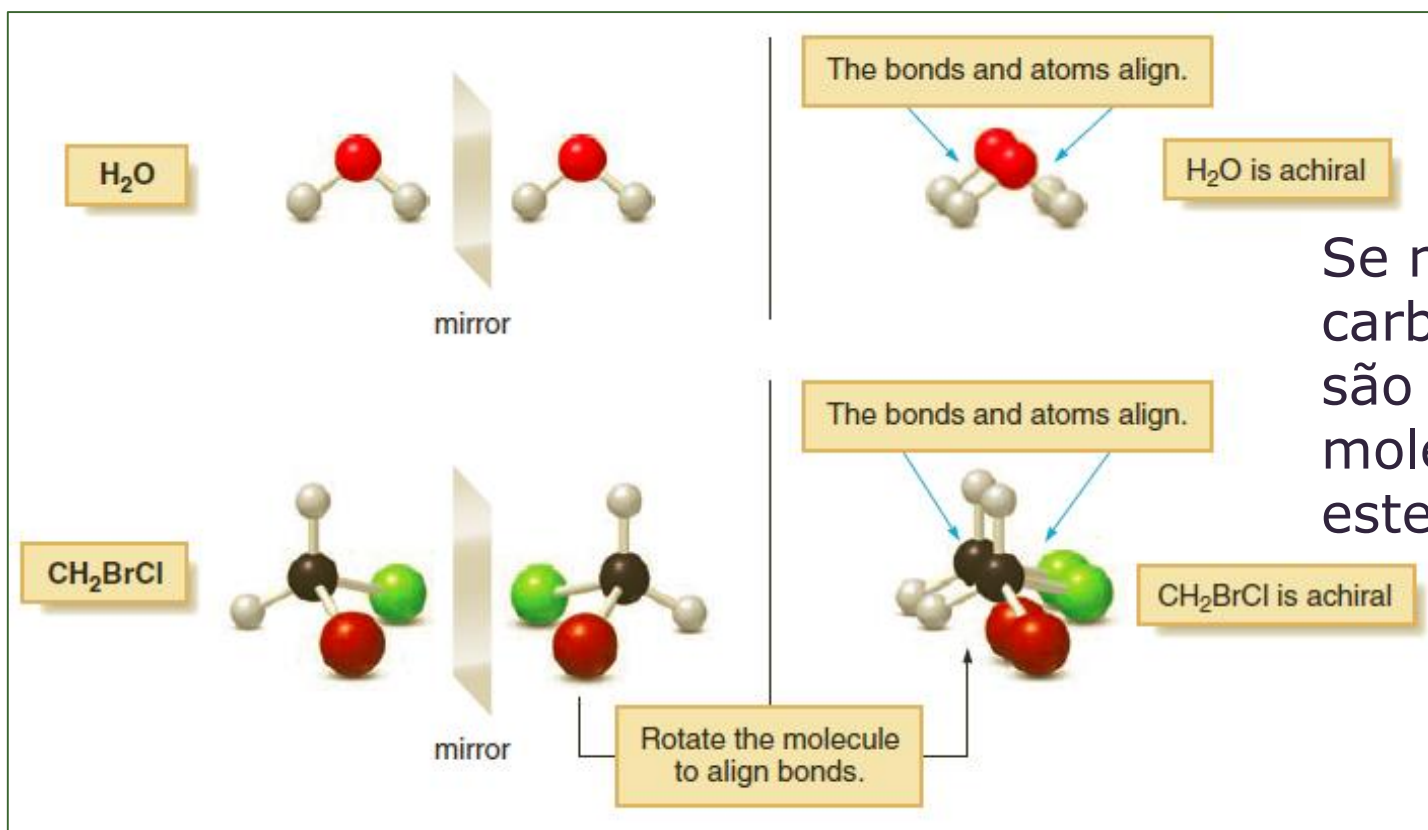
Moléculas quirais têm
um carbono assimétrico
(C com 4 substituintes
diferentes)

Organic Chemistry Lesson:
Stereochemistry 1

<http://www.youtube.com/watch?v=4-4K5OJv3ik>

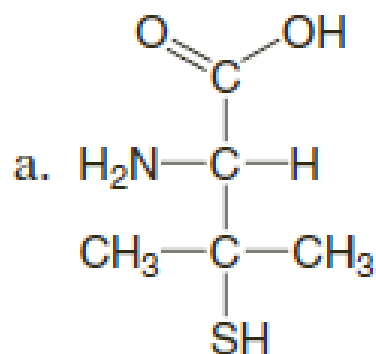
Estereoisómeros

Compostos constituídos pelos mesmos tipos e números de átomos, ligados entre si na mesma sequência, mas com arranjos espaciais diferentes.

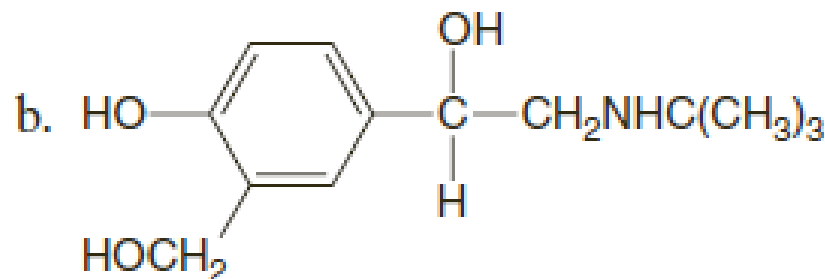


Se não existir carbono assimétrico são a mesma molécula não há estereoisomeria

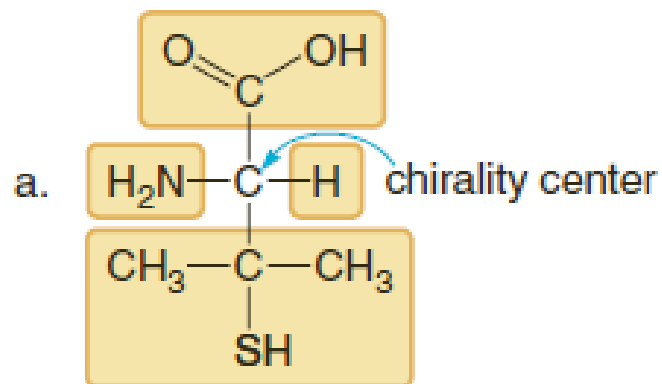
Identificar os carbonos assimétricos (centro de quiralidade) das seguintes moléculas:



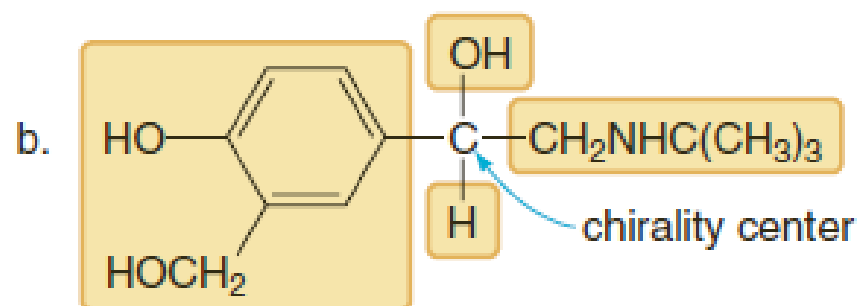
penicillamine



albuterol

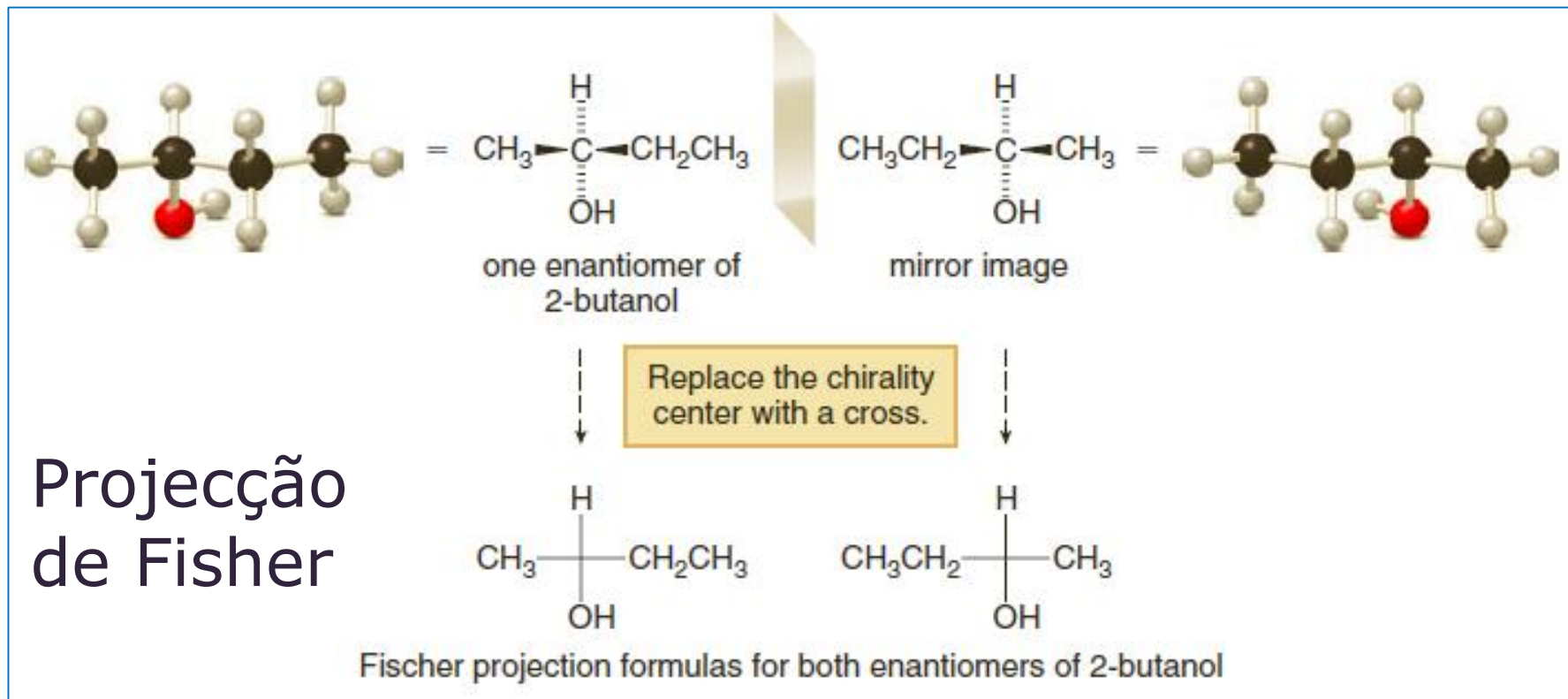
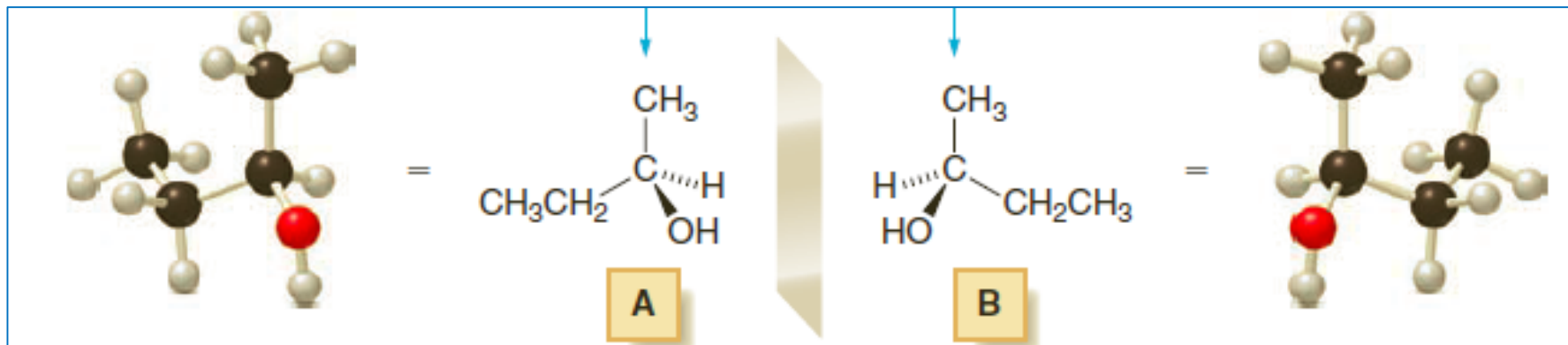


