Química Orgânica

BIOTECNOLOGIA

Miriam Sannomiya

NOMENCLATURA DE COMPOSTOS ORGÂNICOS

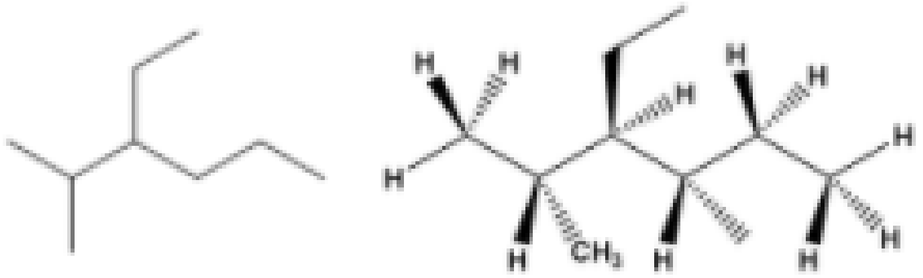
ORGANIC vs. INORGANIC COMPOUNDS

- Estimated $9x10^6$ vs. $5x10^5$ inorganic compounds (18:1)
- Organic compounds form mostly covalent bounds, while inorganic compounds are more polarized and ionic

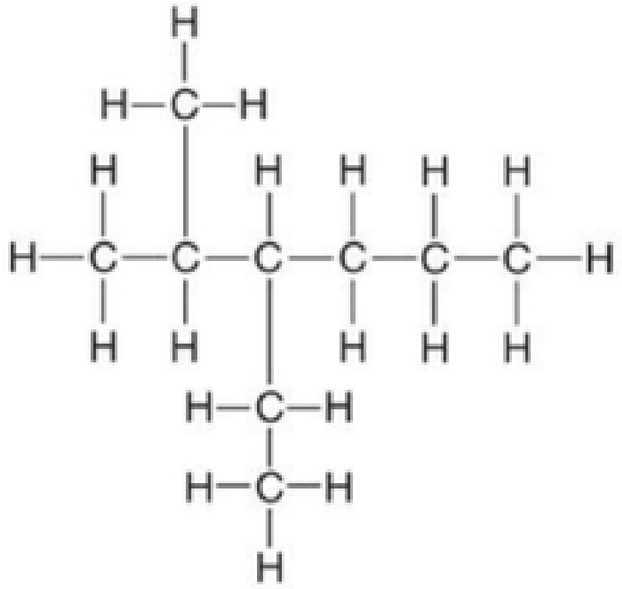
ORGANIC vs. INORGANIC COMPOUNDS

Comparison of Organic and Inorganic Properties		
Properties	**Organic**	**Inorganic**
Bonding	Covalent	Ionic
Forces between molecules	Generally weak	Usually strong
Physical State	G, L, low MP S	High MP solid
Flammability	Often flammable	usually non-flammable
Solubility in H_2O	low	High
Conductivity	non-conductor	Conductor
Rate of Reactions	slower	Faster

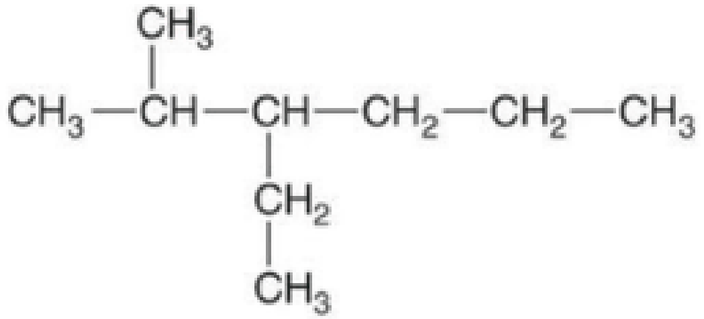
FÓRMULAS QUÍMICAS DOS COMPOSTOS ORGÂNICOS

Fórmula molecular	Indica apenas os elementos que formam o composto e o número de átomos de cada elemento.	C_9H_{20}
Zigue-zague		

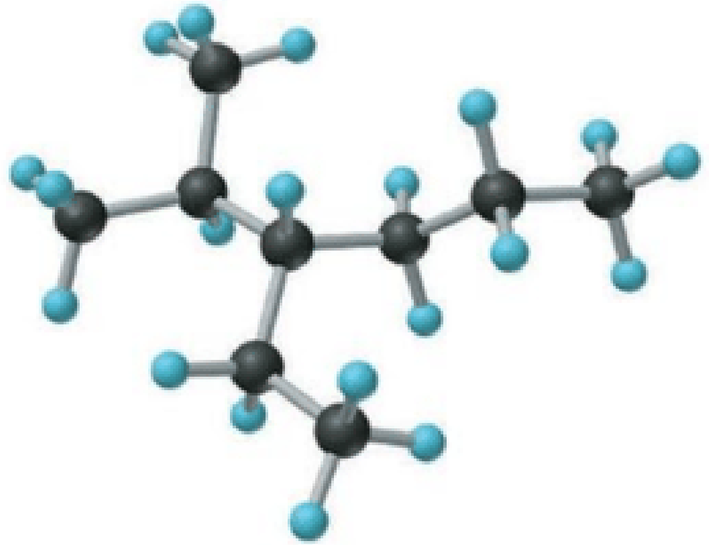
ESTRUTURAS DE KEKULÉ



Expanded formula



Condensed formula

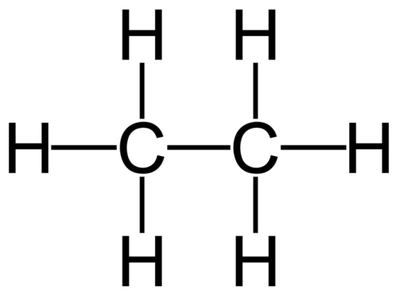


Ball-and-stick model

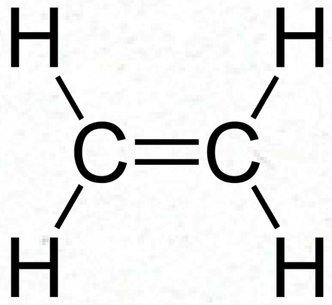
CARBONO é o CARA

forma ligações múltiplas

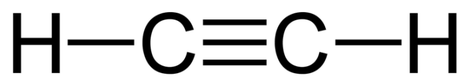
SIMPLES



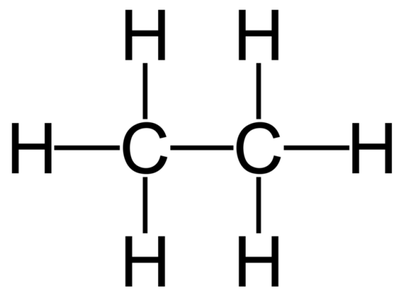
DUPLA

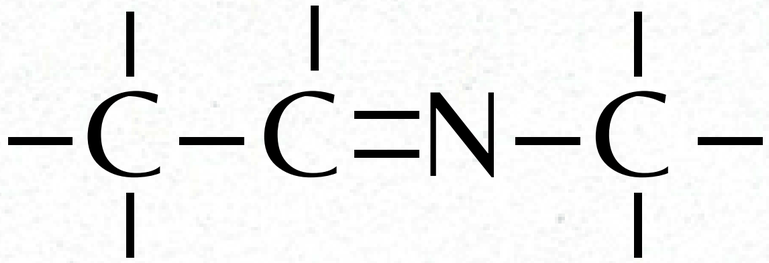


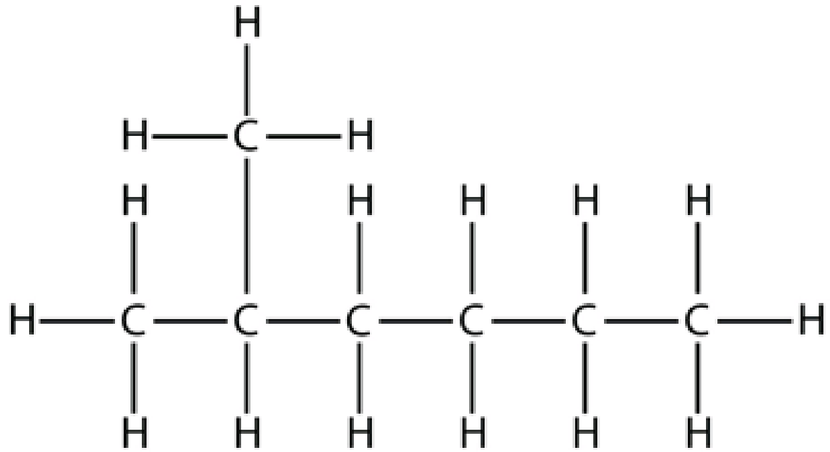
TRIPLA



CARBONO forma cadeias



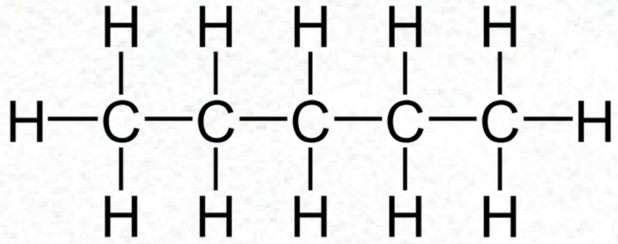


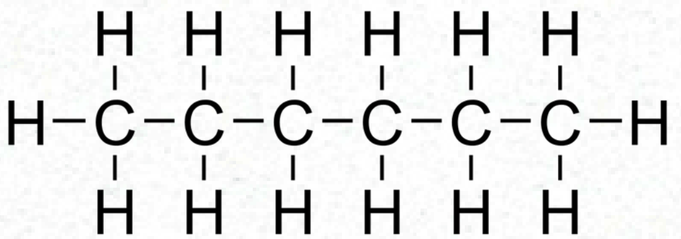


CLASSIFICAÇÃO:
TIPOS DE CADEIA ORGÂNICA

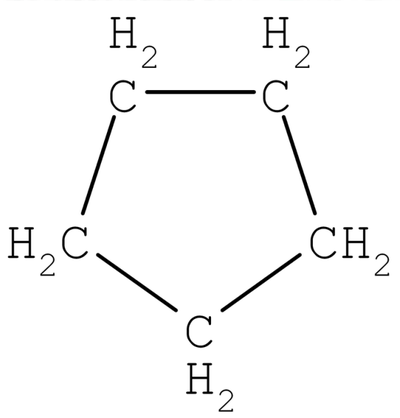
QUANTO AO FECHAMENTO DA CADEIA

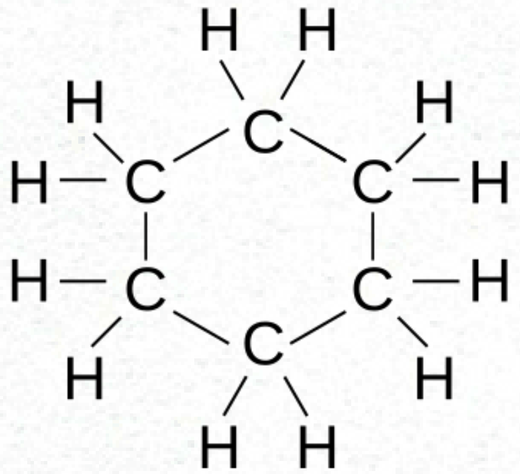
ABERTA





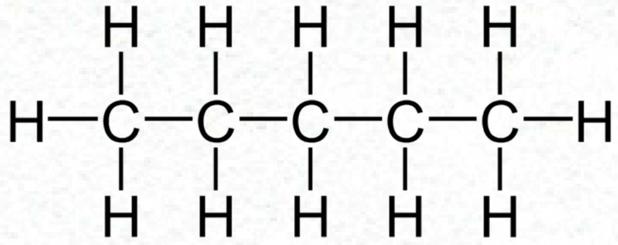
CÍCLICA
OU
FECHADA

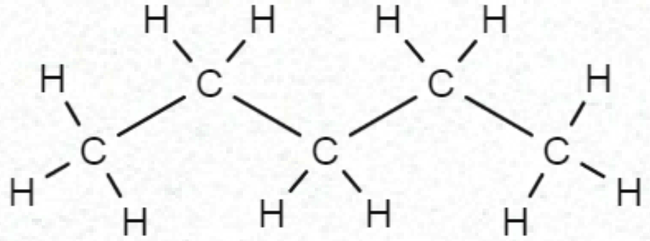




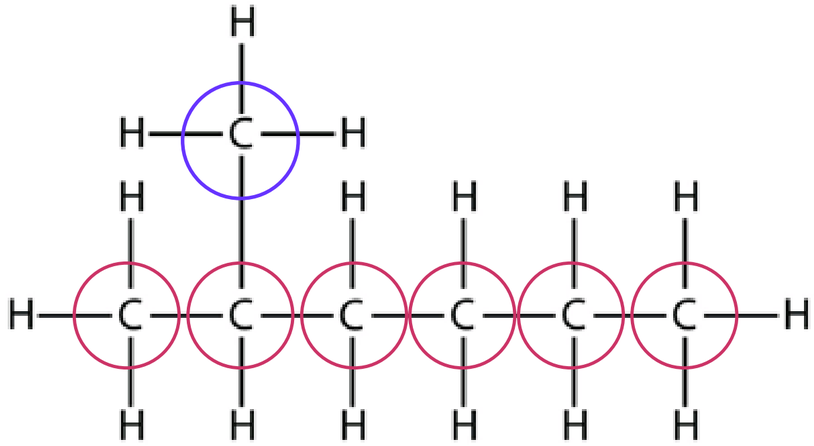
QUANTO À DISPOSIÇÃO DOS ÁTOMOS

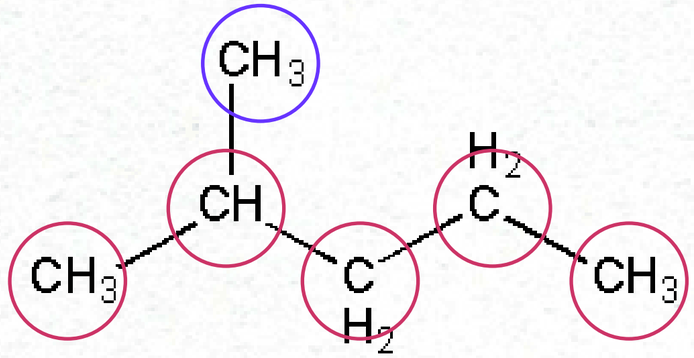
NORMAL





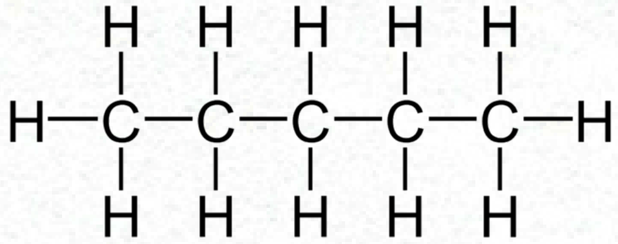
RAMIFICADA

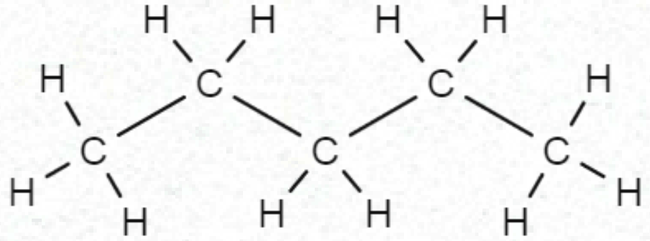




QUANTO AOS TIPOS DE LIGAÇÕES

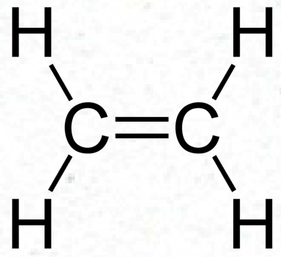
SATURADA

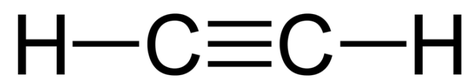




INSATURADA

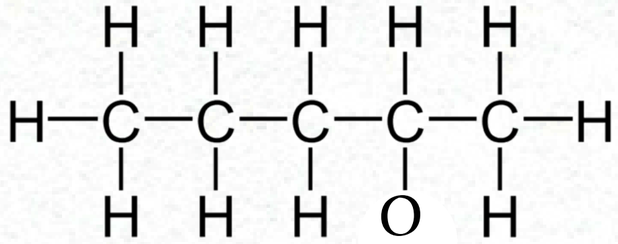
Ligação sigma e π/ Dupla
Ligação sigma, π e π/ Tripla

