QFL1221 (aula 02)

Ligações químicas e grupos funcionais.
Nomenclatura e representação de moléculas orgânicas.
Hidrocarbonetos (alcanos, alcenos e acetilenos)

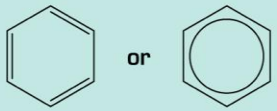
Number of organic compounds
(9.8 – 23 million of compounds)

Structures, names, functional groups,
physical properties,
conformation and stereochemistry

Physico-chemical properties

Reactivity and biological properties

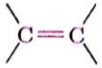
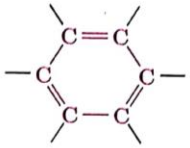
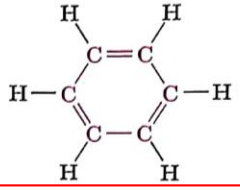
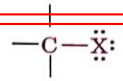
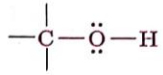
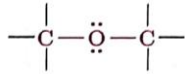
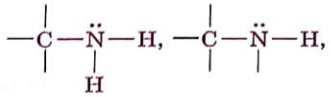
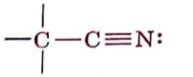
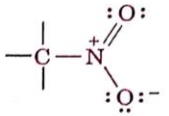
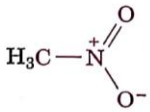
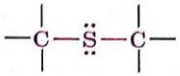
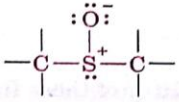
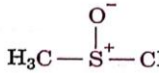
Hydrocarbons

Family	Key Feature	Class	Example	Name
Alkanes	Atoms joined by single bonds only	Saturated	$CH_3CH_2CH_3$	Propane
Alkenes	At least one carbon–carbon double bond	Unsaturated	$CH_2{=}CHCH_3$	Propene
Alkynes	At least one carbon–carbon triple bond	Unsaturated	$HC{\equiv}CCH_3$	Propyne
Aromatic compounds	Contains a ring of alternating single and double bonds	Unsaturated		Benzene

Localized bonds

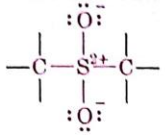
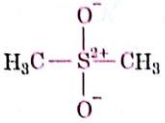
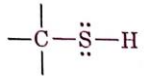
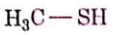
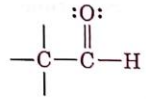
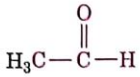
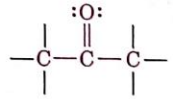
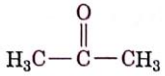
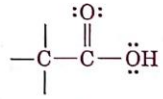
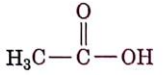
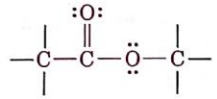
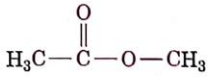
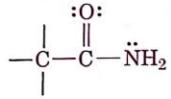
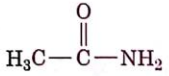
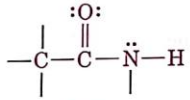
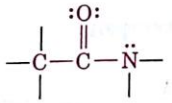
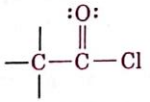
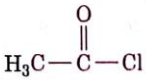
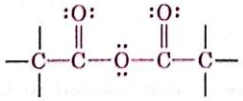
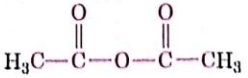
delocalized bonds

Functional groups

Family name	Functional group structure[a]	Simple example	Name ending
Alkane	(Contains only C—H and C—C single bonds)	CH_3CH_3	*-ane* Ethane
Alkene		$H_2C{=}CH_2$	*-ene* Ethene (Ethylene)
Alkyne		$H{-}C{\equiv}C{-}H$	*-yne* Ethyne (Acetylene)
Arene			None Benzene
Halide	 (X = F, Cl, Br, I)	$H_3C{-}Cl$	None Chloromethane
Alcohol		$H_3C{-}O{-}H$	*-ol* Methanol
Ether		$H_3C{-}O{-}CH_3$	*ether* Dimethyl ether
Amine		$H_3C{-}NH_2$	*-amine* Methylamine
Nitrile		$H_3C{-}C{\equiv}N$	*-nitrile* Ethanenitrile (Acetonitrile)
Nitro			None Nitromethane
Sulfide		$H_3C{-}S{-}CH_3$	*sulfide* Dimethyl sulfide
Sulfoxide			*sulfoxide* Dimethyl sulfoxide

Functional groups

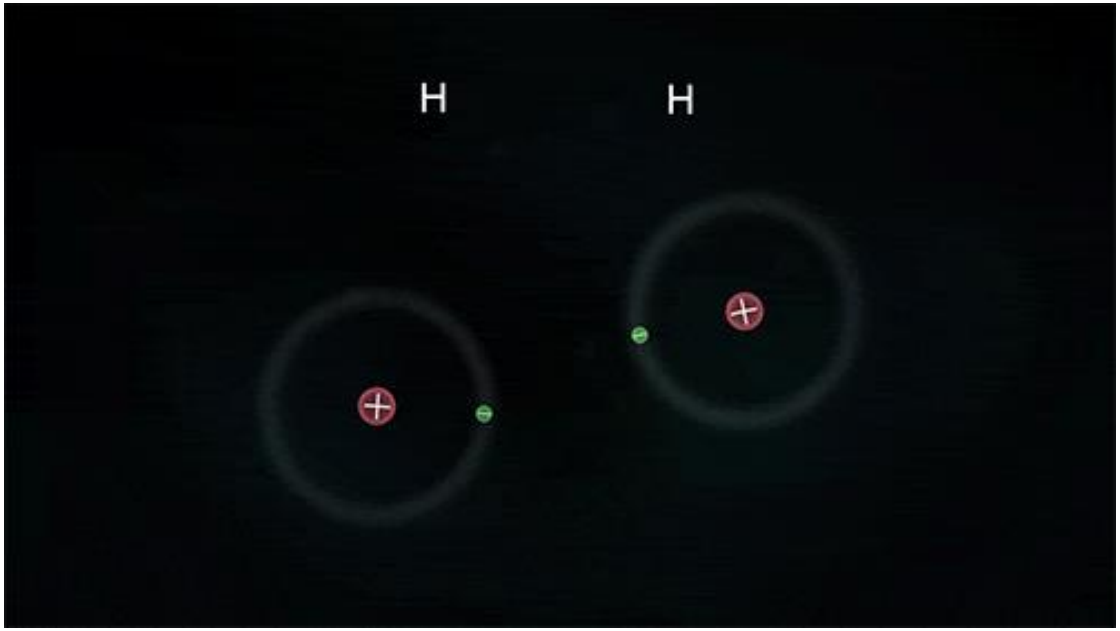
Carbonyl derivatives

Family name	Functional group structure[a]	Simple example	Name ending
Sulfone			*sulfone* Dimethyl sulfone
Thiol			*-thiol* Methanethiol
Carbonyl, 			
Aldehyde			*-al* Ethanal (Acetaldehyde)
Ketone			*-one* Propanone (Acetone)
Carboxylic acid			*-oic acid* Ethanoic acid (Acetic acid)
Ester			*-oate* Methyl ethanoate (Methyl acetate)
Amide			*-amide* Ethanamide (Acetamide)
			
			
Carboxylic acid chloride			*-oyl chloride* Ethanoyl chloride (Acetyl chloride)
Carboxylic acid anhydride			*-oic anhydride* Ethanoic anhydride (Acetic anhydride)

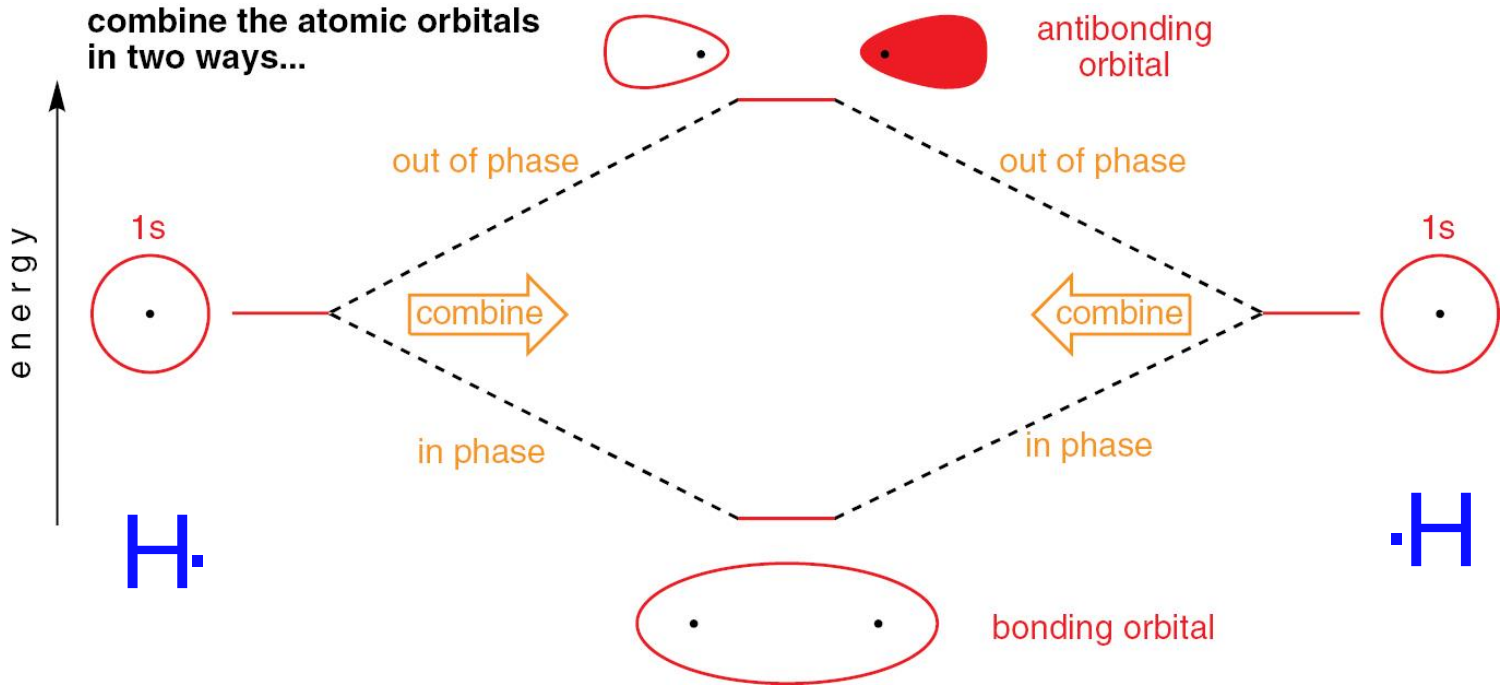
Chemical bonds in organic compounds

NONPOLAR COVALENT BONDS

when electrons are shared *equally*



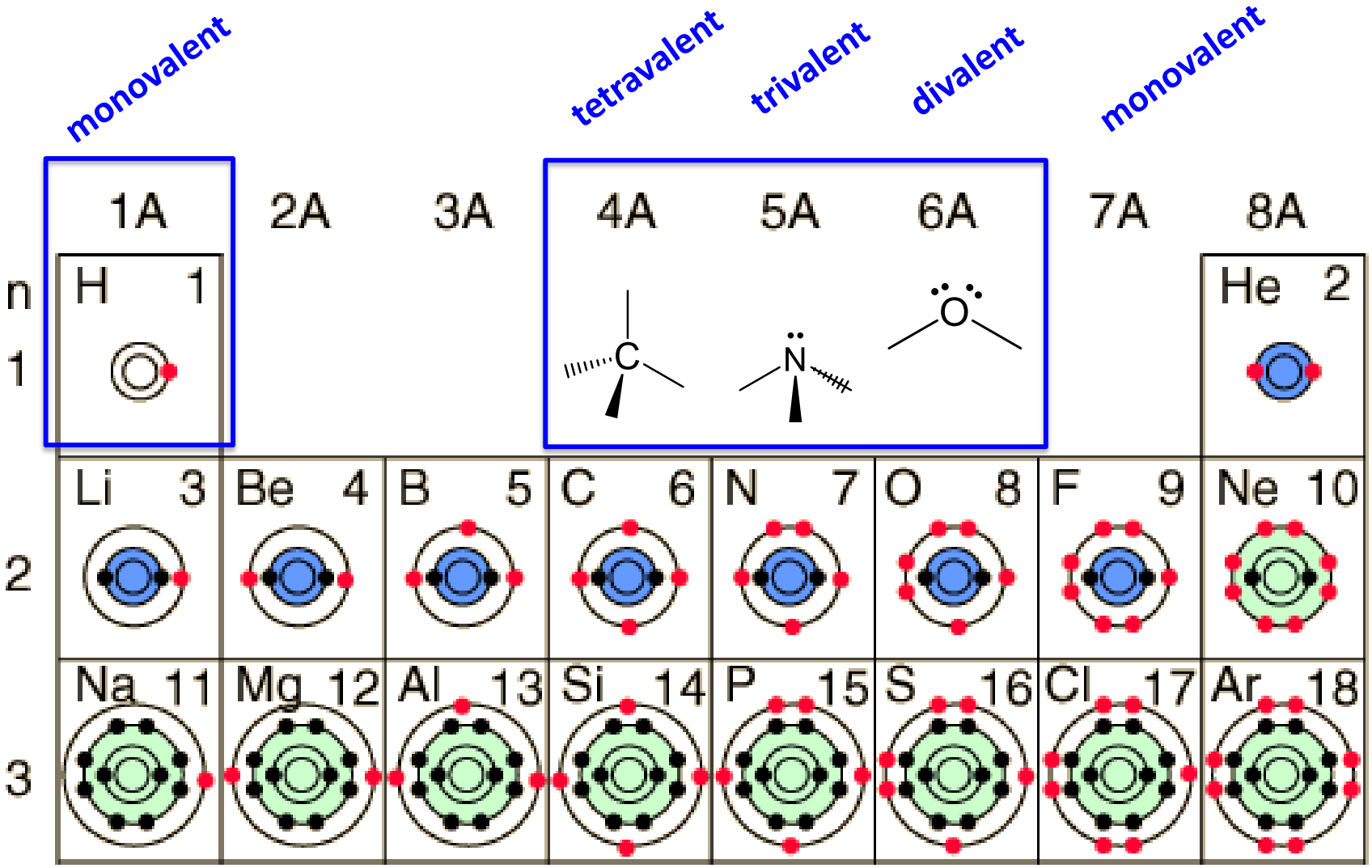
Molecular Orbital Description for H_2



H:H

2 $\bar{e}$ gives to hydrogen configuration analogous to helium.