penicillamine



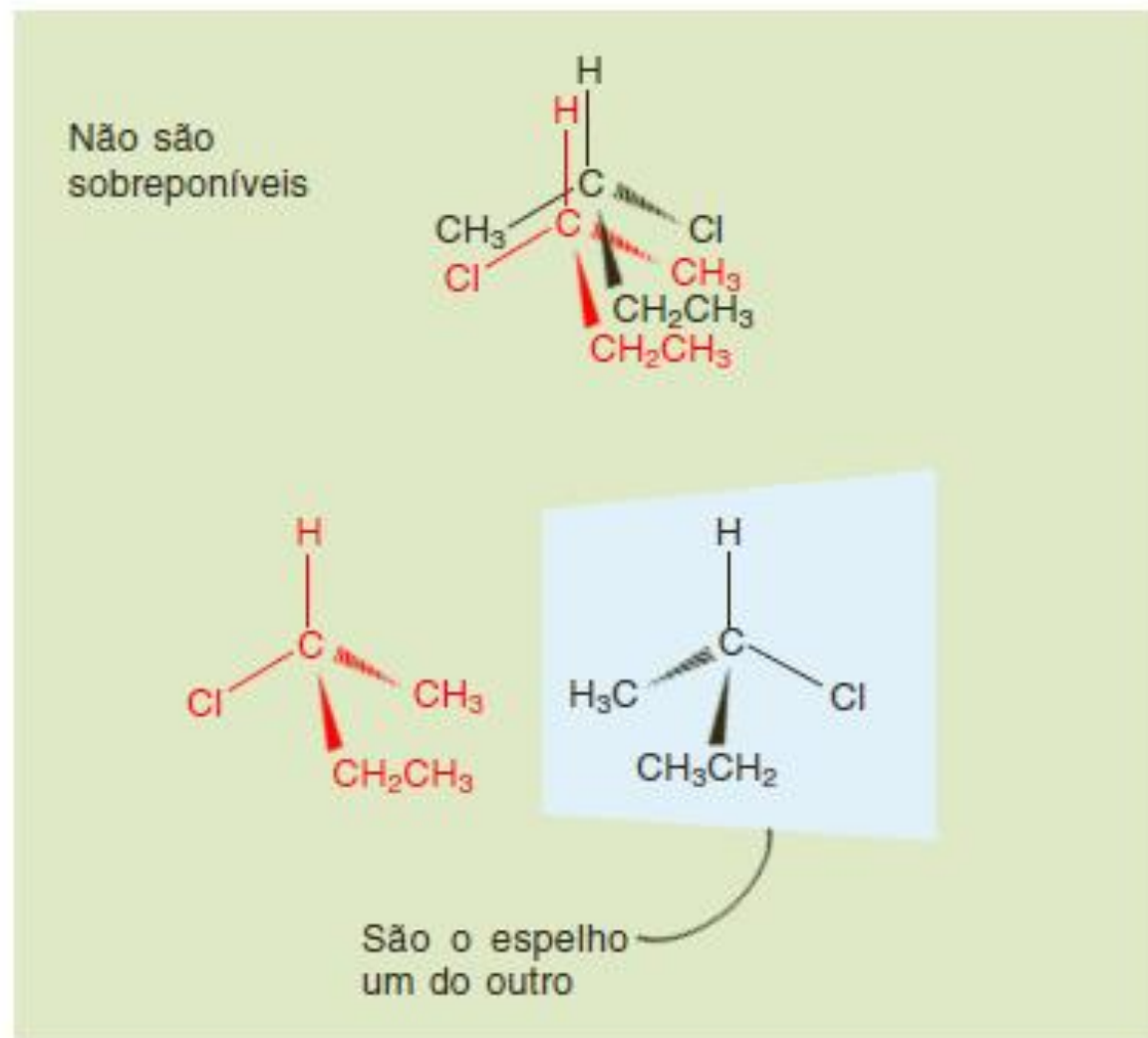
albuterol

Enantiómeros



Projeção
de Fisher

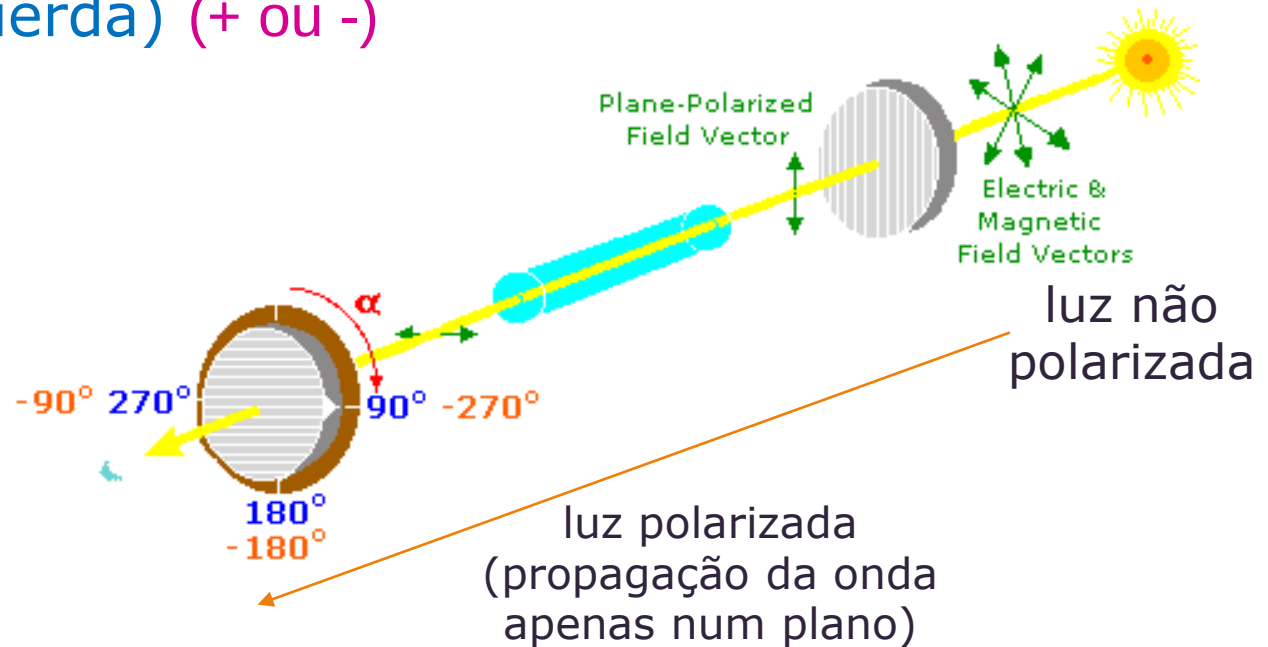
Exemplos de enantiómeros



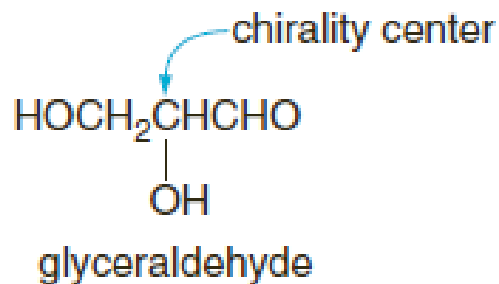
Estereoisómeros são substâncias opticamente ativas

- Apresentam diferente atividade ótica (capacidade de desviar o plano da luz polarizada de forma característica)
- Desviam o plano da luz polarizada num dado sentido (direita ou esquerda) (+ ou -)

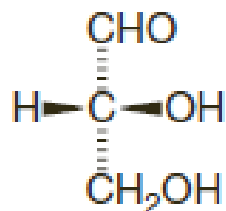
diferenciam-se pelo desvio causado no plano da luz polarizada que incide numa molécula



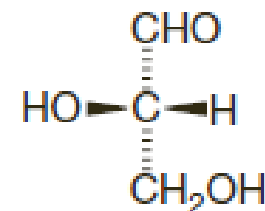
Enantiómeros D e L



Draw the compound.

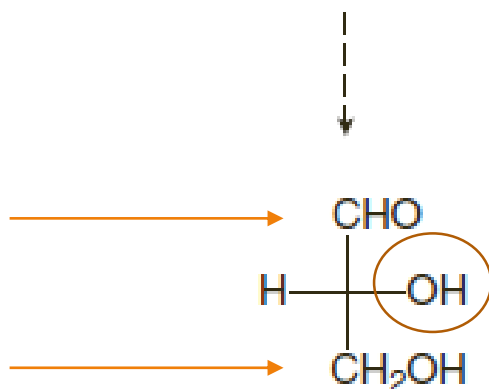


Then, draw the mirror image.

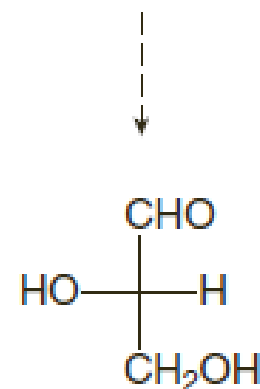


- Horizontal bonds come forward.
- Vertical bonds go back.

Projecção de Fisher



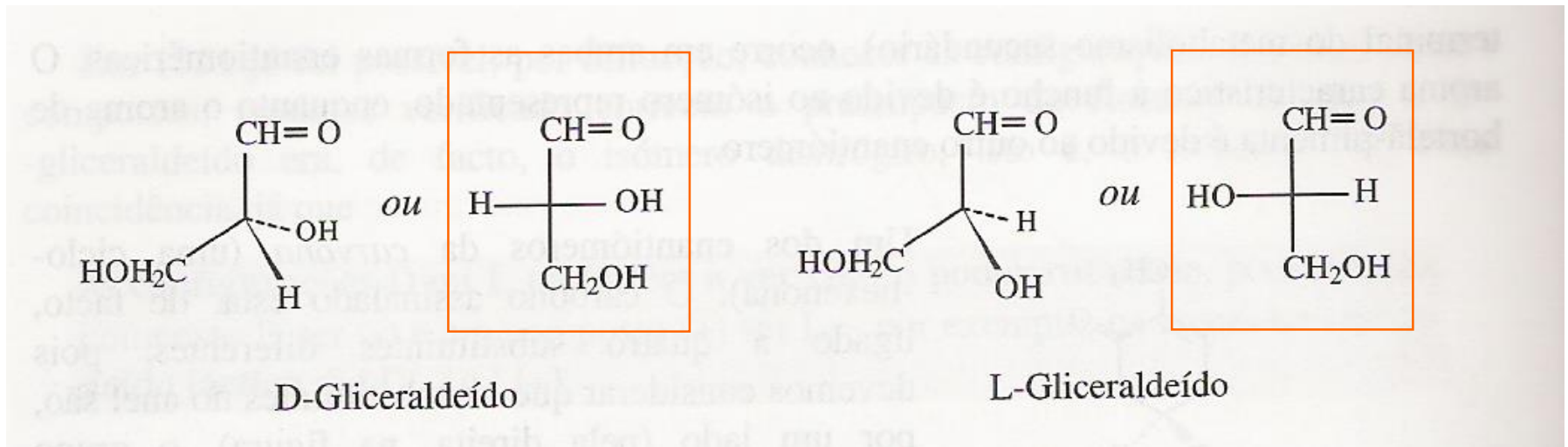
Fischer projection of one enantiomer



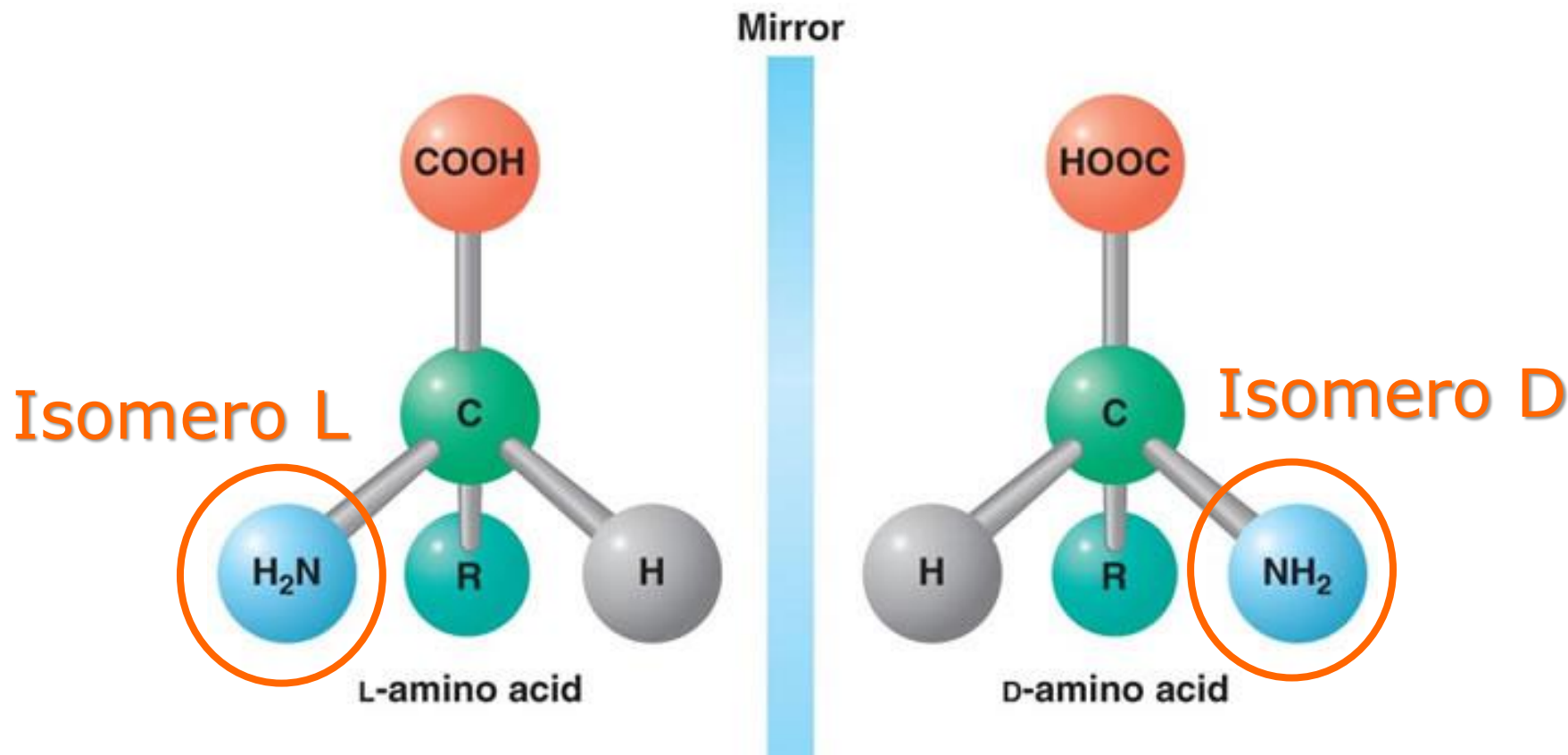
Fischer projection of the second enantiomer