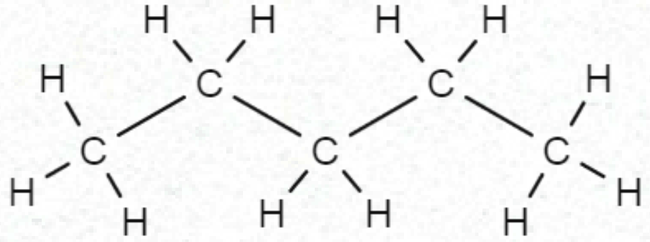




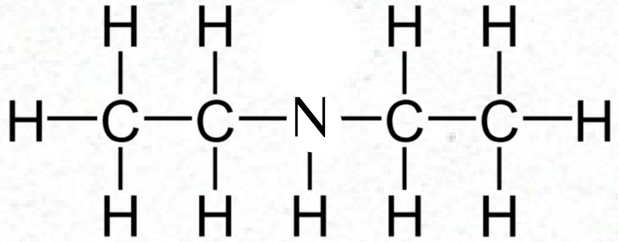
QUANTO À NATUREZA DOS ÁTOMOS

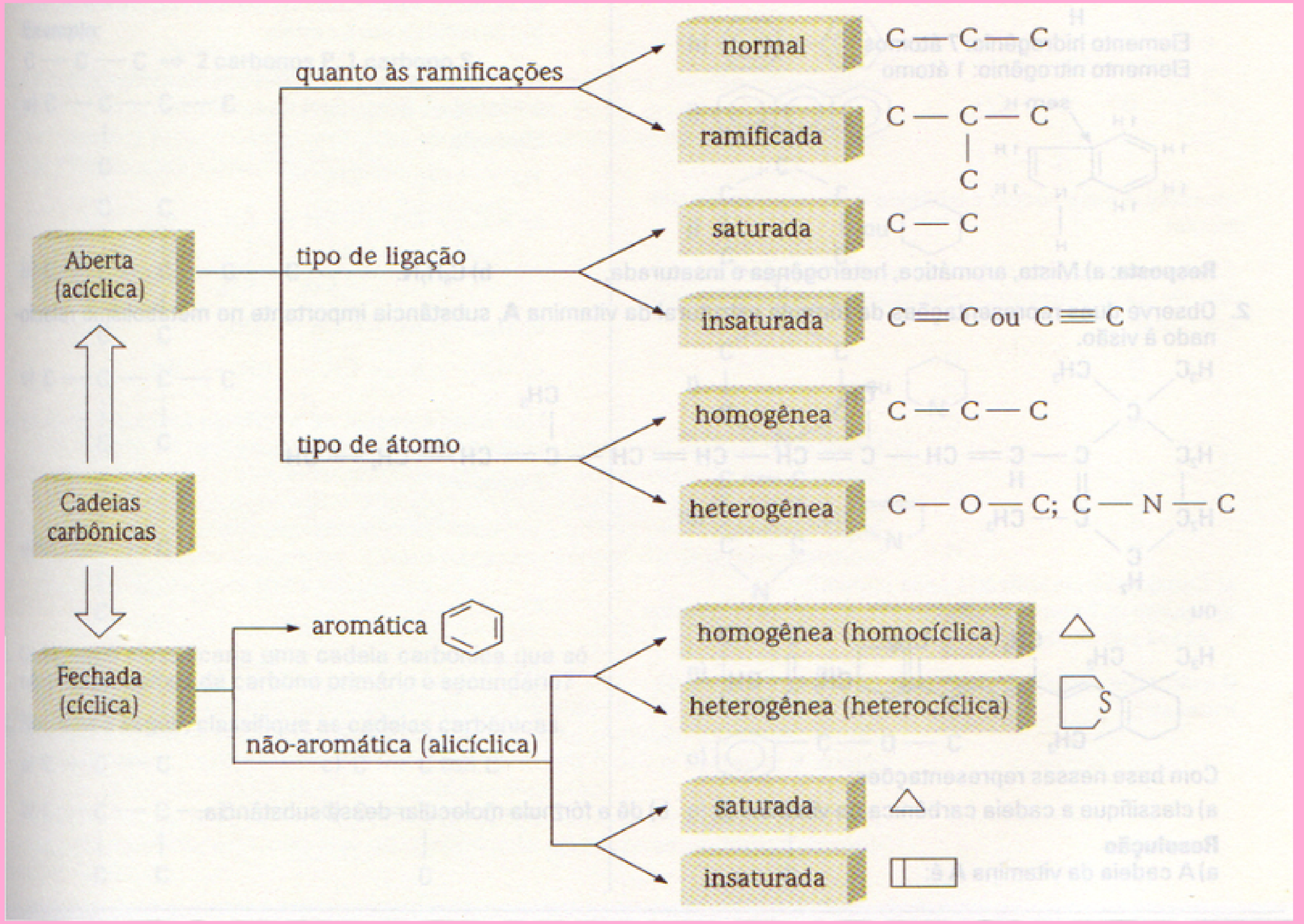
HOMOGÊNEA



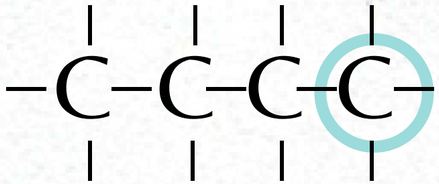


HETEROGÊNEA

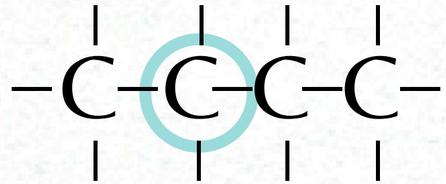



Cadeias carbônicas
Aberta (acíclica)
quanto às ramificações
normal
C — C — C
ramificada
C — C — C
C
tipo de ligação
saturada
C — C
insaturada
C ═ C ou C ≡ C
tipo de átomo
homogênea
C — C — C
heterogênea
C — O — C; C — N — C
Fechada (cíclica)
aromática
não-aromática (alicíclica)
homogênea (homocíclica)
heterogênea (heterocíclica)
S
saturada
insaturada

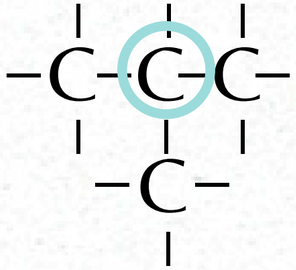
CLASSIFICAÇÃO DOS CARBONOS NA CADEIA



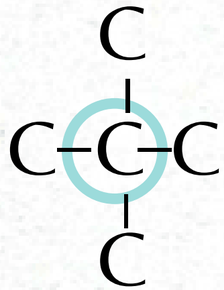
PRIMÁRIO



SECUNDÁRIO



TERCIÁRIO



QUATERNÁRIO

NOMENCLATURA

COMO DAR NOME AOS $9X10^6$ DE MOLÉCULAS QUE JÁ EXISTEM?

Regras?
São necessárias?

Será que se não houvessem, todos ao redor do mundo entenderiam de que composto estamos nos referindo?

IUPAC
INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

ASSIM....

- Identificar a **cadeia carbônica central/principal** mais longa

- **Numeração** dos átomos de carbono desta cadeia será de forma que a numeração da ramificação/radical ou grupo funcional seja o **MENOR** possível.
  - Nome do radical trocando “ano” por “il/ila”.
  - Quando houver mais de um tipo de radical (etil/etila e metil/metila, por exemplo), nomeie por ordem alfabética
  - Use prefixos para indicar múltiplos radicinais

NOMENCLATURA DE COMPOSTOS ORGÂNICOS

PREFIXO: Onde estão os substituintes?

CADEIA PRINCIPAL: Quantos átomos de carbono?

SUFIXO: Qual é a função química?

<**PREFIXO**> <**CADEIA PRINCIPAL**> <**SUFIXO**>

NOMENCLATURA DE COMPOSTOS ORGÂNICOS

O do nome está relacionado com o número de átomos de carbono na **cadeia principal.**

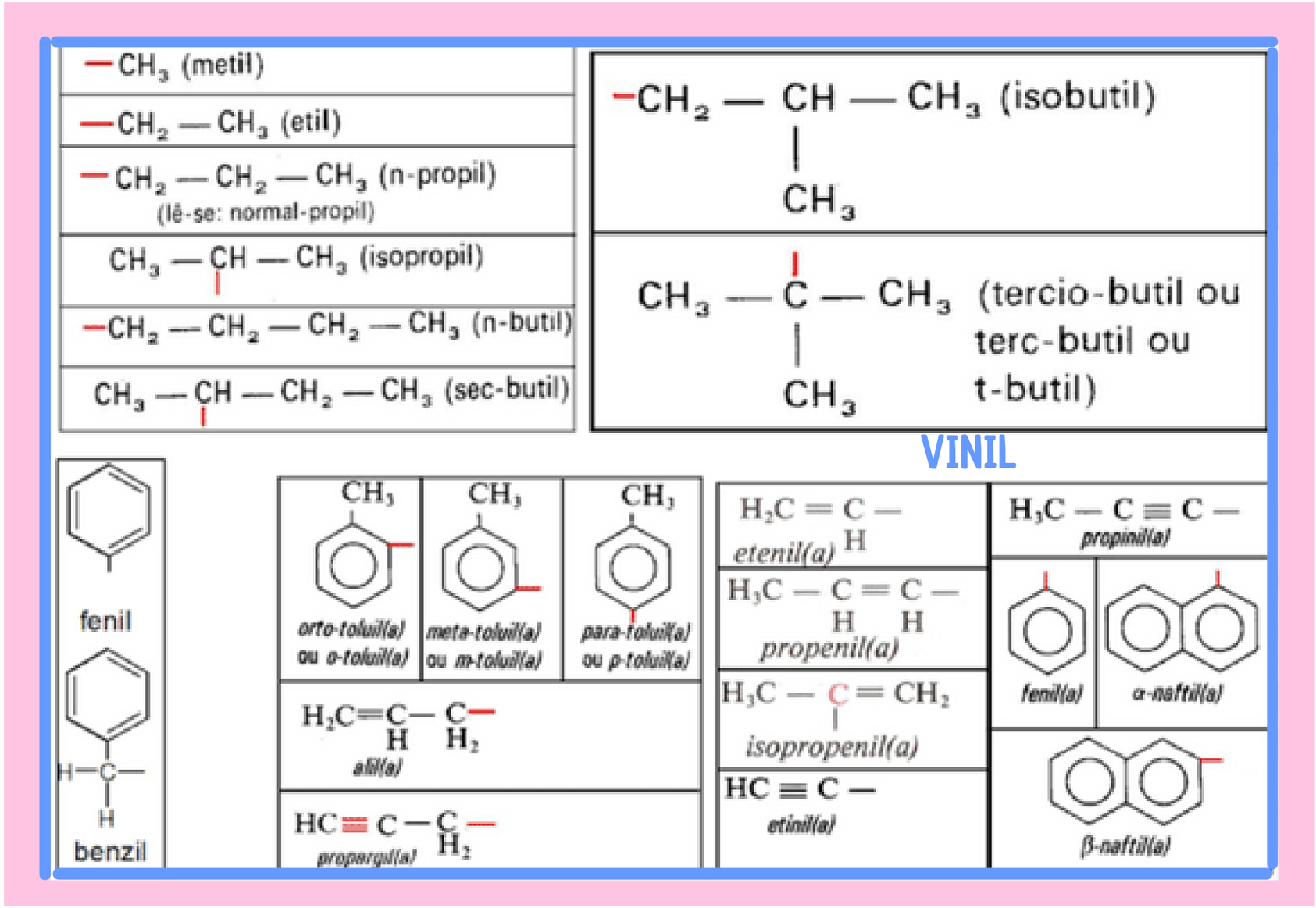
1	MET	6	HEX
2	ET	7	HEPT
3	PROP	8	OCT
4	BUT	9	NON
5	PENT	10	DEC

11	undec
12	dodec
13	tridec
14	tetradec
15	pentadec
16	hexadec
17	heptadec
18	octadec
19	nonadec
20	eicos

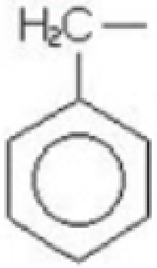
21	heneicos
22	docos
23	tricos
24	tetracos
25	pentacos
26	hexacos
27	heptacos
28	octacos
29	nonacos
30	triacont

31	hentriacont
32	dotriacont
33	tritriacont
34	tetratriacont
35	pentatriacont
36	hexatriacont

ALGUNS RADICAIS ORGÂNICOS E SEUS NOMES



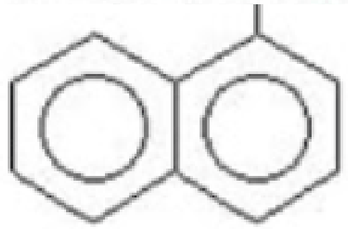
Alguns grupos orgânicos substituintes derivados de compostos insaturados e compostos aromáticos



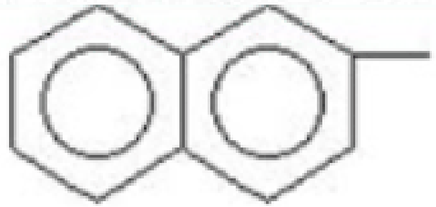
Benzil

Fenil

Vinil



α-naftil



β-naftil

SIMPLES	**AN**
DUPLA	**EN**
TRIPLA	**IN**
DUAS DUPLAS	**DIEN**
DUAS TRIPLAS	**DIIN**
UMA DUPLA E UMA TRIPLA	**ENIN**

SUFIXO

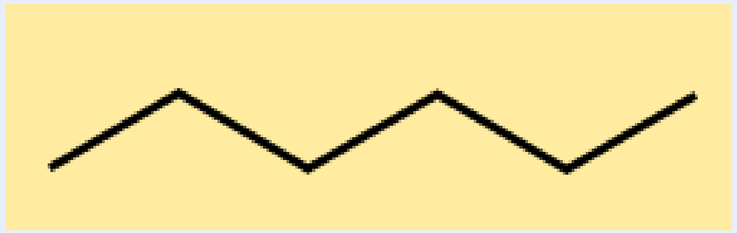
SUFIXO: relacionado com a função orgânica a qual pertence o composto orgânico.

Inicialmente, considere apenas: “**HIDROCARBONETOS**” e “**ÁLCOOIS**”

HIDROCARBONETOS → O
Substâncias formadas apenas por carbono e hidrogênio.

ÁLCOOIS → OL
Substâncias que apresentam o grupo OH (hidroxila) ligado a um carbono que apresenta apenas ligações simples