Atomic number and valence



Formação de Ligações Químicas

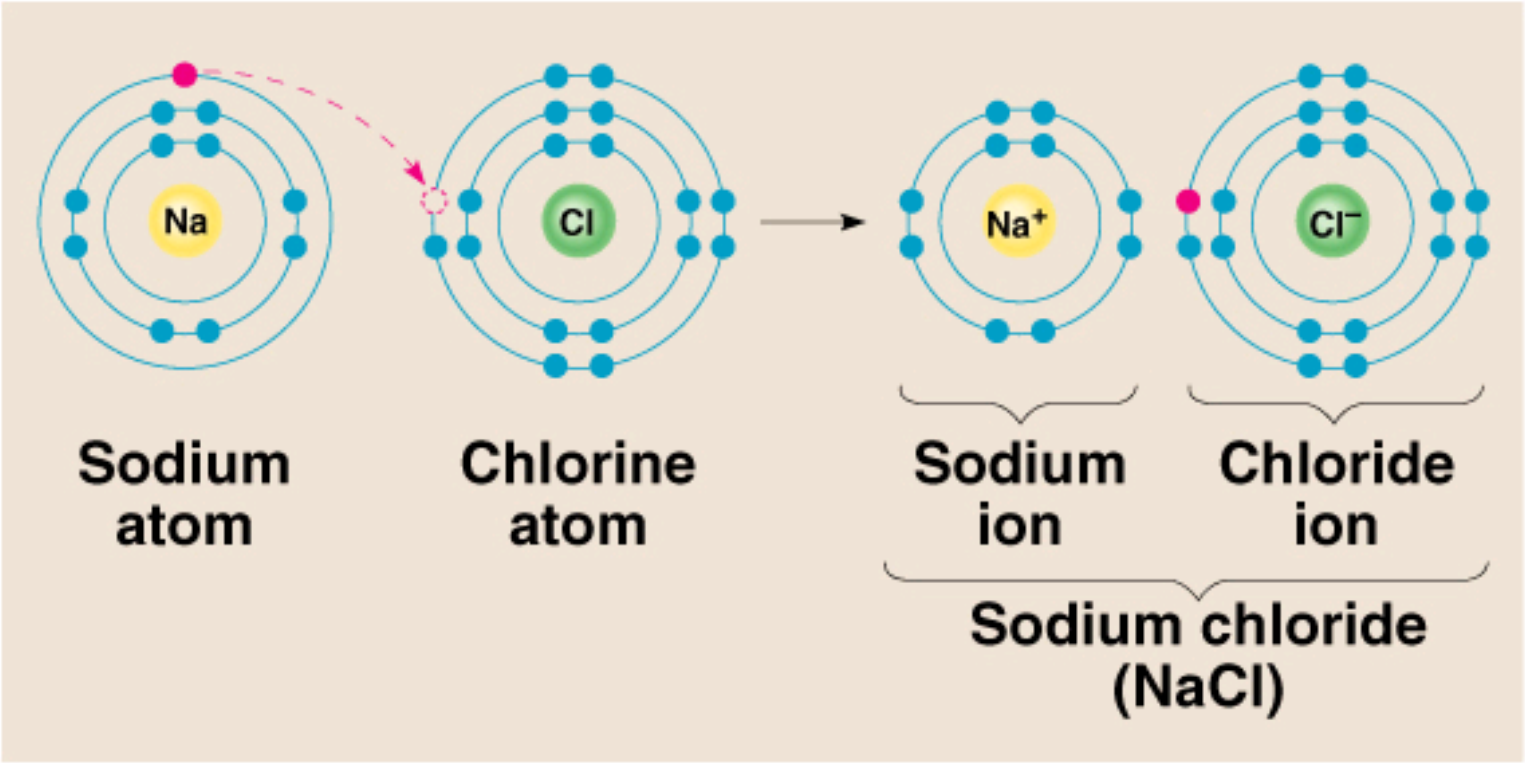
- Tendem a adquirir a configuração eletrônica do gás nobre mais próximo na Tabela Periódica

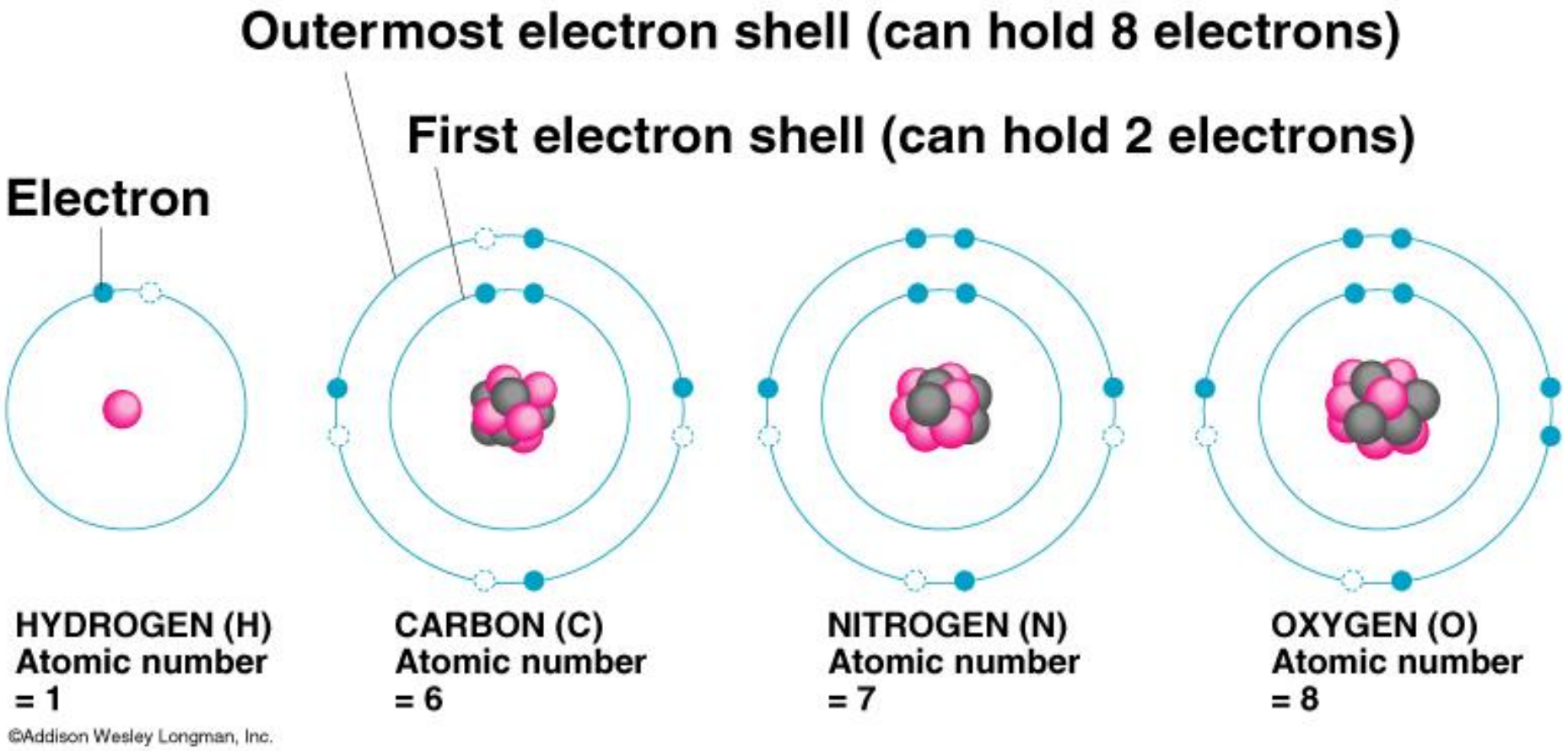
- Dois extremos de ligações
  - **ligação iônica:** ligação química resultante da atração eletrostática entre um ânion e um cátion.

    Ex. Na(11) + F (7) -> $Na^{+}F^{-}$

  - **ligação covalente:** ligação química resultante do compartilhamento de um ou mais pares de elétrons entre dois átomos. Ex. H + H -> H-H

1) **Ionic bond** – electron from Na is transferred to Cl, this causes a charge imbalance in each atom. The Na becomes (Na+) and the Cl becomes (Cl-), charged particles or ions.





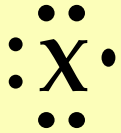
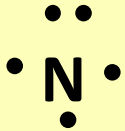
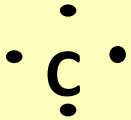
Octet Rule = atoms tend to gain, lose or share electrons so as to have 8 electrons

How many electrons C, N and O require to fill up the valence shell?

Valence electrons and number of bonds

Step #3 (# of Bond) Determine the number of bonds in the compound

Recall the number of bonds at atom prefers depending on the number of valence electrons

Family		# Covalent Bonds*
Halogens F, Br, Cl, I		1 bond often
Calcogens O, S		2 bond often
Nitrogen N, P		3 bond often
Carbon C, Si		4 bond always

In general, these are the number of bonds formed by these atoms.

Hydrocarbons:
Simplest organic compounds

Alkanes - Nomenclature

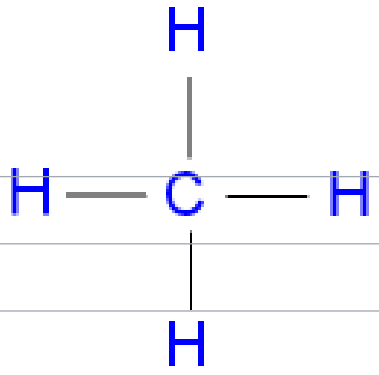
Suffix – Our first functional group is alkane, so the suffix is –ane

For later functional groups we will drop the –ane root suffix for others

Alkane chain	# Carbons	Name
CH_4	1	methane
CH_3CH_3	2	ethane
$CH_3CH_2CH_3$	3	propane
$CH_3CH_2CH_2CH_3$	4	butane
$CH_3CH_2CH_2CH_2CH_3$	5	pentane
$CH_3CH_2CH_2CH_2CH_2CH_3$	6	hexane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$	7	heptane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	8	octane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	9	nonane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	10	decane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	11	undecane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	12	dodecane

Methane CH_4

Greek "*methy*" (alcohol from wood)

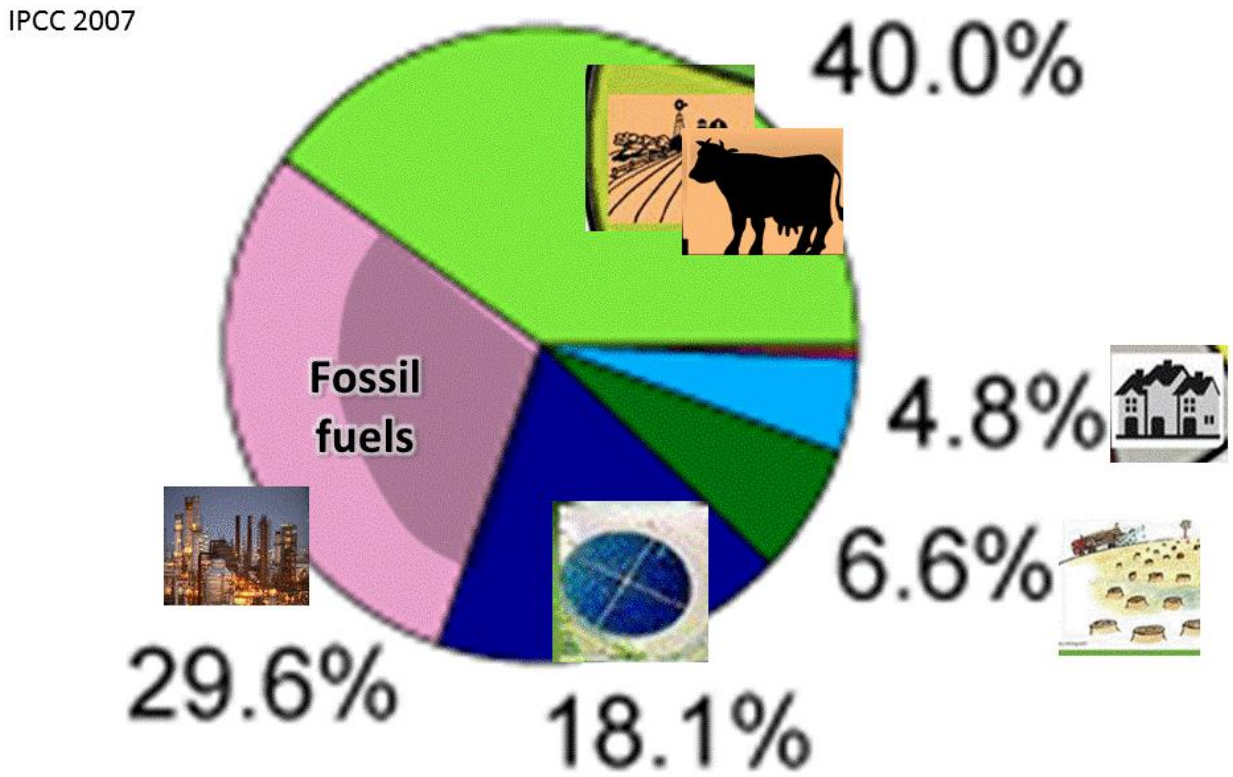


Chemical formula	CH_4
Molar mass	16.04 g·mol^{-1}
Appearance	Colorless gas
Odor	Odorless
Density	•0.657 g·L^{-1} (gas, 25 °C, 1 atm) •0.717 g·L^{-1} (gas, 0 °C, 1 atm) •422.62 g·L^{-1} (liquid, −162 °C)
Melting point	−182.5 °C;
Boiling point	−161.50 °C;
Solubility in water	22.7 mg·L^{-1}
Solubility	Soluble in ethanol, diethyl ether, benzene, toluene, methanol, acetone

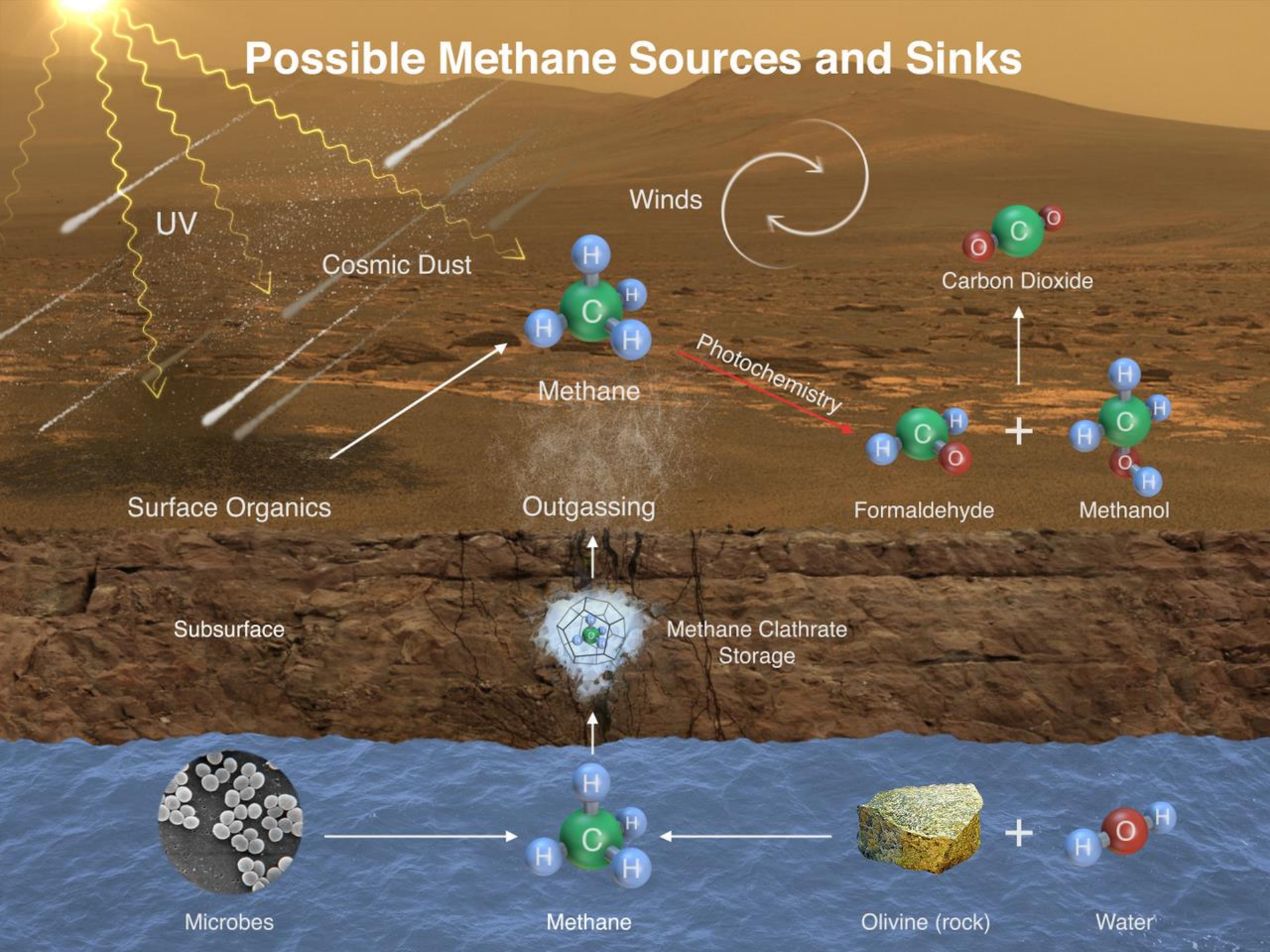
The name "methane" was coined in 1866 by the German chemist August Wilhelm von Hofmann.

Methane was first identified in 1776 by Italian physicist Alessandro Volta in the marshes of Lake Maggiore straddling Italy and Switzerland.