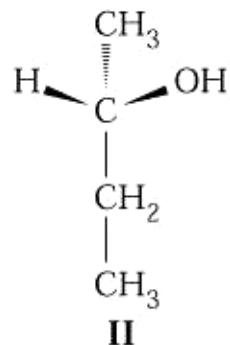
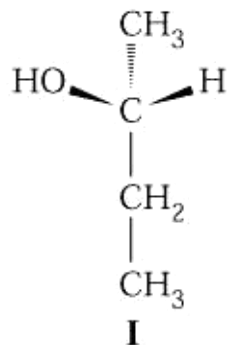
Representação de Fisher

- Tem regras próprias



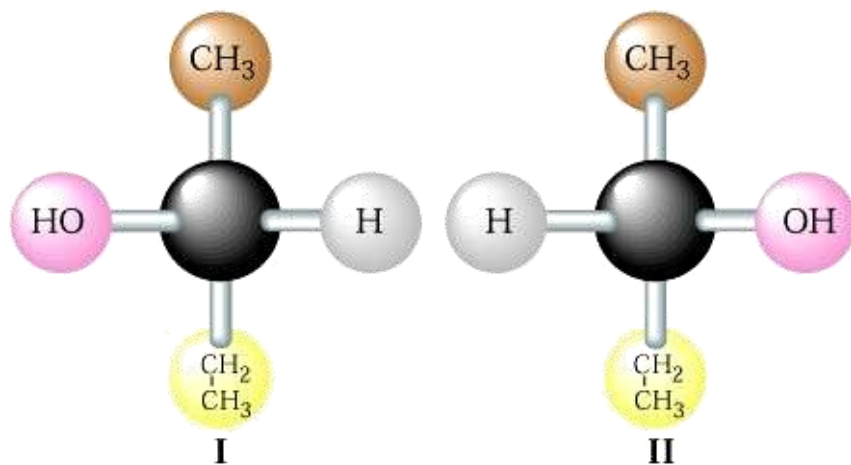
- Nos aminoácidos há estereoisomeria
- Os aminoácidos proteicos são isómeros L



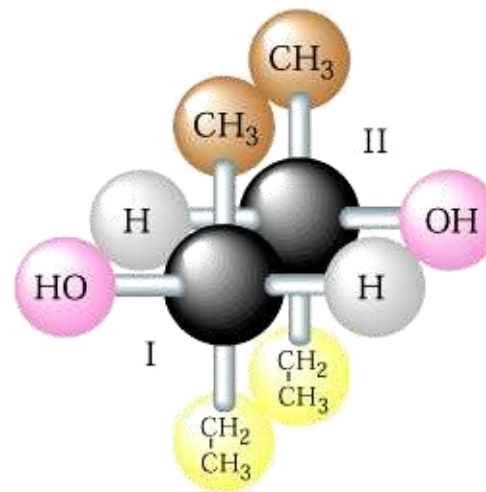


I e II são enantiómeros

(a)



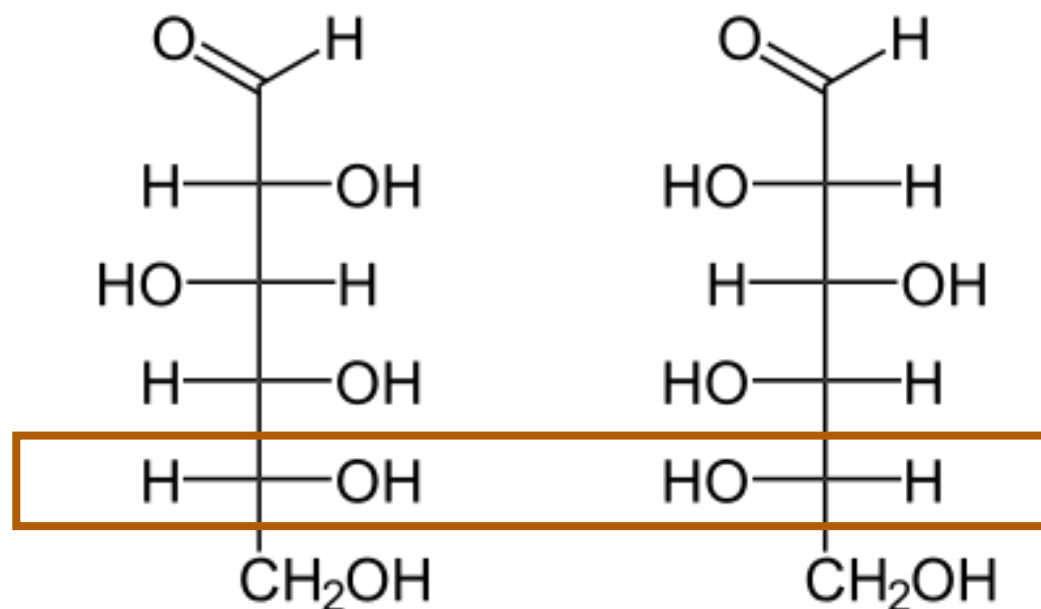
(b)



(c)

Uma mesma molécula pode conter mais do que um carbono assimétrico: o caso dos glúcidos

Glúcidos
simples
são
isómeros D

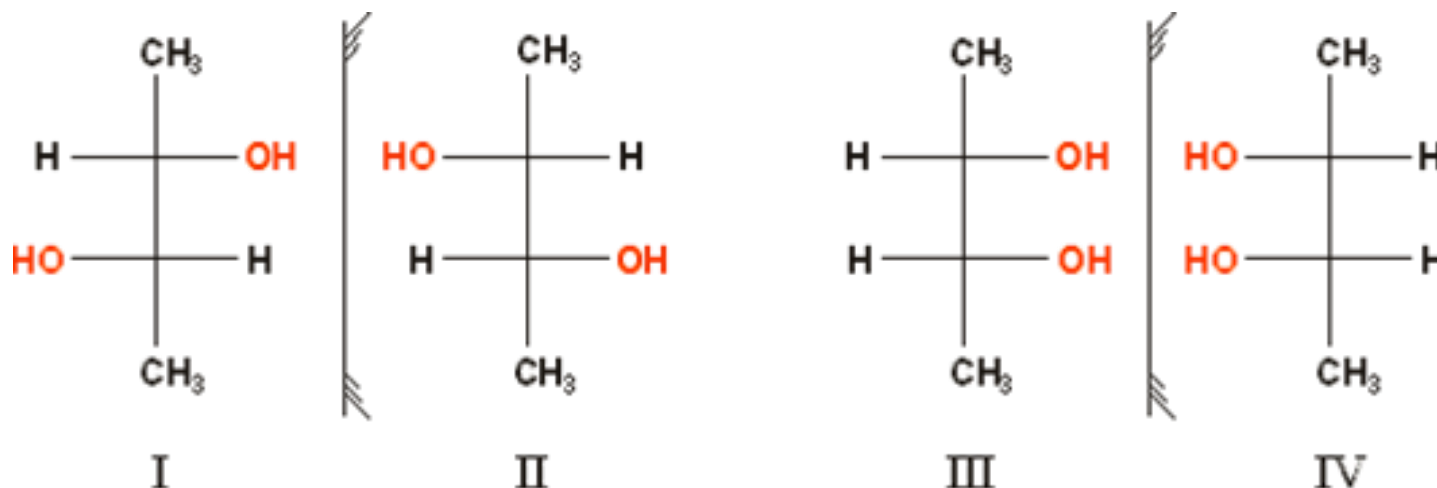


D-Glucose

L-Glucose

A presença de ambos os enantiómeros
designa-se mistura racémica

Uma mesma molécula pode conter mais do que um carbono assimétrico



I e II são **enantiómeros**,
não são sobreponíveis

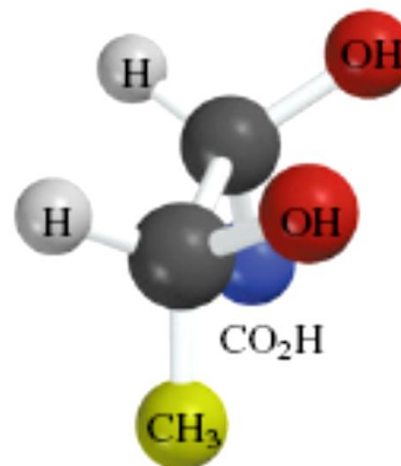
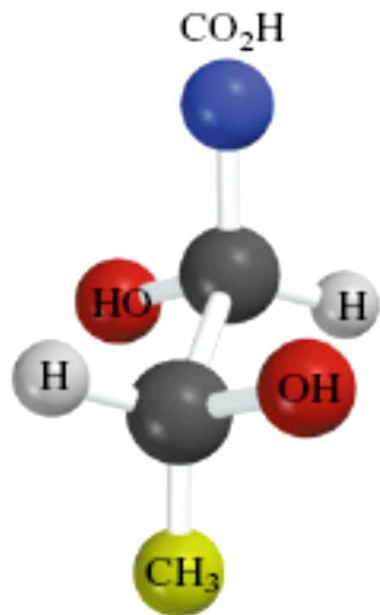
Compare III e IV:
São a mesma estrutura
ou são diferentes???

Compare a estrutura III com I e com II.

A estrutura III não tem relação objecto-imagem, nem com I nem com II.

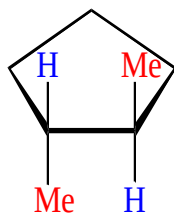
Dizemos que **I e III** (ou **II e III**) são **diastereómeros**.

a) e b) são diastereómeros

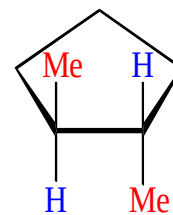


Estereoisómeria em ciclos:

Enantiómeros são estereoisómeros cujas moléculas **são imagens não sobreponíveis *uma da outra***

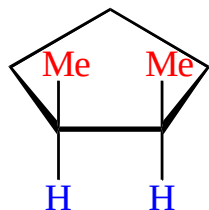


trans-1,2-
Dimetilciclopentano (C_7H_{14})

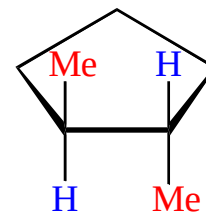


trans-1,2-
Dimetilciclopentano (C_7H_{14})

Diastereómeros são estereoisómeros cujas moléculas **não são imagem uma da outra num espelho**

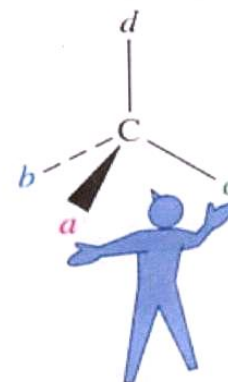
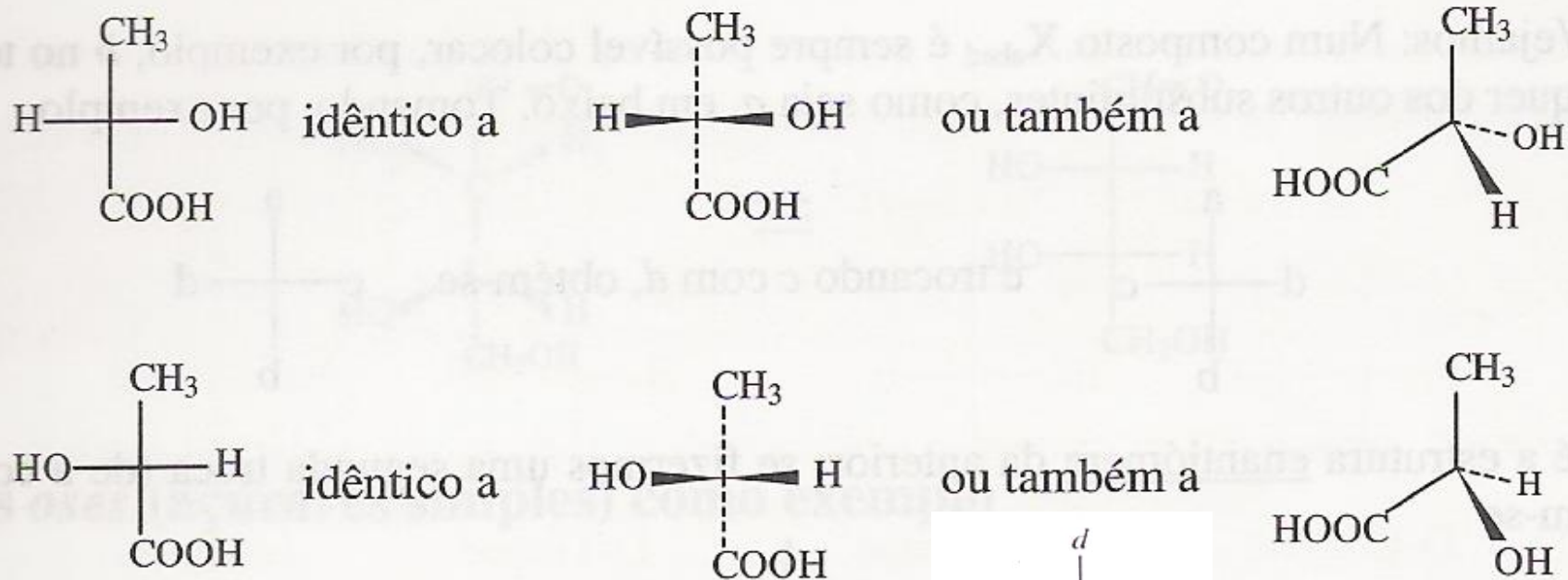


cis-1,2-Dimetilciclopentano
(C_7H_{14})