EXEMPLO



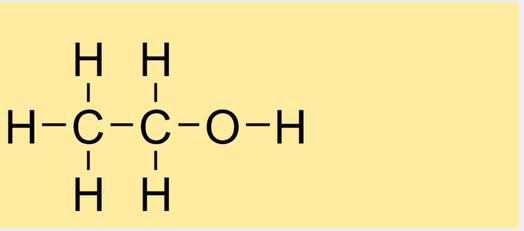
HEXANO

ANÁLISE

HEX	6 CARBONOS
AN	LIGAÇÃO SIMPLES ENTRE ÁTOMOS DE CARBONO
O	HIDROCARBONETO

EXEMPLO

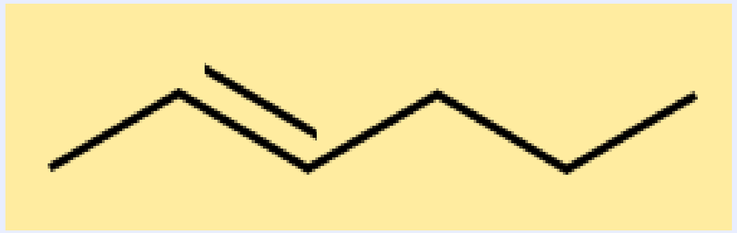
ANÁLISE



ETANOL

ET	2 CARBONOS
AN	LIGAÇÃO SIMPLES ENTRE ÁTOMOS DE CARBONO
OL	ÁLCOOL

EXEMPLO



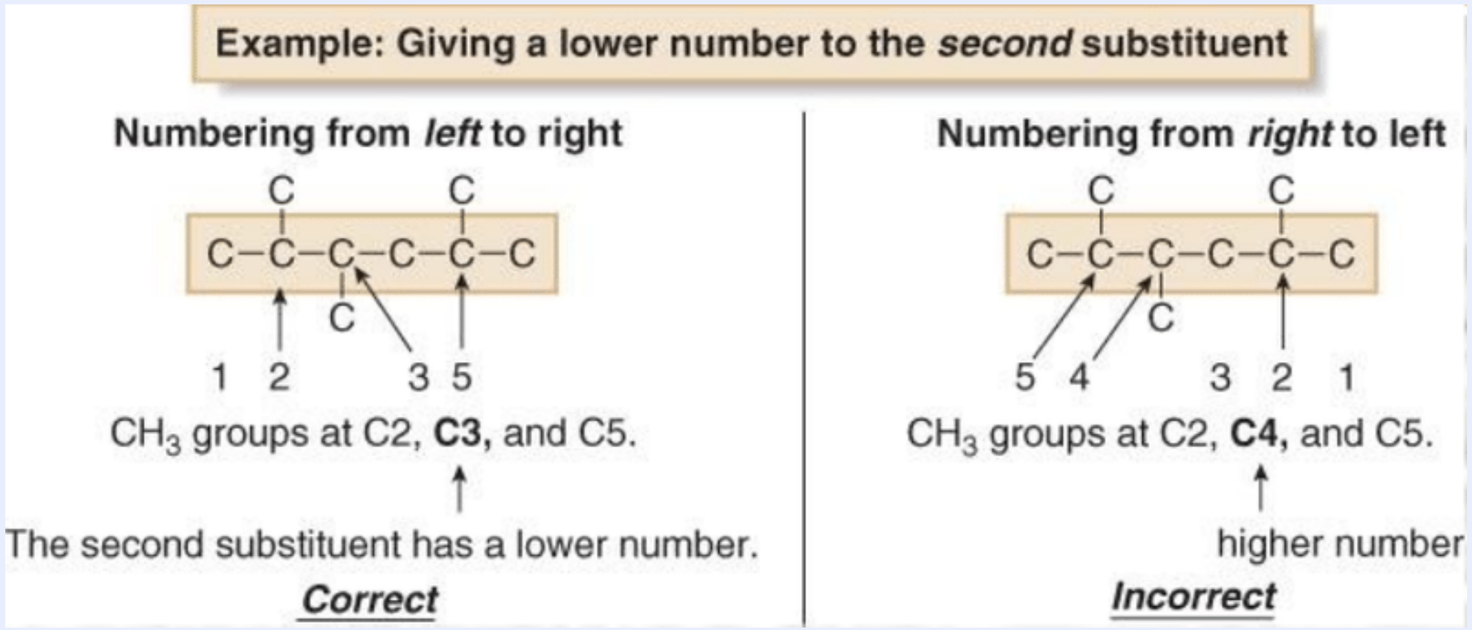
HEX-2-ENO

ANÁLISE

HEX	6 CARBONOS
EN	LIGAÇÃO DUPLA ENTRE ÁTOMOS DE CARBONO
O	HIDROCARBONETO

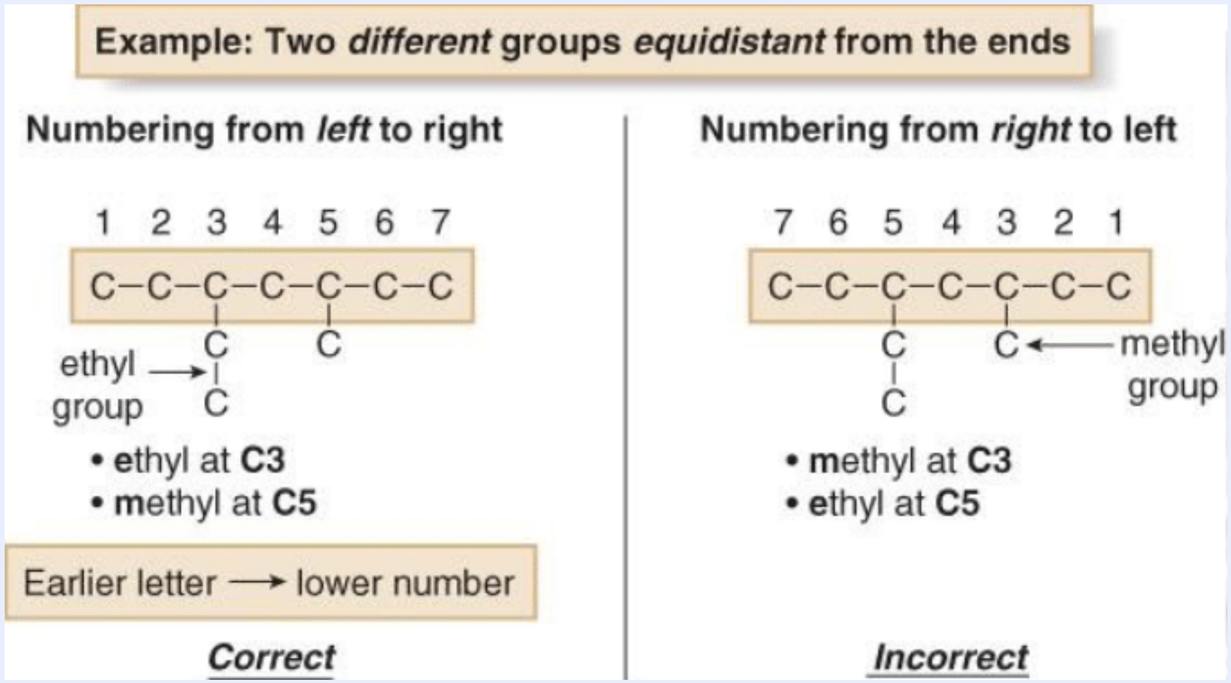
ALCANOS

- Se o primeiro substituinte tiver a **mesma distância** em qualquer um dos lados da cadeia principal, enumere de tal modo que o **segundo substituinte** leve a **menor** numeração

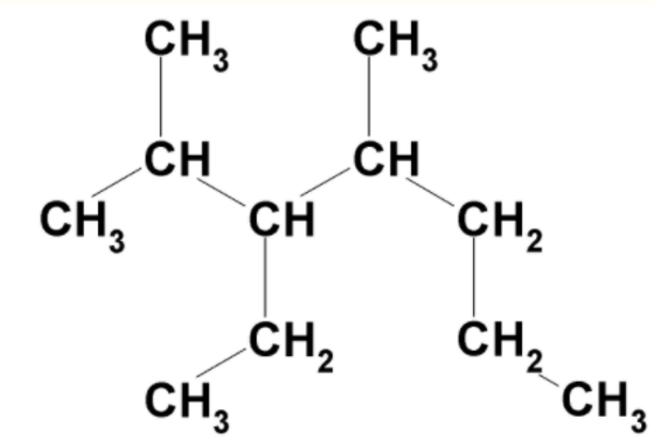


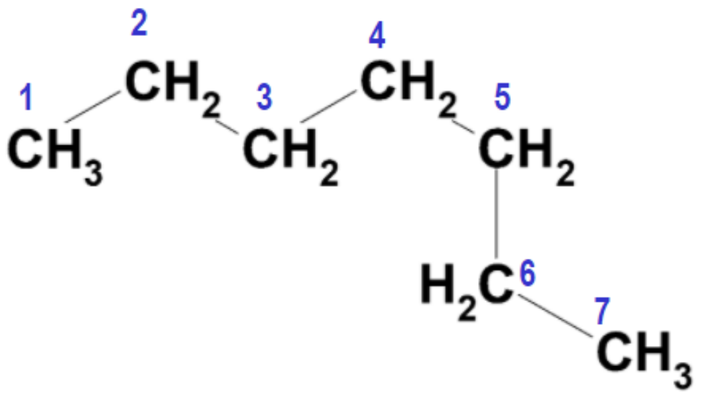
ALCANOS

Quando houver grupos **equidistantes** a partir do final de uma cadeia principal, atribua o **menor** número levando em consideração a **ordem alfabética** do substituinte.



EXEMPLO: 3-etil-2,4-dimetilheptano





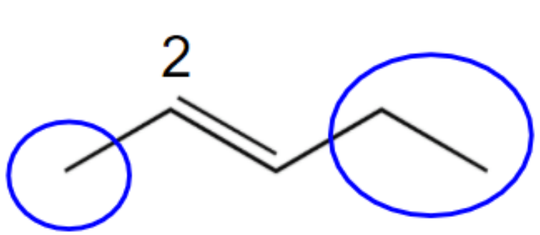
ANÁLISE

“3-etil-” mostra a presença de um radical etila no carbono 3.

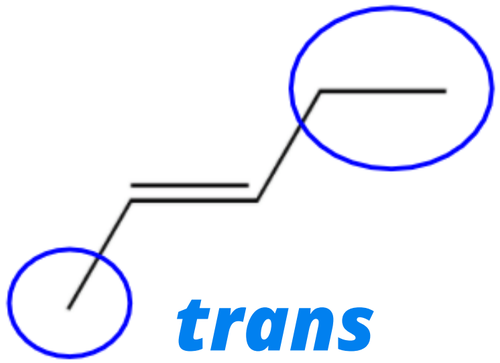
“2,4-dimetil” indica 2 grupos metílicos ou metila ligados nos carbonos de Nº 2 e 4

Cadeia carbônica central com 7 átomos de carbono- “heptano”

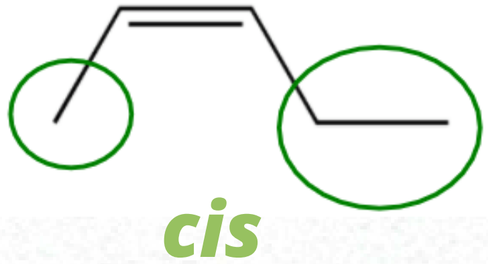
ISOMERIA GEOMÉTRICA



pent-2-eno



(2E)-pent-2-eno



(2Z)-pent-2-eno

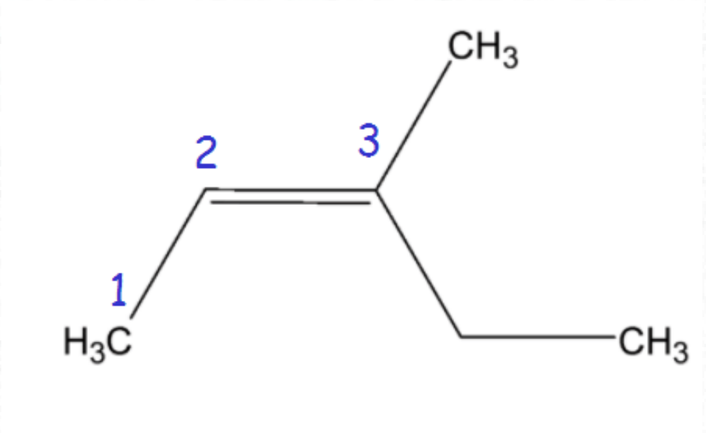
E/Z notação

Se houverem três ou quatro grupos substituintes diferentes na dupla ligação

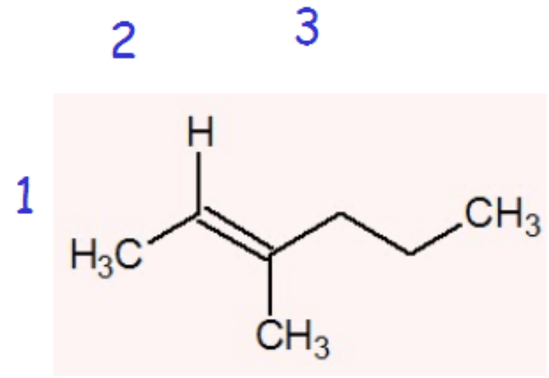
E : opostos → *trans*

Z : juntos → *cis*

EXEMPLOS



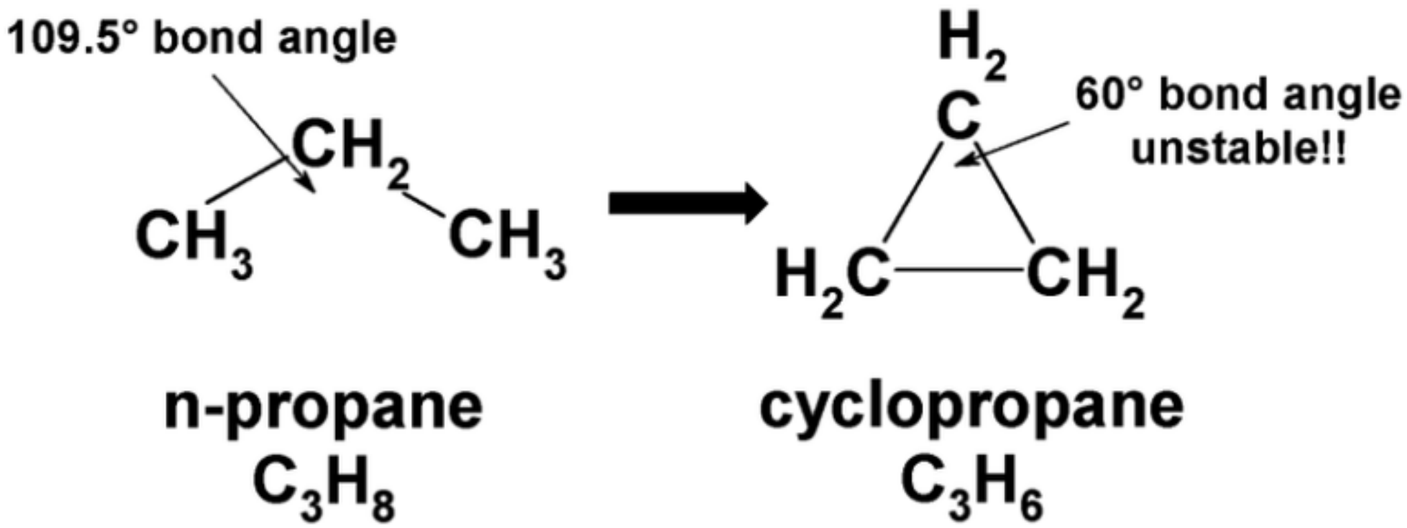
(2Z)-3-metilpent-2-eno



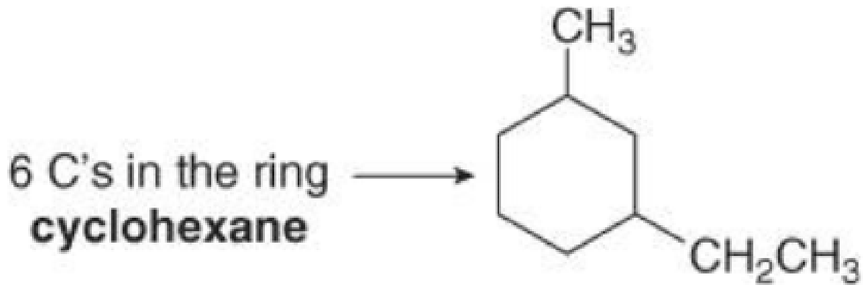
(2E)-3-metil-hexen-2-eno

CICLOALCANOS

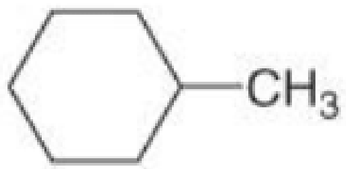
- Cadeia carbônica formando um “**anel**”
- Note a **perda de átomos de H** para obter o **fechamento do anel**



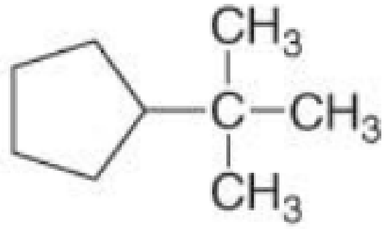
1. Find the parent cycloalkane.



2. Name and number the substituents. No number is needed to indicate the location of a single substituent.



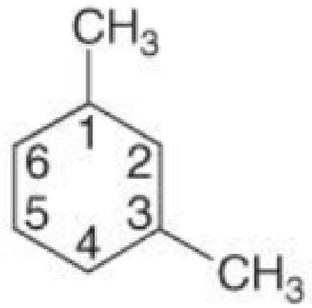
methylcyclohexane



tert-butylcyclopentane

Para anéis com mais de um substituinte: Enumere um substituinte e o segundo será de tal modo que este tenha o menor numeração.

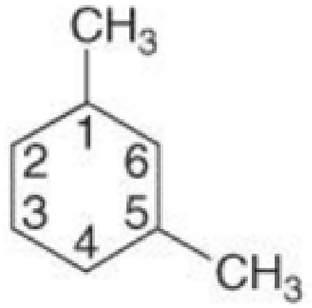
numbering clockwise



CH_3 groups at C1 and **C3**
The 2nd substituent has a lower number.

Correct: **1,3-dimethylcyclohexane**

numbering counterclockwise

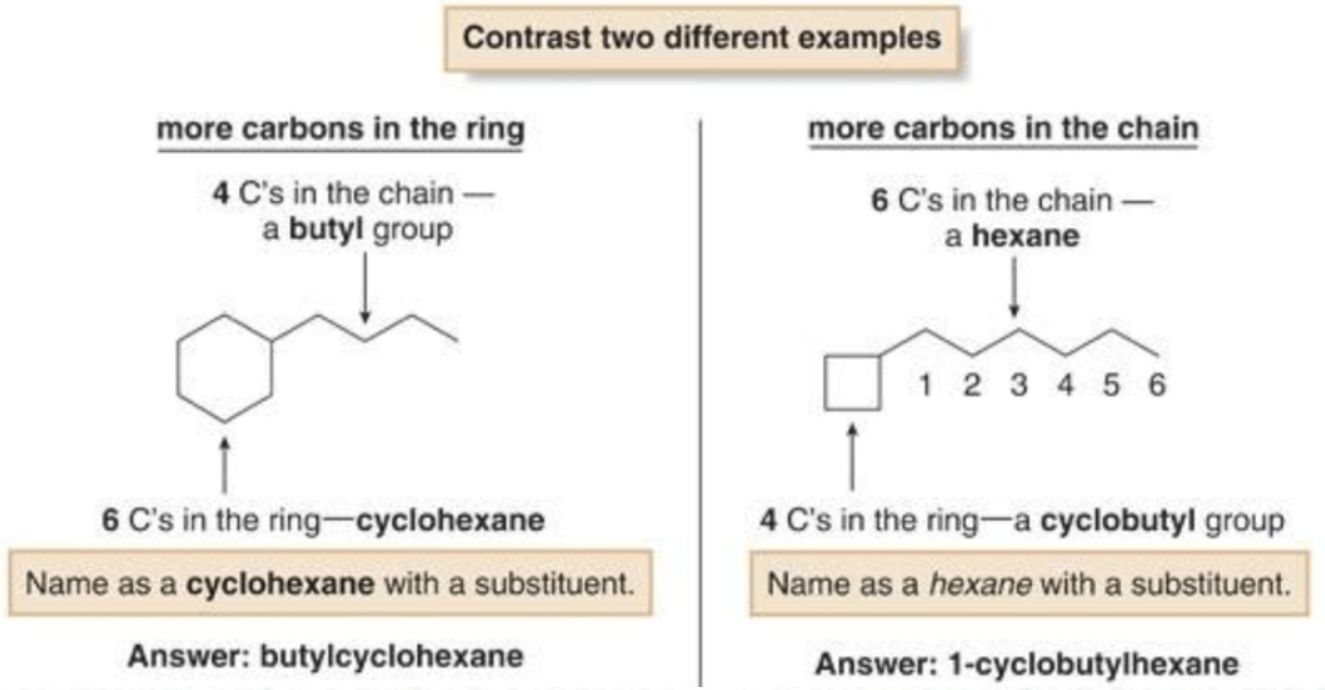


CH_3 groups at C1 and **C5**

Incorrect: 1,5-dimethylcyclohexane

Quando o alcano for composto de um anel e de uma cadeia carbônica:

Se o **número** de carbonos **do anel for maior ou igual** ao **número de carbonos da maior cadeia carbônica**, o composto será denominado **cicloalcano**.