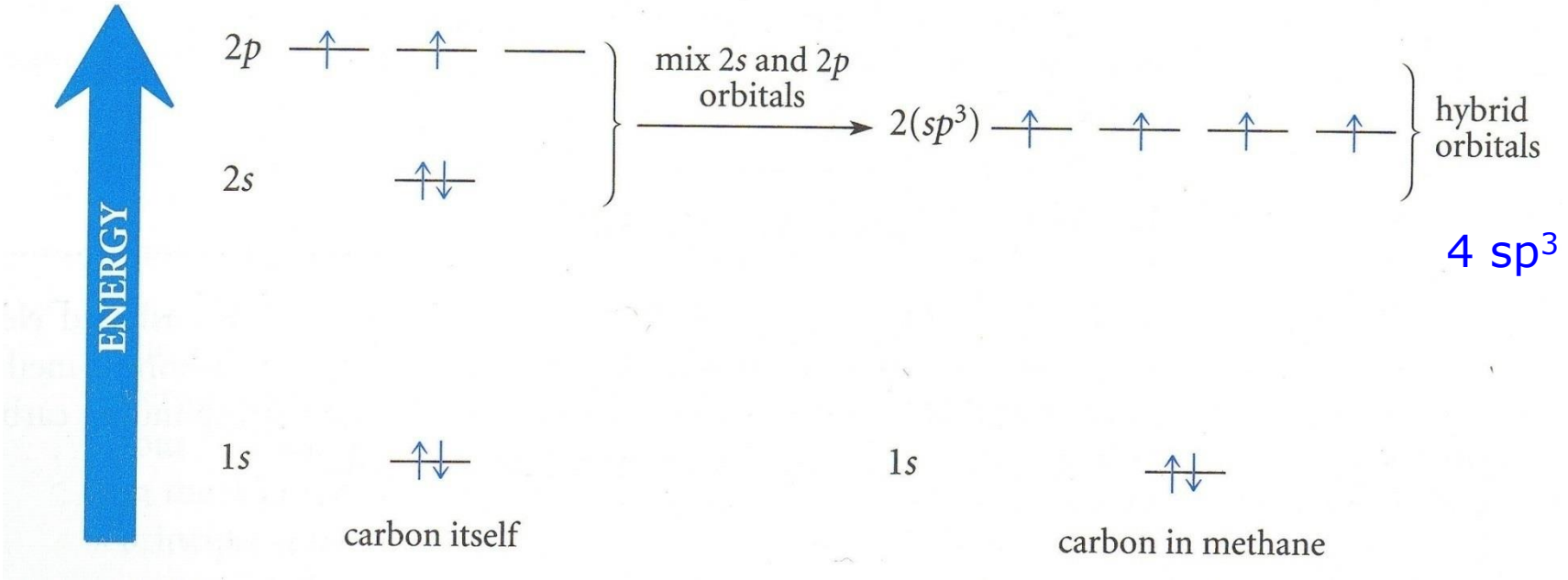
Global methane emissions 18% of total



Methane is an important greenhouse gas with a global warming potential of 34 compared to CO_2 (potential of 1).


Possible Methane Sources and Sinks
UV
Cosmic Dust
Winds
Carbon Dioxide
Methane
Photochemistry
Surface Organics
Outgassing
Formaldehyde
Methanol
Subsurface
Methane Clathrate
Storage
Microbes
Methane
Olivine (rock)
Water

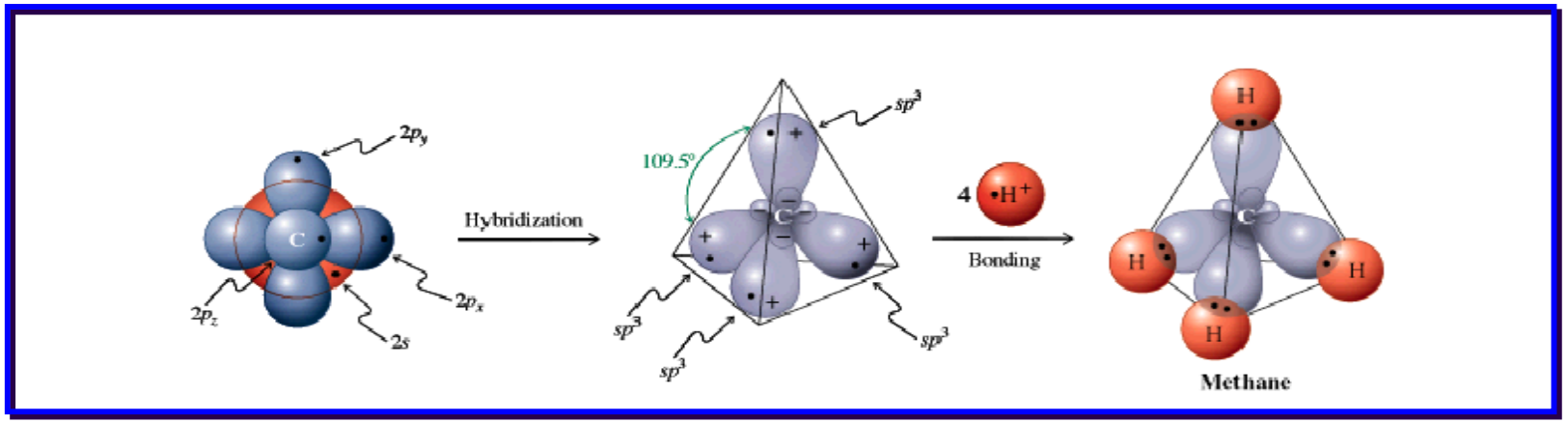
Metano

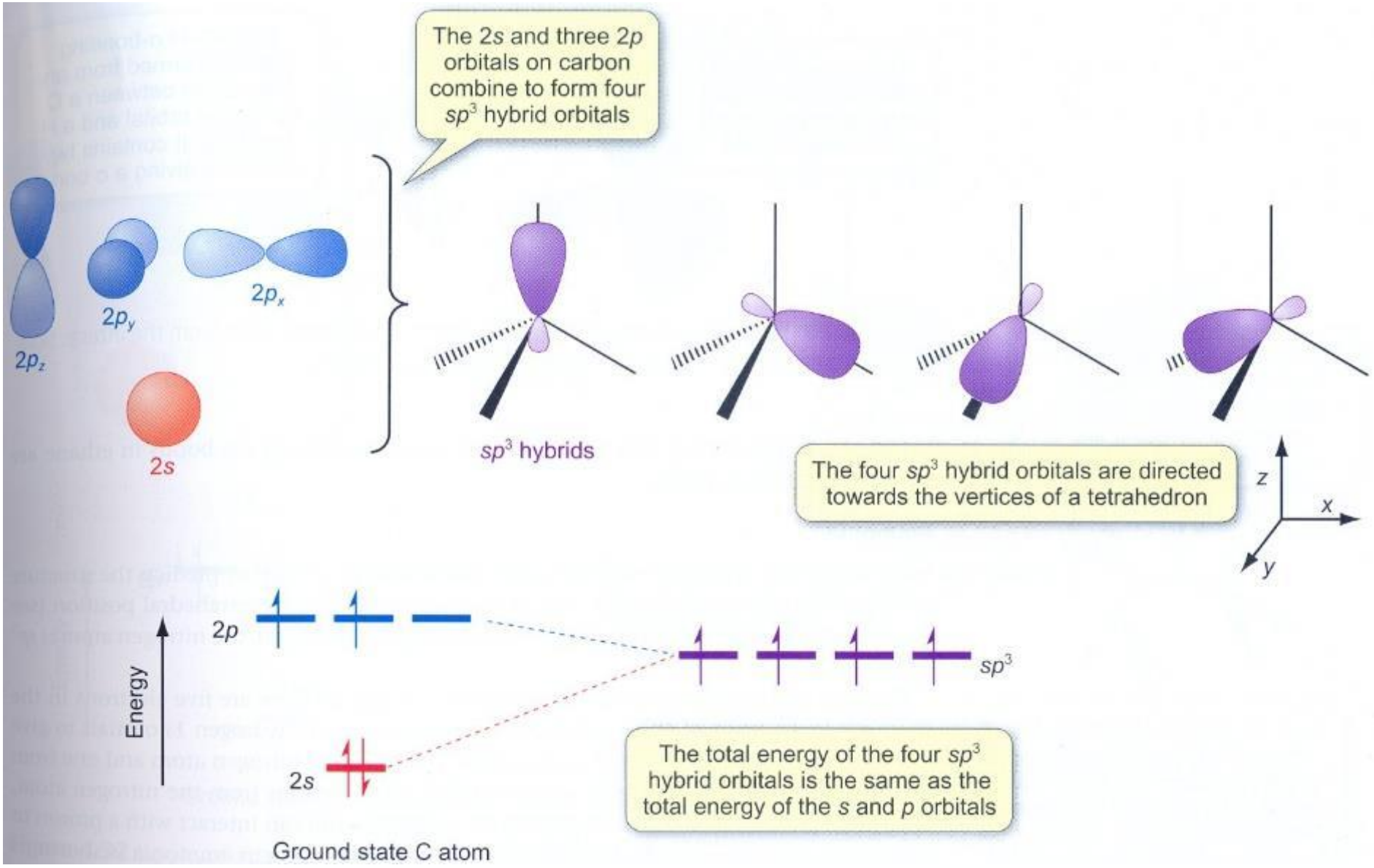


4 sp^3

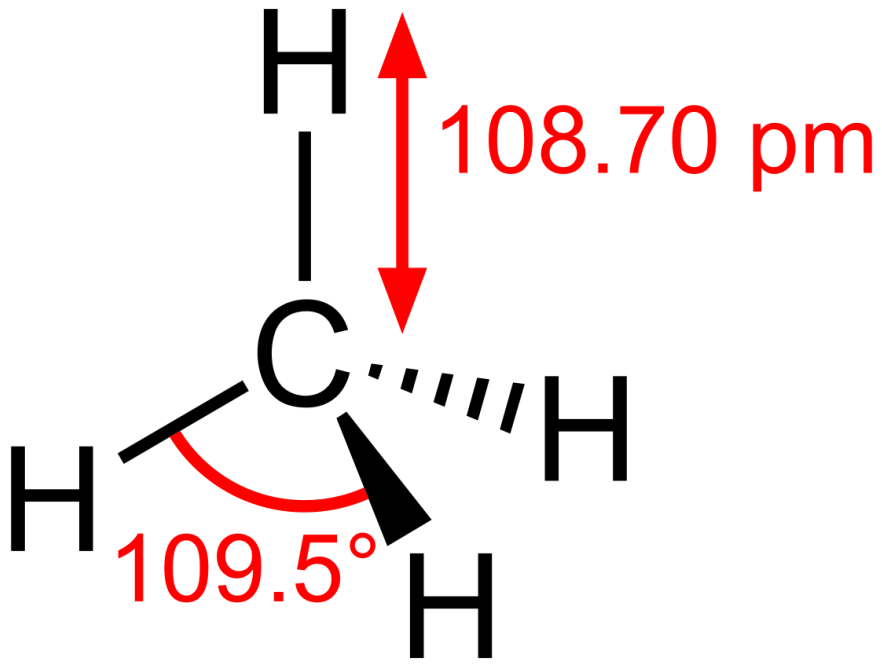
C (nº atômico: 6):

$1s^2\ 2s^2\ 2p_x^1\ 2p_y^1$




The 2s and three 2p orbitals on carbon combine to form four sp^3 hybrid orbitals
$2p_z$
$2p_y$
$2p_x$
2s
sp^3 hybrids
The four sp^3 hybrid orbitals are directed towards the vertices of a tetrahedron
z
x
y
Energy
2p
2s
sp^3
The total energy of the four sp^3 hybrid orbitals is the same as the total energy of the s and p orbitals
Ground state C atom

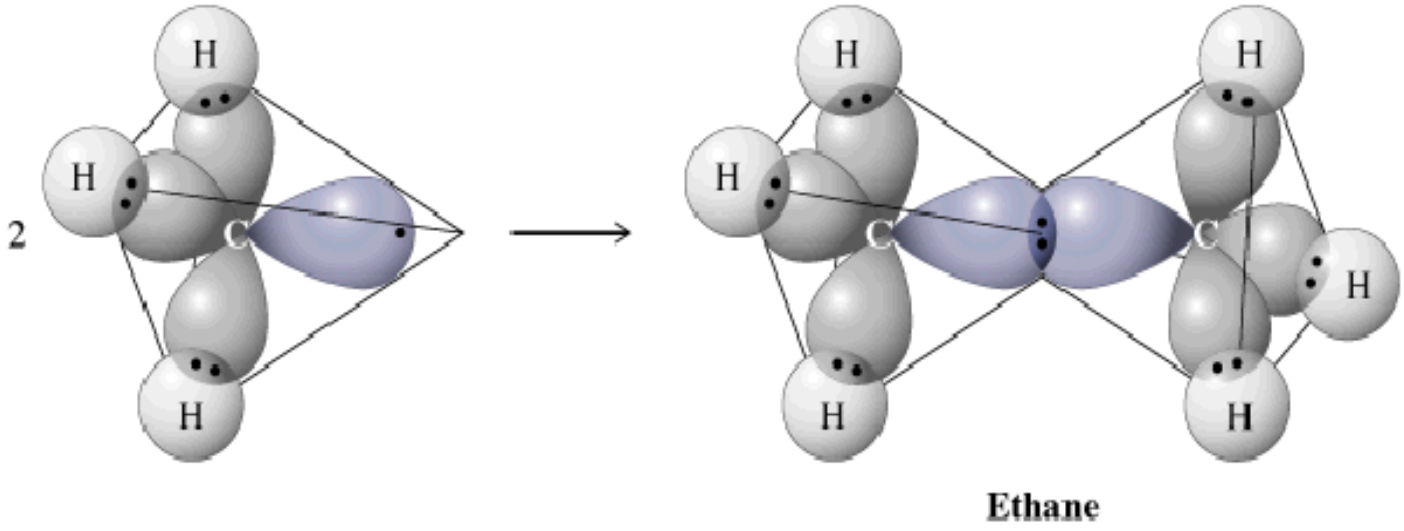
Tetrahedral structure of Methane (neutral molecule)



https://www.worldofmolecules.com/3D/methane_3d.htm

Etano

- ✓ Uma ligação sigma (σ) é uma ligação covalente em que a sobreposição dos orbitais de uma ligação ocorre ao longo do eixo dos dois núcleos.
- ✓ De modo geral, os esqueletos das moléculas orgânicas são formados de átomos unidos por ligações sigma.



Ethane

IUPAC INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

IUPAC was formed in 1919 by chemists from industry and academia, who recognized the need for international standardization in chemistry.

- Nomenclature of inorganic and organic chemistry;
- Standardization of atomic weights;
- Standardization of physical constants;
- Editing tables of properties of matter;
- Establishing a commission for the review of work;
- Standardization of the formats of publications;
- Measures required to prevent repetition of the same papers.