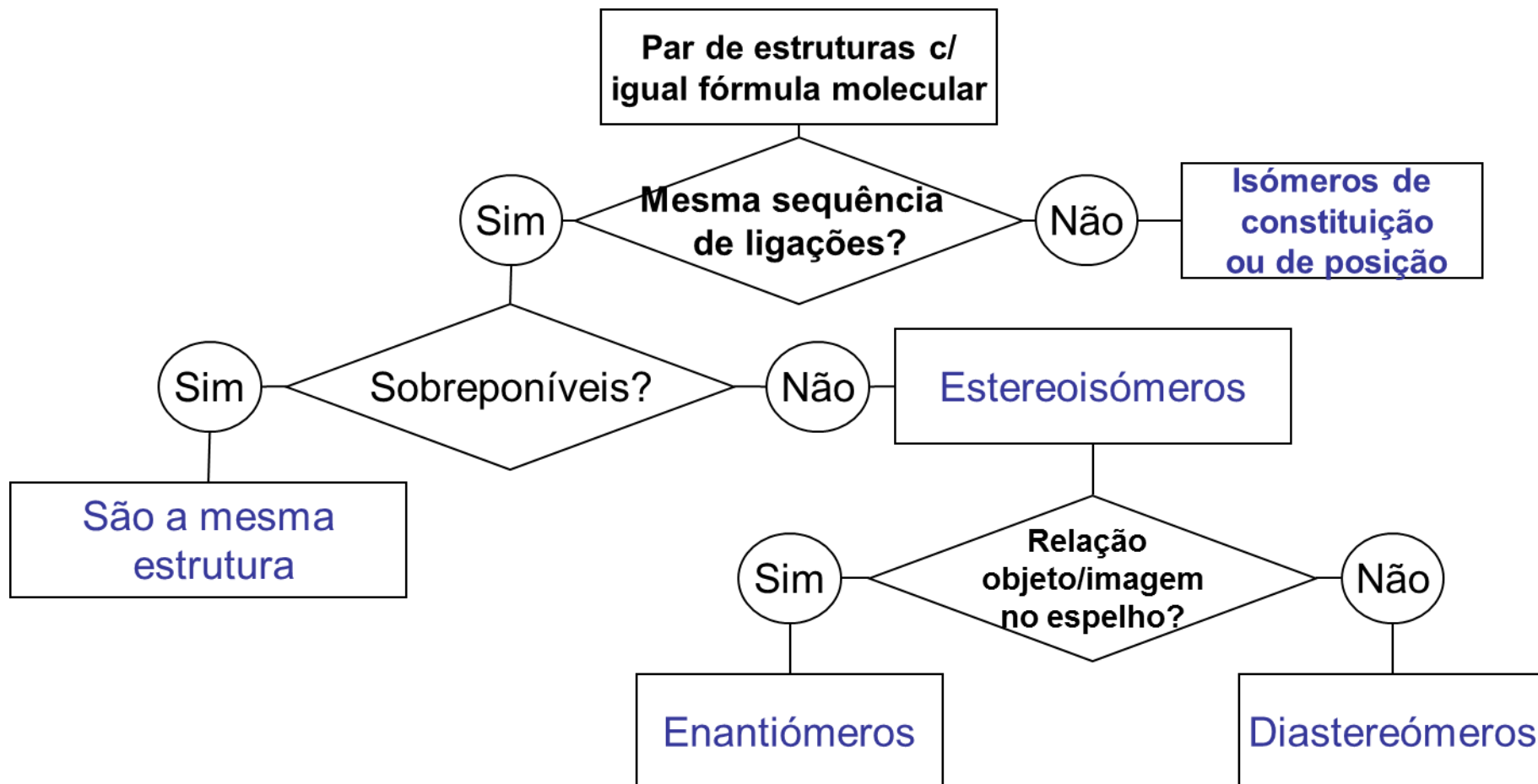


trans-1,2-Dimetilciclopentano
(C_7H_{14})

Representação de dois isómeros do ácido láctico

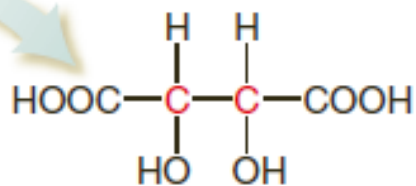


Representação em perspetiva

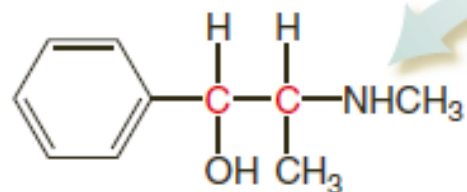


Moléculas orgânicas no nosso dia-a-dia

Larger organic molecules can have two, three, or even hundreds of chirality centers. Tartaric acid, isolated from grapes, and ephedrine, isolated from the herb ma huang (used to treat respiratory ailments in traditional Chinese medicine), each have two chirality centers. Once a popular drug to promote weight loss and enhance athletic performance, ephedrine use has now been linked to episodes of sudden death, heart attack, and stroke.



tartaric acid



ephedrine
(bronchodilator, decongestant)



[Chirality centers are labeled in red.]

Moléculas orgânicas no nosso dia-a-dia

- O caso dramático da talidomida

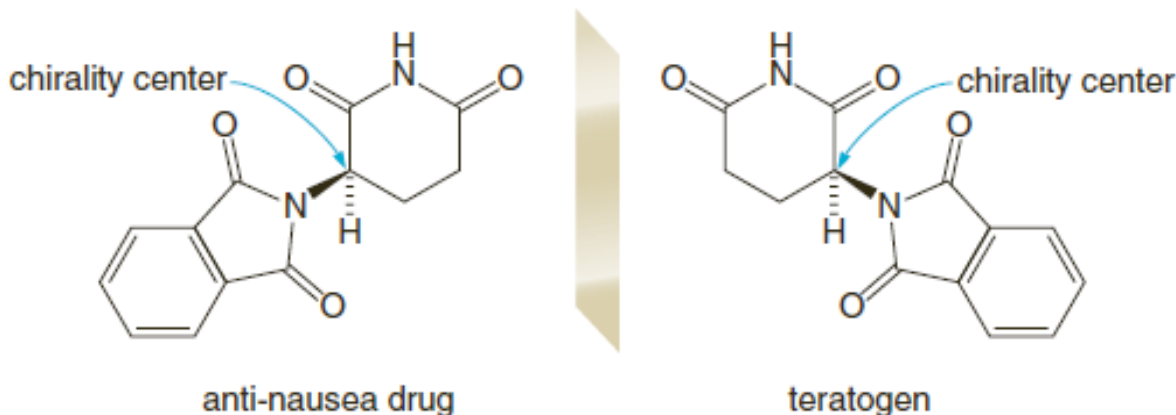
15.4B FOCUS ON HEALTH & MEDICINE

THE UNFORGETTABLE LEGACY OF THALIDOMIDE



Many biologically active compounds contain one or more chirality centers on ring carbons. For example, **thalidomide**, which contains one such chirality center, was once used as a sedative and anti-nausea drug for pregnant women in Europe and Great Britain from 1959–1962.

Two enantiomers of thalidomide

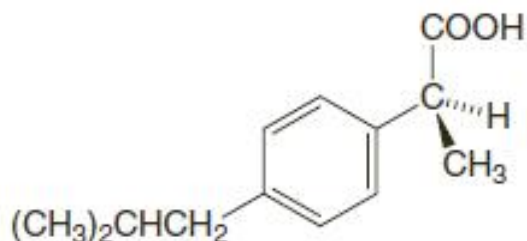


Unfortunately, thalidomide was sold as a mixture of its two enantiomers, and each of these stereoisomers has a different biological activity, a property not uncommon to chiral drugs, as we will see in Section 15.5. While one enantiomer has the desired therapeutic effect, the other enantiomer was responsible for thousands of catastrophic birth defects in children born to women who took the drug during pregnancy. Thalidomide was never approved for use in the United States due to the diligence of Frances Oldham Kelsey, a medical reviewing officer for the Food and Drug Administration, who insisted that the safety data on thalidomide were inadequate.

Moléculas orgânicas no nosso dia-a-dia

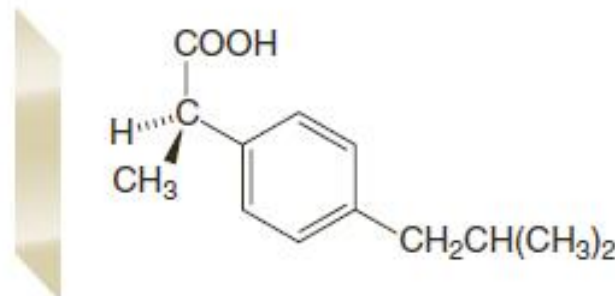
Ibuprofen and naproxen are nonsteroidal anti-inflammatory drugs (NSAIDs) that illustrate how two enantiomers can have different biological activities. Both drugs are common over-the-counter remedies that relieve pain and fever, and reduce inflammation.

Ibuprofen is the generic name for the pain relievers known as Motrin and Advil. Ibuprofen has one chirality center, and thus exists as a pair of enantiomers. Only one enantiomer, labeled **A**, is an active anti-inflammatory agent. Its enantiomer **B** is inactive. **B**, however, is slowly converted to **A** in the body. Ibuprofen is sold as a mixture of both enantiomers. An equal mixture of two enantiomers is called a *racemic mixture* (pronounced ra-see'-mik).



ibuprofen
active anti-inflammatory agent

A



inactive enantiomer

B

Polarização das ligações covalentes

A polaridade de uma ligação covalente resulta da diferença de **eletronegatividade** dos átomos que a formam

Escala de eletronegatividade de Pauling

Grupo	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Período																		
1	H 2,1																	He
2	Li 1,0	Be 1,5											B 2,0	C 2,5	N 3,0	O 3,5	F 4,0	Ne
3	Na 0,9	Mg 1,2											Al 1,5	Si 1,8	P 2,1	S 2,5	Cl 3,0	Ar
4	K 0,8	Ca 1,0	Sc 1,3	Ti 1,5	V 1,6	Cr 1,6	Mn 1,5	Fe 1,8	Co 1,9	Ni 1,8	Cu 1,9	Zn 1,6	Ga 1,6	Ge 1,8	As 2,0	Se 2,4	Br 3,0	Kr
5	Rb 0,8	Sr 1,0	Y 1,2	Zr 1,4	Nb 1,6	Mo 1,8	Tc 1,9	Ru 2,2	Rh 2,2	Pd 2,2	Ag 1,9	Cd 1,7	In 1,7	Sn 1,8	Sb 1,9	Te 2,1	I 2,5	Xe
6	Cs 0,7	Ba 0,9	*	Hf 1,3	Ta 1,5	W 1,7	Re 1,9	Os 2,2	Ir 2,2	Pt 2,2	Au 2,4	Hg 1,9	Tl 1,8	Pb 1,9	Bi 1,9	Po 2,0	At 2,2	Rn
7	Fr 0,7	Ra 0,9	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo

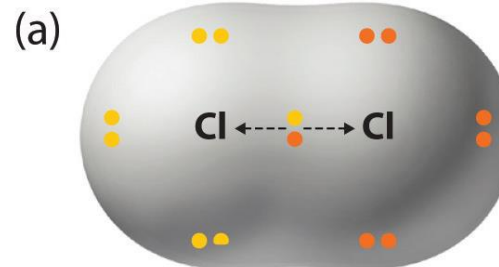
É a tendência de um átomo para atrair os eletrões numa ligação

Polarização das ligações covalentes

Ligação covalente apolar

-não constitui dipolo elétrico

-forma-se entre átomos com eletronegatividade igual ou semelhante



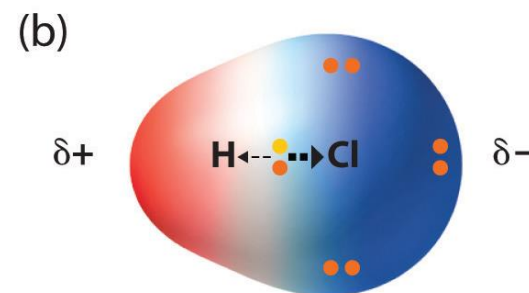
Nonpolar covalent bond

Bonding electrons shared equally between two atoms.
No charges on atoms.

