

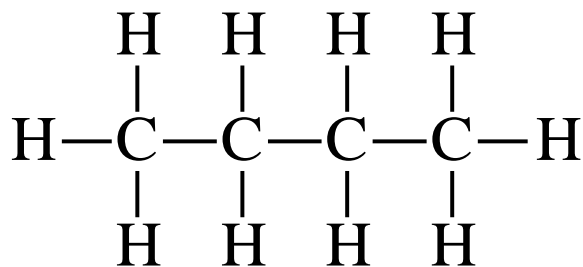


COMPOSTOS ORGÂNICOS: ALCANOS E CICLOALCANOS Nomenclatura

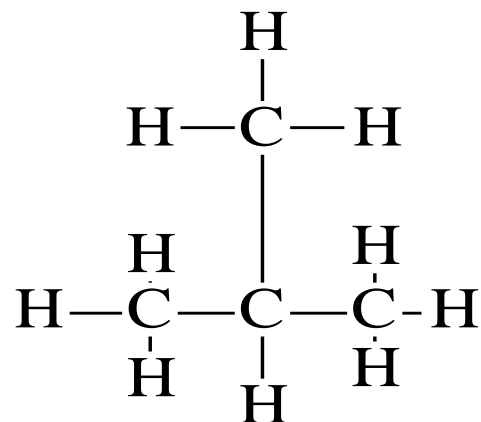
Prof. Gustavo Pozza Silveira
gustavo.silveira@iq.ufrgs.br

NOMENCLATURA E GRUPO FUNCIONAL: ALCANOS

- Todas as ligações C-C são saturadas (símples)
- Fórmula geral: C_nH_{2n+2}
- Alcanos podem apresentar ramificação



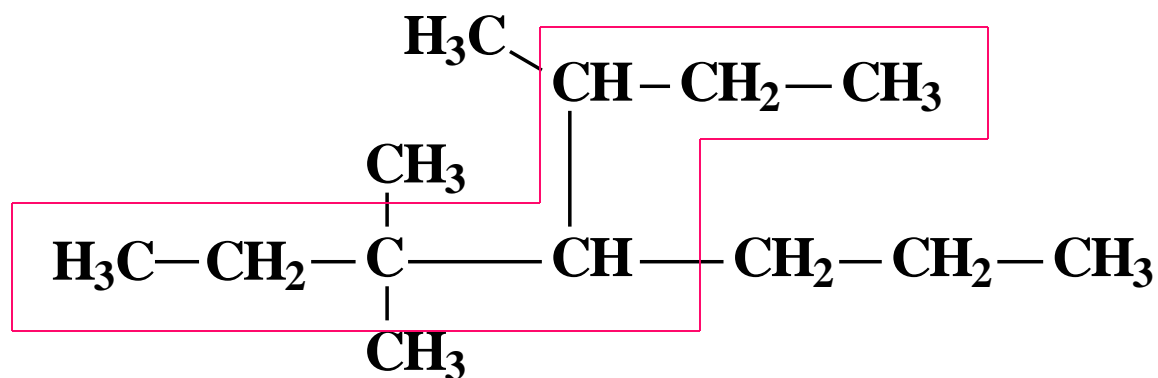
Butane, C_4H_{10}



Isobutane, C_4H_{10}

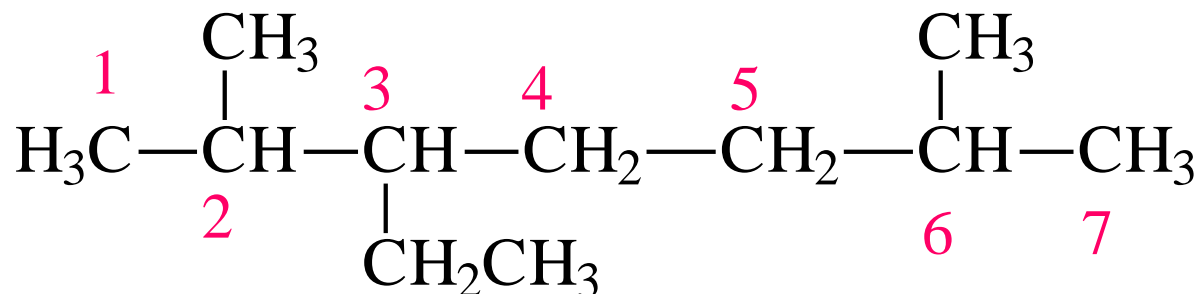
NOMENCLATURA ALCANOS: CADEIA PRINCIPAL

- Ache a cadeia com o maior número de átomos de carbono.
- Se houver duas possibilidades de cadeia principal com o mesmo número de átomos de carbono, escolha a que conter o maior número de ramificações.



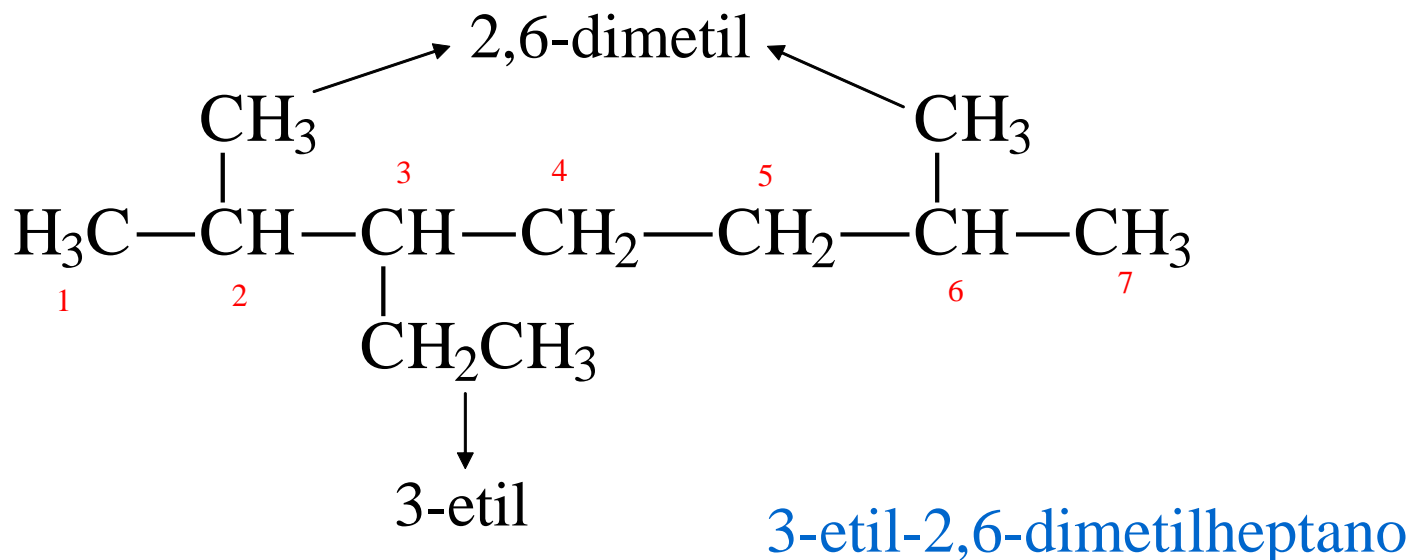
NOMENCLATURA ALCANOS: NUMERAÇÃO

- Comece a numeração o mais próximo da primeira ramificação.
- Se os dois primeiros substituintes estão equidistantes, procure pela próxima ramificação.



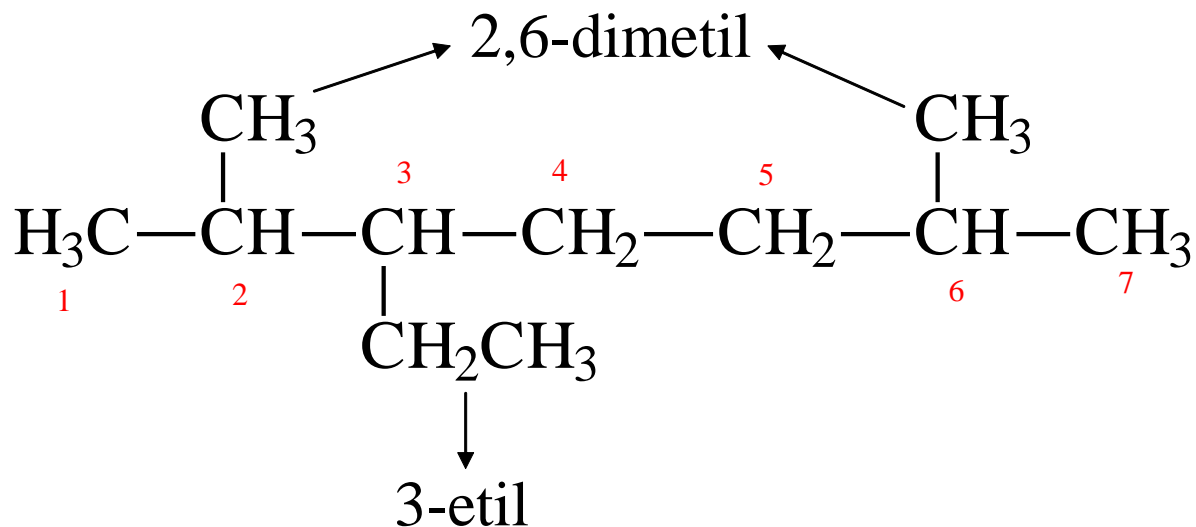
NOMENCLATURA ALCANOS: NOME IUPAC

- Coloque de ordem alfabética os substituintes.
- Não considere os indicadores de quantidade (di, tri, etc).