46th World Chemistry Congress - July 7 to 13, 2017 - São Paulo - Brazil
40ª Reunião Anual da Sociedade Brasileira de Química
July 9 to 14, 2017 - São Paulo - Brazil
Sustainability & Diversity through Chemistry

Regras para nomear compostos orgânicos

1) Determine a cadeia carbônica mais longa;

2) Identifique (com nomes) os substituíntes ligados a cadeia;

3) Numere a cadeia principal tendo a ramificação a menor numeração;

4) Designe as posições dos substituíntes pelos números onde se encontram;

5) Escreva o nome completo da substância, listando os substituíntes em order alfabética;

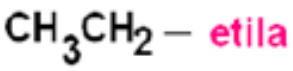
Os prefixos di-, tri-, tetra-, sec- e terc- não são considerados na priorização;

Mas Iso-, ciclo- e neo- são considerados na ordem alfabética

Nomes de substituíntes alquílicos

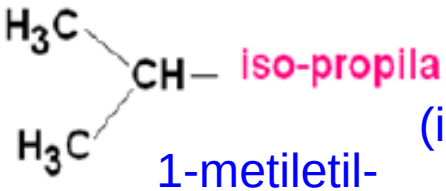
(não use o termo radical, que deve ser utilizado para espécie reativa)

(Me)



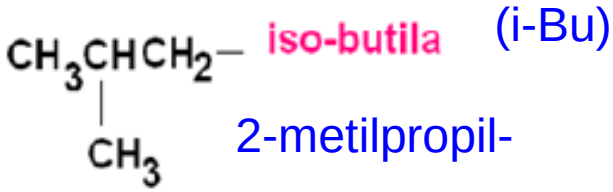
(Et)

(Pr)



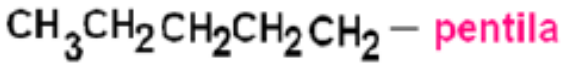
(i-Pr)

1-metiletil-



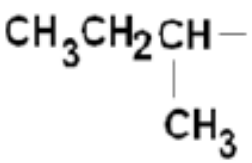
(i-Bu)

2-metilpropil-

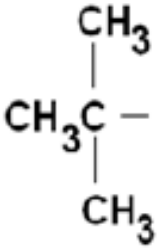


(pent)

1-metilpropil-

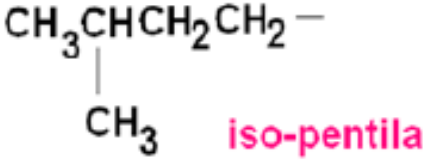


(sec-Bu)

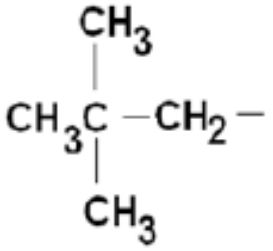


(t-Bu)

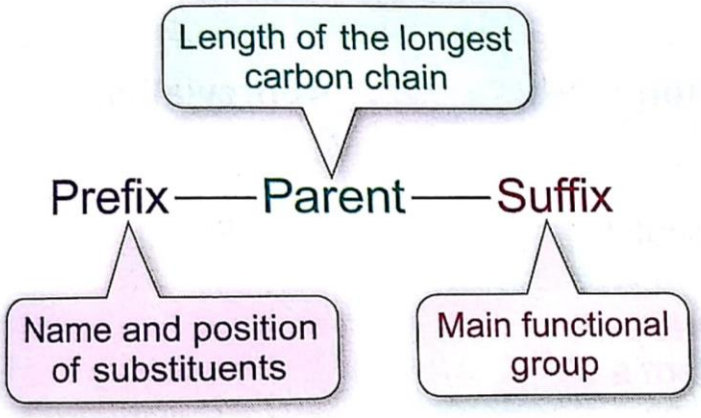
1,1-dimetiletil-

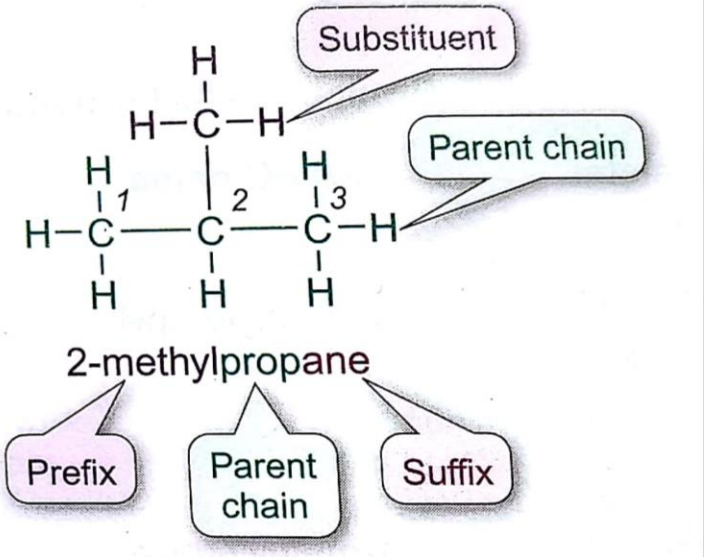


(i-pent)



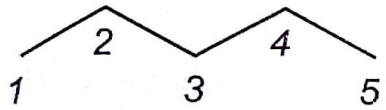
(neo-pent)



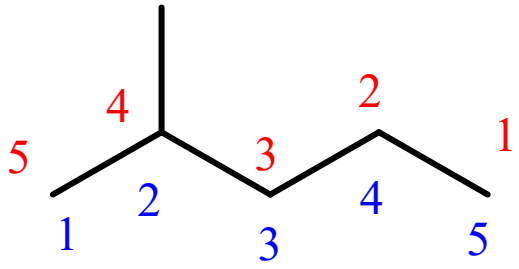


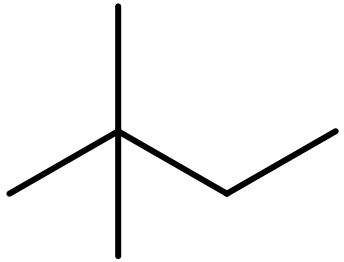
Nome IUPAC:
2-metilpropano

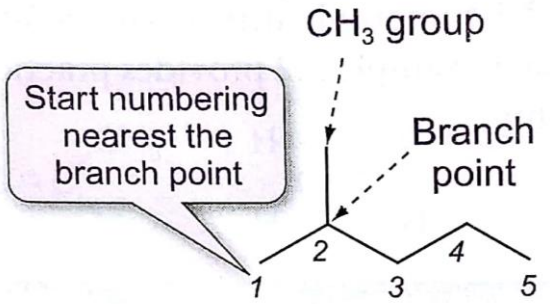
Nome comum:
isobutano



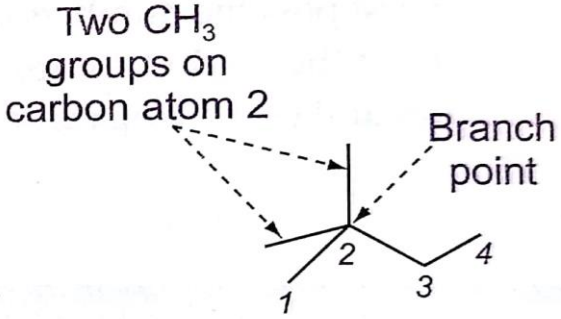
pentane







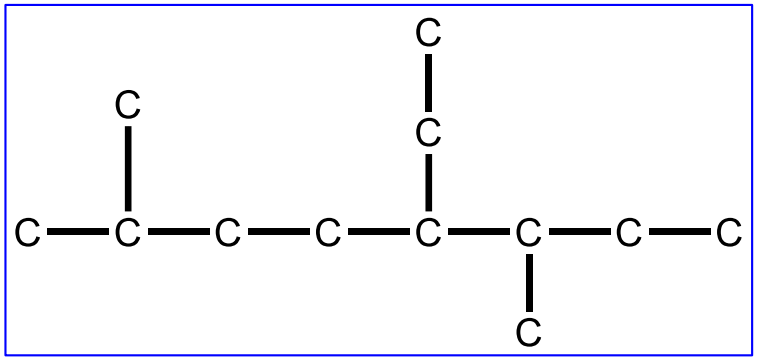
2-methylpentane



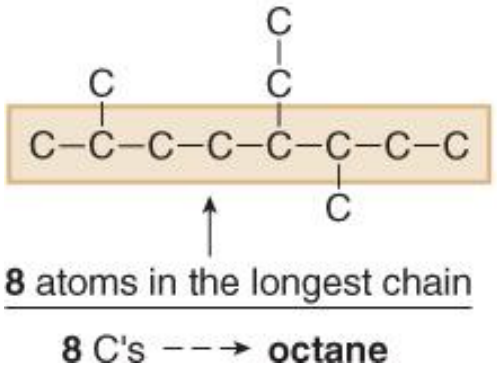
2,2-dimethylbutane

Rules to name branched alkanes

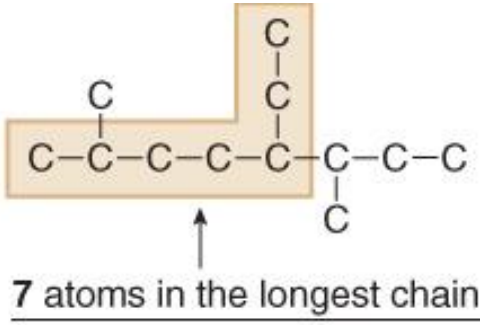
1. Find the longest parent carbon chain and add the suffix.



corrrect

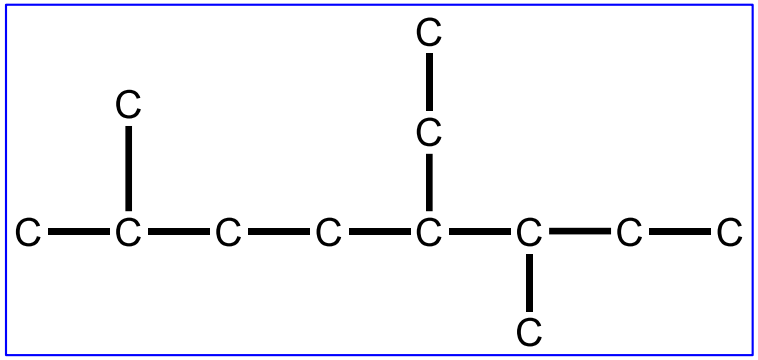


uncorrrect

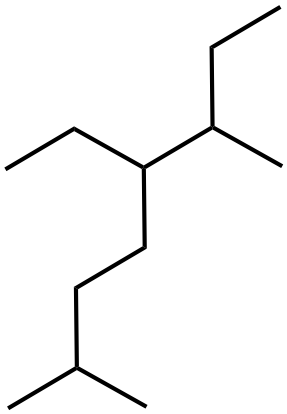


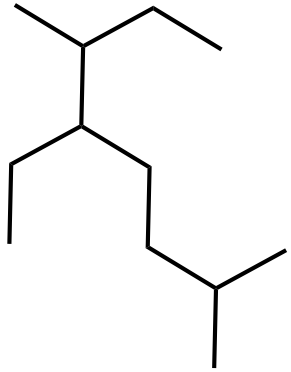
Rules to name branched alkanes

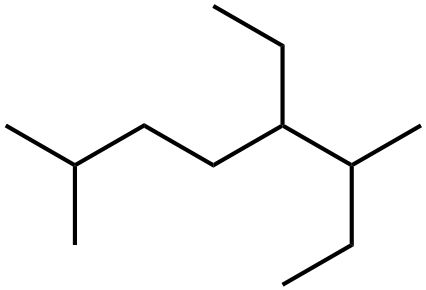
1. Find the parent carbon chain (**C-8**) and add the suffix.

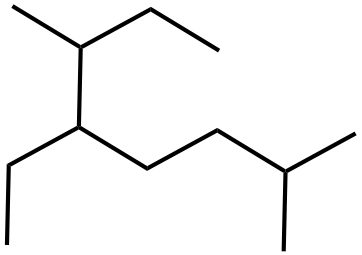


Does not matter if the chain is straight or it bends.

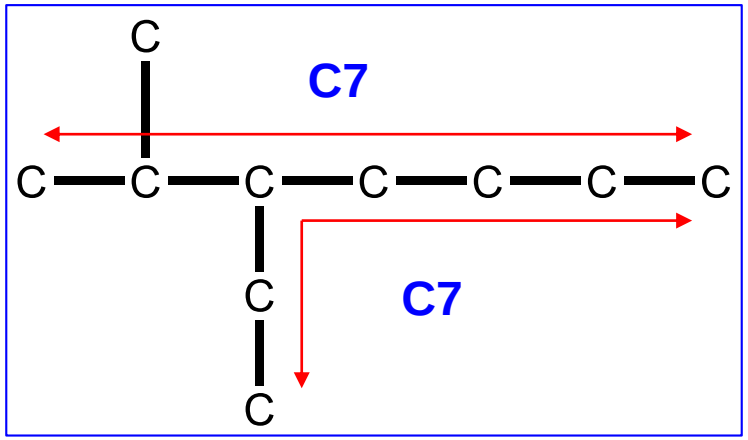


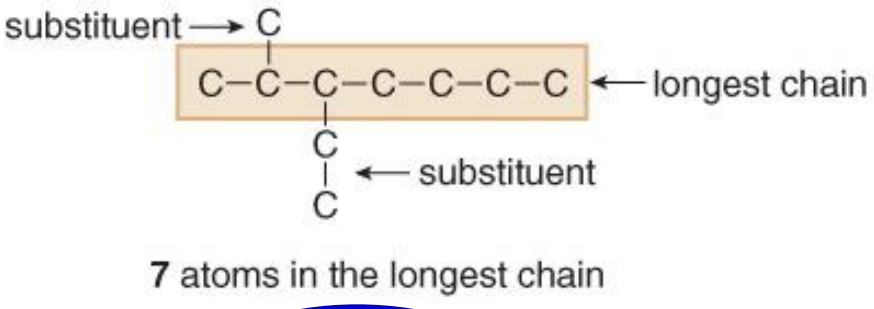


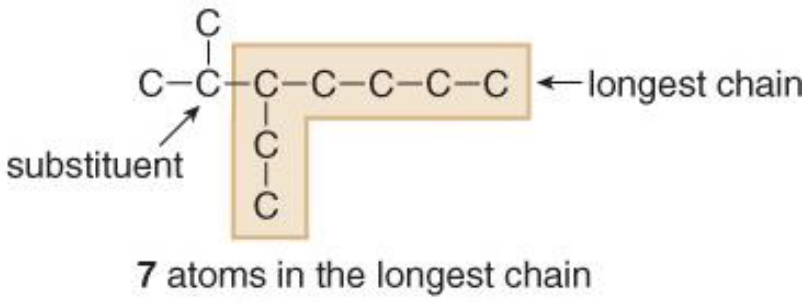




In case of having two different longest chains of **same length (C7):**







2 substituents

more substituents

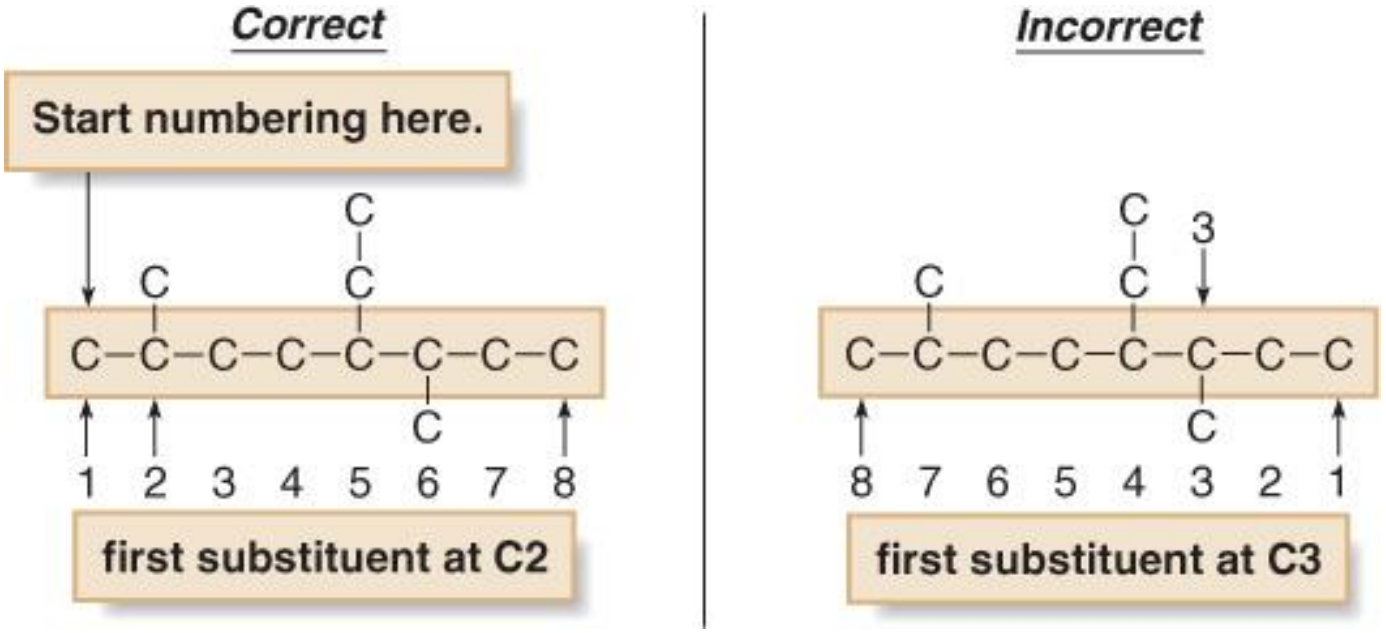
Correct

only 1 substituent

fewer substituents

Incorrect

2. Number the atoms in the carbon chain to give the first substituent the lowest number.

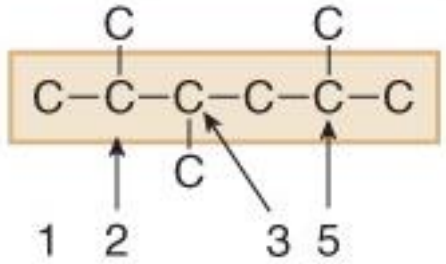


Primeiro substituinte em C-2

Primeiro substituinte em C-3 (errado)

Give the second substituent the lower number.

Numbering from *left* to right

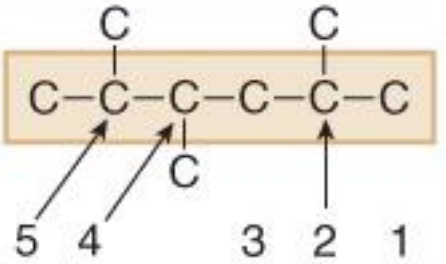


CH_3 groups at C2, **C3**, and C5.