Ligação covalente polar

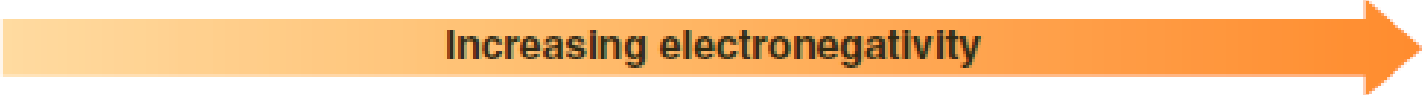
Constitui um dipolo elétrico

Forma-se quando as eletronegatividades dos elementos ligados são bastante diferentes



Polar covalent bond

Bonding electrons shared unequally between two atoms.
Partial charges on atoms.

Increasing electronegativity 

1A		2A												3A		4A		5A		6A		7A		8A	
H 2.1																									
Li 1.0		Be 1.5												B 2.0	C 2.5	N 3.0	O 3.5	F 4.0							
Na 0.9		Mg 1.2												Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0							
K 0.8		Ca 1.0												Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8							
Rb 0.8		Sr 1.0												In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5							

Increasing electronegativity 

Polarização das ligações covalentes

As ligações C-C e C-H não têm polarização

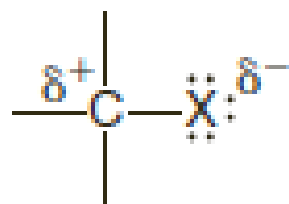
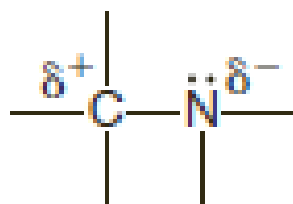
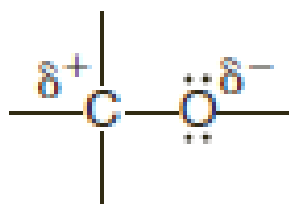


a eletronegatividades dos átomos ligados é semelhante, não origina dipolos eléctricos

As ligações C-O e C-N têm polarização



a eletronegatividades dos átomos ligados é diferente, a ligação covalente origina dipolos eléctricos



A ligação covalente polar origina um dipolo eléctrico

X = halogen

na ligação covalente polar surgem pólos distintos (representados pela letra δ)

$\delta+$ carga parcial positiva (elemento menos eletronegativo)

$\delta-$ carga parcial negativa (elemento mais eletronegativo)

A ligação covalente polar ocorre:

- entre elementos de eletronegatividade diferente
- o mais eletronegativo apresenta maior capacidade de atrair o par de eletrões
- cria-se nesse extremo uma maior densidade eletrónica

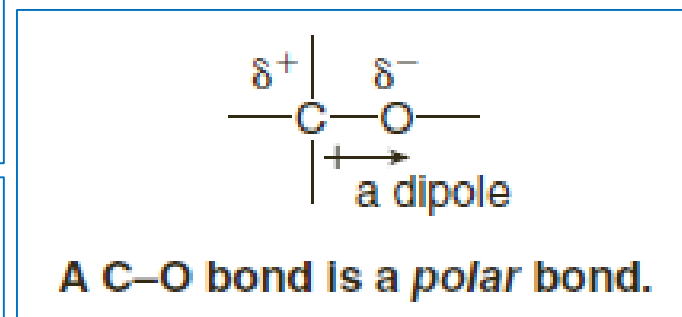
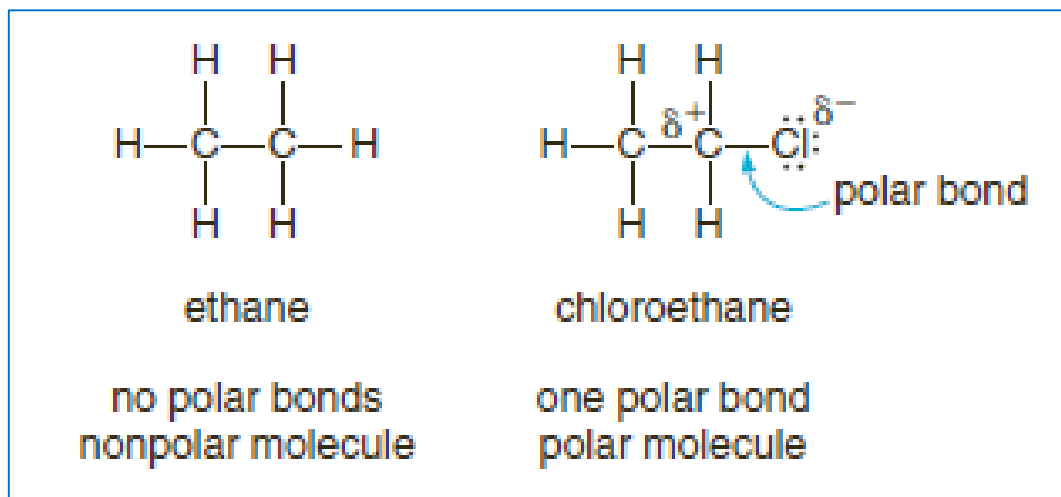
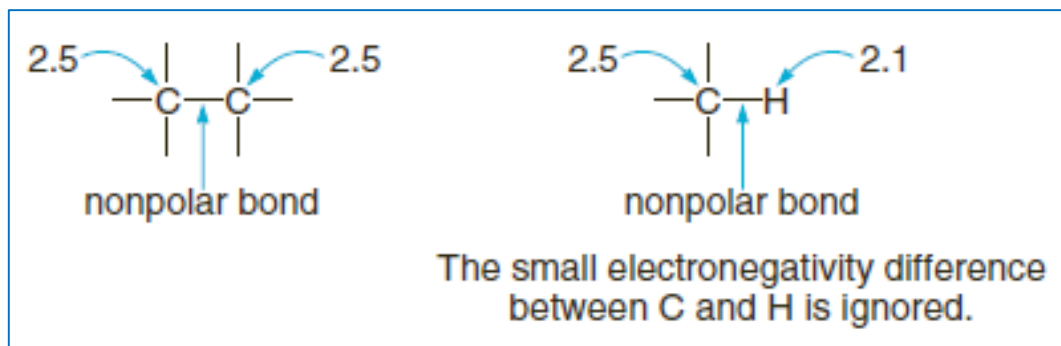
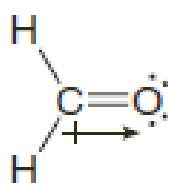


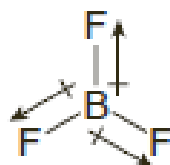
TABLE 4.3 Electronegativity Difference and Bond Type

Electronegativity Difference	Bond Type	Electron Sharing
Less than 0.5 units	Nonpolar	Electrons are equally shared.
0.5–1.9 units	Polar covalent	Electrons are unequally shared; they are pulled towards the more electronegative element.
Greater than 1.9 units	Ionic	Electrons are transferred from the less electronegative element to the more electronegative element.



one polar bond

polar molecule



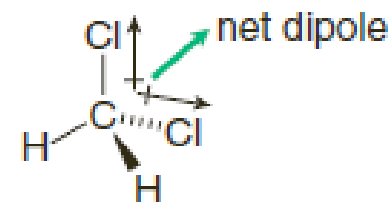
three polar bonds
All dipoles cancel.
NO net dipole

nonpolar molecule



three polar bonds
All dipoles reinforce.

polar molecule



two polar bonds
Two dipoles reinforce.

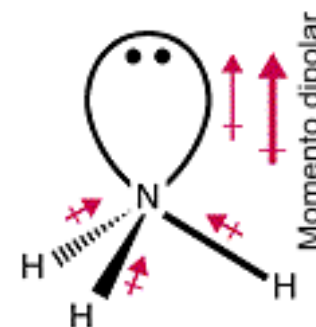
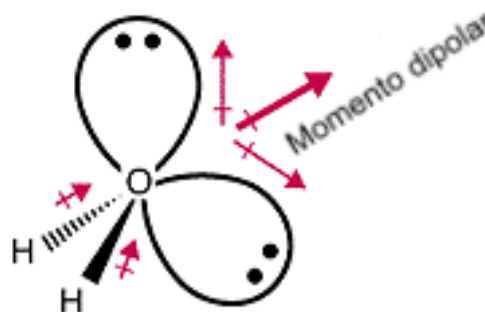
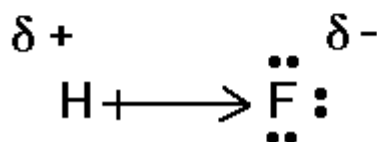
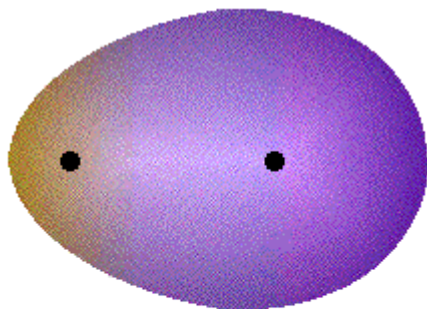
polar molecule

Momento dipolar

Magnitude do caráter polar da ligação covalente

Momento dipolar = carga x distância

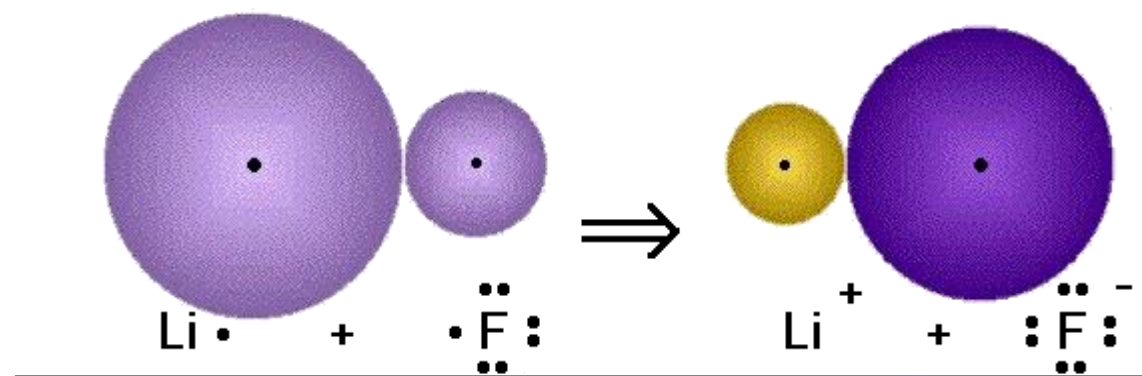
$$\mu = e \times d$$



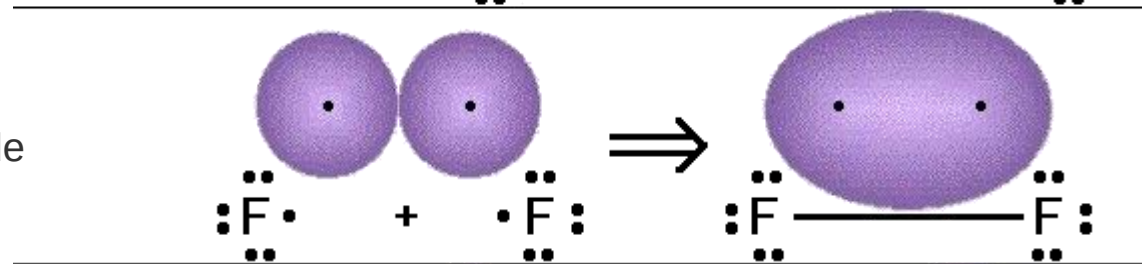
- Origina cargas parciais (δ), $0 < |\delta| < 1$
- Origina a formação de dipolos permanentes (na maior parte das moléculas orgânicas)