REGRAS PARA NOMEAR CICLOALCANOS

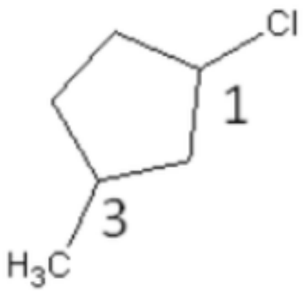
cyclopropane

cyclobutane

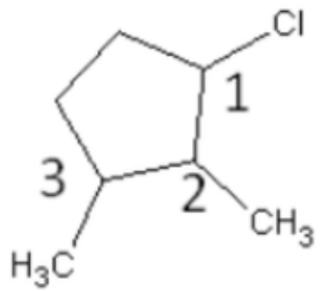
cyclopentane

cyclohexane

- Substituents are named so that the first one is determined **alphabetically**
- After the first one is identified, the others are numbered to get the **lowest** possible sequence of numbers



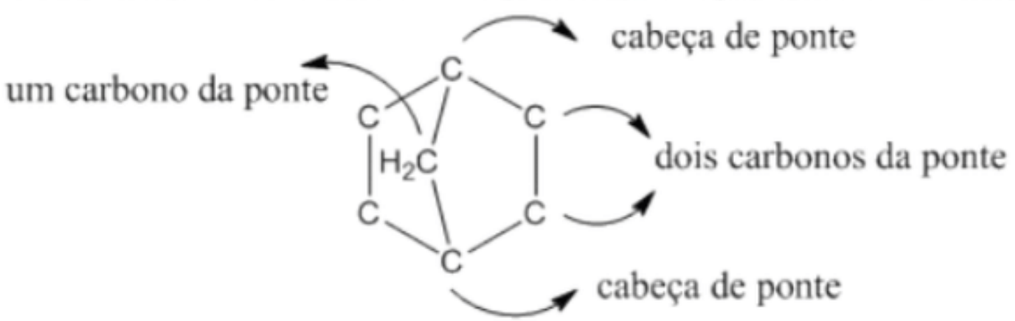
chloro-3-methylcyclopentane

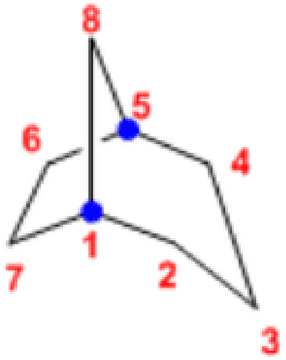


chloro-2,3-dimethylcyclopentane

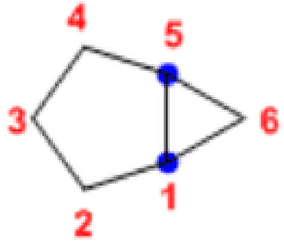
NOMENCLATURA DE BICICLOS

Na sequência é interposto **entre colchetes** o nome que denota o **número de átomos de carbono em cada ponte** (em ordem decrescente de comprimento), **anéis fundidos tem zero átomos** de carbono na ponte

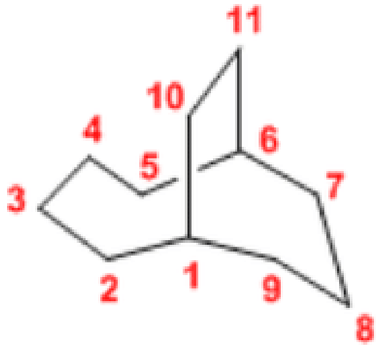




Biciclo[3.2.1]octano



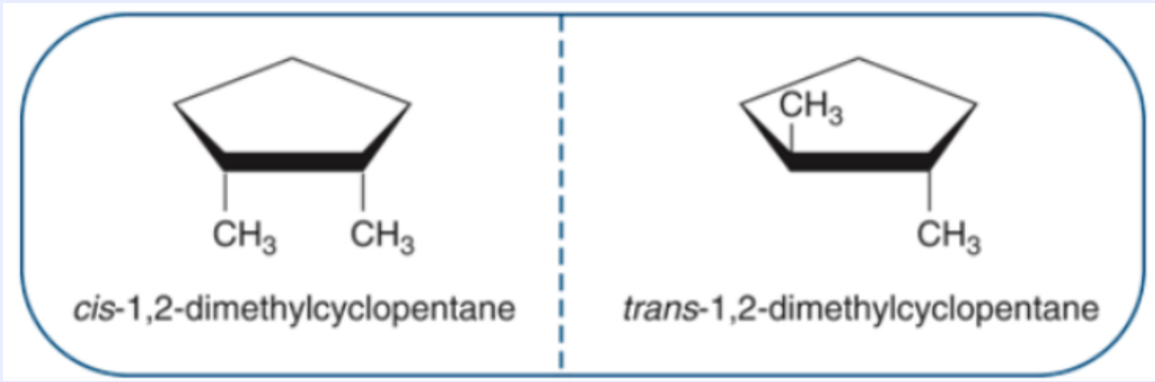
Biciclo[3.1.0]hexano



Biciclo[4.3.2]undecano

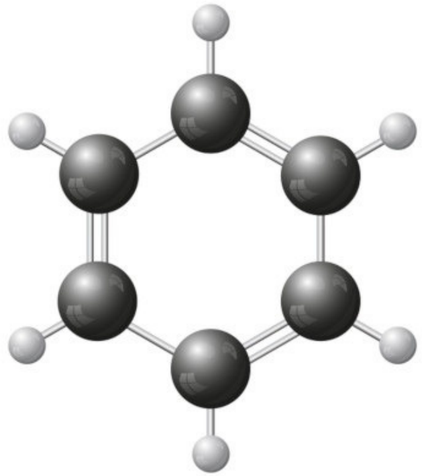
ISOMERISM AND CYCLOALKANES

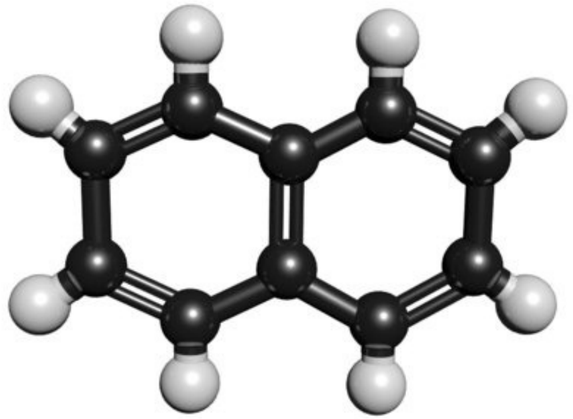
- **Structural isomers:** same formula, different arrangement
- **Stereoisomers:** same formula, same arrangement, different 3D orientation
- **Geometric isomers:** stereoisomers of cyclic atoms
  -Rotation about C-C single bonds occurs in open-chain compounds but not within rings
  -***Cis:*** substituents on the same side
  -***Trans:*** substituents on the opposite side



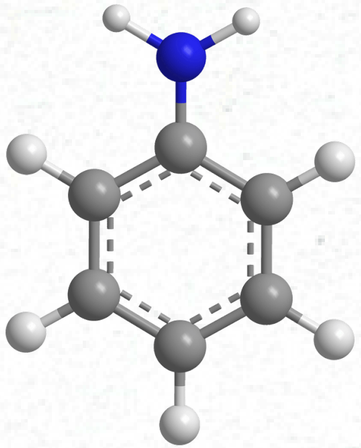
COMPOSTOS AROMÁTICOS

- **Benzeno (C_6H_6):** entre os 25 produtos químicos mais produzidos
- Ponto de partida para obtenção de milhares de outros compostos

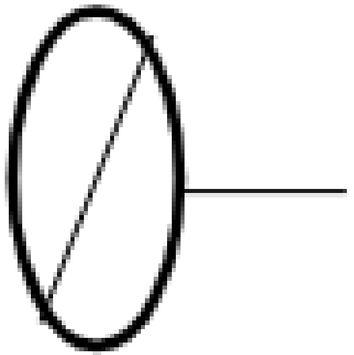




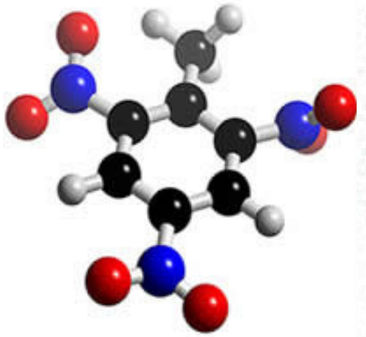
Naftaleno



Anilina



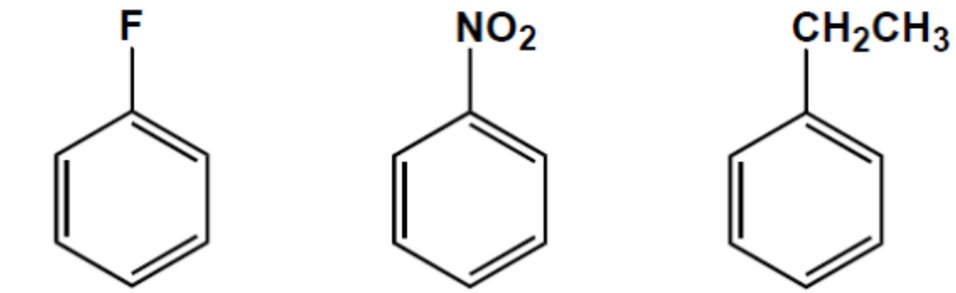
Radical: Ar---



TNT
Trinitrotolueno

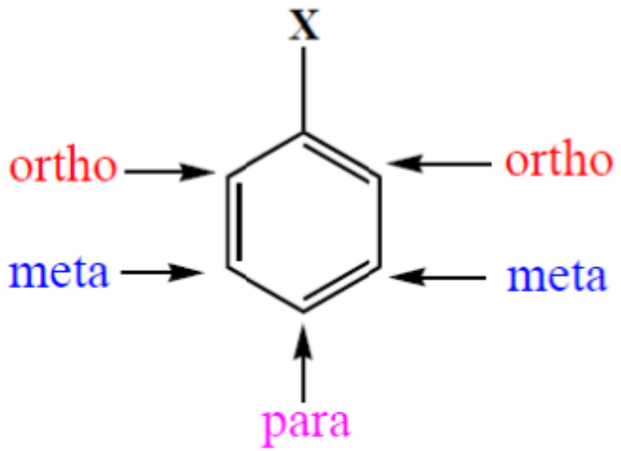
MONOSUBSTITUTED BENZENES (IUPAC)

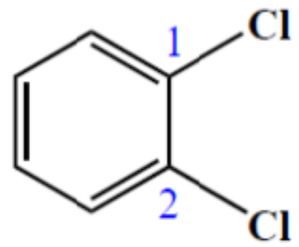
- Monosubstituted aromatics are named using ***-benzene*** as the parent name
- Alkyl substituted benzenes are named according to the chain length of the alkyl group
- If the alkysubstituted has six carbons or fewer, it will be named as ***alkylbenzene***



Fluorobenzene **Nitrobenzene** **Ethylbenzene**

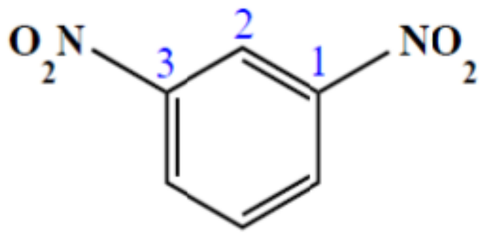
AROMÁTICOS DISSUBSTITUÍDOS





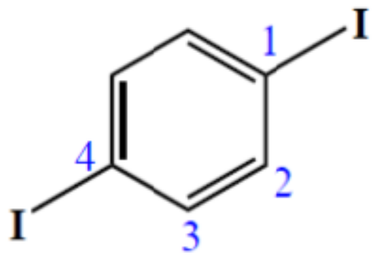
***ortho*-Dichlorobenzene**

1,2-Dichlorobenzene



***meta*-Dinitrobenzene**

1,3-Dinitrobenzene



***para*-Diiodobenzene**

1,4-Diiodobenzene

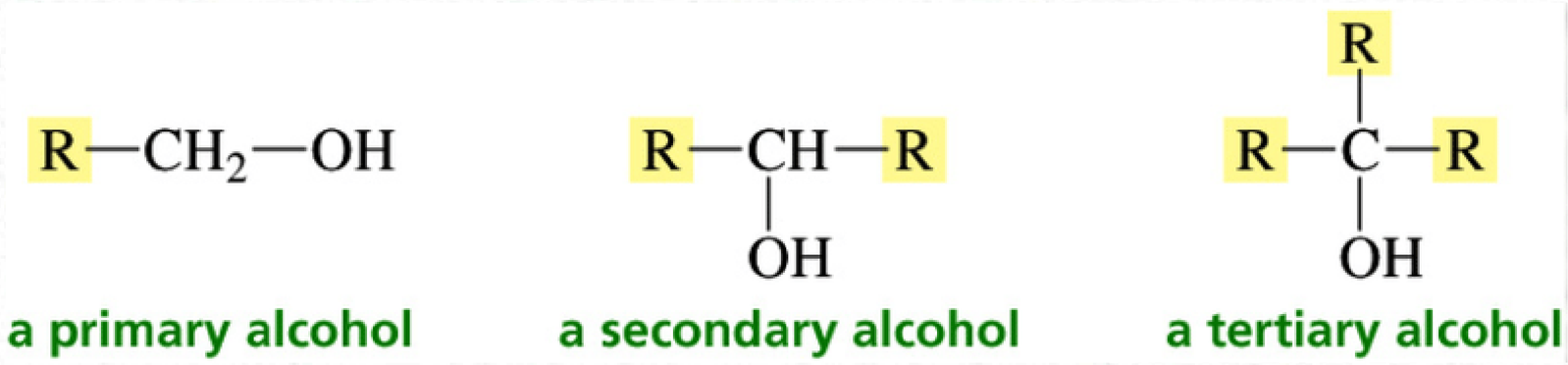
COMPOSTOS OXIGENADOS: DERIVADOS DE HIDROCARBONETOS

- Hidrocarbonetos onde um ou mais hidrogênios são substituídos por grupos funcionais (**cadeiras heterogêneas**)
- Grupos funcionais possuem O, que confere **propriedades diferentes** aos compostos

OH	ROH	Álcool	CH_3CH_2OH – etanol
OR'	ROR'	Éter	$(CH_3CH_2)_2O$ – éter dietílico
CHO	RCHO	Aldeído	CH_3CHO – etanal
COOH	RCOOH	Ácido carboxílico	CH_3CO_2H – ácido etanóico

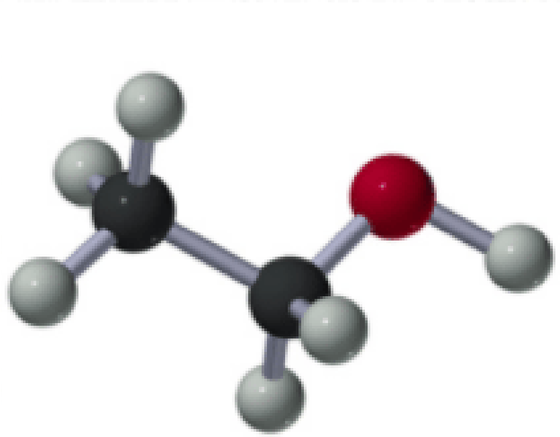
NOMENCLATURA DE ÁLCOOIS

Podem ser classificados como **primários, secundários** ou **terciários**

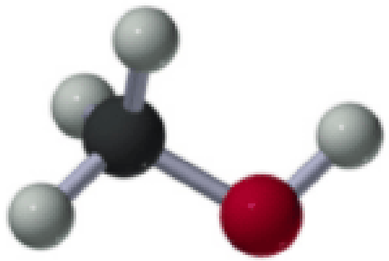


NOMENCLATURA DE ÁLCOOIS

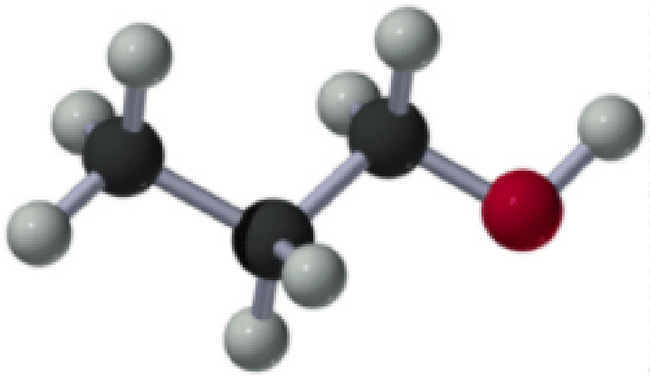
Nome comum- Nome do grupo **alquílico** seguido da palavra “**álcool**”



ethyl alcohol



methyl alcohol



propyl alcohol

NOMENCLATURA DE ÁLCOOIS

Essa função orgânica é denotada pelo sufixo **“ol”**

Metanol, CH_3OH

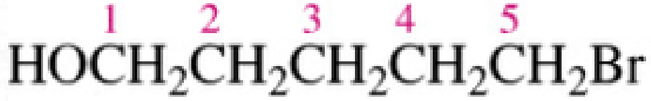
Etanol, CH_3CH_2OH

NOMENCLATURA DE ÁLCOOIS - IUPAC

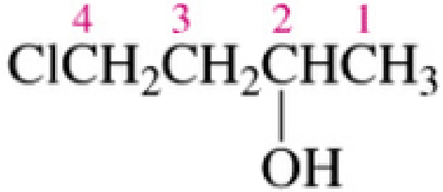
- A **cadeia principal** será aquela que houver **maior número** de carbonos e contiver o grupo **–OH**
- A **numeração** será aquela na qual o **grupo funcional** tenha o **menor número**
- Se houver um **substituinte e um grupo funcional** presente, leva o **menor** número o **grupo funcional.**