NOMENCLATURA ALCANOS: NOME IUPAC

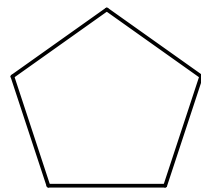
- Escreva o prefixo do nº de átomos de carbono da cadeia principal + terminação ano.



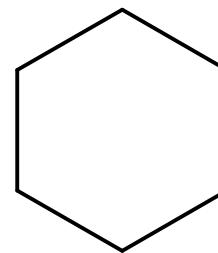
3-etil-2,6-dimetilheptano

NOMENCLATURA ALCANOS: CICLOALCANOS

- Verifica-se o número de carbonos que formam o ciclo (este dará o nome do composto)



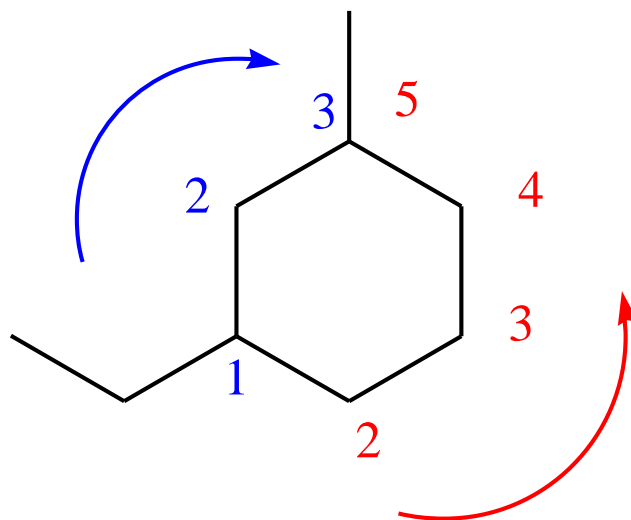
Ciclopentano



Ciclohexano

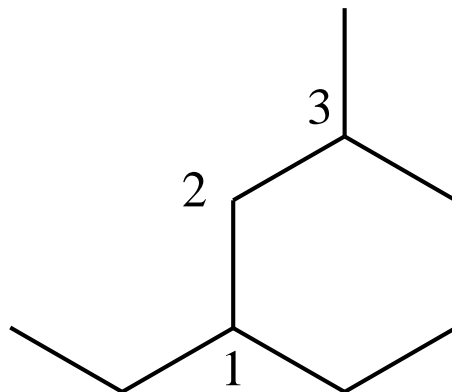
NOMENCLATURA ALCANOS: CICLOALCANOS

- Numera-se os substituintes de modo a obterem a menor numeração possível e por prioridade alfabética



NOMENCLATURA ALCANOS: CICLOALCANOS

- Nomeia-se os substituintes em ordem alfabética usando numeração
- Escreva ciclo + prefixo n^o átomos de C da cadeia principal + ano.

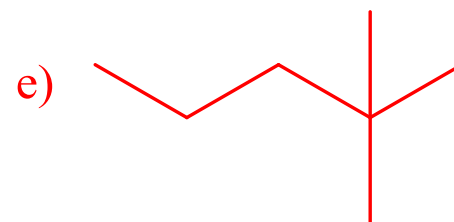
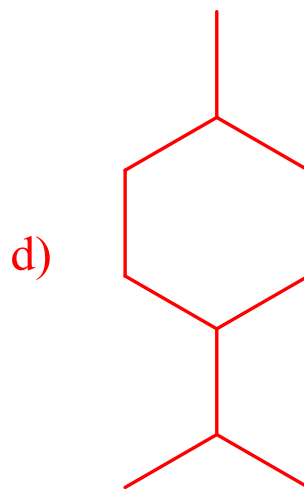
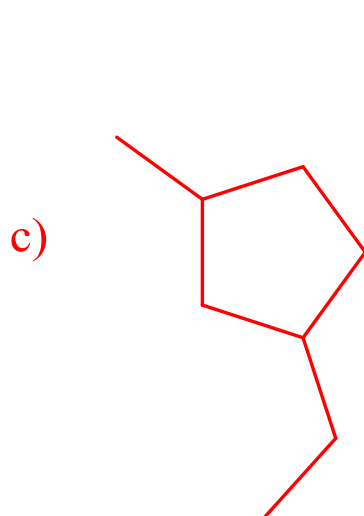
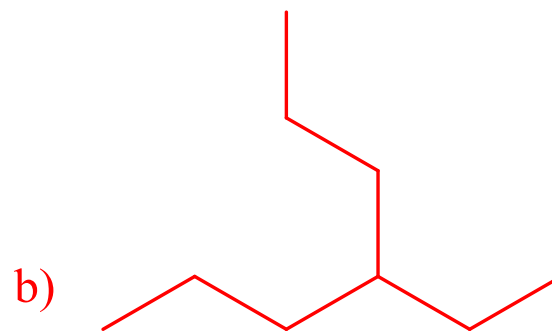
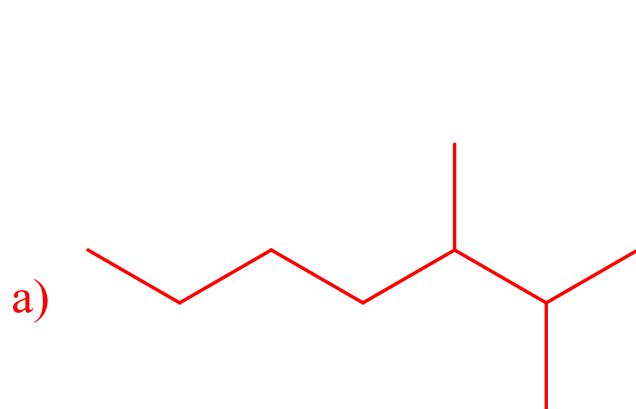


1-etil-3-metil-ciclohexano

NOMENCLATURA ALCANOS: RESUMO

- Encontre a mais longa cadeia de carbono contínua
- Numere os carbonos começando o mais próximo possível da primeira ramificação
- Nomeie os grupos ligados aos átomos de carbono, usando a numeração como indicador de posição
- Ordene os substituintes em ordem alfabética
- Use di-, tri-, etc., para mais de 1 do mesmo substituinte

Exercícios: Dê a nomenclatura IUPAC para os seguintes hidrocarbonetos

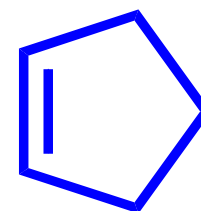
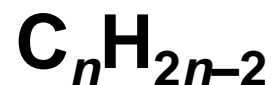


Fórmula Molecular dos Alcenos

Alcenos Acíclicos:



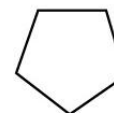
Alcenos Cíclicos:



an alkane



an alkene



a cyclic alkane



a cyclic alkene

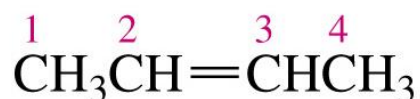


Nomenclatura Sistemática de Alcenos

- A cadeia mais longa de carbonos deve conter o grupo funcional (ligação dupla).



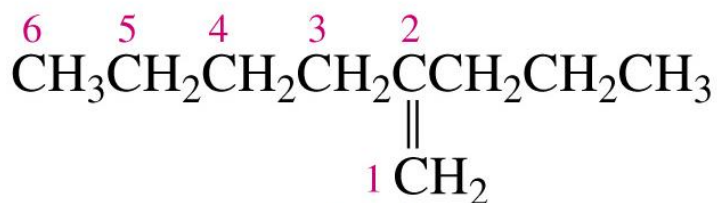
1-butene



2-butene



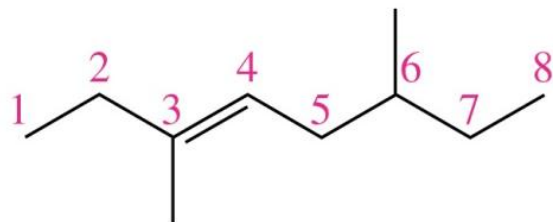
2-hexene



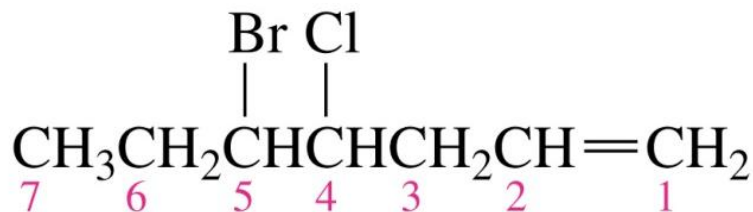
2-propyl-1-hexene

the longest continuous chain has eight carbons but the longest continuous chain containing the functional group has six carbons, so the parent name of the compound is hexene