Tipo de ligação em função da diferença de **eletronegatividade** entre os átomos

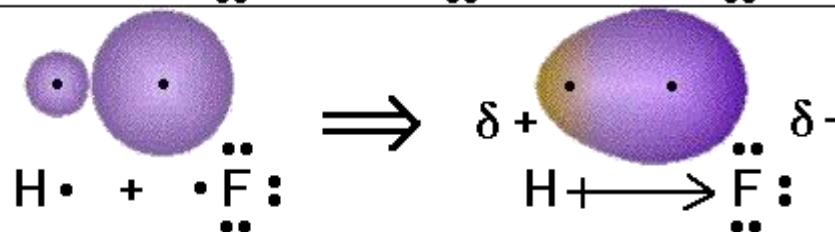
IÓNICA
Maior que 2



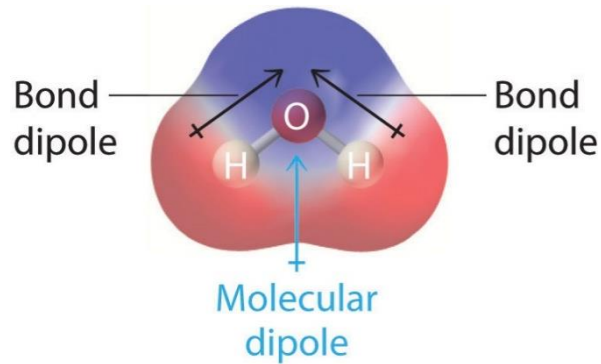
COVALENTE
(**apolar** – eletronegatividade
semelhante)



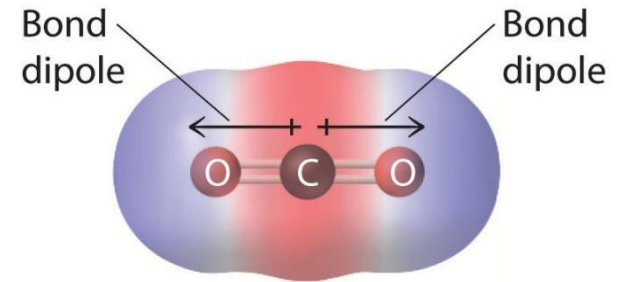
COVALENTE
(**polarizada** – diferente
eletronegatividade)



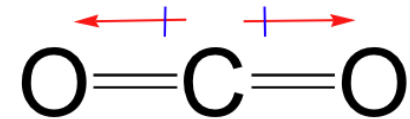
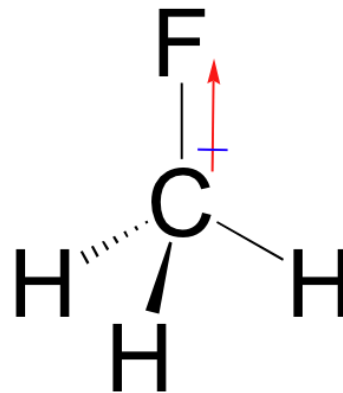
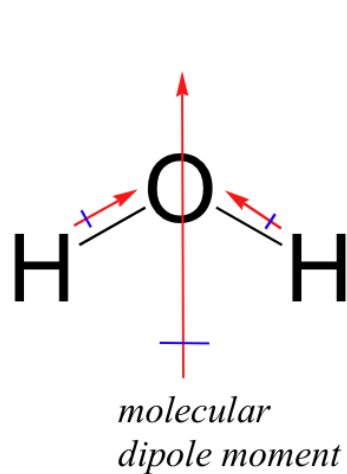
Polarização das moléculas



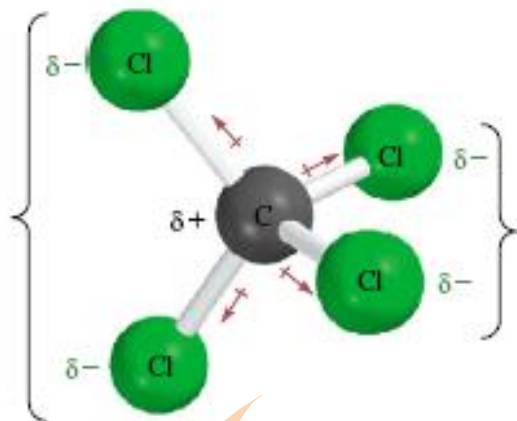
(b) Net dipole moment



(a) No net dipole moment



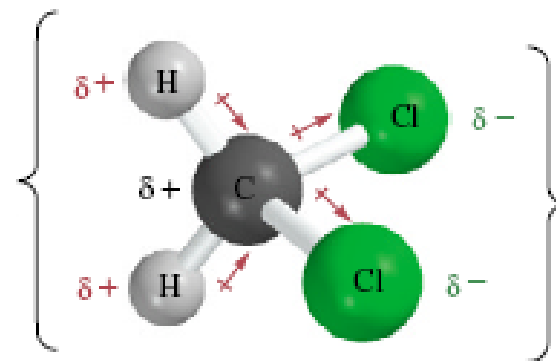
Polarização e momento dipolar das moléculas



$$\mu = 0$$

Os vetores dos momentos dipolares de cada ligação podem anular-se, resultando uma molécula sem momento dipolar

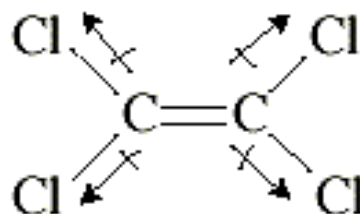
A contribuição das ligações C-H é desprezável, sendo o momento dipolar praticamente devido à ligação C-Cl



$$\mu = 1,87 \text{ D}$$

Explique porque é que a molécula $\text{CCl}_2 = \text{CCl}_2$ não apresenta **momento dipolar**

A soma dos vetores é zero pois anulam-se dois a dois, tal como se pode observar na representação:



O MOMENTO
DIPOLAR das
moléculas
determina
propriedades
específicas

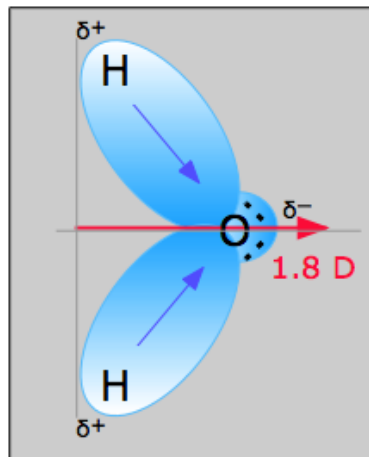
REATIVIDADE
ESTADO FÍSICO
SOLUBILIDADE

Molécula	Geometria	Momento dipolar
HF	Linear	1,92
HCl	Linear	1,08
HBr	Linear	0,78
HI	Linear	0,38
H ₂ O	Angular	1,87
H ₂ S	Angular	1,10
NH ₃	Piramidal	1,46
SO ₂	Angular	1,60

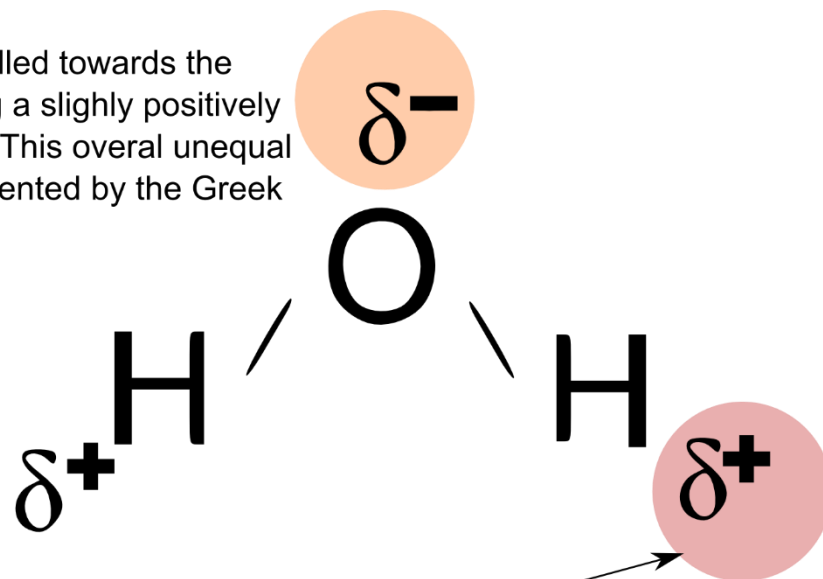
MOMENTO DIPOLAR DE ALGUMAS MOLECULAS ORGÂNICAS

Molécula	μ (D)	Molécula	μ (D)
CH ₄	0	CHCl ₃	1,02
CH ₃	1,87	CCl ₄	0
CH ₂ Cl ₂	1,55	NH ₃	1,47

O caso da água:



electrons are pulled towards the oxygen, creating a slightly positively charged region. This overall unequal charge is represented by the Greek delta, for dipole



electrons are pulled away from the hydrogen towards the oxygen, creating a slightly positively charged region

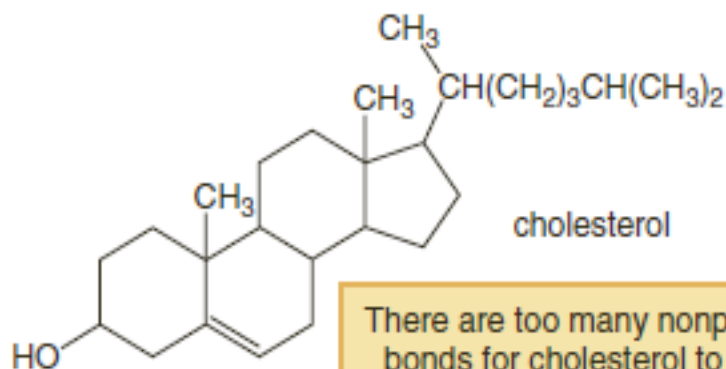
Comparar propriedades físico-químicas da água e outros compostos:

MOLECULE	DIPOLE MOMENT (D)	MELTING POINT (°C)	BOILING POINT (°C)
H ₂ O	1.85	0	100
NH ₃	1.47	- 78	- 33
HCl	1.08	- 115	- 85
HBr	0.80	- 88	- 67
HI	0.42	- 51	- 35

Solubilidade é determinada por interações intermoleculares

TABLE 11.7 The Solubility Characteristics of Three Representative Organic Molecules

Compound	Solubility in an Organic Solvent	Solubility in Water
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ Hexane	Soluble	Insoluble
$\text{CH}_3\text{CH}_2\text{OH}$ Ethanol	Soluble	Soluble
Cholesterol	Soluble	Insoluble

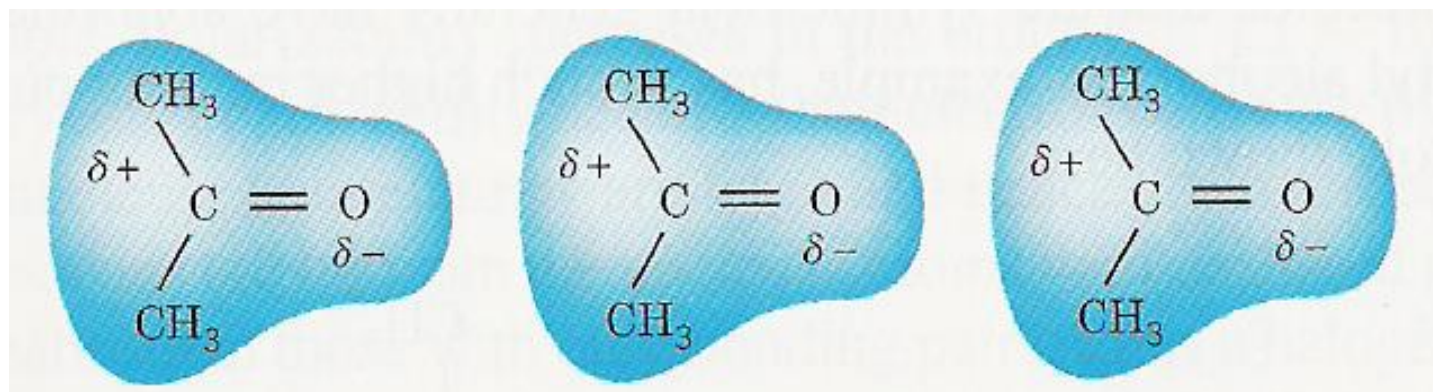


As propriedades físicas dependem do *tipo* e *intensidade* das forças intermoleculares

- Interações iónicas
- Interações dipolo-dipolo
- Pontes de hidrogénio
- Forças de van der Waals

Interações dipolo-dipolo

Ex: cetonas e aldeídos (grupo carbonilo é dipolo permanente)



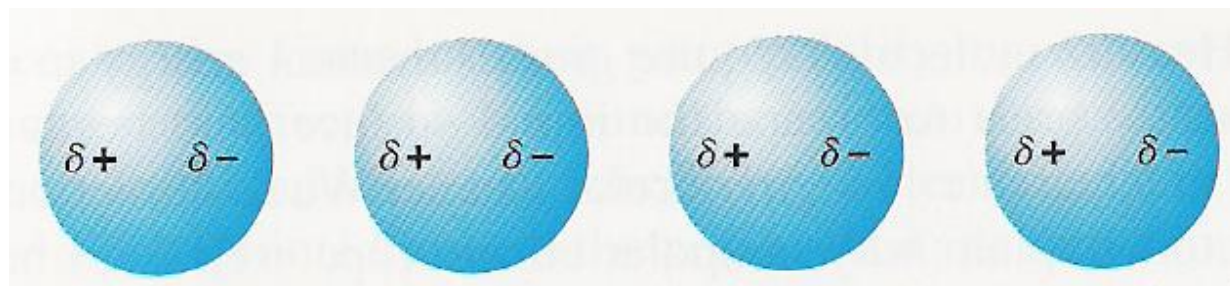
**** -17: Dipole Forces:** <https://www.youtube.com/watch?v=cERb1d6J4-M&list=PLlIVwaZQkS2op2kDuFifhStNsS49LaxkZ&index=17>