The second substituent has a lower number.

Correct

Numbering from *right* to left



CH_3 groups at C2, **C4**, and C5.

higher number

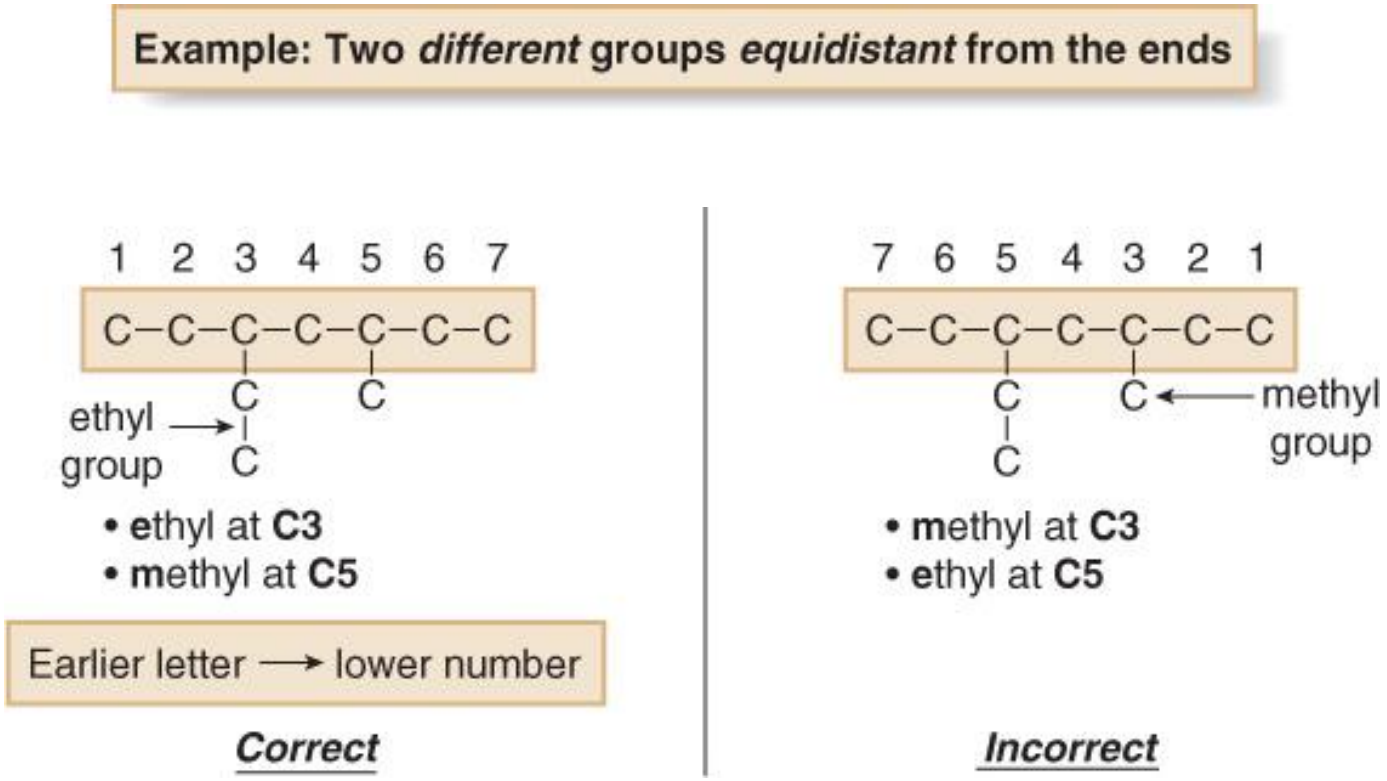
Incorrect

2, 3, 5

Menor número para
o segundo substituínte

2, 4, 5

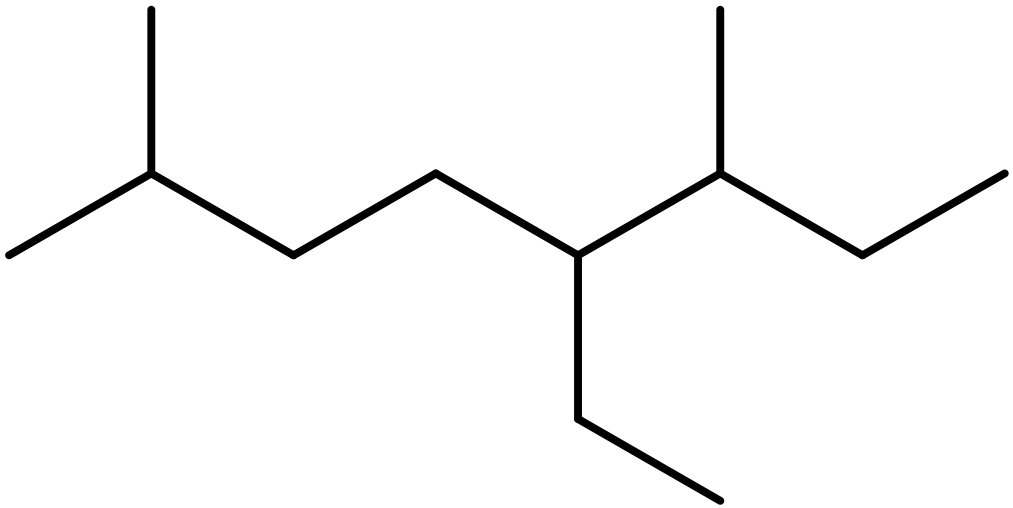
When numbering a carbon chain results in the same numbers from either end of the chain (**C3, C5 or C5, C3)**, assign the lower number alphabetically to the first substituent.



3-etil-5-metileptano

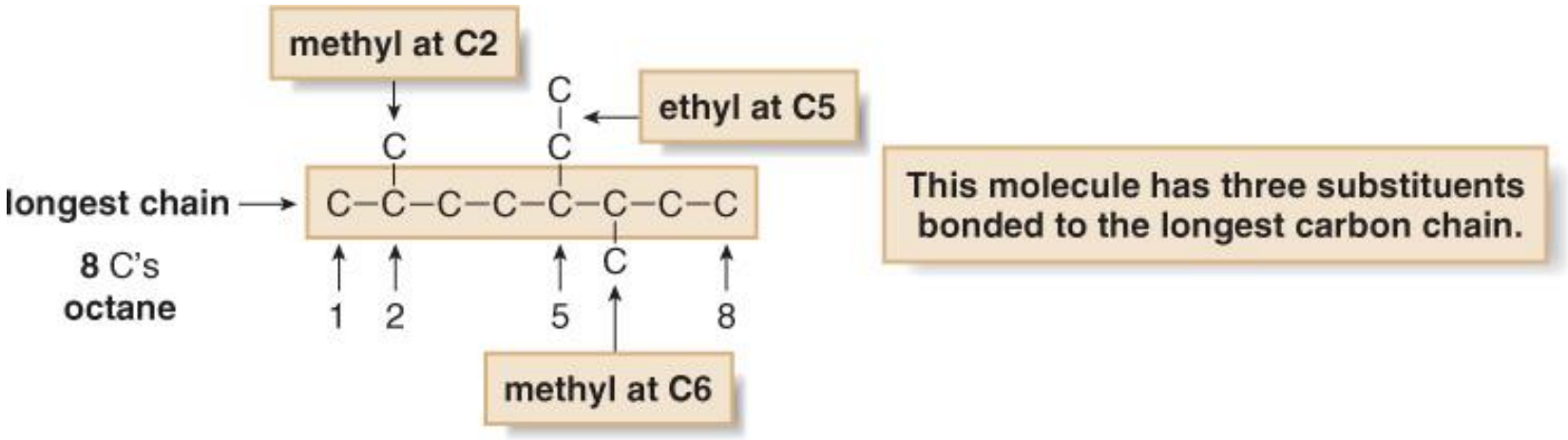
5-etil-3-metileptano

What is the name for this compound?



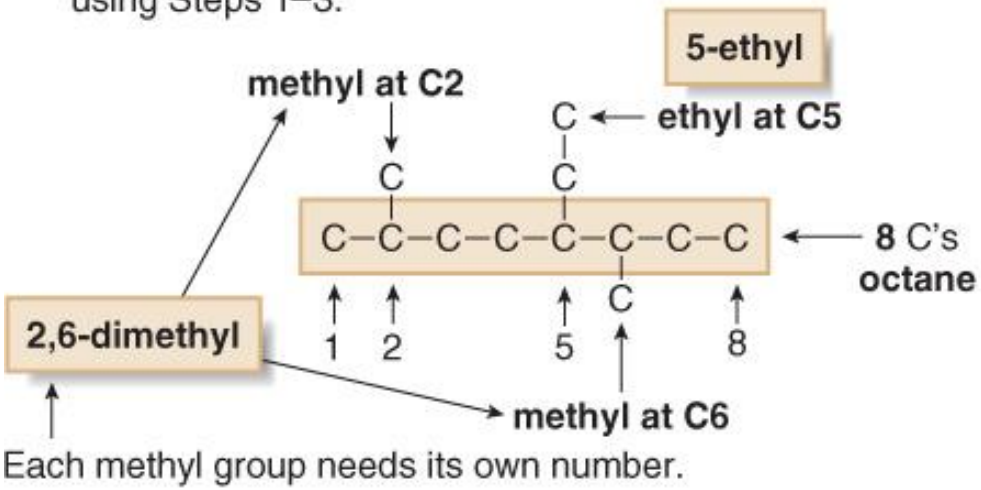
Name and number the substituents.

- Name the substituents as alkyl groups.
- Each substituent needs its own number.
- Use prefixes to indicate how many identical groups are present: di-, tri-, tetra- and so forth.

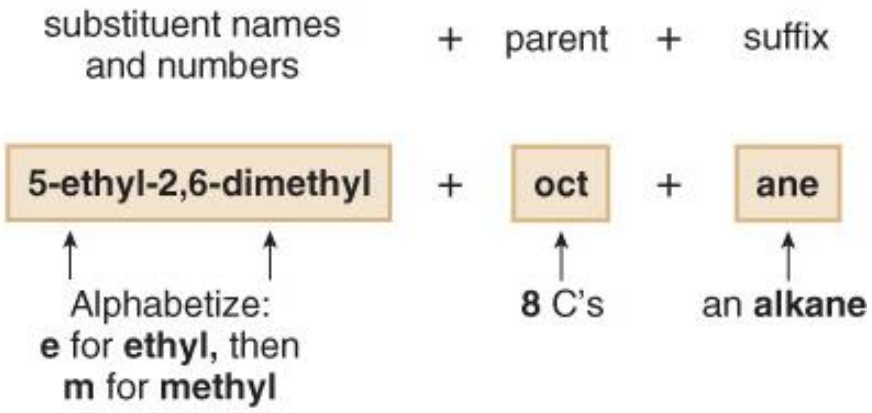


4. Combine substituent names and numbers + parent and suffix.

[1] Identify all the pieces of a compound, using Steps 1–3.



[2] Then, put the pieces of the name together.

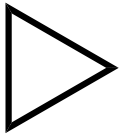


5-ethyl-2,6-dimethyl-octane

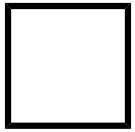
Lembrem-se que o **di** Não conta.

Nomenclature for cycloalkanes

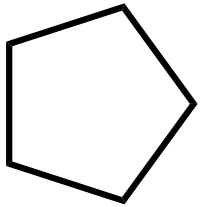
Use prefix cyclo- immediately precedes the name of the parent.



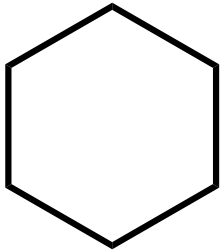
cyclopropane



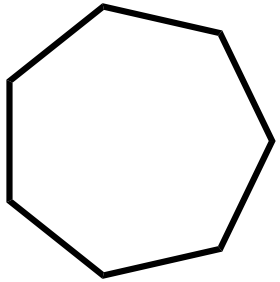
cyclobutane



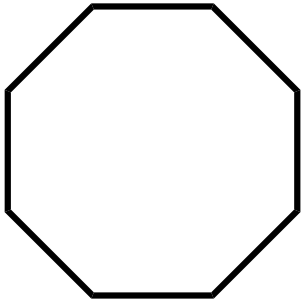
cyclopentane



cyclohexane



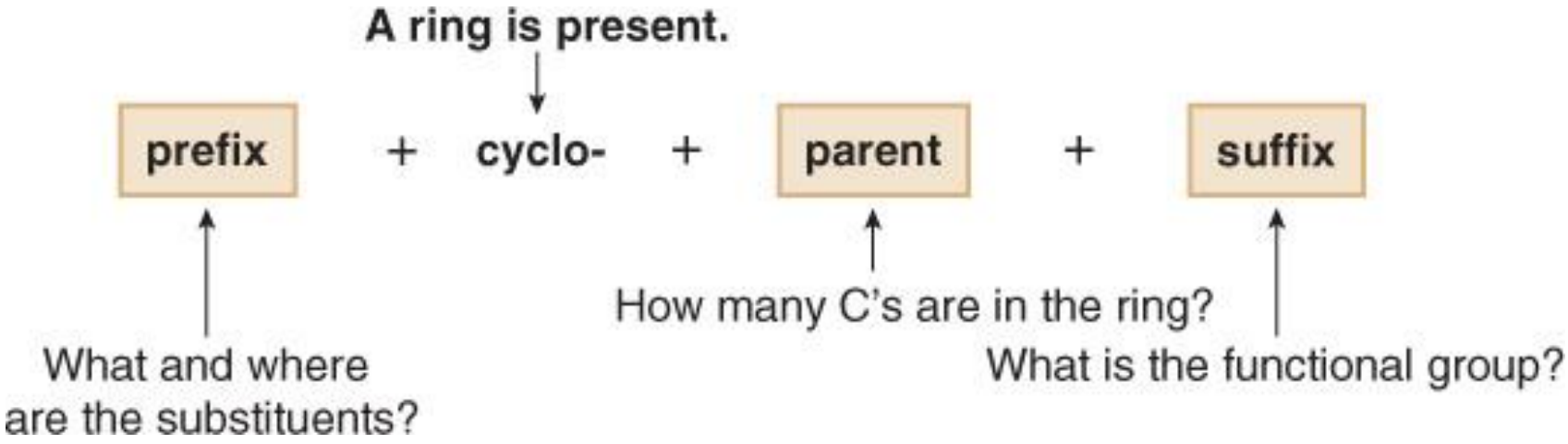
cycloheptane



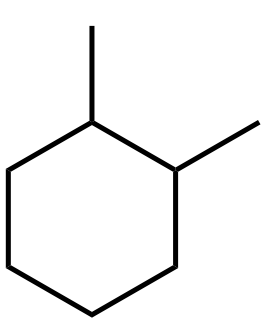
cyclooctane

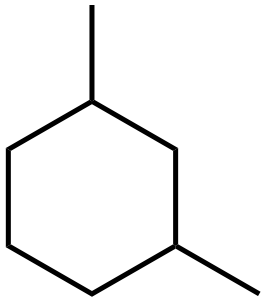
Nomenclature for cycloalkanes

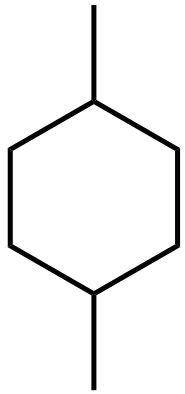
Use prefix cyclo- immediately precedes the name of the parent.

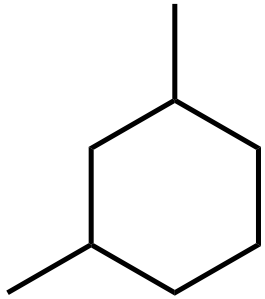



SAY
MY
NAME



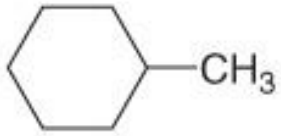




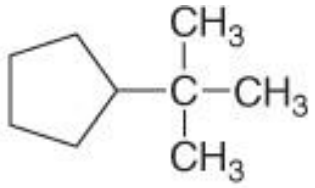


2. Name and number the substituents.

Single substituent: No number is needed to indicate its location.