Citar os substituintes em ordem alfabética

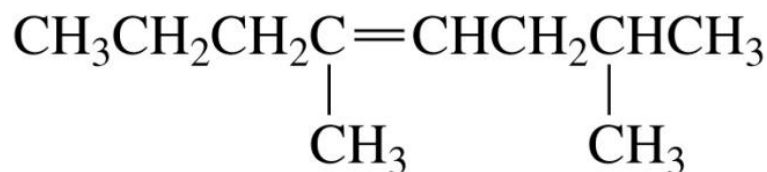


3,6-dimethyl-3-octene



5-bromo-4-chloro-1-heptene

Numere os grupos presentes com os menores números possíveis

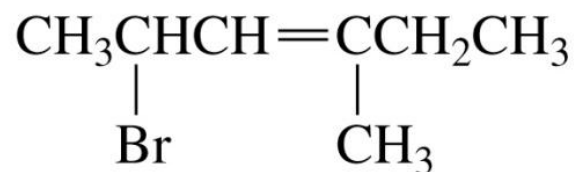


2,5-dimethyl-4-octene

not

4,7-dimethyl-4-octene

because 2 < 4



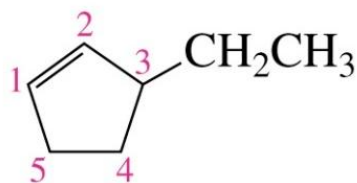
2-bromo-4-methyl-3-hexene

not

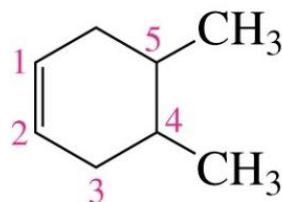
5-bromo-3-methyl-3-hexene

because 2 < 3

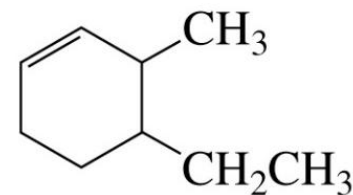
Não há necessidade de numerar o grupo funcional em um alceno cíclico



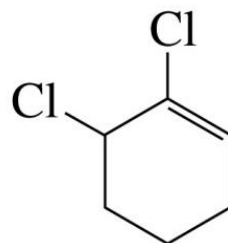
3-ethylcyclopentene



4,5-dimethylcyclohexene



4-ethyl-3-methylcyclohexene



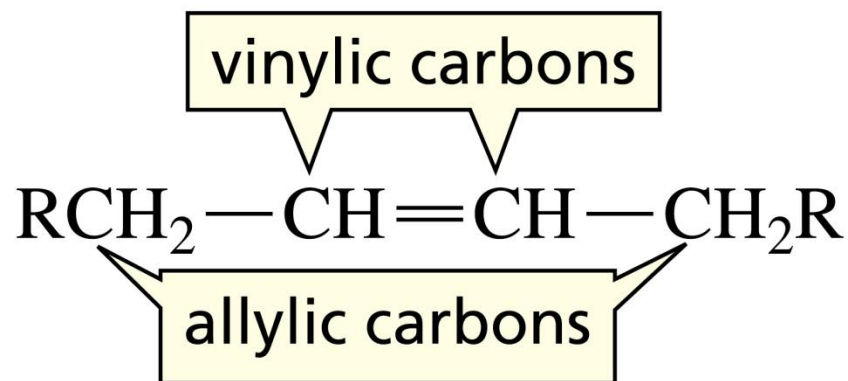
1,6-dichlorocyclohexene

not

2,3-dichlorocyclohexene

because $1 < 2$

Nomenclatura Especial



$\text{H}_2\text{C}=\text{CH}-$
the vinyl group

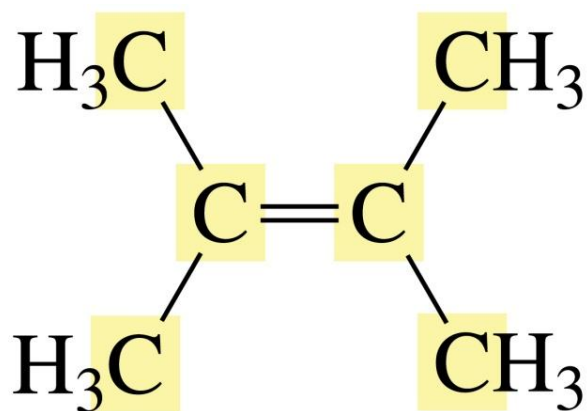
$\text{H}_2\text{C}=\text{CHCH}_2-$
the allyl group

systematic name:
common name:

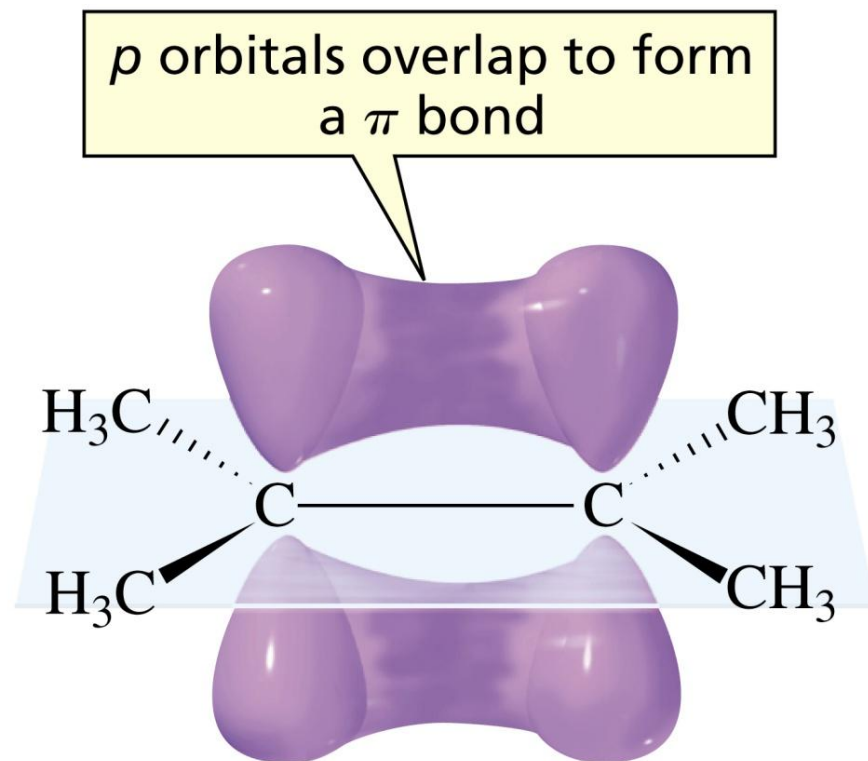
$\text{H}_2\text{C}=\text{CHCl}$
chloroethene
vinyl chloride

$\text{H}_2\text{C}=\text{CHCH}_2\text{Br}$
3-bromopropene
allyl bromide

Estrutura de Alcenos

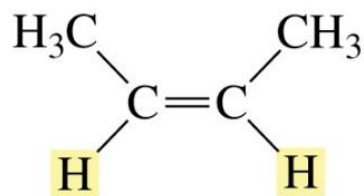
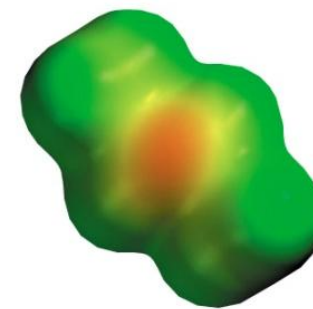
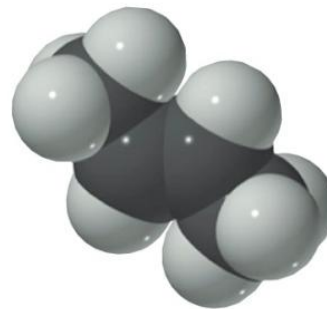
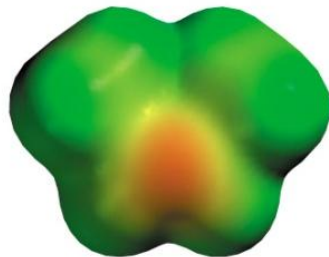
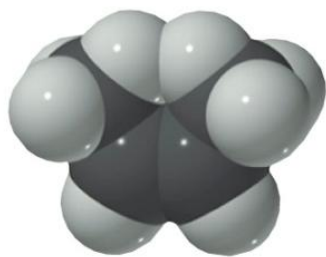
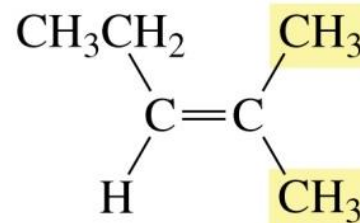
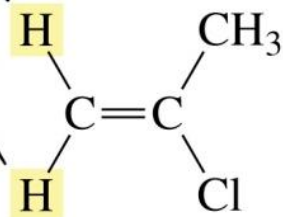