Forças de van der Waals (ou forças de London)

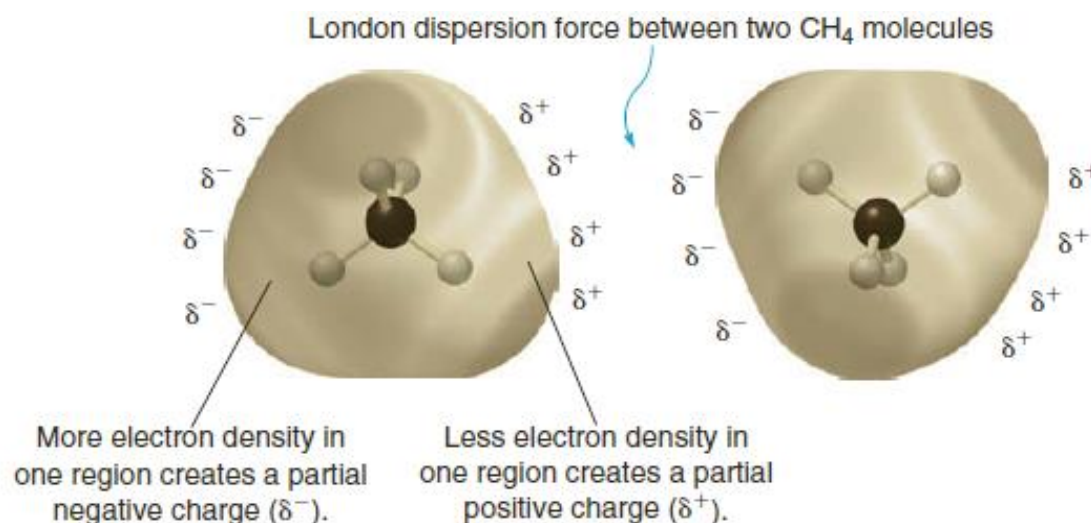
Dipolos temporários
em moléculas não
polares causam
distribuição não
uniforme dos eletrões
num dado instante)

Ex: alcanos

dipolos temporários
geram forças atrativas
entre moléculas
(forças fracas)



(dipolos instantâneos-dipolos induzidos)



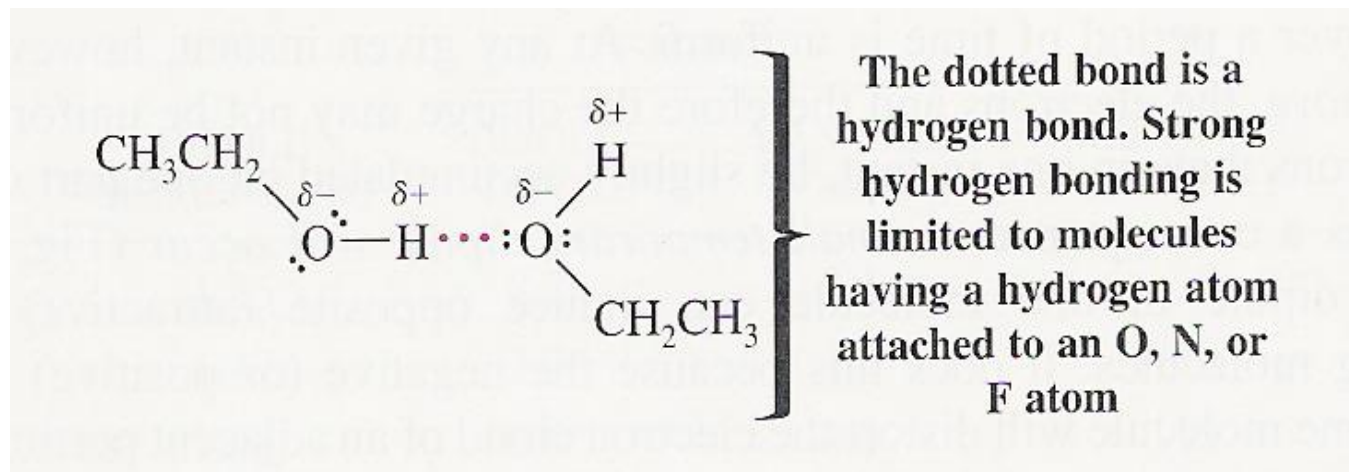
**** -16: London Dispersion Forces:**

<https://www.youtube.com/watch?v=1iYKajMsYPY&list=PLlIVwaZQkS2op2kDuFifhStNsS49LaxkZ&index=16>



Pontes de hidrogénio:

H ligado a um elemento fortemente eletronegativo



Ex: Comparação entre propriedades físicas de 2 isómeros $\text{C}_2\text{H}_6\text{O}$:



etanol ($P_{\text{ebulição}} = 78,5^\circ\text{C}$)

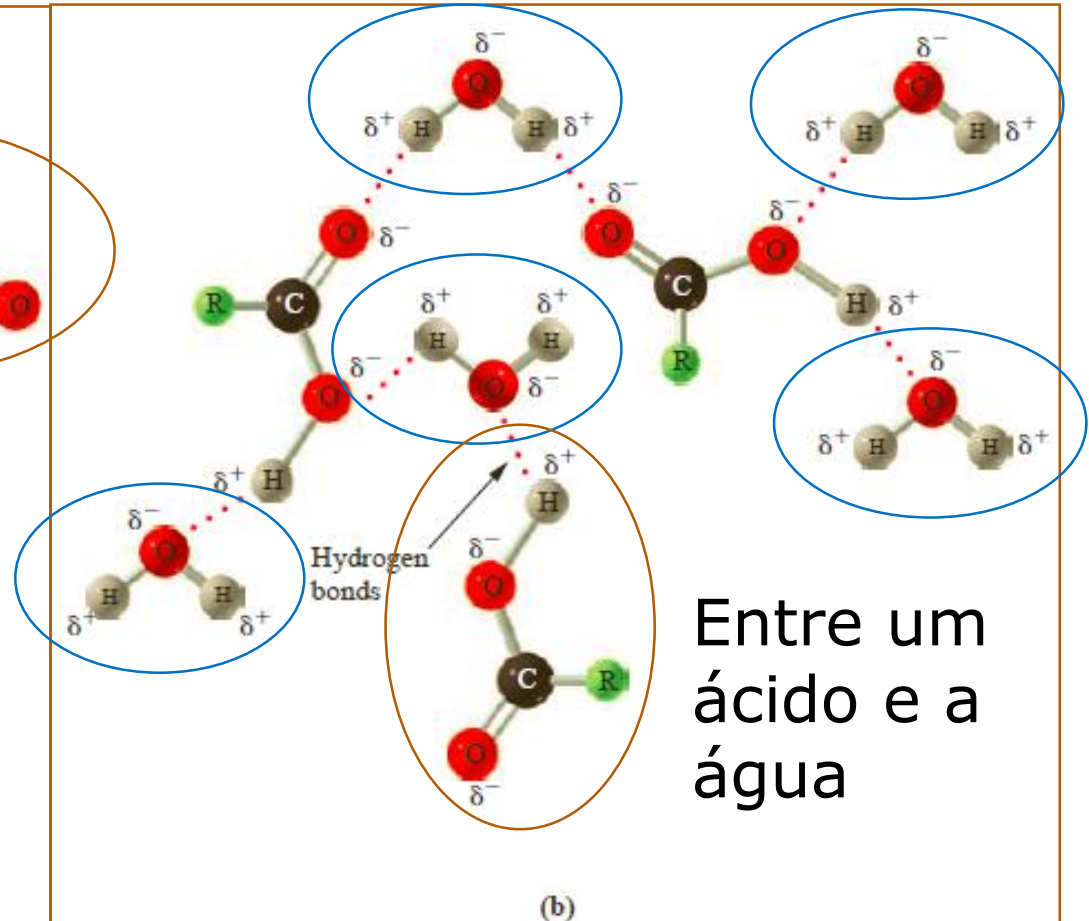
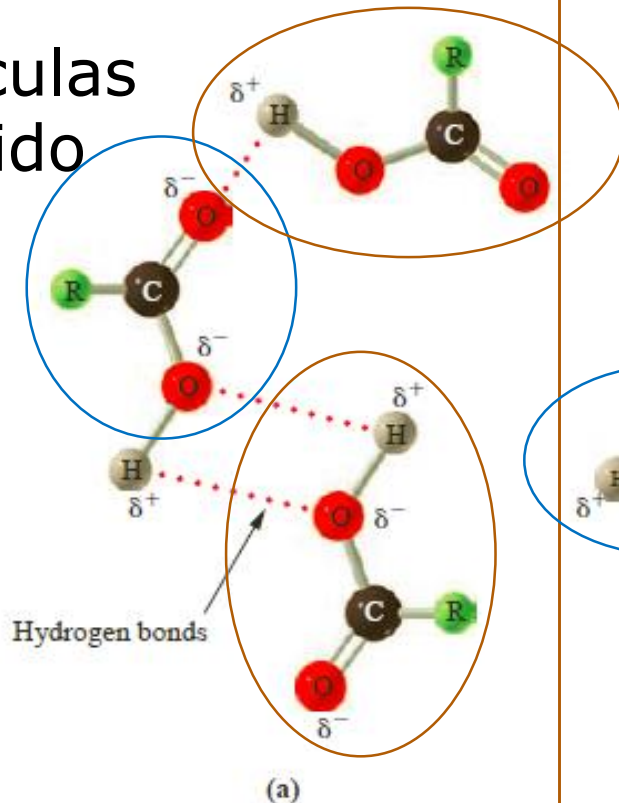


éter dimetílico ($P_{\text{ebulição}} = -24,9^\circ\text{C}$)



Pontes de hidrogénio:

Entre
moléculas
de ácido



Entre um
ácido e a
água

Interações iónicas:

Forças de atração entre compostos com cargas positivas (+) e negativas (-)