NOMENCLATURA DE ÁLCOOIS - IUPAC

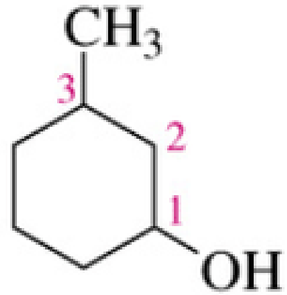
- Se o grupo funcional tem o **mesmo número** em **ambas direções**, use a direção na qual o **substituinte tenha o menor número**
- Se houver **mais de um** substituinte, coloque-os em **ordem alfabética**
- [**SUBSTITUINTE**] + [**CADEIA CARBÔNICA PRINCIPAL**] + [**GRUPO FUNCIONAL**]



5-bromo-1-pentanol

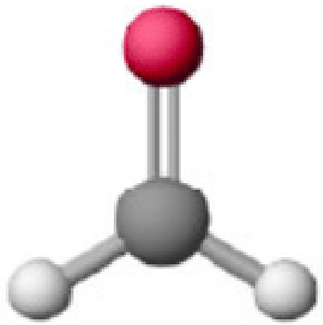


4-chloro-2-butanol



3-methylcyclohexanol

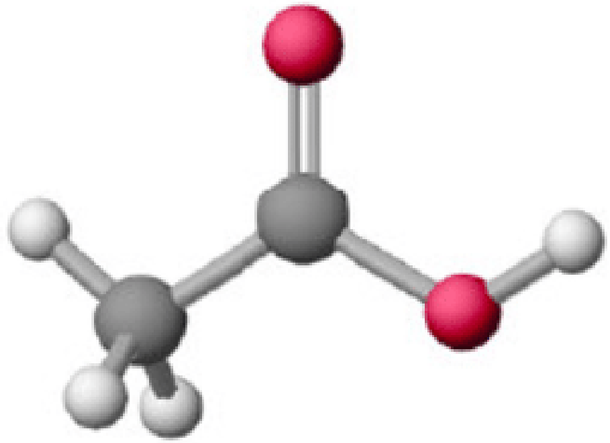
COMPOSTOS COM GRUPO CARBONILA



Formaldeído

CH_2O

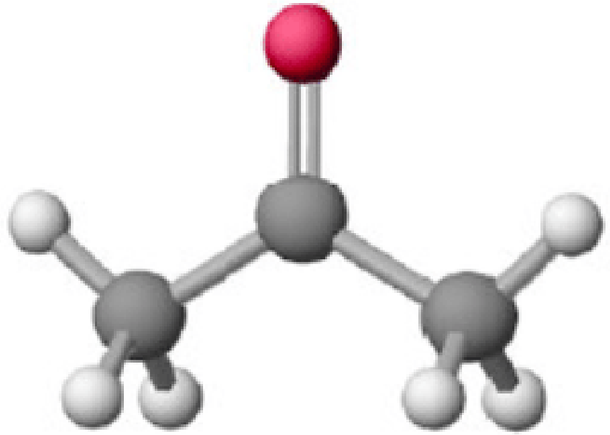
Aldeídos



Ácido Acético

CH_3CO_2H

Ácidos carboxílicos



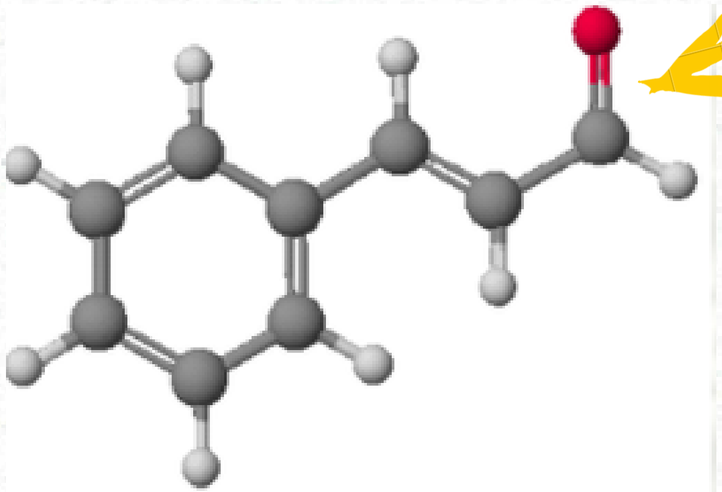
Acetona

CH_3COCH_3

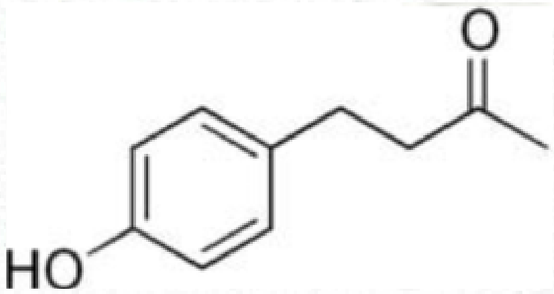
Cetonas

ALDEÍDOS E CETONAS

Cinamaldeído

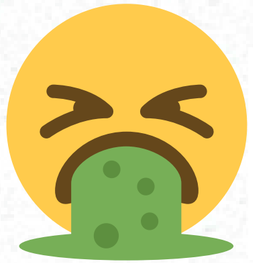


p-hidroxifenil-2-butanona

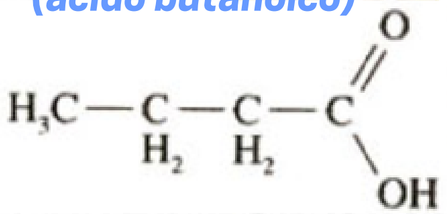


Odores agradáveis

ÁCIDOS CARBOXÍLICOS

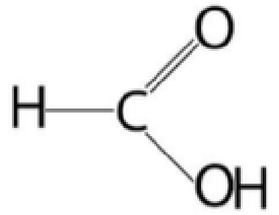


Ácido butírico
(ácido butanóico)



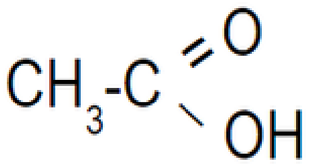
Butyrum (latim)
manteiga

Ácido metanóico

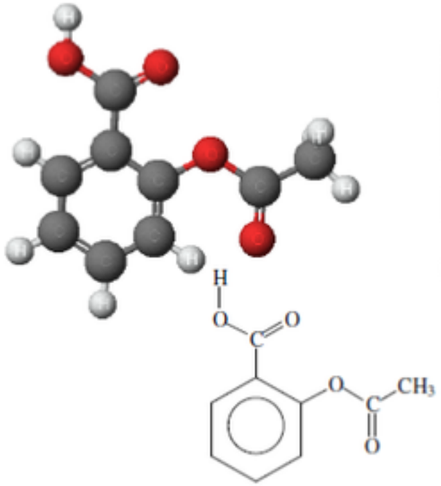


Formica (latim)
formiga

Ácido etanóico
Ácido etanóico

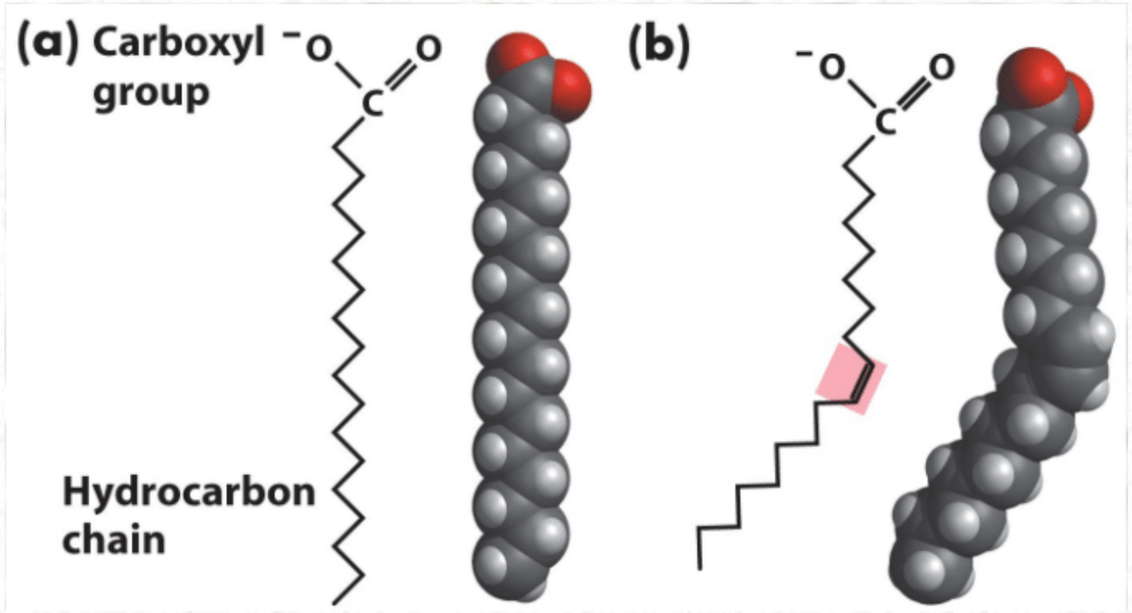


Ácido 2-acetoxibenzóico

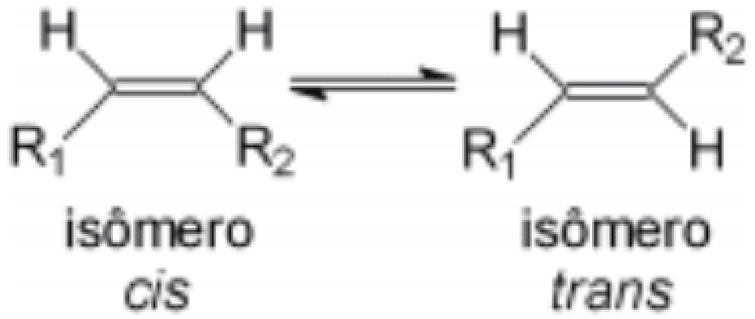


ÁCIDOS GRAXOS

A cadeia R tem geralmente **12 a 18 C** de comprimento e pode incluir uma ou mais ligações duplas.



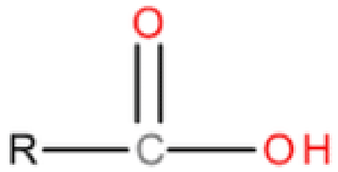
Ácido graxo saturado *Ácido graxo insaturado*



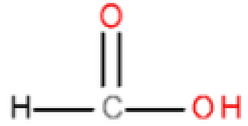
Reação de isomerização *cis-trans*

ESTRUTURA DOS ÁCIDOS CARBOXÍLICOS E SEUS DERIVADOS

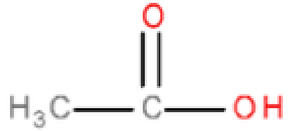
FÓRMULA GERAL



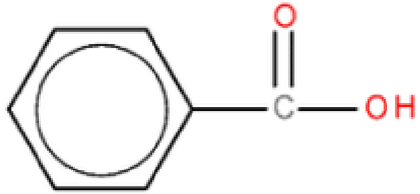
ÁCIDOS CARBOXÍLICOS SIMPLES



formic acid
IUPAC: methanoic acid



acetic acid
IUPAC: ethanoic acid

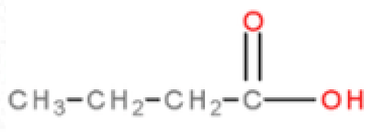


IUPAC: benzoic acid

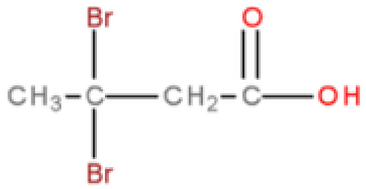
NOMENCLATURA DOS ÁCIDOS CARBOXÍLICOS IUPAC

Para **ácidos monocarboxílicos** (um único grupo –COOH):

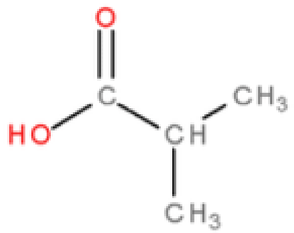
- Selecionar a cadeia carbônica principal que **contenha o grupo carboxil**. Esta será a **cadeia principal e o grupo –COOH será designado como o C-1.**
- **Inicie** o nome **com** a palavra "**ácido**" seguido do **nome do alcano** e troque a **terminação "ano"para "óico"**.
- Indique a **localização dos substituintes** na cadeia principal



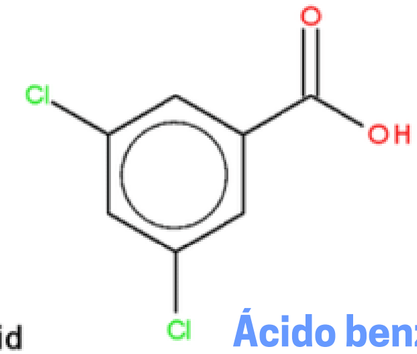
Butanoic acid



3,3-Dibromobutanoic acid



2-Methylpropanoic acid



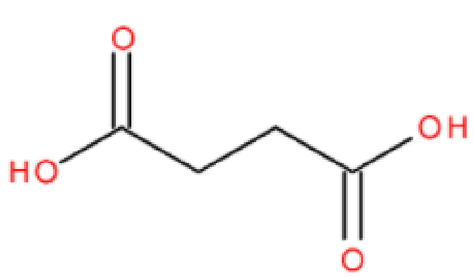
Ácido benzóico

3,5-Dichlorobenzoic acid

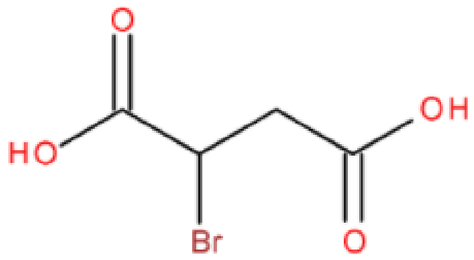
NOMENCLATURA DOS ÁCIDOS CARBOXÍLICOS IUPAC

Para **ácidos dicarboxílicos**:

- Os **finais da cadeia** carbônica terminam com um grupo**–COOH.**
- **Iniciar com a palavra ácidos** seguido do **nome do alcano** da cadeia principal terminado com "**dióico**".



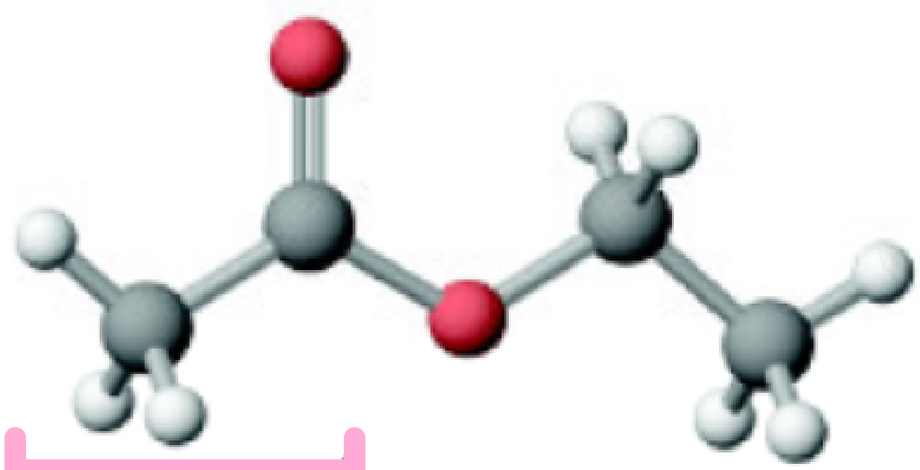
Butanedioic acid
(Succinic acid)



Bromobutanedioic acid
(Bromosuccinic acid)

ÁCIDOS + ÁLCOOIS = ÉSTERES!