**the six carbon atoms
are in the same plane**

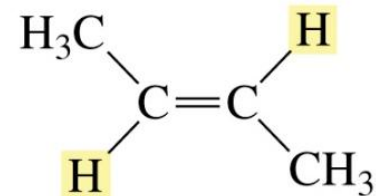


Isômeros de Alcenos

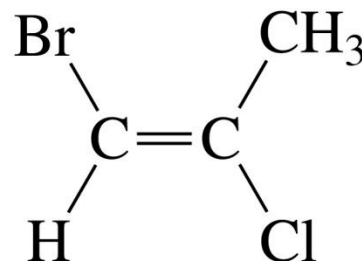
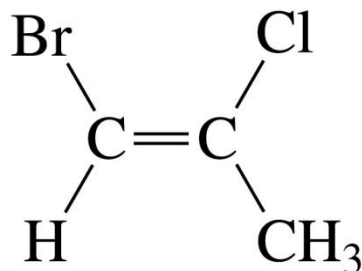
cis and trans isomers are not possible for these compounds because two substituents on an sp^2 carbon are the same



cis-2-butene

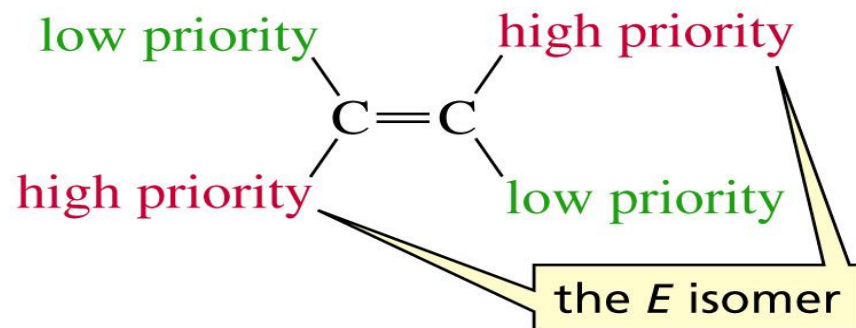
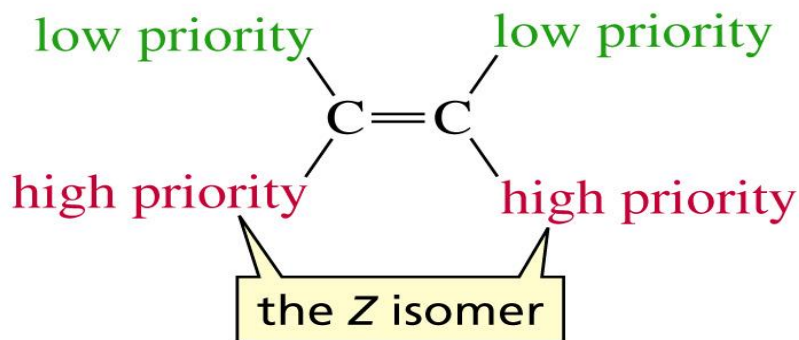


trans-2-butene



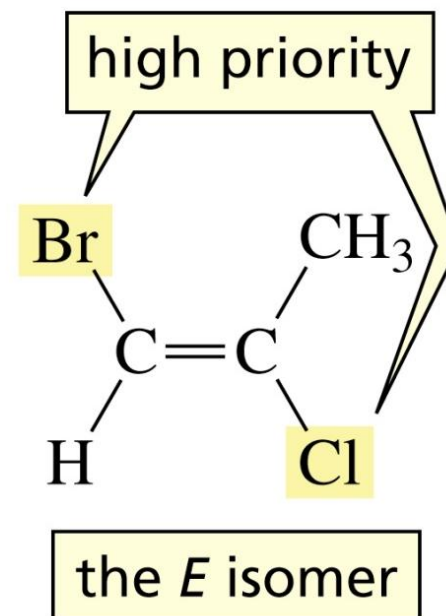
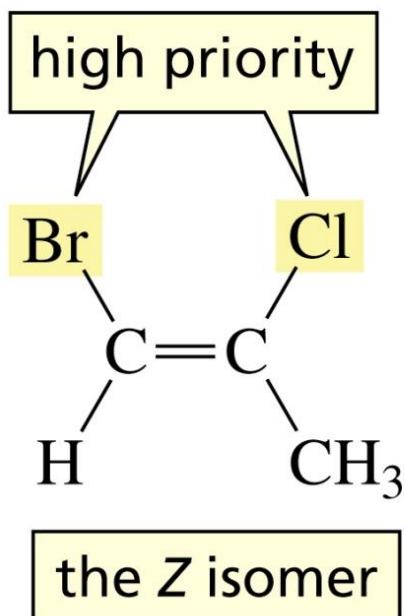
Which isomer is cis and which is trans?

Isômeros *E* e *Z*

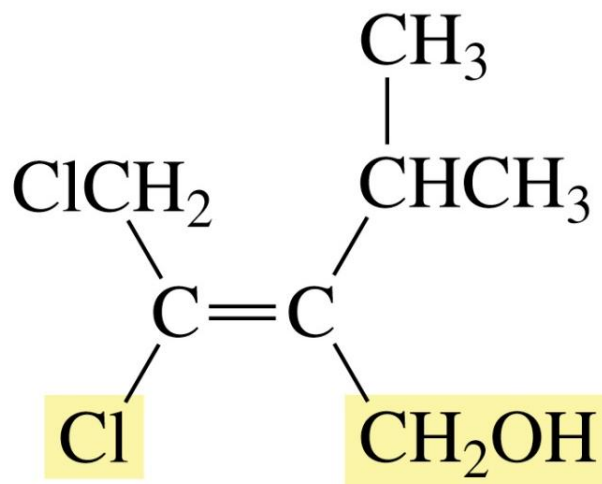


Nomeando pelo Sistema *E,Z*

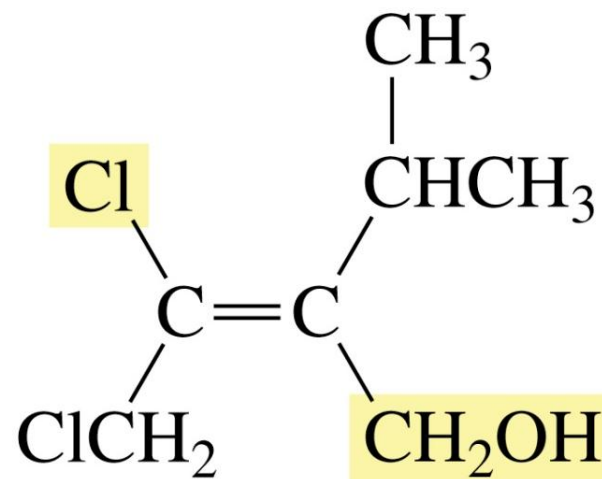
Regra 1: Considere o número atômico do átomo ligado diretamente ao carbono sp^2 . Maior número atômico, maior a prioridade.



Regra 2: Se houver ramificações, considere os átomos ligados e veja qual possui maior número atômico.



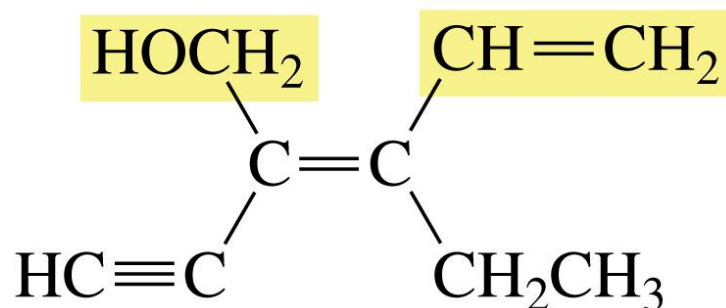
the Z isomer



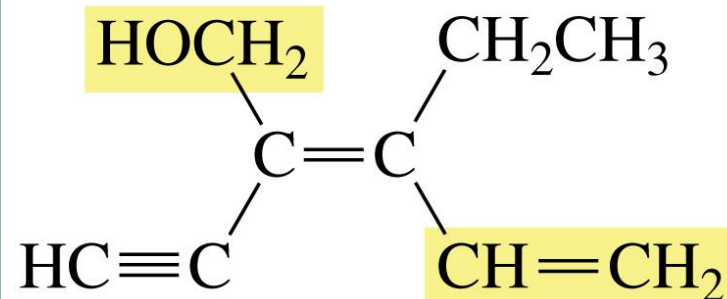
the E isomer

...não podemos somar os números atômicos; devemos apenas usar o átomo que possuir maior número atômico...