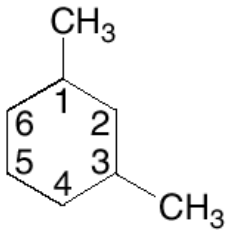
methylcyclohexane



tert-butylcyclopentane

Two substituents

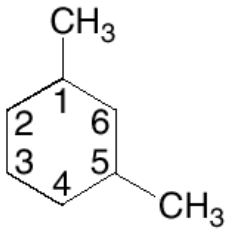
numbering clockwise



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

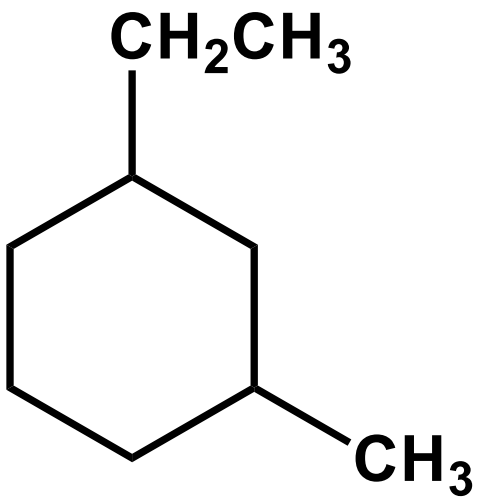
Correct: **1,3-dimethylcyclohexane**

numbering counterclockwise

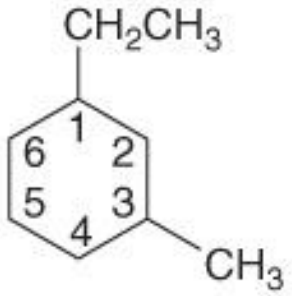


CH_3 groups at C1 and **C5**

Incorrect: 1,5-dimethylcyclohexane


CH2CH3
CH3

Begin numbering at the ethyl group.

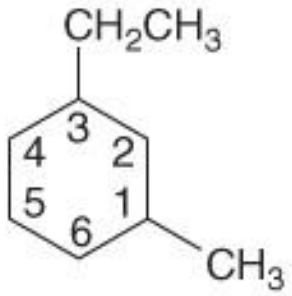


- **e**thyl group at **C1**
- **m**ethyl group at **C3**

earlier letter → lower number

Correct: **1-ethyl-3-methylcyclohexane**

Begin numbering at the methyl group.



- **m**ethyl group at **C1**
- **e**thyl group at **C3**

Incorrect: 3-ethyl-1-methylcyclohexane

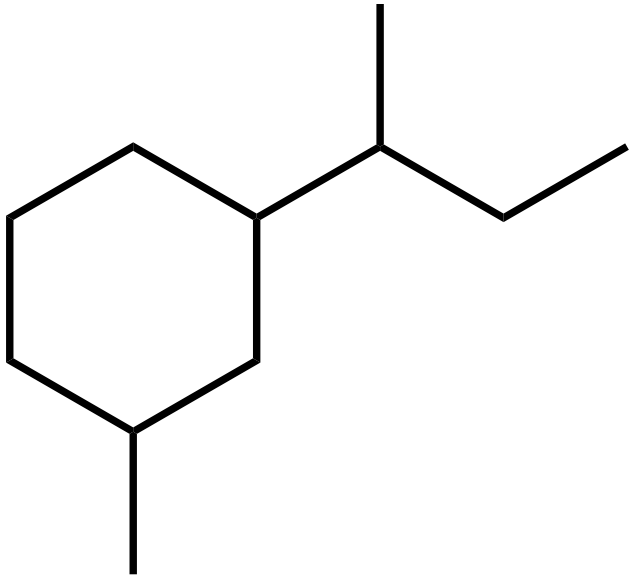
1-etil-3-metilcicloexano

(Certo)

3-etil-1-metilcicloexano

(errado)

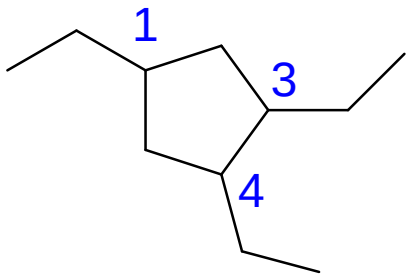
Ordem alfabética e substituinte com menor número !!!

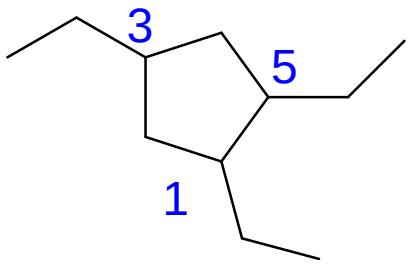


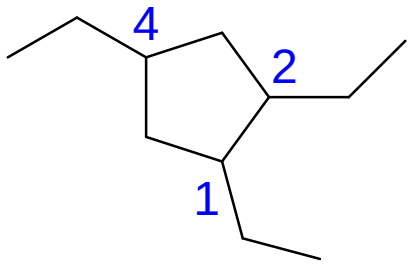
1-*sec*-**b**util-3-**m**etilcicloexano

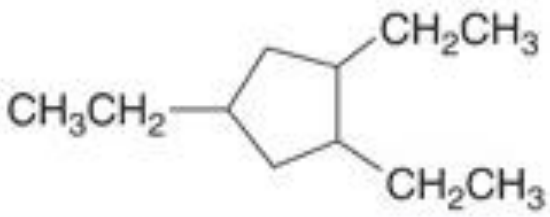
Os prefixos di-, tri-, tetra-, sec- e terc- não são considerados na priorização;

Mas Iso-, ciclo- e neo- são considerados na ordem alfabética





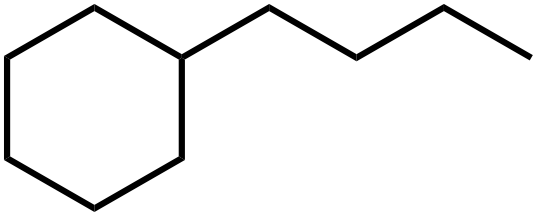


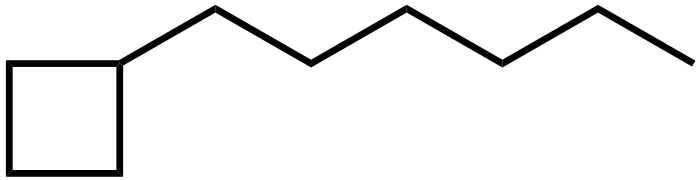


1,2,4-triethylcyclopentane

[Number to give the 2nd CH_3CH_2 group the lower number: 1,2,4- not 1,3,4- or 1,3,5-.]

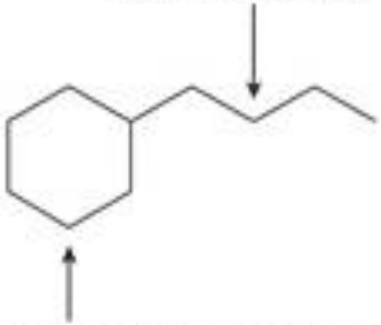
Alkane with a ring and a long chain.





more carbons in the ring

4 C's in the chain —
a **butyl** group



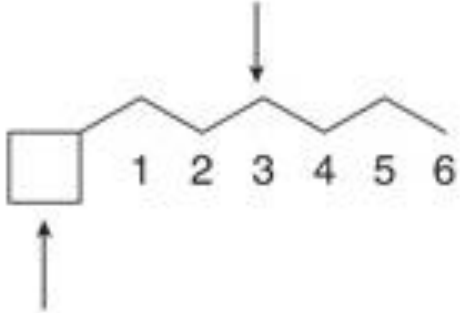
6 C's in the ring—**cyclohexane**

Name as a **cyclohexane** with a substituent.

Answer: butylcyclohexane

more carbons in the chain

6 C's in the chain —
a **hexane**

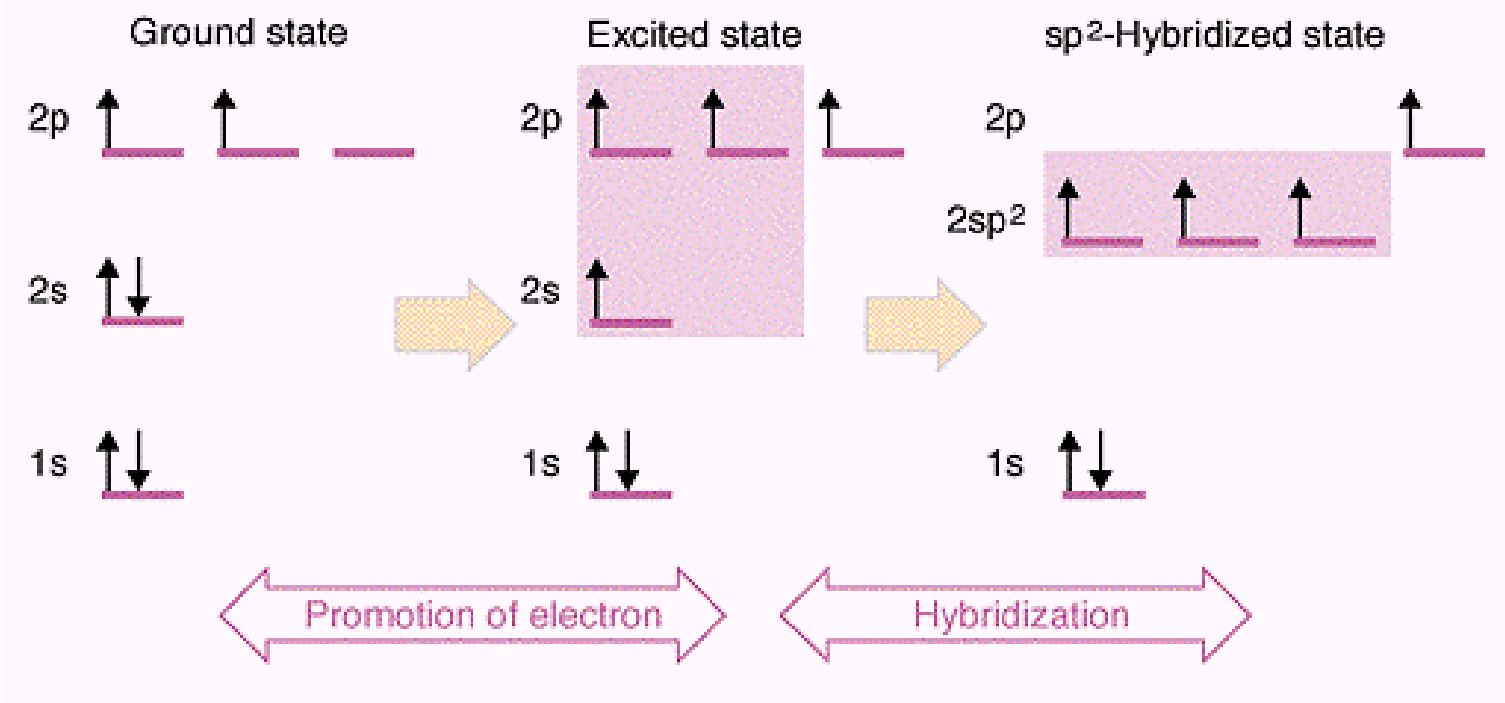


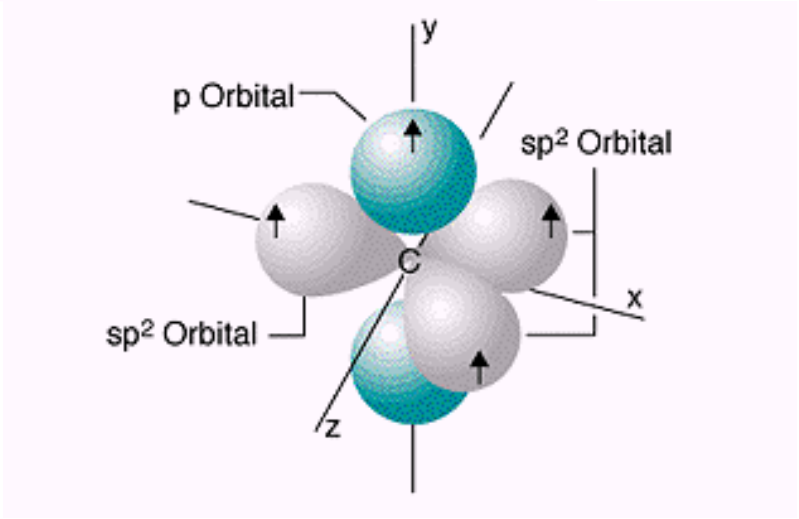
4 C's in the ring—a **cyclobutyl** group

Name as a *hexane* with a substituent.

Answer: 1-cyclobutylhexane

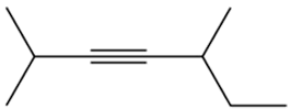
Obtaining sp2-hybridized carbon atoms



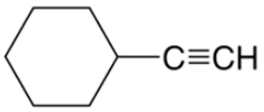


Alkynes - Nomenclature

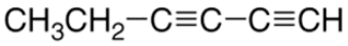
- Compounds with two triple bonds are named as diynes, those with three are named as triynes and so forth.
- Compounds with both a double and triple bond are named as enynes.
- The chain is numbered to give the first site of unsaturation (either C=C or C≡C) the lower number.