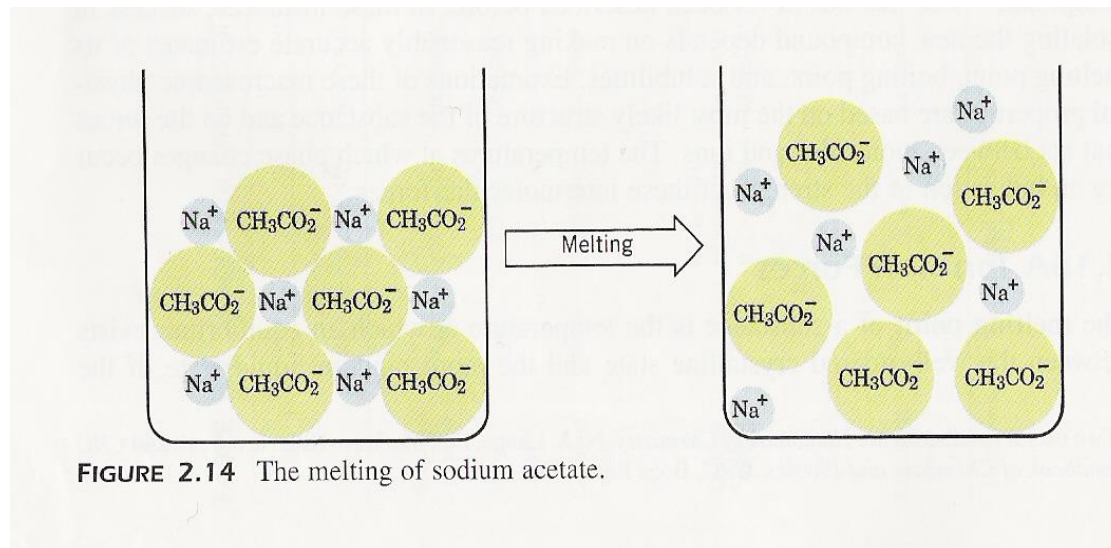
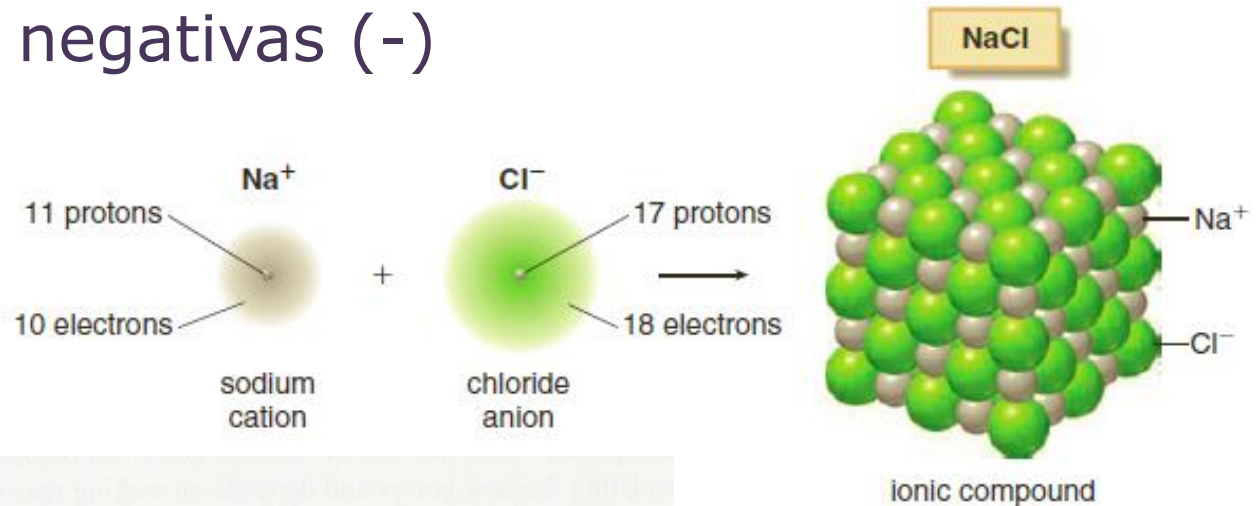
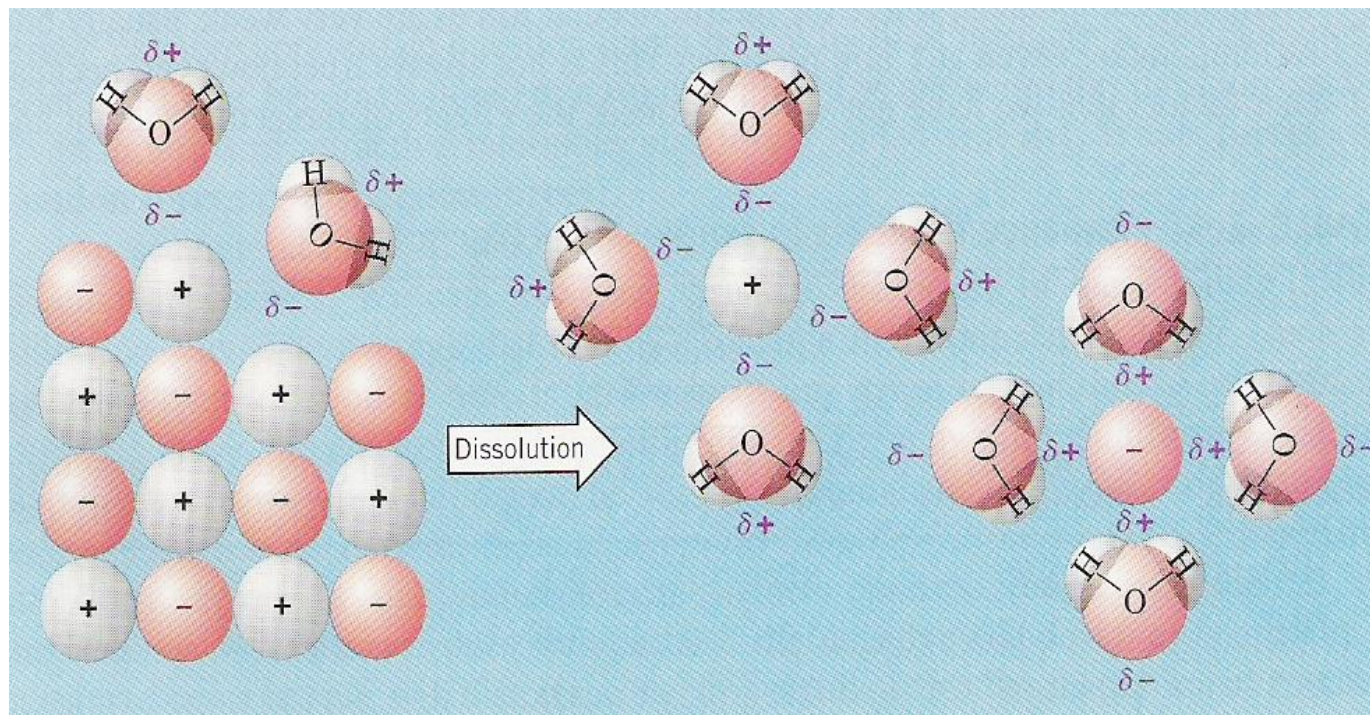


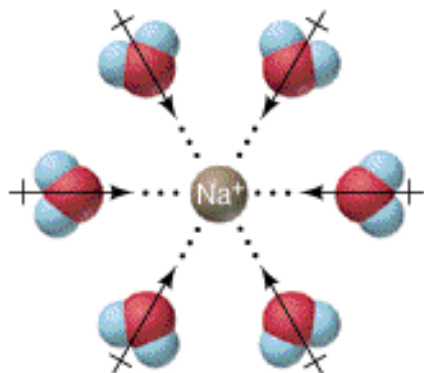
FIGURE 2.14 The melting of sodium acetate.

Ex:
solubilidade do
acetato de sódio

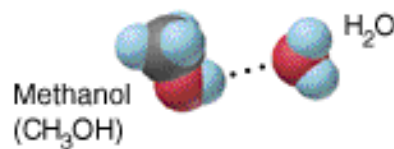
Solubilidade de um sal iónico em água:

Solvatação do NaCl

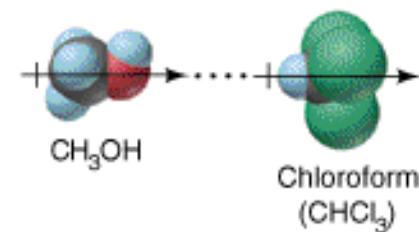




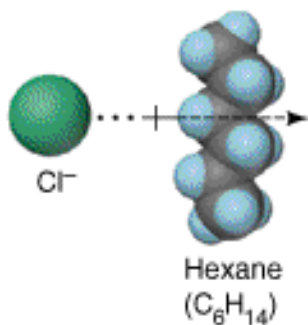
Interações iónicas



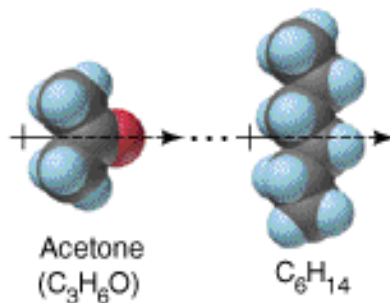
Ponte de hidrogénio



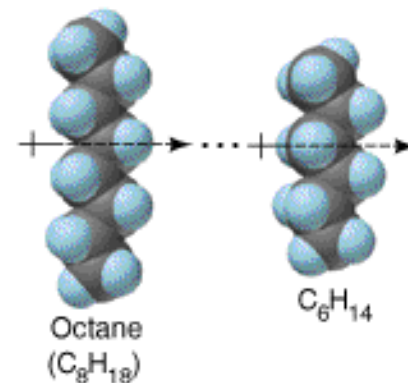
Dipolo induzido



Dipolo induzido

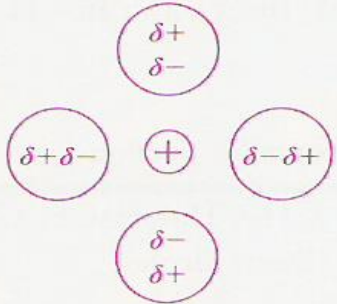
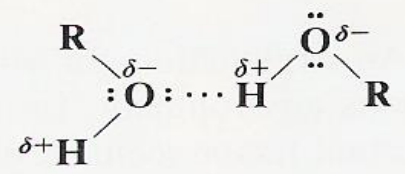
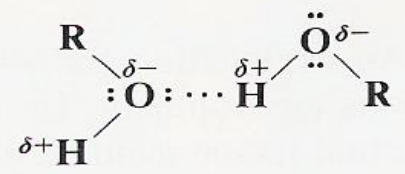


Dipolo induzido



Dipolo induzido

TABLE 2.5 Attractive electric forces

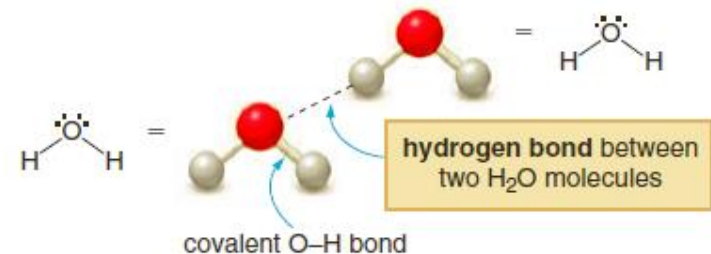
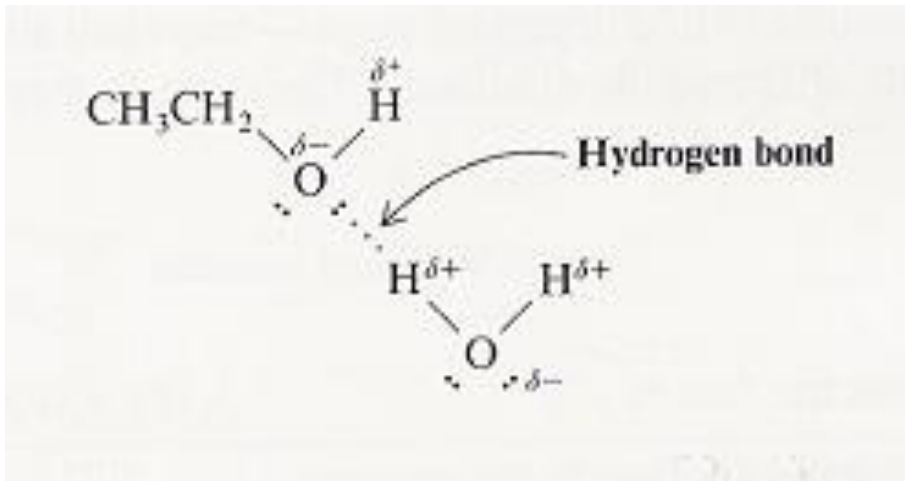
ELECTRIC FORCE	RELATIVE STRENGTH	TYPE	EXAMPLE
Cation–anion (in a crystal)	Very strong	$\oplus \quad \ominus$	Lithium fluoride crystal lattice
Covalent bonds	Strong (36–125 kcal mol ⁻¹)	Shared electron pairs	H—H (104 kcal mol ⁻¹) CH ₃ —CH ₃ (88 kcal mol ⁻¹) I—I (36 kcal mol ⁻¹)
Ion–dipole	Moderate		Na ⁺ in water (see Fig. 2.18)
Dipole–dipole (including hydrogen bonds)	Moderate to weak (1–9 kcal mol ⁻¹)	$\overset{\delta-}{\text{Z}} \cdots \overset{\delta+}{\text{H}}$ and  and 	 Interactions between methane molecules
van der Waals	Variable	Transient dipole	Interactions between methane molecules

Solubilidade de ácidos e álcoois em água

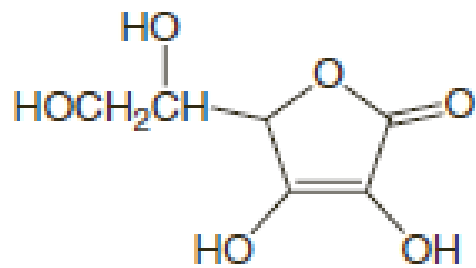
- H ligado a um elemento eletronegativo pode formar **pontes de hidrogénio**

Solubilidade do etanol em água

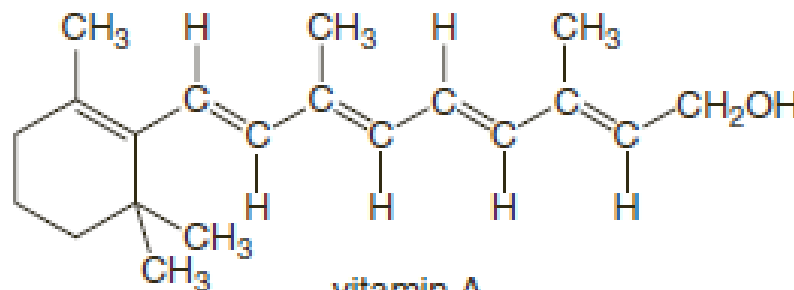
$\text{CH}_3\text{CH}_2\text{OH}$



É solúvel em água?



vitamin C
(ascorbic acid)



vitamin A

**** -16: London Dispersion Forces:**

<https://www.youtube.com/watch?v=1iYKajMsYPY&list=PLlIVwaZQkS2op2kDuFifhStNsS49LAXkZ&index=16>

**** -17: Dipole Forces:** <https://www.youtube.com/watch?v=cERb1d6J4-M&list=PLlIVwaZQkS2op2kDuFifhStNsS49LAXkZ&index=17>

**** -18: Intermolecular Forces:** <https://www.youtube.com/watch?v=-QqTwJzi7Wo&index=18&list=PLlIVwaZQkS2op2kDuFifhStNsS49LAXkZ>

**** -19: Covalent Bonding:**

<https://www.youtube.com/watch?v=Mo4Vfqt5v2A&index=19&list=PLlIVwaZQkS2op2kDuFifhStNsS49LAXkZ>

**** -20: Ionic Bonding:**

https://www.youtube.com/watch?v=hiyTfhjeF_U&list=PLlIVwaZQkS2op2kDuFifhStNsS49LAXkZ&index=20