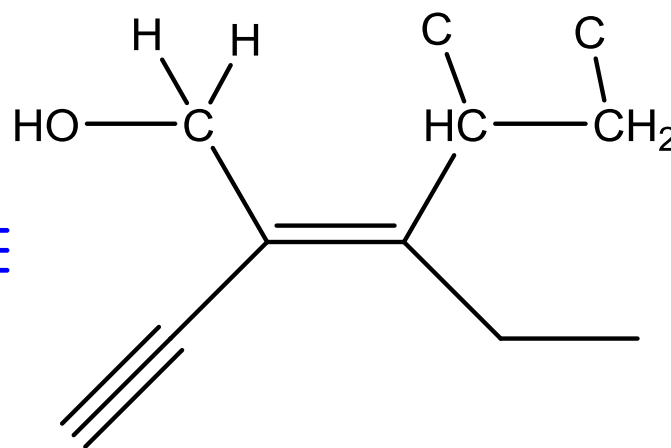
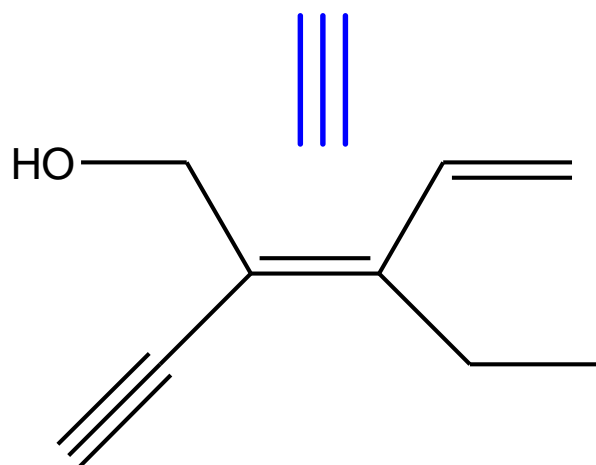
Regra 3: Se um átomo está ligado duplamente com outro átomo, o sistema de prioridades trata como se estivesse usando ligações simples a dois daqueles átomos. Se um átomo está ligado triplamente com outro átomo, o sistema de prioridades trata como se estivesse usando ligações simples a três daqueles átomos



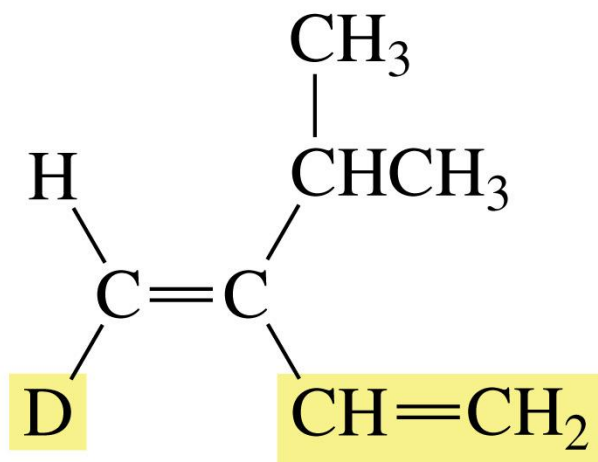
the *Z* isomer



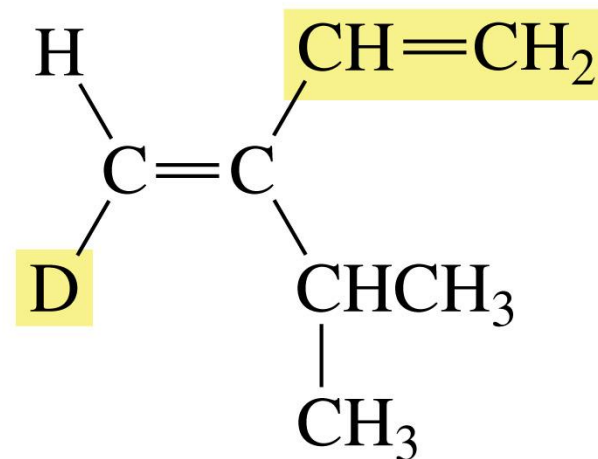
the *E* isomer



Regra 4: O isótopo de maior massa tem prioridade.



the Z isomer



the E isomer

Outras regras de Nomenclatura

Quando os grupos funcionais são uma ligação dupla e uma ligação tripla, a cadeia é numerada de modo a fornecer o menor número possível ao nome da substância, independente de qual grupamento funcional adquire o menor número.



5-hepten-1-yne

not 2-hepten-6-yne

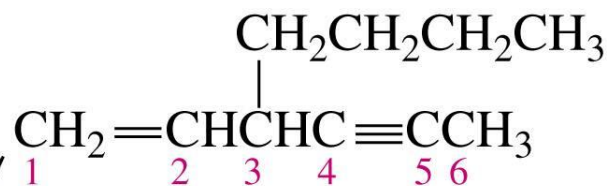
because $1 < 2$



1-hepten-5-yne

not 6-hepten-2-yne

because $1 < 2$



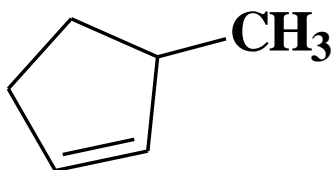
3-butyl-1-hexen-4-yne

the longest continuous chain has eight carbons, but the 8-carbon chain does not contain both functional groups; therefore, the compound is named as a hexenyne because the longest continuous chain containing both functional groups has six carbons

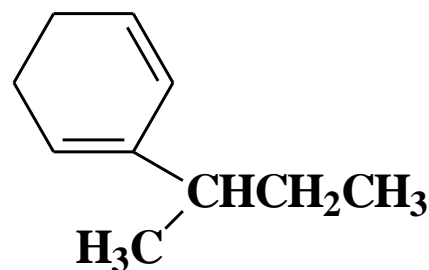
Se ocorrer empate entre uma ligação dupla e uma ligação tripla, a ligação dupla adquire o menor número.

NOMENCLATURA ALCENOS: CICLOALCENOS

No caso de alcenos cíclicos, utiliza-se a numeração 1 e 2 correspondente aos carbonos da ligação dupla levando em consideração a proximidade dos substituintes seguintes.



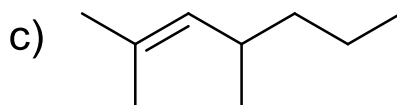
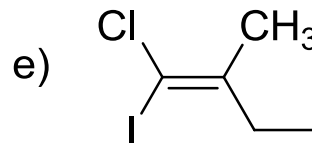
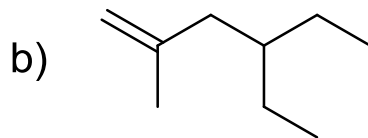
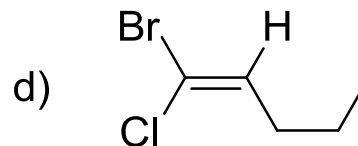
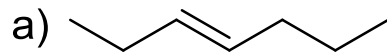
3-metilciclopenteno



2-sec-butil-1,3-ciclohexadieno

Exercícios:

1. Dê o nome IUPAC para os seguintes alcenos:



2. Escreva a fórmula estrutural (cavalete) para:

a) 3,4-dimetilciclopenteno

c) trans-2-hexeno

b) cis-3-octeno

d) vinilciclopentano

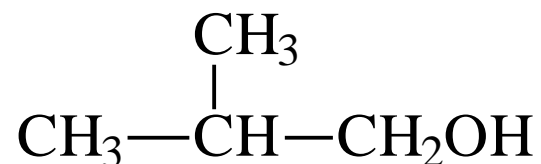
e) 1,2-diclorociclohexeno

Compostos Orgânicos Oxigenados: Nomenclatura

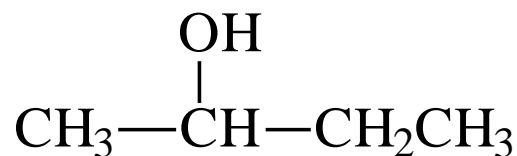
**•Álcoois, Éteres, Epóxidos e
Compostos Análogos de Enxofre**

NOMENCLATURA ÁLCOOIS: CLASSIFICAÇÃO

- Primário: carbono com -OH é ligado a um carbono

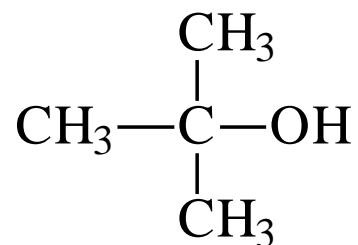


- Secundário: carbono com -OH é ligado a dois carbonos

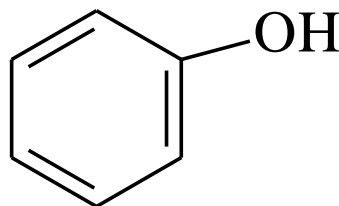


NOMENCLATURA ÁLCOOIS: CLASSIFICAÇÃO

- Terciário: carbono com –OH é ligado a três carbonos.

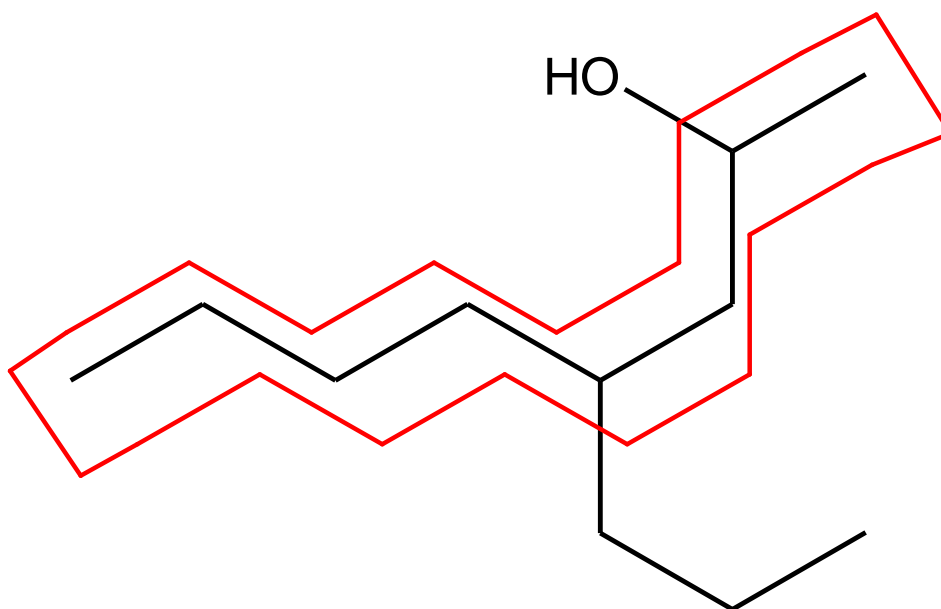


- Aromático (fenol): –OH é ligado a um grupo arila.