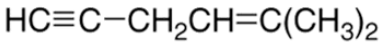
2,5-dimethyl-3-heptyne



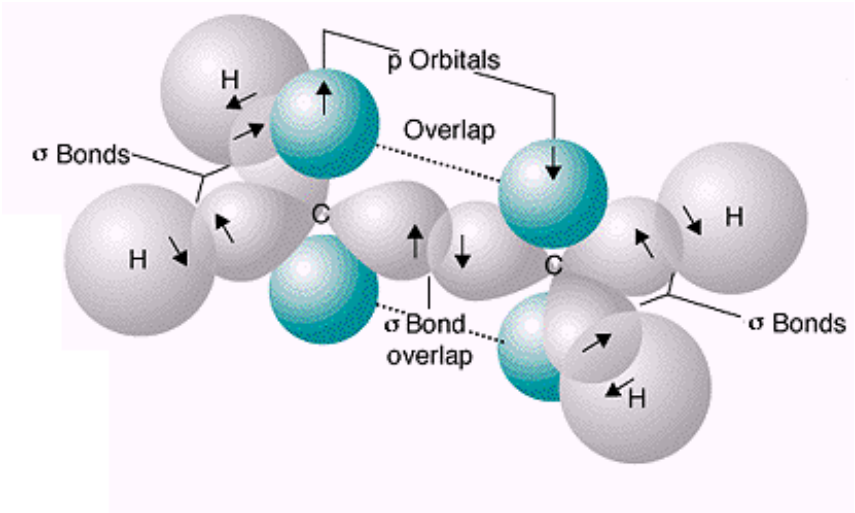
ethynylcyclohexane

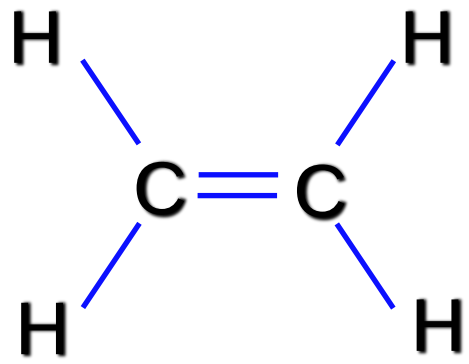


1,3-hexadiyne



5-methyl-4-hexen-1-yne


p Orbitals
H
Overlap
σ Bonds
C
H
C
H
σ Bond
overlap
σ Bonds
H

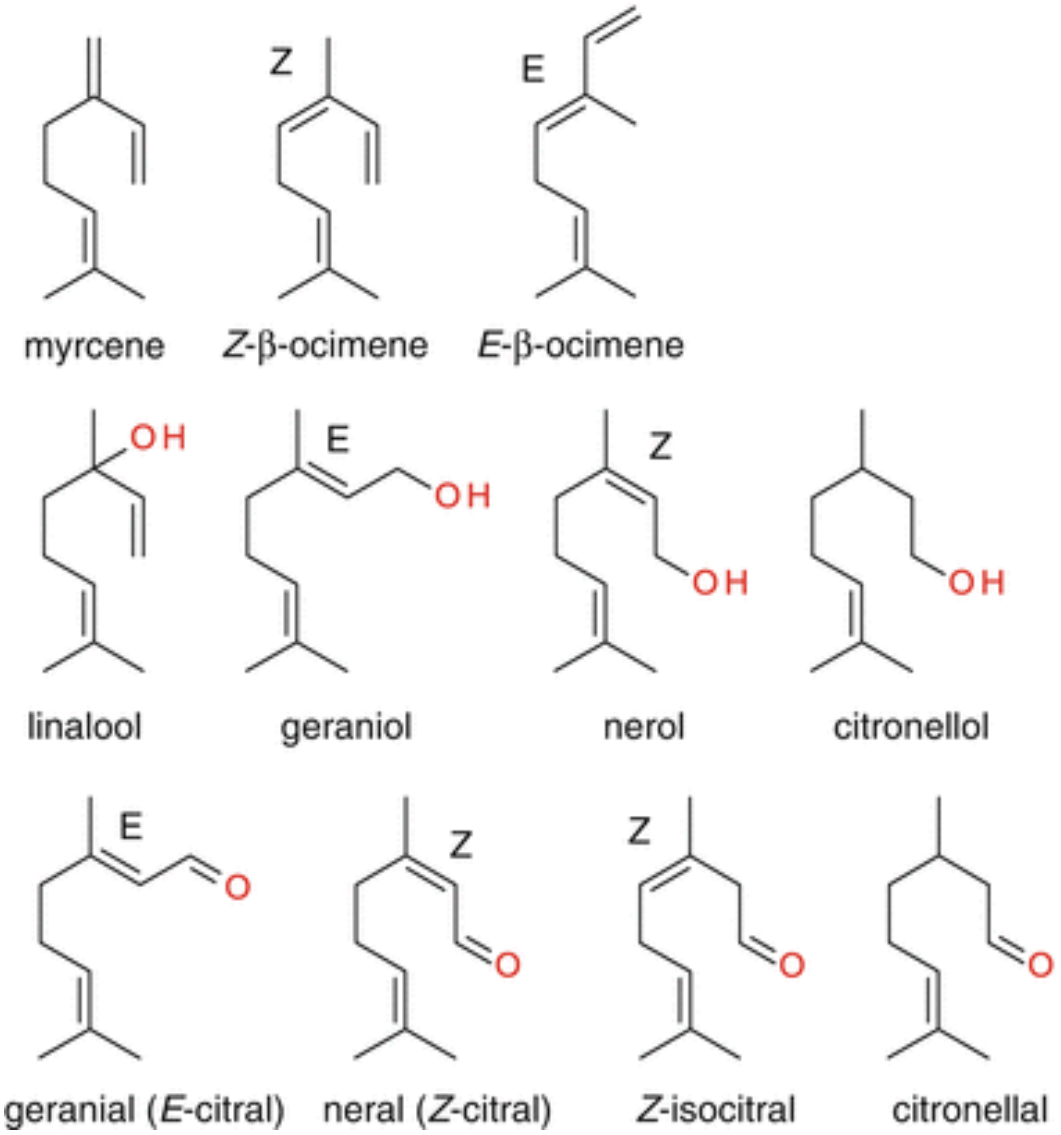

H
H
C
C
H
H

Ethylene

- In terms of quantity produced, ethylene is the most important organic chemical
- Ranked # 4 among all chemicals after
  - 1. Sulfuric acid
  - 2. Nitrogen
  - 3. Oxygen

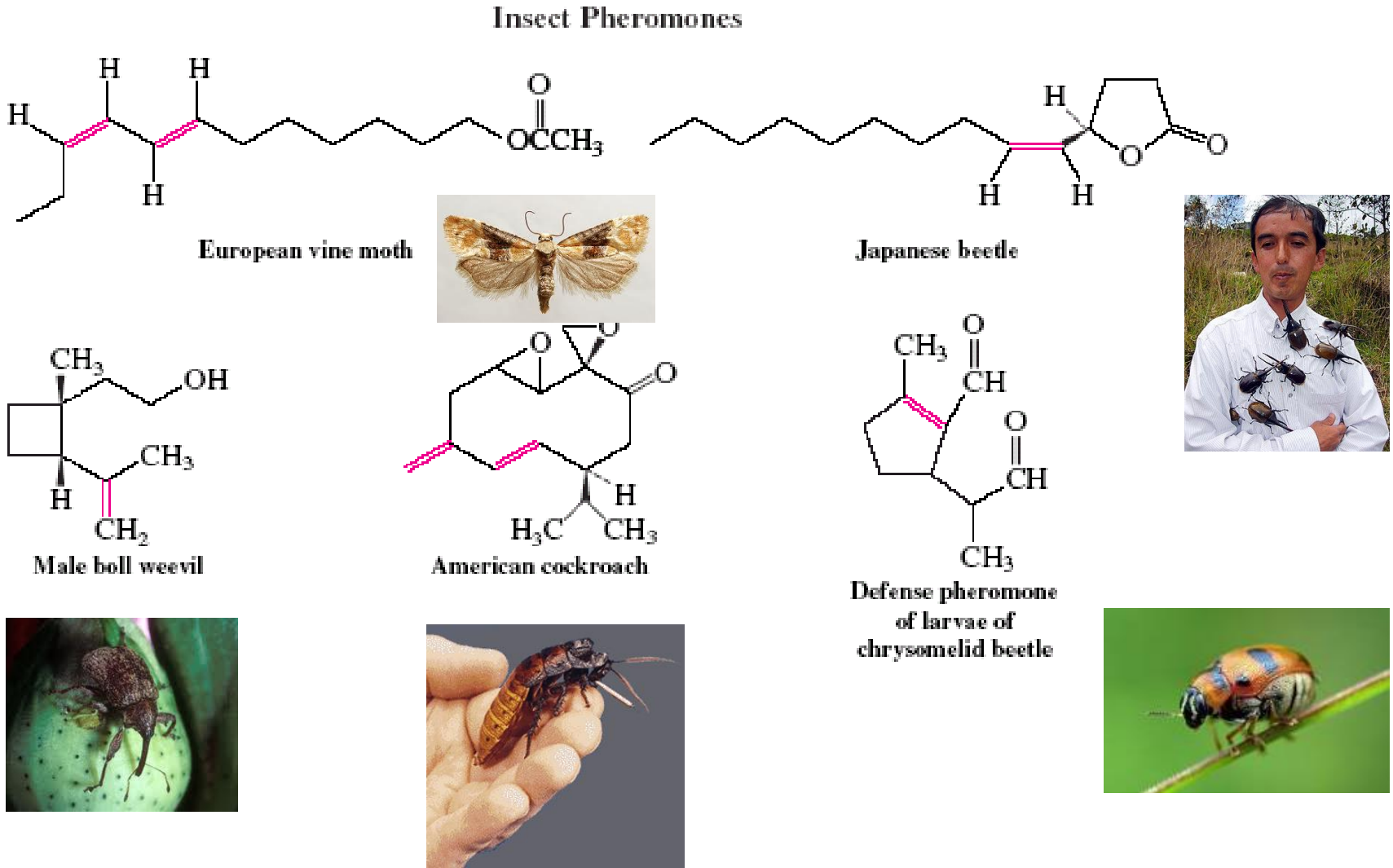
Ethylene Uses

- Polyethylene 55%
- Ethylene dichloride, 16%
- Ethylene glycol, 13%
- Ethylbenzene, 6 %
- Linear alcohols, 4%
- Vinyl acetate, 2%
- Miscellaneous, 4%


myrcene
Z
Z-β-ocimene
E
E-β-ocimene
OH
linalool
E
OH
geraniol
Z
OH
nerol
OH
citronellol
E
O
geranial (E-citral)
Z
O
neral (Z-citral)
Z
O
Z-isocitral
O
citronellal

Alkenes in Nature: Insect Pheromones

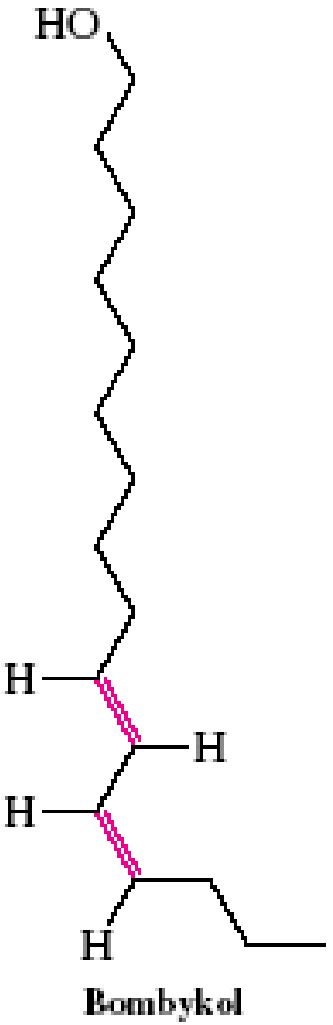
Pheromones are chemical substances used for communication within a living species. Pheromones are used for sex, trail, alarm, and defense signaling, to name a few uses.



The sex attractant for the male silkworm moth is

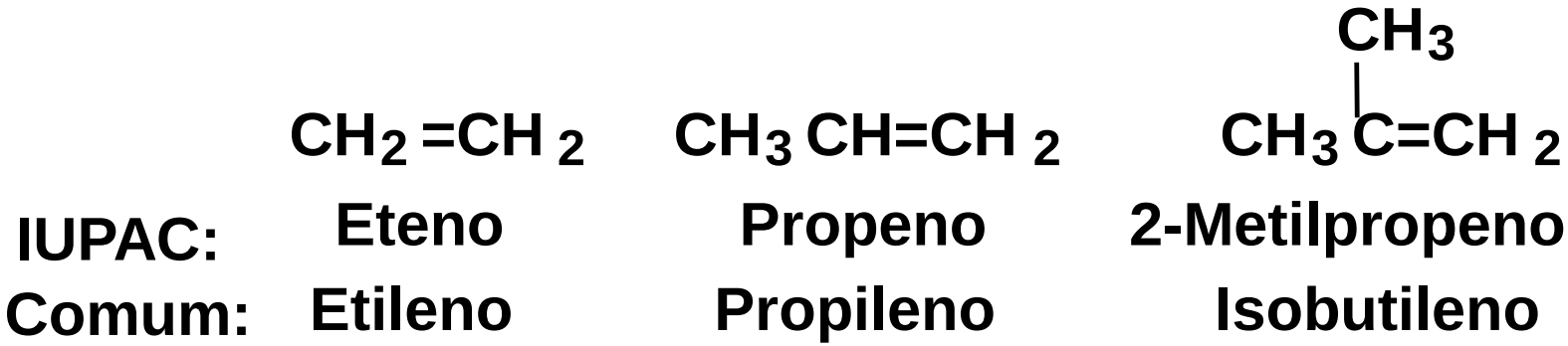
10-*trans*-12-*cis*-hexadecadien-1-ol (bombykol)

The natural pheromome is 10 billion times more active in eliciting a response than is the 10-*cis*-12-*trans* isomer, and 10 trillion times more active than the *trans, trans* isomer.

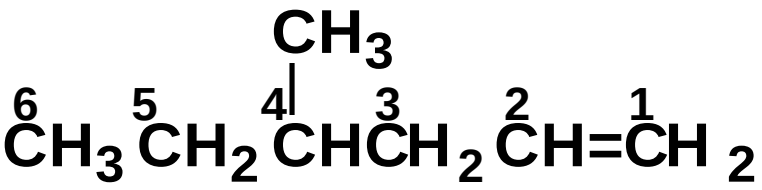


Nomes Comuns

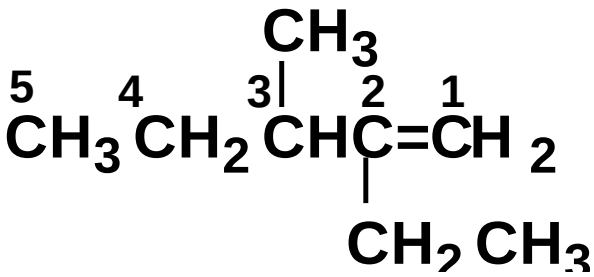
- Apesar da precisão e da aceitação universal da nomenclatura IUPAC, alguns alcenos, particularmente os de baixa massa molecular, são conhecidos quase que exclusivamente por seus nomes comuns



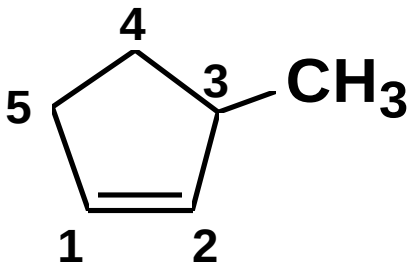
Nomenclatura IUPAC para olefinas



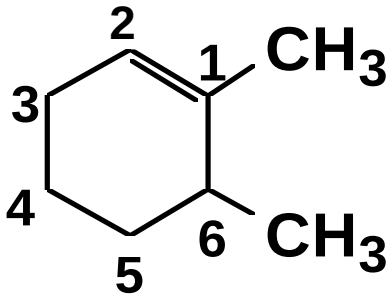
4-Metil-1-hexeno



2-Etil-3-metil-1-penteno



3-Metilciclopenteno

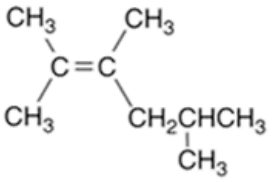


1,6-Dimetilciclohexeno

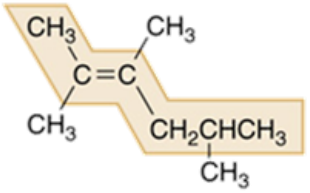
Alkenes - Nomenclature

HOW TO Name an Alkene

Example Give the IUPAC name of the following alkene:



Step [1] Find the longest chain that contains *both* carbon atoms of the double bond.



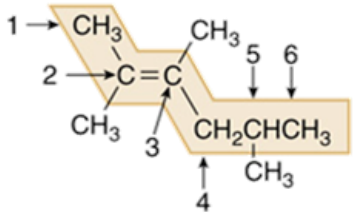
6 C's in the longest chain

hex*ane* ----→ **hex*ene***

- Change the ***-ane*** ending of the parent alkane to ***-ene.***

Step [2] Number the carbon chain to give the double bond the lower number, and apply all other rules of nomenclature.

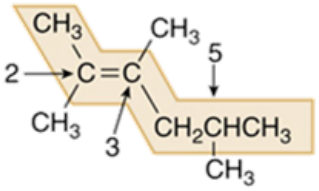
a. **Number** the chain, and name using the ***first*** **number** assigned to the C=C.



- Number the chain to put the C=C at C2, not C4.

2-hexene

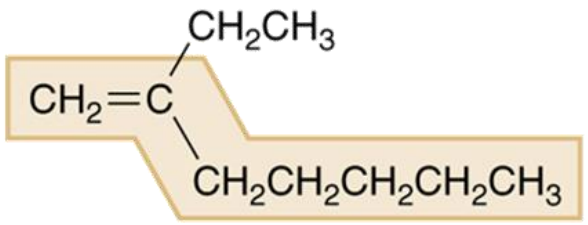
b. **Name** and **number** the substituents.



three methyl groups at C2, C3, and C5

Answer: 2,3,5-trimethyl-2-hexene

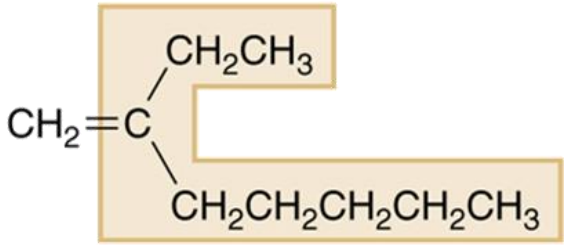
Alkenes - Nomenclature



7 C's ----→ heptene

Both C's of the C=C are contained in this long chain.

***Correct:* 2-ethyl-1-heptene**

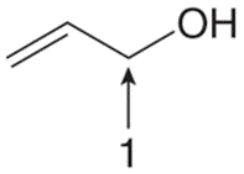


8 C's

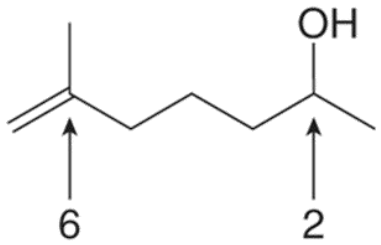
Both C's of the C=C are NOT contained in this long chain.

Incorrect

- Compounds that contain both a double bond and a hydroxy group are named as alkenols and the chain (or ring) is numbered to give the OH group the lower number.



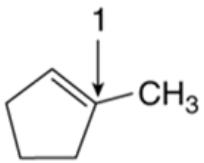
2-propen-1-ol



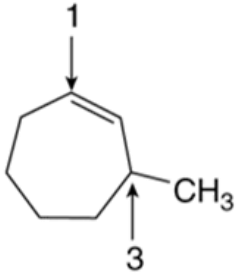
6-methyl-6-hepten-2-ol

Alkenes - Nomenclature

- Compounds with two double bonds are named as dienes by changing the “-ane” ending of the parent alkane to the suffix “-adiene”.
- Compounds with three double bonds are named as trienes, and so forth.
- In naming cycloalkenes, the double bond is located between C1 and C2, and the “1” is usually omitted in the name.
- The ring is numbered clockwise or counterclockwise to give the first substituent the lower number.