Ésteres geralmente promovem odores agradáveis



Grupo Carboxilato: porção que veio do ácido acético

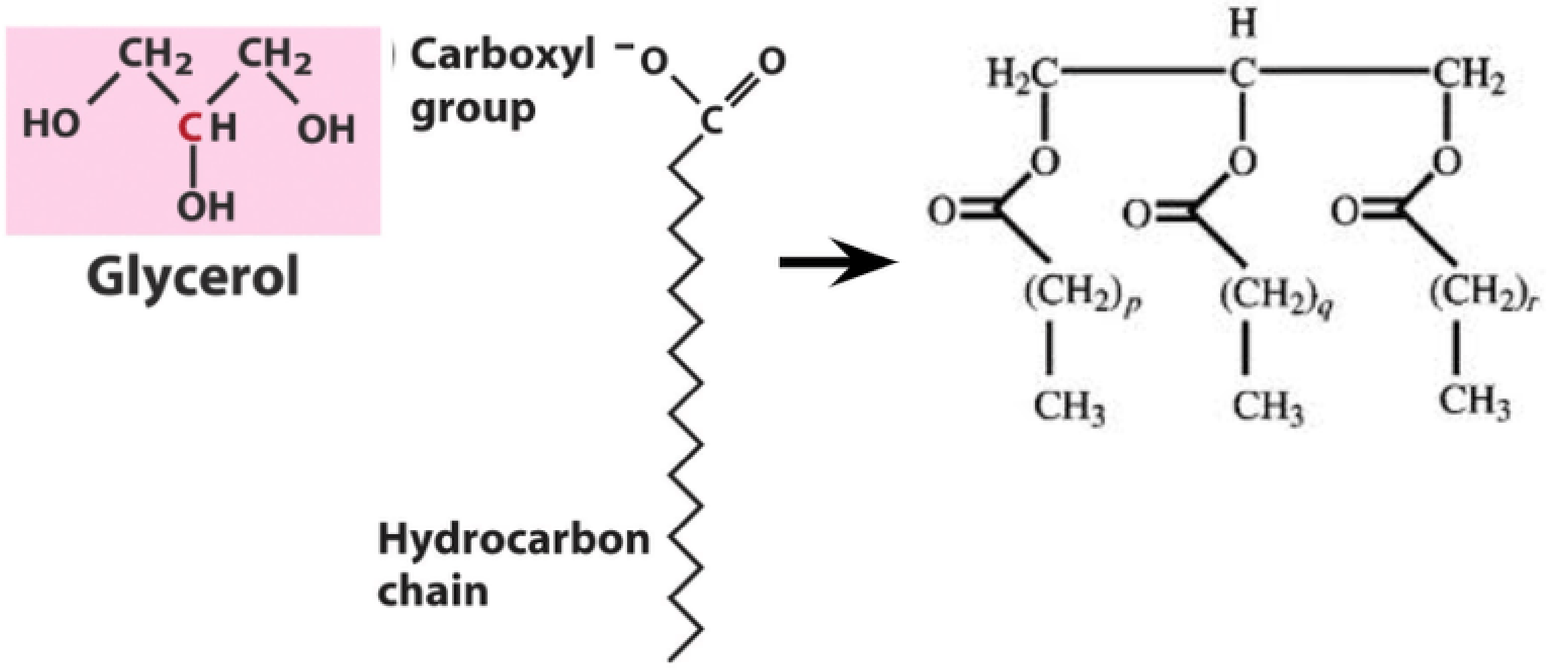
Porção que veio do etanol

$CH_3CO_2CH_2CH_3$

Acetato de etila, um éster!

ÁCIDOS + ÁLCOOIS = ÉSTERES!

Triglicerídeos são os principais constituintes de gorduras (sólidos) e óleos (líquidos) e são triésteres formados por:



AMIDAS

Urea

Aspartame

Saccharin

Antitérmico

Phenacetin

Tylenol analgésico e antitérmico

Acetaminophen

Luminal (phenobarbital)

Nembutal (pentobarbital)

Valium (diazepam)

Sedativos

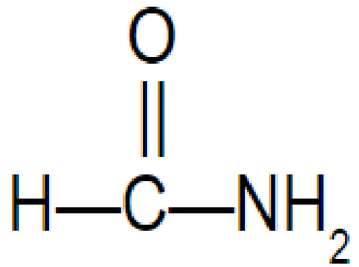
Seconal (secobarbital)

Equanil (meprobamate)

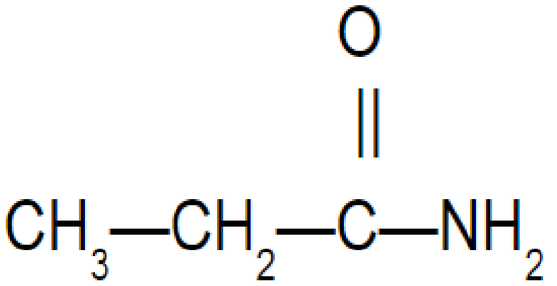
Antiansiolítico

AMIDAS

Chamadas de alcanamidas.



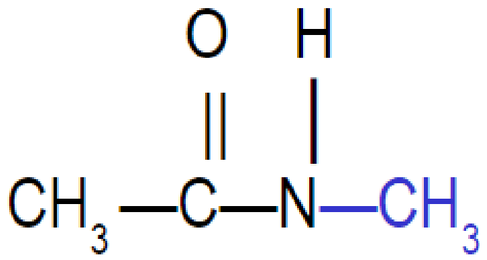
Metanamida (IUPAC)
Formamida (comum)



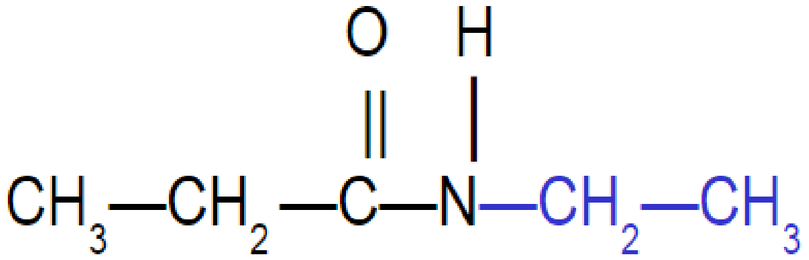
Propanamida (IUPAC)
Propionamida (comum)

AMIDAS COM N GRUPOS

Um grupo alquil ligado ao átomo de N é chamado de ***N*-alquil** no nome da amida



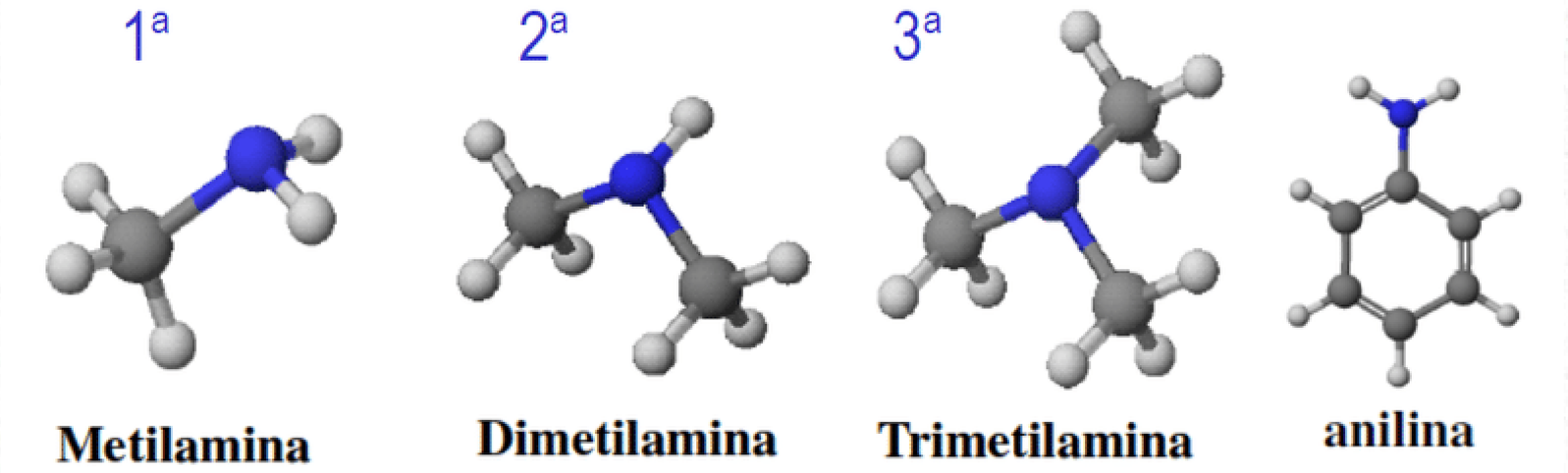
***N*-metiletanamida (IUPAC)**
***N*-metilacetamida (comum)**



***N*-etilpropanamida (IUPAC)**
***N*-etilpropionamida (comum)**

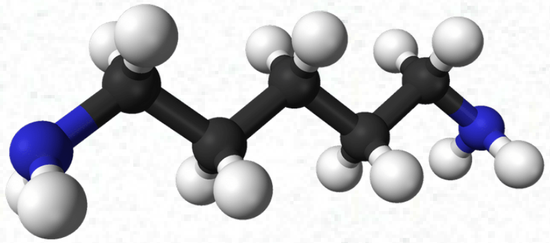
AMINAS

- Aminas são derivadas de **NH_3**
- Um ou mais H ligados ao N são **substituídos** por um grupo orgânico.
- Aminas, assim como o **NH_3**, são **bases**.

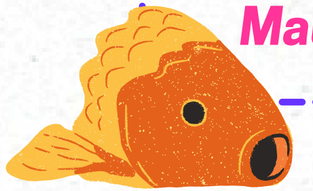


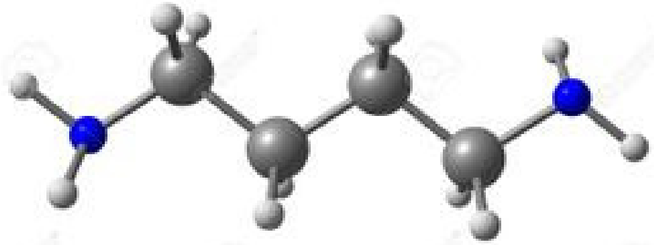
AMINAS

Geralmente tem odores **horríveis**!



Peixe podre
Urina
Maú hálito

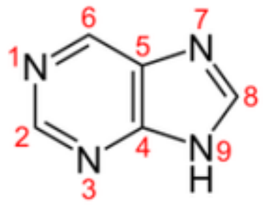




Cadaverina

Putrescina

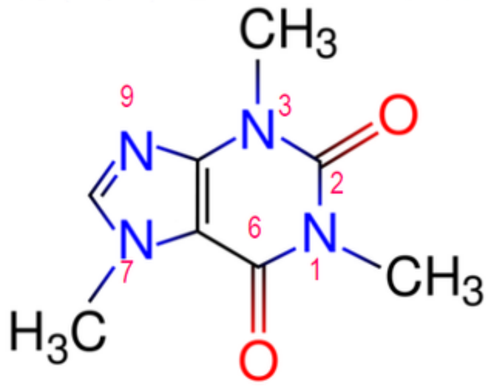
AMINAS

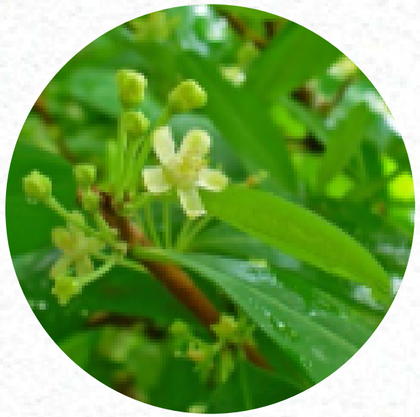


PURINA

CAFEÍNA

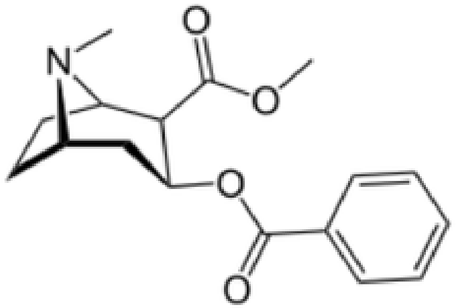
1,3,7-trimetil- 1H-purino-2,6(3H,7H)-diona





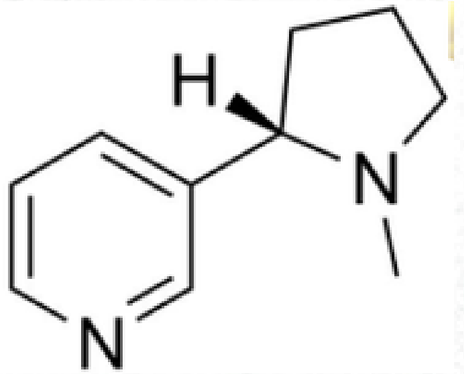
COCAÍNA

3-benzoiloxi-8-metil-8-azabiciclo.[3.2.1]octano-4-carboxilato



NICOTINA

(S)-3-(1-Methyl-2-pyrrolidinyl)pyridine



NOMENCLATURA DE AMINAS

- **IUPAC** – O grupo **NH_2** é grupo funcional
- O grupo funcional é o sufixo : “**amina**”
- Final “**o**” do alcano mais longo é substituído pelo sufixo “**amina**”

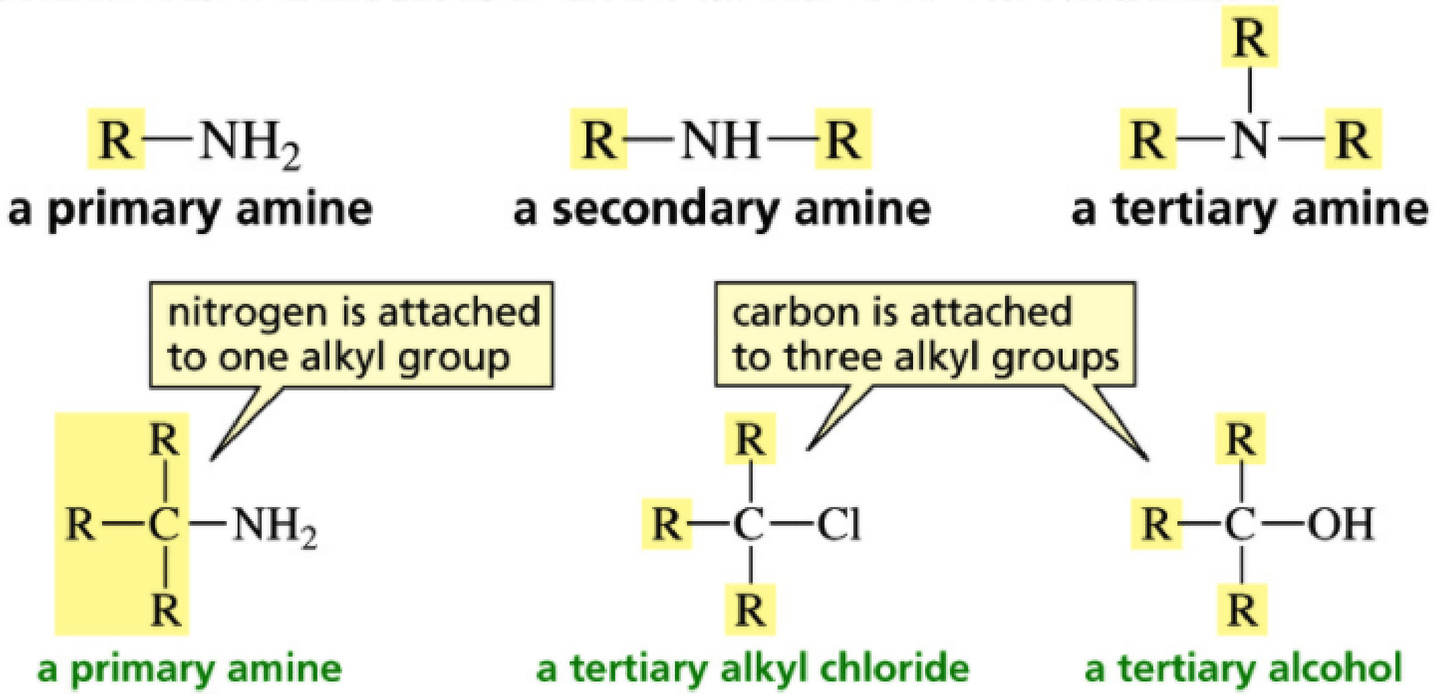
$CH_3CH_2CH_2CH_2NH_2$

1-butanamine

butan-1-amine

AMINAS

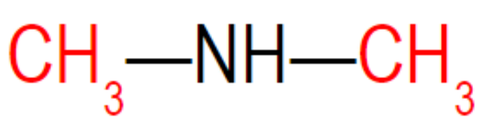
Classificadas como **primárias, secundárias e terciárias** dependendo do **número de grupos alquilas ligados** ao átomo de **N**.



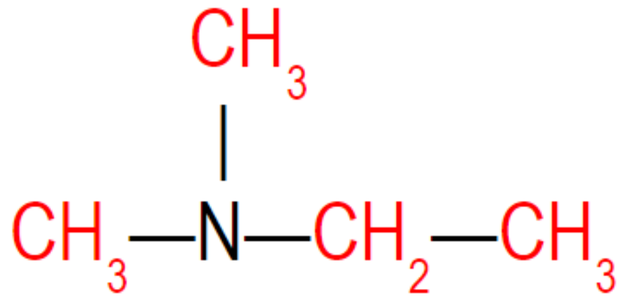
AMINAS SIMPLES

Listar os **grupos alquilas** ligados ao átomo de N em **ordem alfabética** na frente da palavra "**amina**".