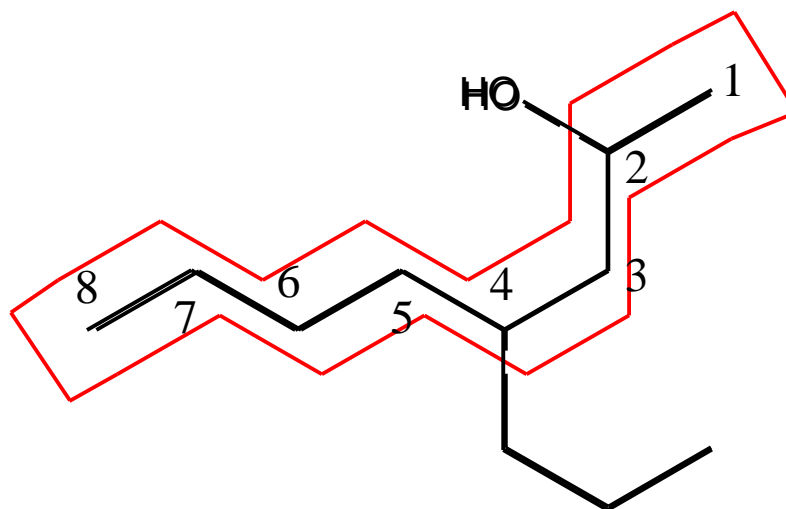
NOMENCLATURA ÁLCOOIS: CADEIA PRINCIPAL

- Encontre a mais longa cadeia de carbono cont nua que contenha o grupo -OH .



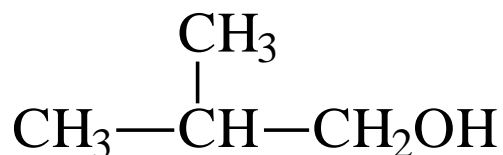
NOMENCLATURA ÁLCOOIS: NUMERAÇÃO

- Numere os carbonos começando o mais próximo possível da função $-OH$

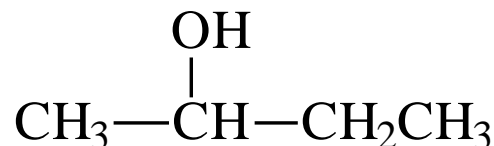


NOMENCLATURA ÁLCOOIS: NOME DO COMPOSTO

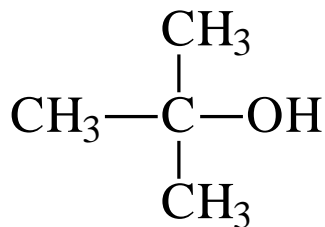
Exercício: dê o nome para os seguintes álcoois:



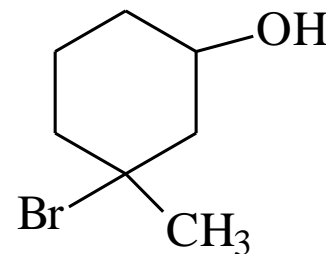
2-metil-1-propanol



2-butanol



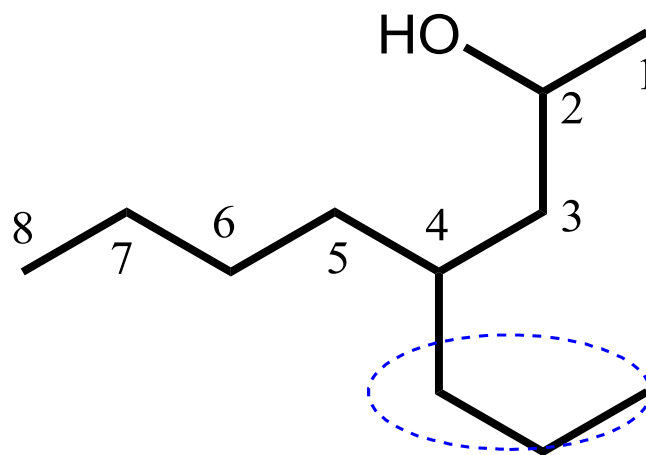
2-metil-2-propanol



3-bromo-3-metil-ciclohexanol

NOMENCLATURA ÁLCOOIS: NOME DO COMPOSTO

- Nomeie os grupos ligados a cadeia principal em ordem alfabética e usando a numeração como indicador de posição. Troque a terminação o do HC correspondente por *ol*.



4-propil-2-octanol

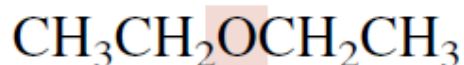
NOMENCLATURA ÁLCOOIS INSATURADOS: NOME DO COMPOSTO

- Grupo hidroxila tem prioridade. Numere a cadeia mais próxima da hidroxila.
- Use o nome do HC correspondente (alceno ou do alcino).



4-penten-2-ol

ÉTERES



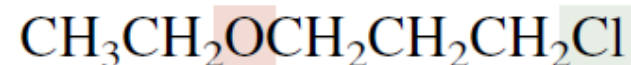
Ethoxyethane
Diethyl ether

IUPAC



Methoxyethane
Ethyl methyl ether

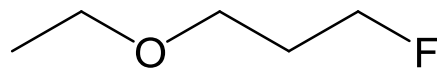
IUPAC



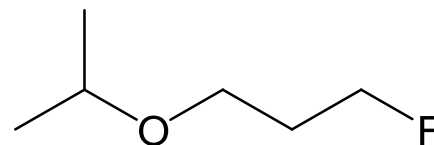
1-Chloro-3-ethoxypropane
3-Chloropropyl ethyl ether

IUPAC: menor cadeia carbônica ligada ao oxigênio = alquilóxi.

Maior cadeia = aquilano. Prioridade na numeração depende da ordem alfabética.



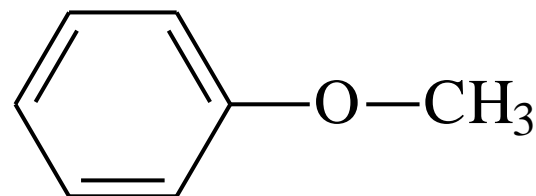
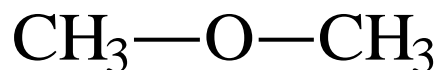
1-ethoxy-3-fluoropropane



1-fluoro-3-isopropoxypropane

NOMENCLATURA E GRUPO FUNCIONAL: ÉTERES

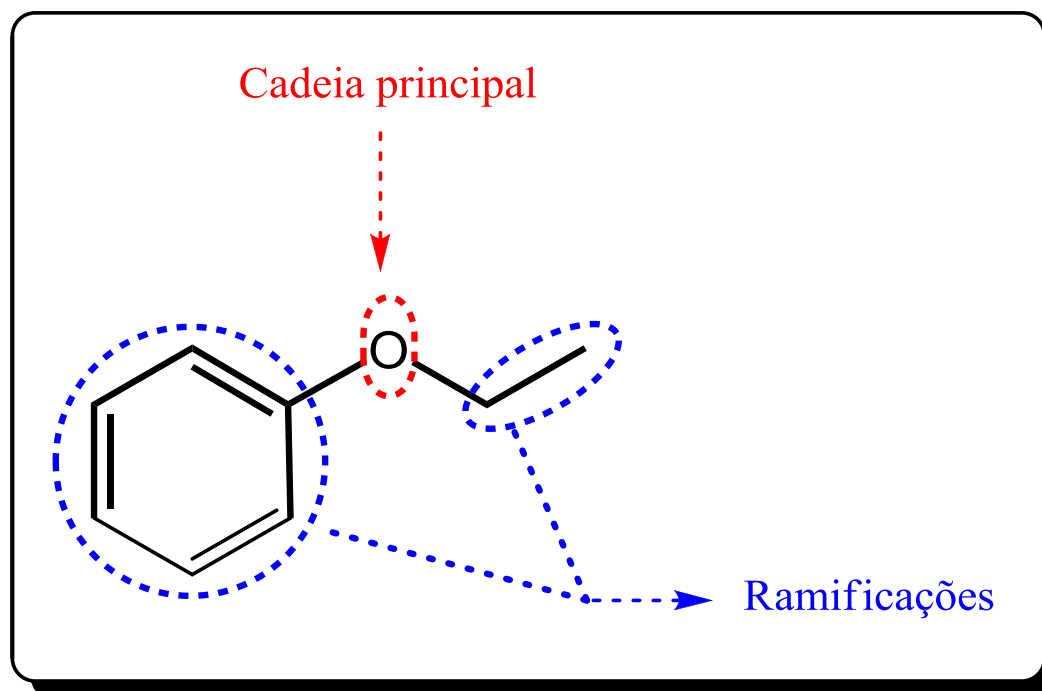
- Fórmula R-O-R onde R é alquila ou arila.
- Simétrico ou não-simétrico
- Exemplos:



anisol

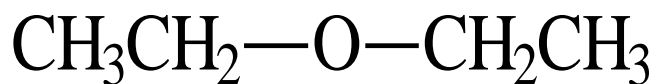
NOMENCLATURA ÉTERES: CADEIA PRINCIPAL

- Apresenta um átomo central (O)
- Grupos ligados ao “O” são as ramificações

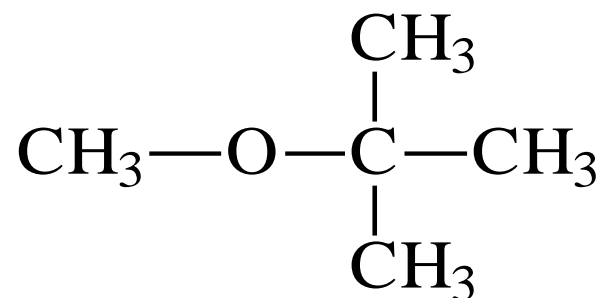


NOMENCLATURA ÉTERES: NOME DO COMPOSTO - RESUMO

- Alquil-alquil éter ou éter alquil-alquílico (usual)
- Ordene o nome por ordem alfabética
- Simétricos: use dialquil ou somente alquil éter.
- Nomenclatura sistemática (IUPAC): cadeia menor + óxi + alcano.



dietil éter ou
Éter dietílico
Etóxi-etano (IUPAC)

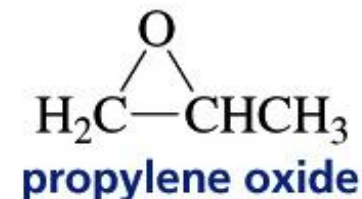
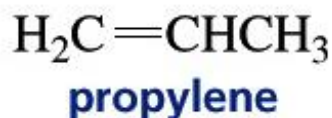
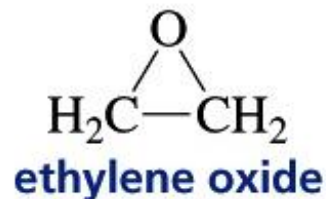
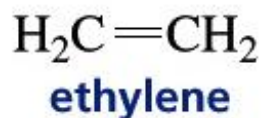


Metil *t*-butil éter ou
Éter metil-*t*-butílico
Metóxi-2-metil-propano (IUPAC)

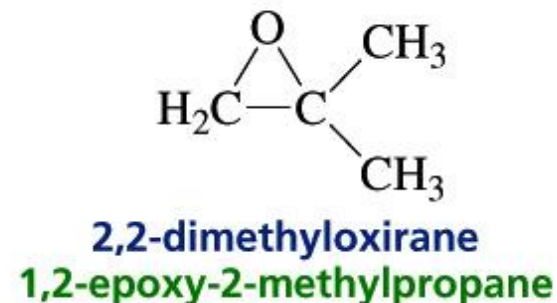
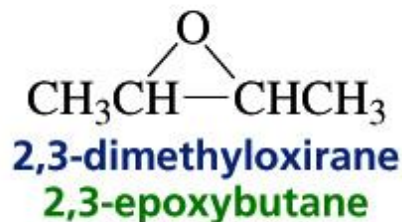
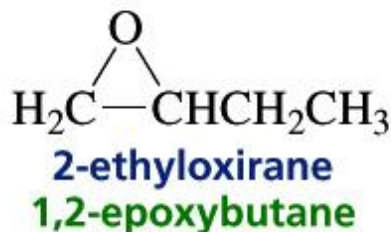
EPÓXIDOS

Epóxidos

Usual



Oxirano - IUPAC



Oxigênio leva a numeração 1

Tiois (RSH)

Odor forte característico. Ex. Cebola – 1-propanotiol.

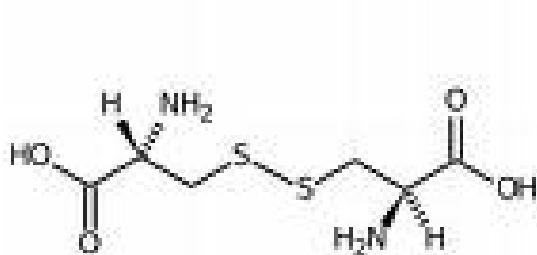


1-propanotiol

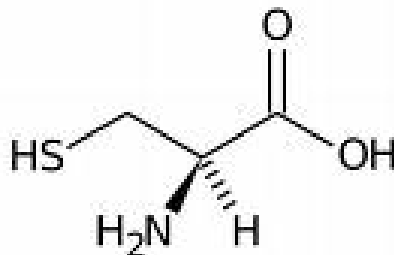
Cheiro de alho = tióis

Odor do gambá = tióis

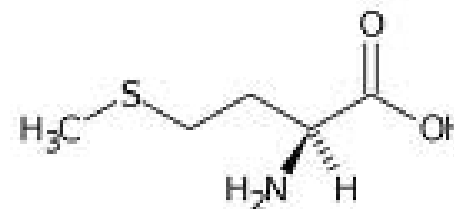
Compostos de enxofre: Tióis e Sulfetos



Cistina
(dissulfeto)

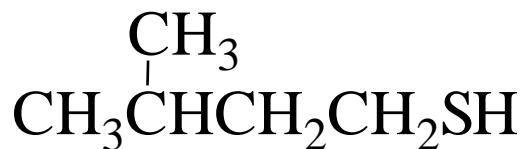


Cisteína
(tiol)



Metionina
(sulfeto)

Nomenclatura (Tiol)