***etil*amina**



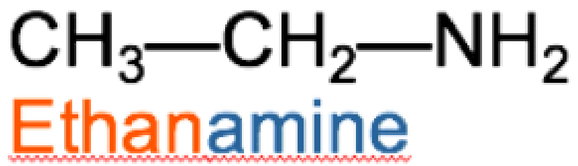
***dimetil*amina**

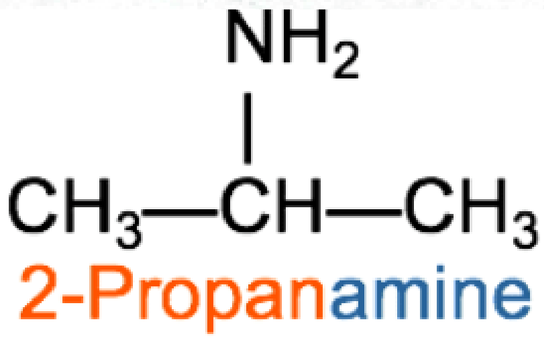


***etildimetil*amina**

AMINAS - IUPAC

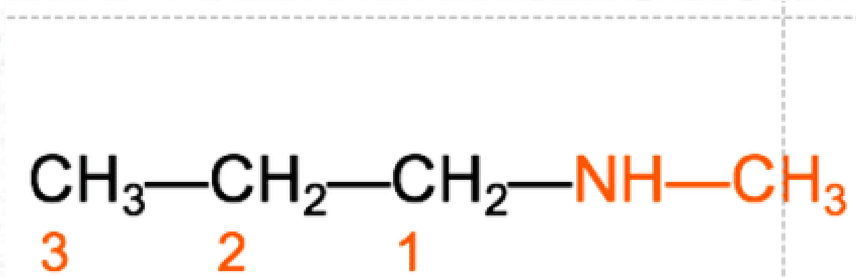
- Chamadas de **alcanaminas**
- A letra “**o**” do nome do **alcano** de **maior cadeia carbônica** será **trocada** por “**amina**".
- A cadeia é **numerada** para **localizar** os **grupos substituintes** na amina.



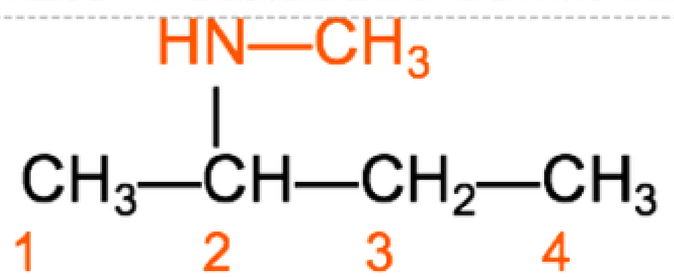


AMINAS SECONDÁRIAS E TERCIÁRIAS

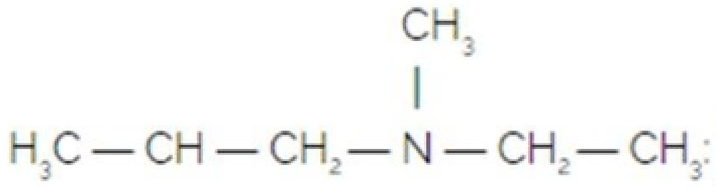
- Enumerar a **cadeia principal**.
- Cada grupo **alquil** ligado ao átomo de N é nomeado de ***N-alquil*** grupo



N-Methyl-1-propanamine

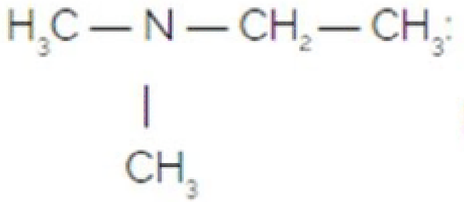


N-Methyl-2-butanamine



etilmetilpropilamina

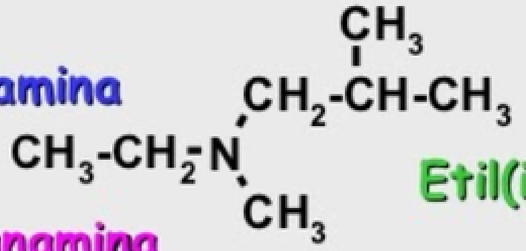
N-etil- N-metilpropanamina



etildimetilamina

NN-dimetiletanamina

N-Etil-*N*-metilisobutilamina

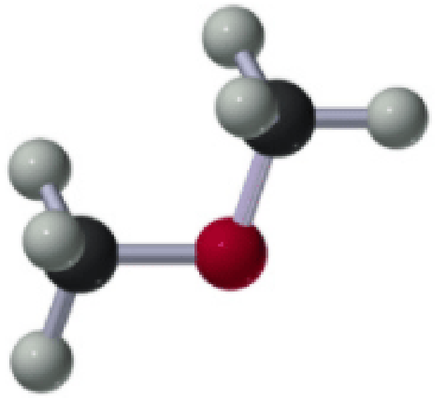


Etil(isobutil)metilamina

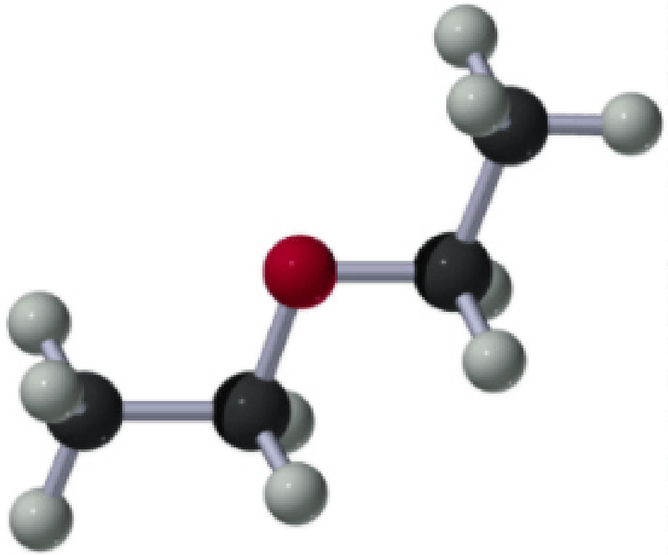
N-Etil-*N*-metilisobutanamina

NOMENCLATURA DE ÉTERES

Nome comum- Nome(s) do(s) grupo(s) alquílicos listados e seguidos da palavra "**éter**"



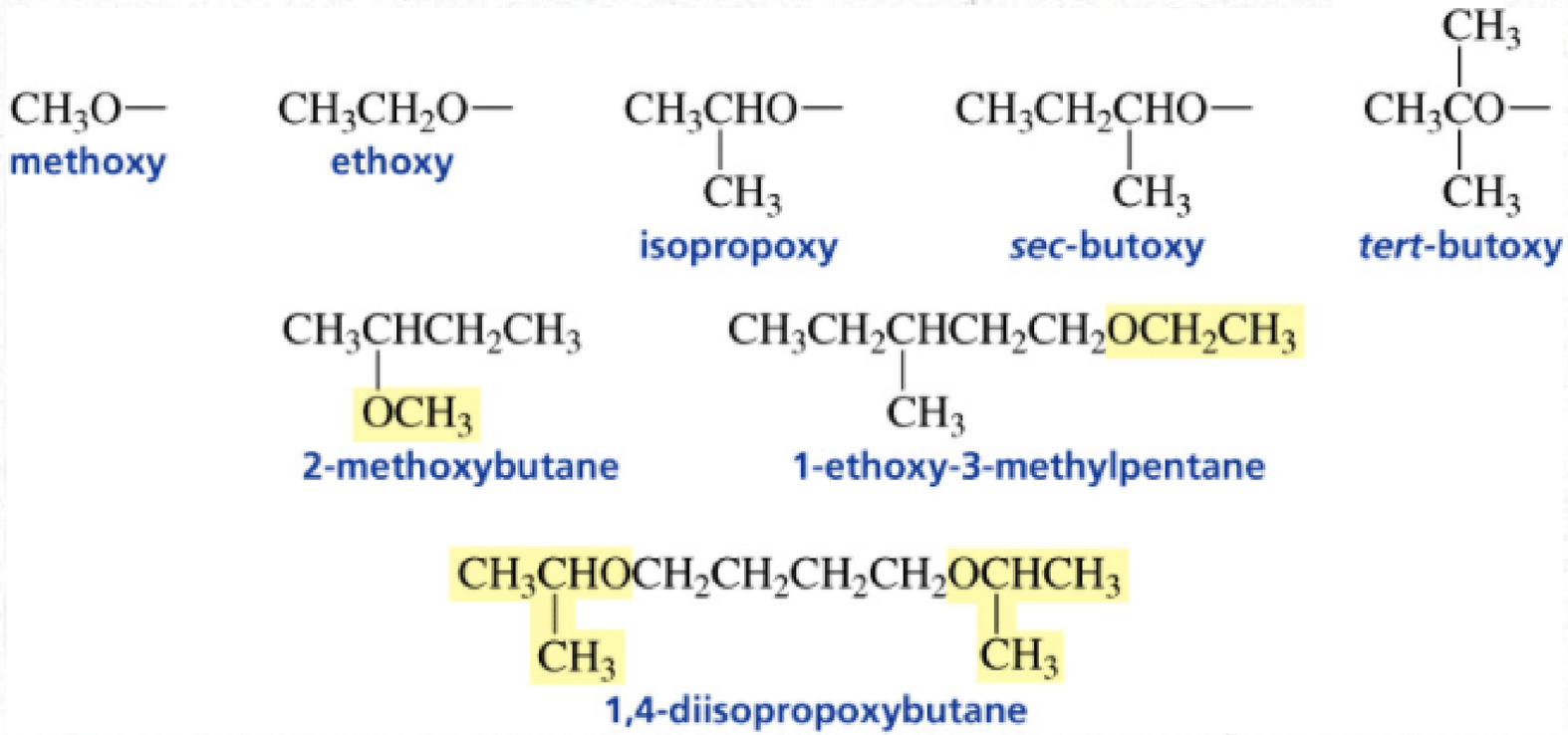
dimethyl ether



diethyl ether

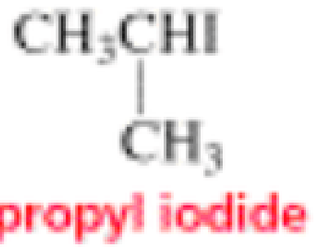
NOMENCLATURA DE ÉTERES

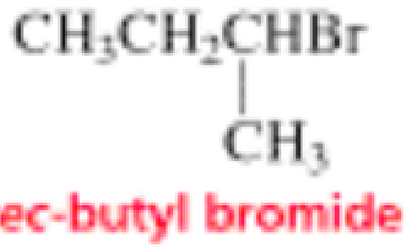
IUPAC – O **menor grupo alquila** é **convertido a ”alcóxi”** e usá-lo como um **substituinte**



HALETOS DE ALQUILA/ ORGÂNICOS

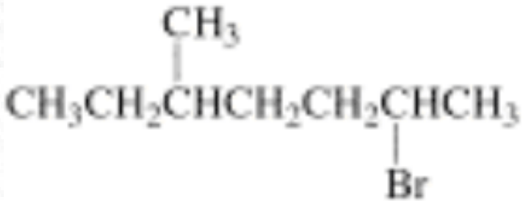
Nome comum – O nome do **primeiro grupo alquílico**, seguido do nome do **halogênio**, usando a terminação ”**eto**"



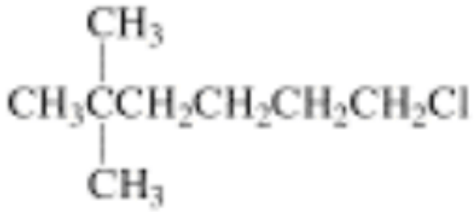


HALETOS DE ALQUILA
NOMENCLATURA

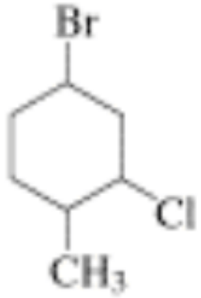
IUPAC - O halogênio é tratado como um substituinte



2-bromo-5-methylheptane

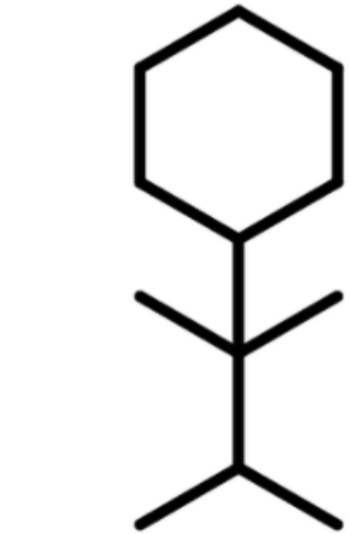


1-chloro-5,5-dimethylhexane

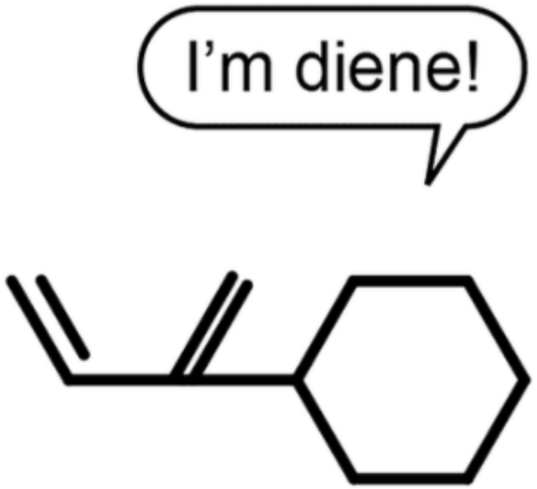


4-bromo-2-chloro-1-methylcyclohexane

DIZEM QUE...



Before Organic Exam



After Organic Exam

PROPRIEDADES FÍSICAS

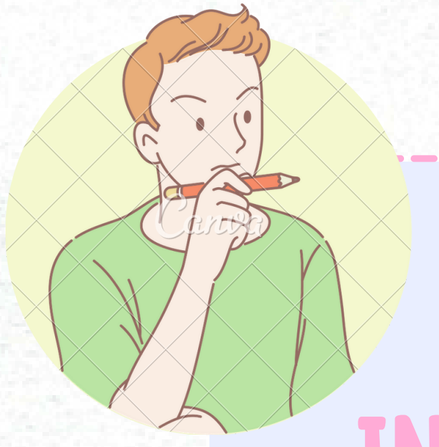
PROPRIEDADES FÍSICAS DE ALCANOS, HALETOS DE ALQUILA, ALCÓOIS, ÉTERES E AMINAS

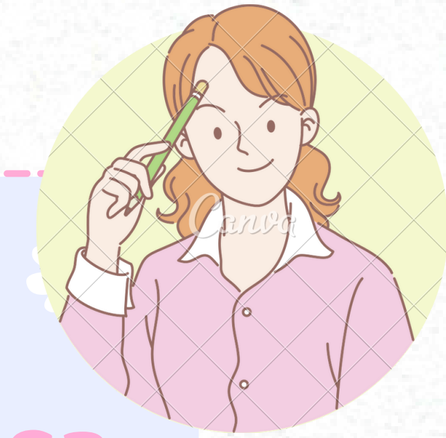
Ponto de ebulição (p.e.)

A **variação do p.e.** de uma substância para outra **está associada às forças que mantêm moléculas** individuais **unidas às outras**.

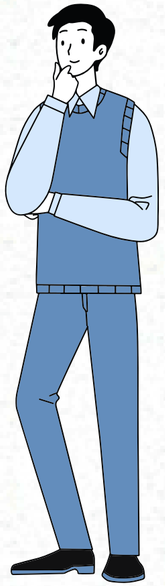
ASSIM SENDO.....

QUE FORÇAS SERIAM ESTAS?





QUAIS SÃO MESMO AS FORÇAS INTERMOLECULARES QUE CONHECEMOS?



COLOQUE-AS EM ORDEM CRESCENTE DE INTERAÇÃO/FORÇA

SAIBA QUE:

EM UMA SÉRIE HOMÓLOGA, OS VALORES DE PONTO DE EBULIÇÃO AUMENTA DE ACORDO COM O AUMENTO DO PESO MOLECULAR.