3-metil-1-butanotiol

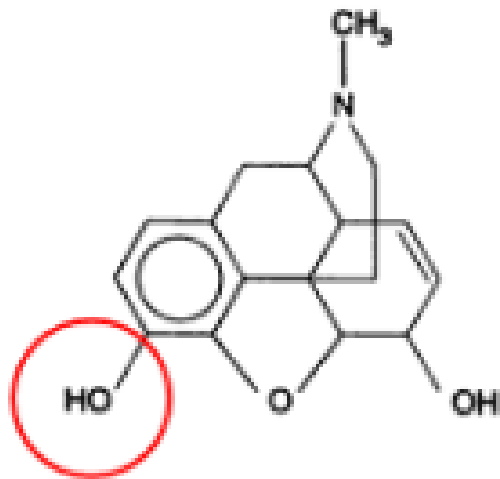


1-propanotiol

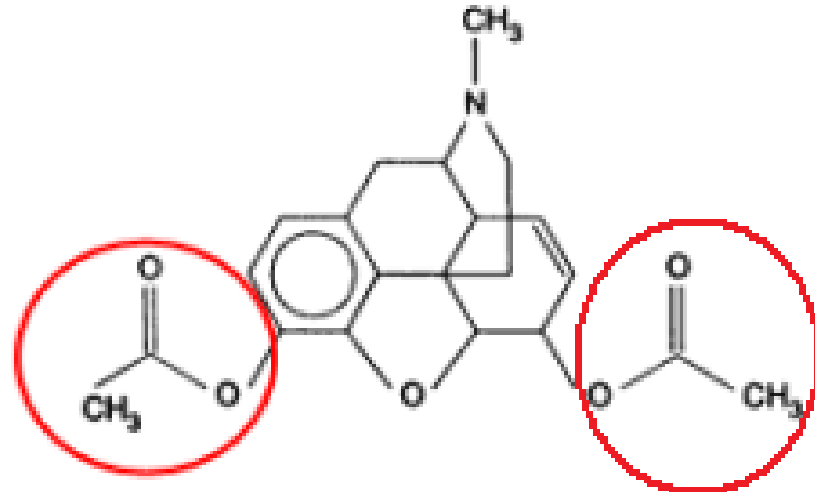


2-mercaptoetanol

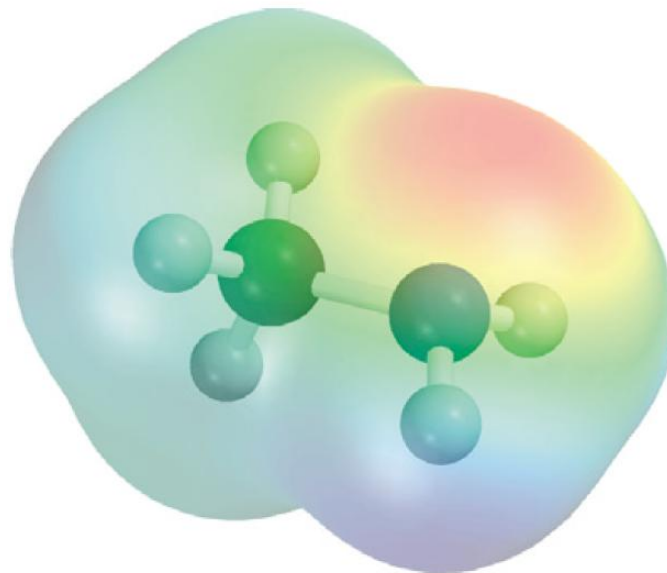
AMINAS



Morfina



Heroína

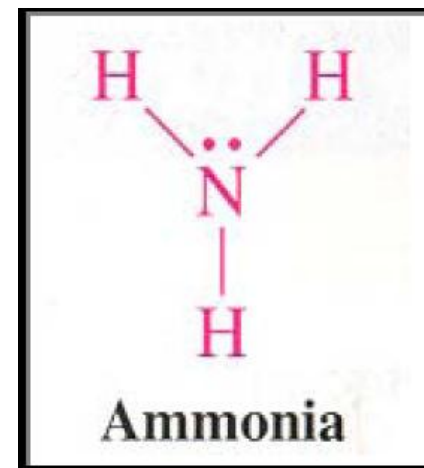


Aminas – podem ser consideradas derivadas da amônia

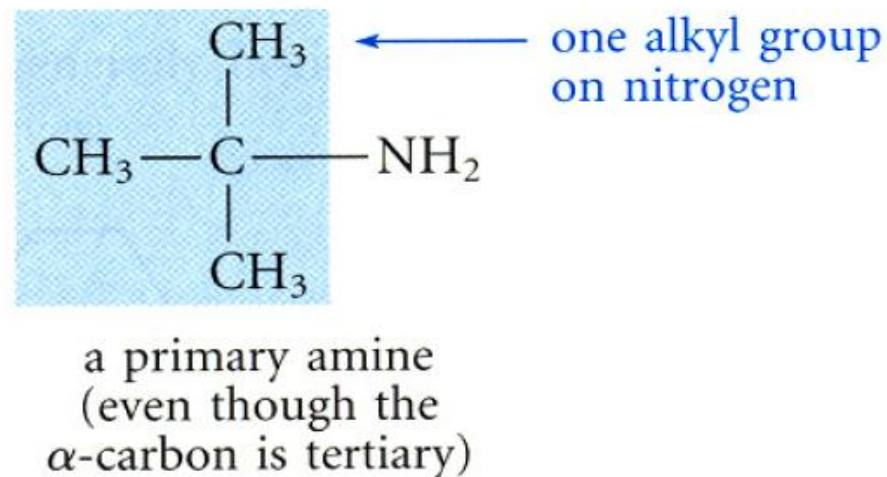
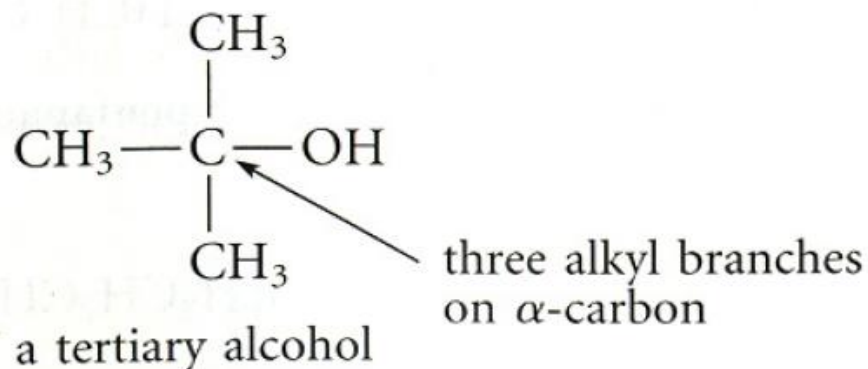
Nomenclatura

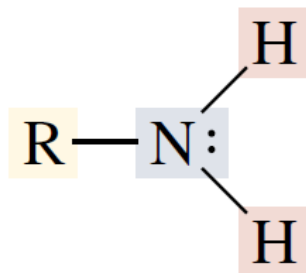
Nomenclatura Comum: Alquilamina.

Nomenclatura IUPAC: sufixo –amina.

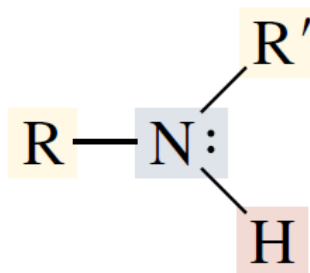


- Aminas podem ser primárias, secundárias e terciárias, de maneira análoga às amidas. Esta classificação é feita de maneira diferente do que com álcoois, haletos, etc. Exemplo:

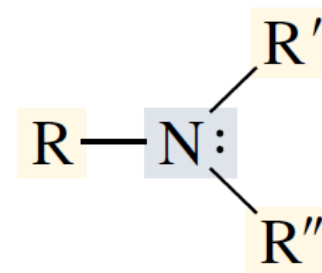




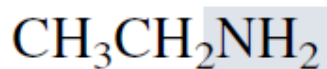
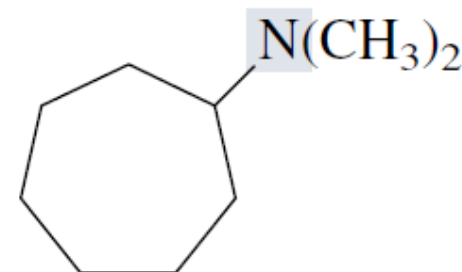
Primary amine



Secondary amine

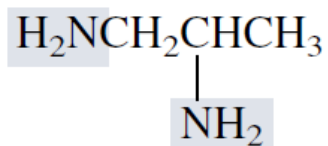


Tertiary amine

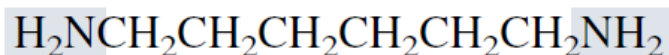
Ethylamine
(ethanamine)*N*-Methylethylamine
(a secondary amine)*N,N*-Dimethylcycloheptylamine
(a tertiary amine)

N + cadeia menor + il + cadeia maior + amina.

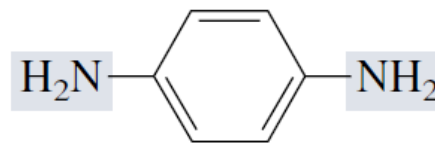
DIAMINAS



1,2-Propanediamine

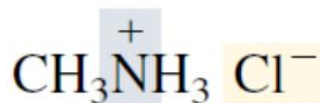


1,6-Hexanediamine

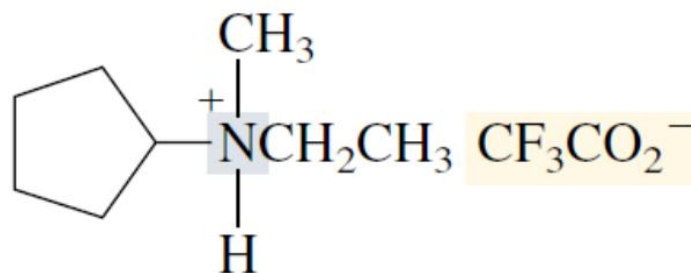


1,4-Benzenediamine

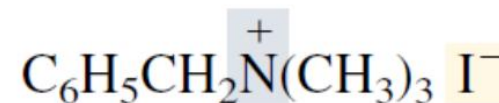
SAIS DE AMÔNIO QUATERNÁRIOS



Cloreto de metilamônio



N-etil-*N*-metilciclopropil-
Amônio trifluoroacetato

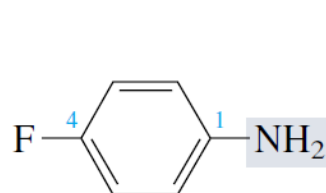
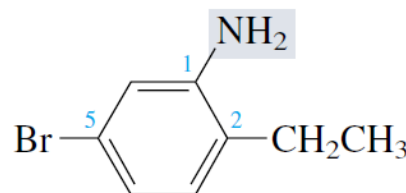


Iodeto de benziltrimetil-
amônio

N - ordem alfabética - *N* - radicais + amônio + contra íon

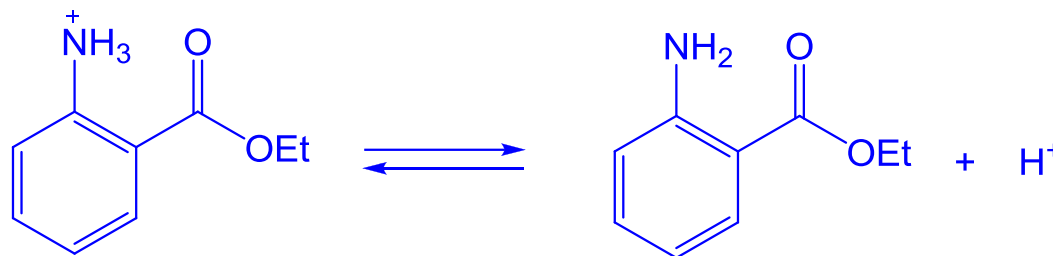
ARILAMINAS

(anilinas)

*p*-Fluoroaniline

5-Bromo-2-ethylaniline

Exemplos em fármacos: muitas estruturas são mais conhecidas pelo nome usual do que IUPAC.



IUPAC: 2-etóxicarbonil anilínio

**Usual: benzocaina protonada
forma ácida**

IUPAC: 2-aminobenzoato de etila

**benzocaina
forma básica**

Exercício: benzocaina ($pK_a = 2,5$). Qual a forma preponderante (ácida ou básica) da benzocaina no estômago ($pH = 1$), intestino ($pH = 8$) e plasma ($pH = 7,4$). Aonde haveria melhor absorção do fármaco?