ÁREA DE CONTATO ENTRE MOLÉCULAS

CADEIAS LINEARES

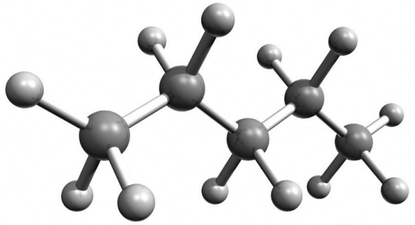
MAIOR SUPERFÍCIE DE CONTATO

MAIOR P.E

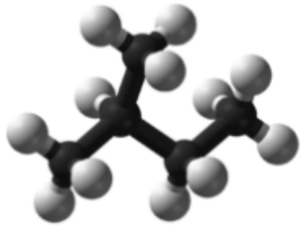
CADEIAS RAMIFICADAS

MENOR SUPERFÍCIE DE CONTATO

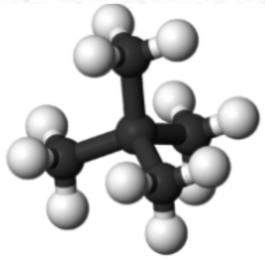
MENOR P.E



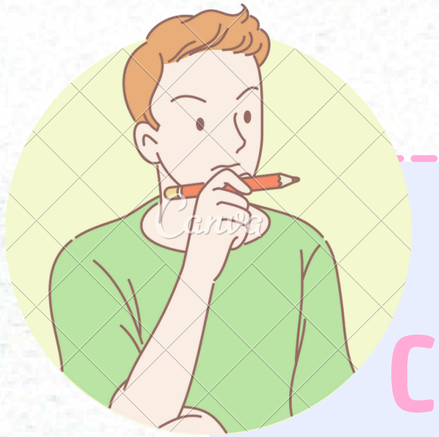
p.e.= 36.1C
pentano

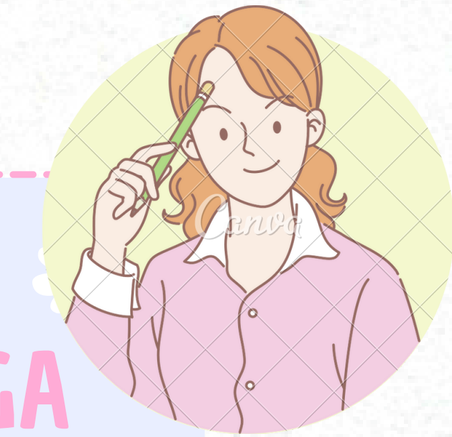


p.e.=27,9C
Isopentano

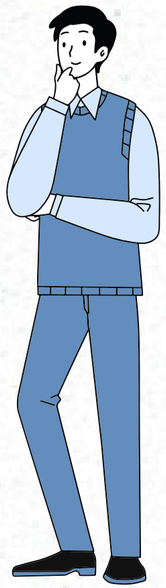


p.e.= 9,5C
neopentano

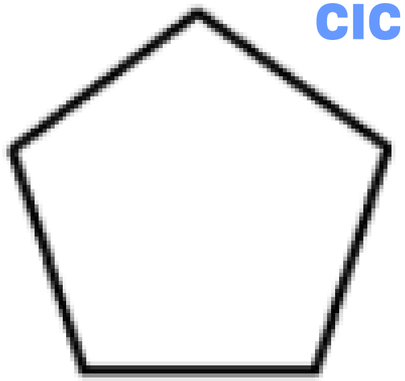


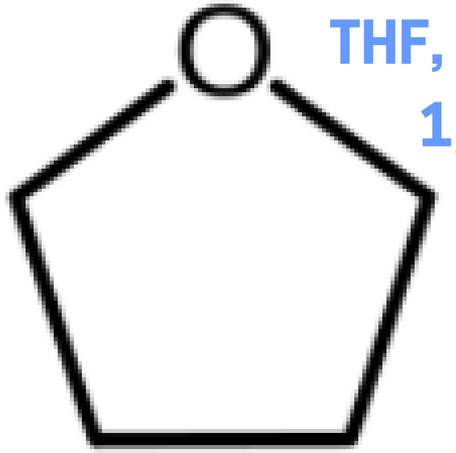


COMPARE OS COMPOSTOS ABAIXO E DIGA QUEM TERIA MAIOR P.E.



ciclopentano

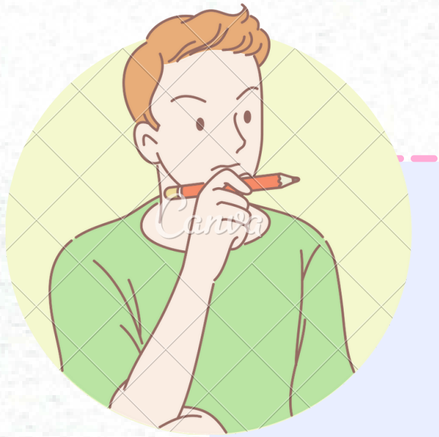


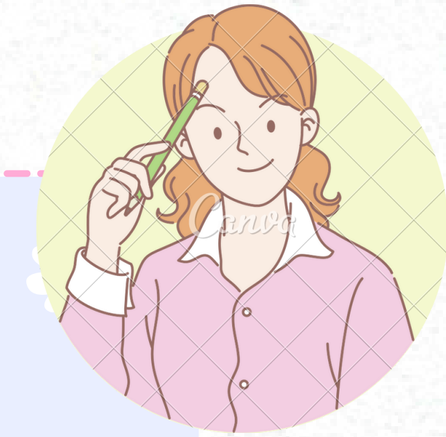


THF, tetraidrofurano ou 1,4-epóxibutano

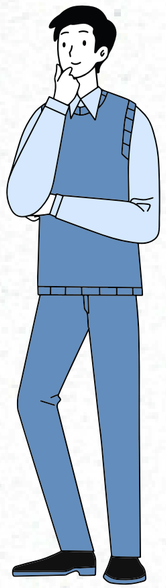
VALORES DE P.E. COMPARATIVOS

Ponto de ebulição (ºC)			
Alcanos	**Éteres**	**Aminas**	**Álcoois**
C_3H_8	H_3COCH_3	$H_3CCH_2NH_2$	H_3CCH_2OH
-42,1	-23,7	16,6	78,0
C_4H_{10}	$H_3COC_2H_5$	$H_3CCH_2CH_2NH_2$	$H_3CCH_2CH_2OH$
-0,5	10,8	47,8	97,4
C_5H_{12}	$H_5C_2OC_2H_5$	$H_9C_4NH_2$	H_9C_4OH
36,1	34,5	77,8	117,3



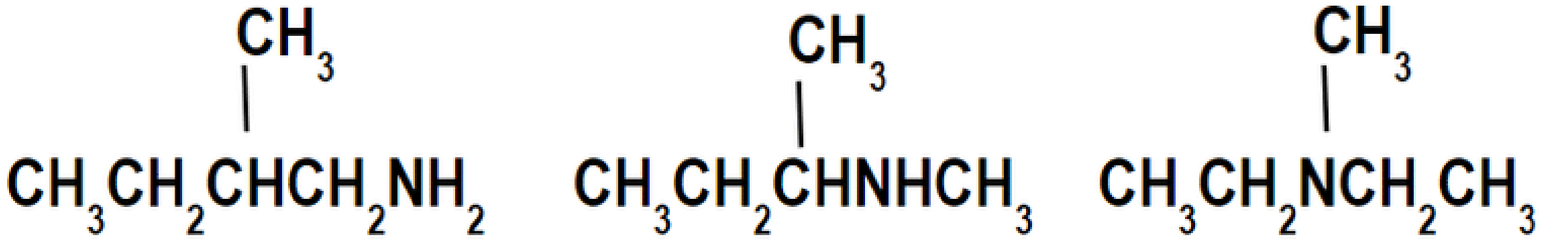


COMPARANDO OS VALORES DE P.E. ENTRE AMINAS

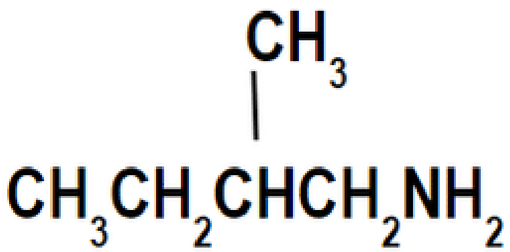


QUE TIPO DE AMINAS TEMOS NESTAS MOLÉCULAS?

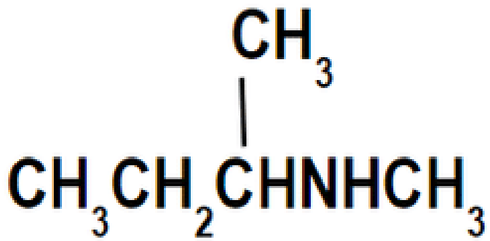
O QUE VOCÊ ACHA QUE DEVE ACONTECER COM O P.E. DA AMINA TERCIÁRIA?



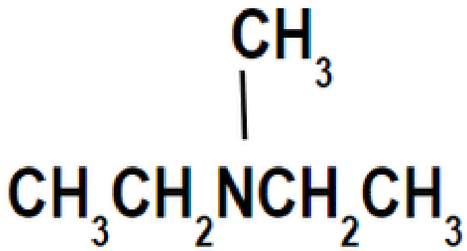
RESPOSTA



amina primária
p.e= 97 C



amina secundária
p.e= 84 C



amina terciária
p.e= 65 C

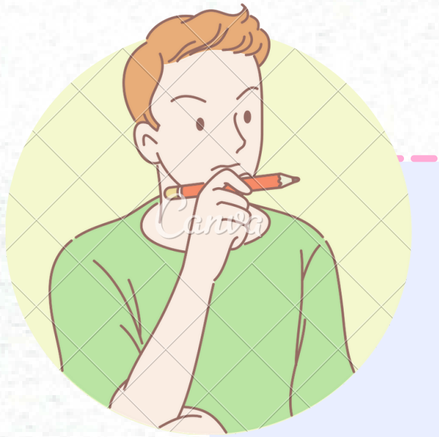
SOLUBILIDADE

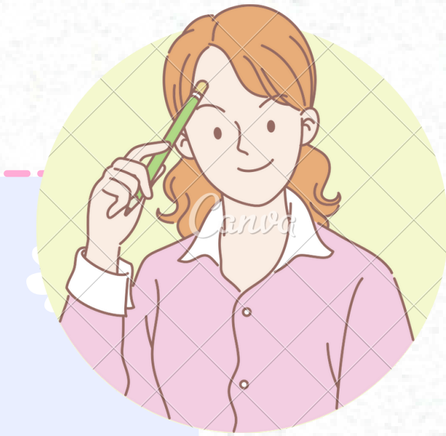
- **Regra geral:** é por **polaridade** das moléculas
- **Frase** : ***"SIMILAR DISSOLVE SIMILAR"***
- Quanto **maior a cadeia carbônica**, **maior seu caráter apolar!**

2C	CH_3OCH_3	Solúvel
3C	$CH_3OCH_2CH_3$	Solúvel
4C	$CH_3CH_2OCH_2CH_3$	Ligeiramente solúvel (10g/100g de H2O)
5C	$CH_3CH_2OCH_2CH_2CH_3$	Pouco solúvel (1,0g/100g de H2O)
6C	$CH_3CH_2OCH_2CH_2CH_2CH_3$	Insolúvel

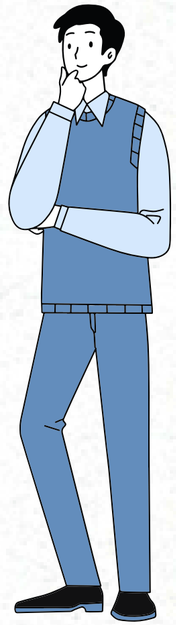
LINK

http://coral.ufsm.br/quimica_organica/images/nomenclat_IUPAC.pdf





EXERCÍCIOS

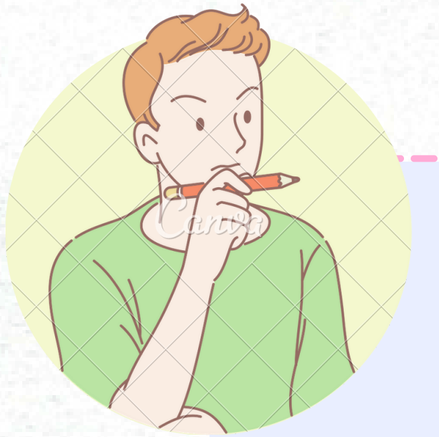


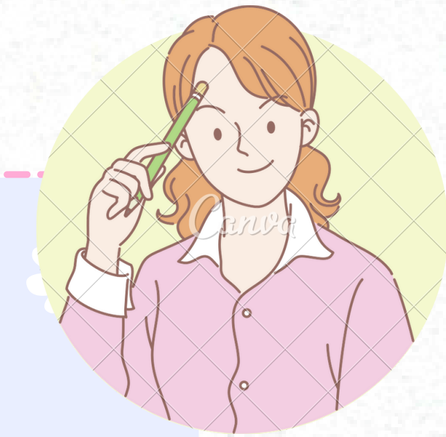
COLOCAR EM ORDEM CRESCENTE DE SOLUBILIDADE EM ÁGUA

$CH_3CH_2CH_2OH$

$CH_3CH_2CH_2CH_2OH$

$CH_3CH_2CH_2CH_2CH_3$



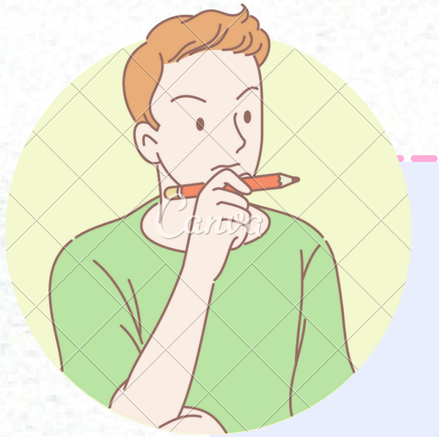


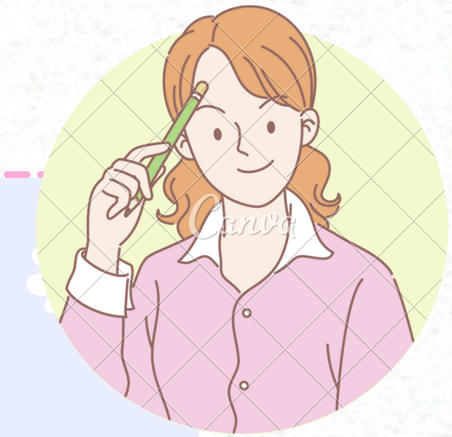
EM QUAIS DOS SOLVENTES ABAIXO, O CICLOPENTANO TERIA MENOR SOLUBILIDADE?

1-PENTANOL

ÉTER DIETÍLICO

HEXANO



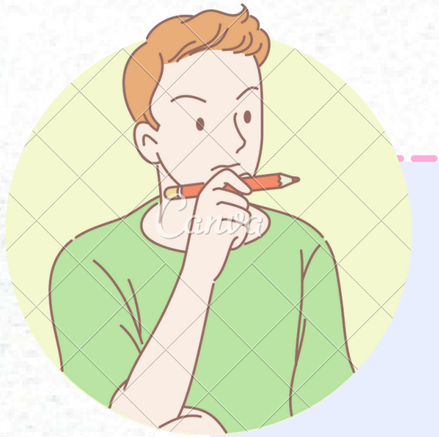


QUEM SÃO ELES?

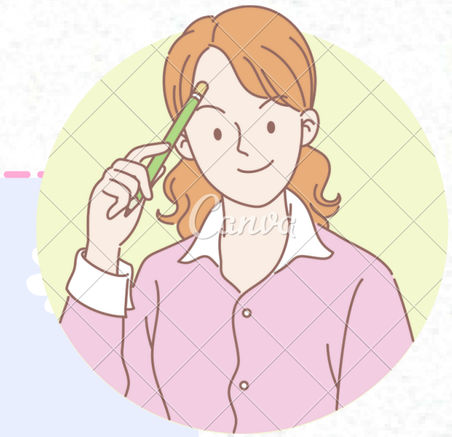
2-METILHEX-2-ENO

CICLOPENTENO

CIS-HEPT-3-ENO

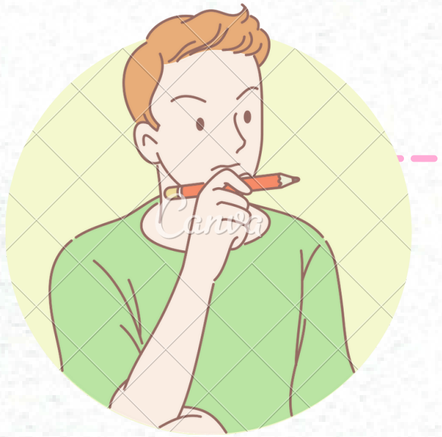


EXERCÍCIOS



1 **REPRESENTE A ESTRUTURA DO COMPOSTO ABAIXO:**

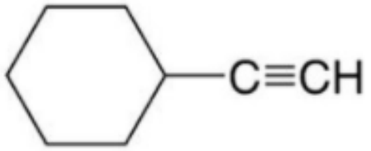
(2E)-5-METILHEX-2-ENO



2

DÊ O NOME DOS COMPOSTOS ABAIXO:

(a)



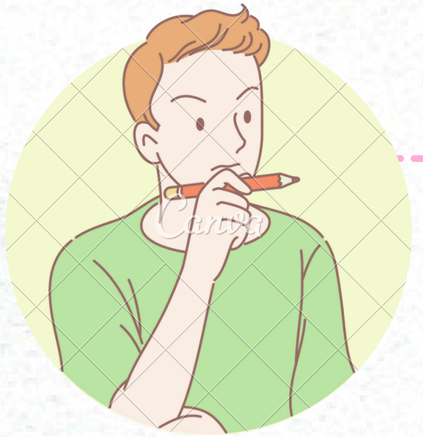
(b)

$CH_3CH_2-C\equiv C-C\equiv CH$

(c)

$HC\equiv C-CH_2CH=C(CH_3)_2$

(d)



3 DÊ O NOME DAS AMINAS ABAIXO:

A) $CH_3—CH_2—CH_2—NH_2$

B) $CH_3—CH_2—N(CH_3)—CH_3$

4 DÊ A ESTRUTURA DOS COMPOSTOS ABAIXO

A) 2-PENTANAMINA

B) N-METIL-1-BUTANAMINA