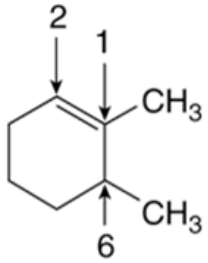


1-methylcyclopentene



3-methylcycloheptene

Number clockwise beginning at the C=C and place the CH_3 at C3.

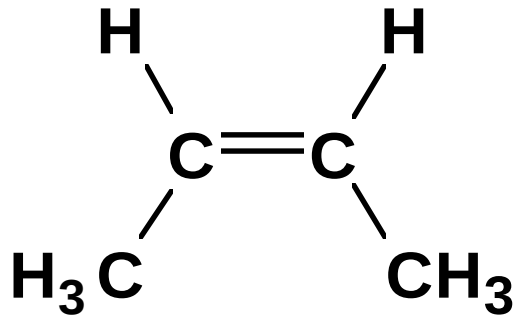


1,6-dimethylcyclohexene

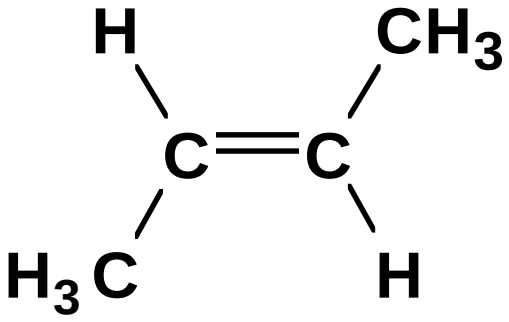
Number counterclockwise beginning at the C=C and place the first CH_3 at C1.

Isomeria *Cis-Trans*

- Devido à restrição de rotação da ligação dupla
  C-C, grupos em carbonos adjacentes podem ser *cis* ou *trans* uns aos outros



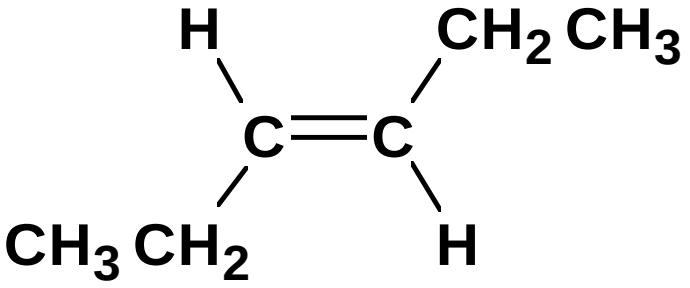
cis-2-Buteno
pf= -139°C, pe= 4°C



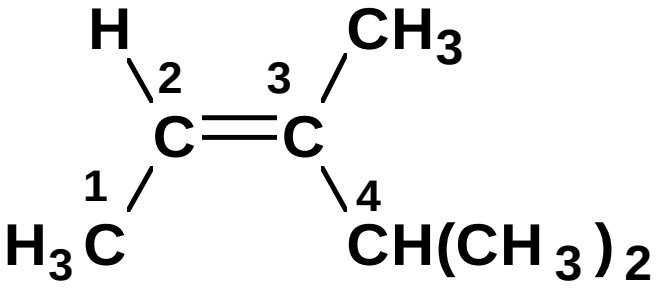
trans-2-Buteno
pf= -106°C, pe= 1°C

Configuração

- O sistema *cis-trans*: a configuração é determinada pela orientação dos átomos da cadeia principal



***trans*-3-Hexeno**



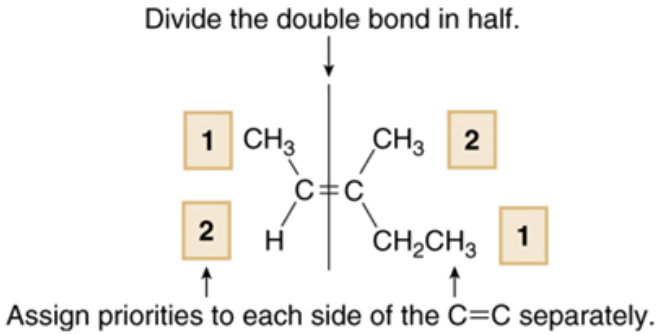
***cis*-3,4-Dimetil-2-penteno**

Alkenes - Nomenclature

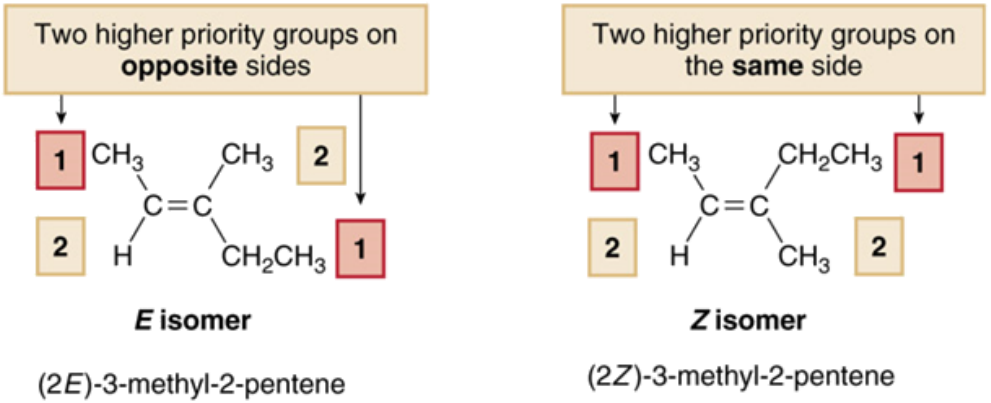
HOW TO Assign the Prefixes *E* and *Z* to an Alkene

Step [1] Assign priorities to the two substituents on each end of the C=C by using the priority rules for *R,S* nomenclature (Section 5.6).

- Divide the double bond in half, and assign the numbers **1** and **2** to indicate the relative priority of the two groups on each end—the higher priority group is labeled **1,** and the lower priority group is labeled **2.**



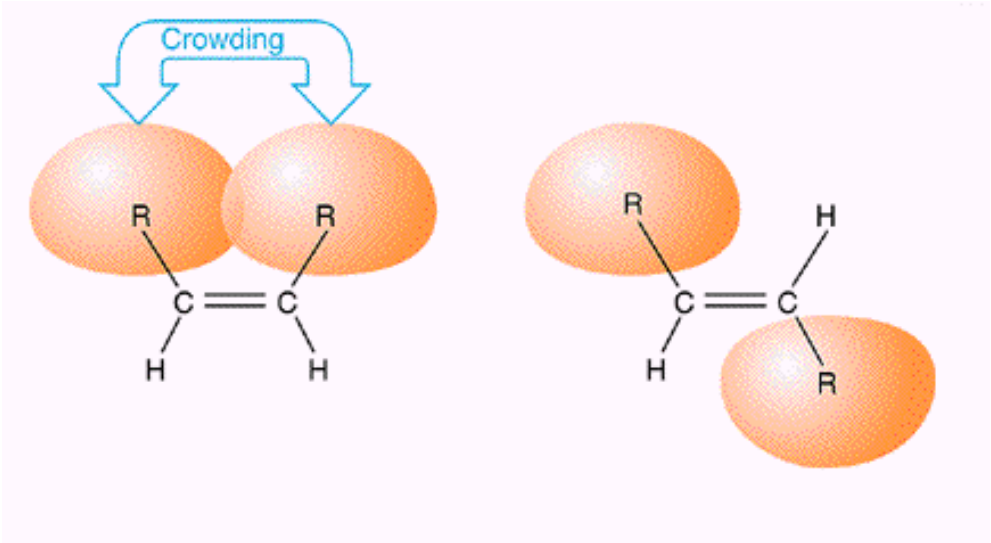
Step [2] Assign *E* or *Z* based on the location of the two higher priority groups (1).



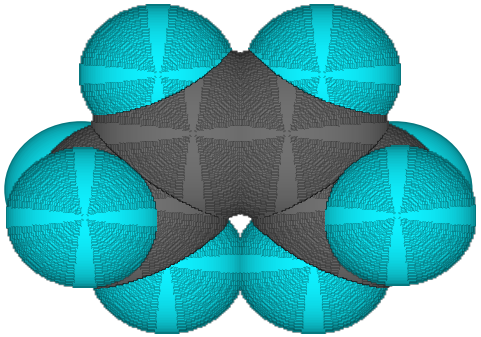
- The ***E*** isomer has the two higher priority groups on the **opposite sides.**
- The ***Z*** isomer has the two higher priority groups on the **same side.**

Estrutura dos Alcenos

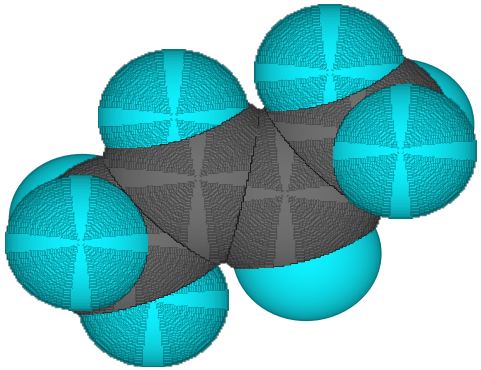
- Os alcenos *trans* são mais estáveis que os *cis* devido a interações não-ligadas (estéricas)



alceno *cis* (*Z*)



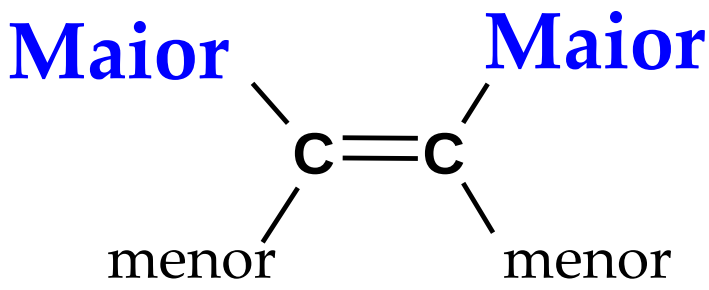
alceno *trans* (*E*)



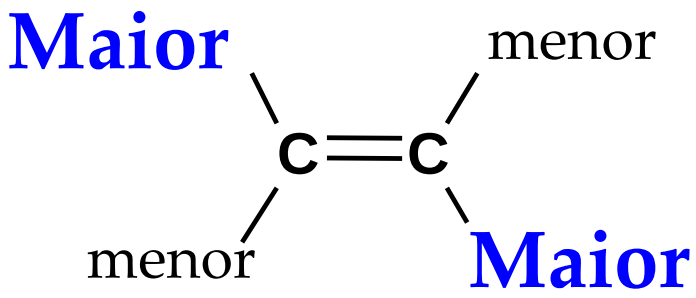
Configuração - E,Z

- O sistema E,Z usa as regras de prioridade
- Se os grupos de maior prioridade estão do mesmo lado, a configuração é Z (em alemão, *zusammen*)
- Se os grupos de maior prioridade estão de lados opostos, a configuração é E (em alemão, *entgegen*)

Configuração - E,Z



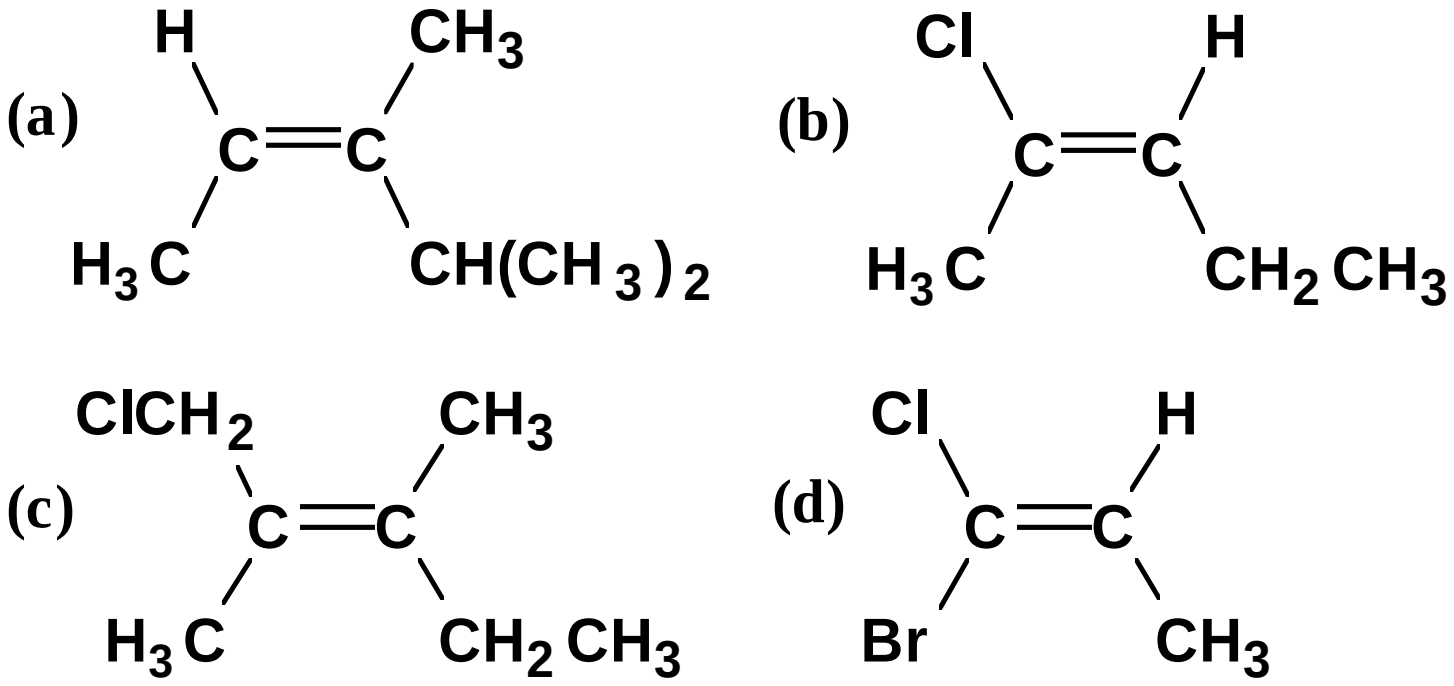
Z (zusammen)



E (entgegen)

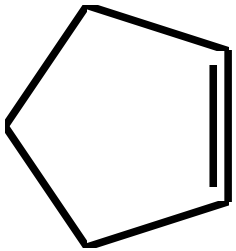
Configuração - *E,Z*

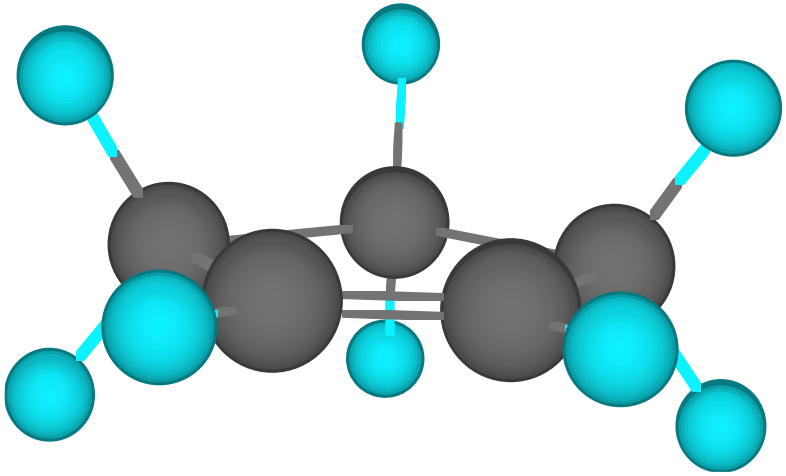
- Exemplo: nomeie cada alceno e especifique sua configuração pelo sistema E,Z



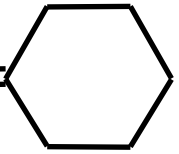
Isomeria *Cis-Trans* em cicloalcenos

- Do ciclopropeno ao cicloheptено a configuração da dupla ligação é sempre *cis*
- O ciclopenteno é planar

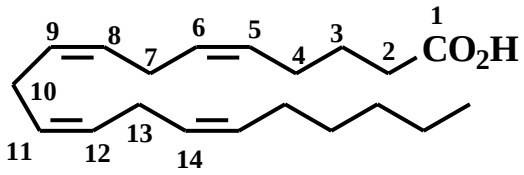




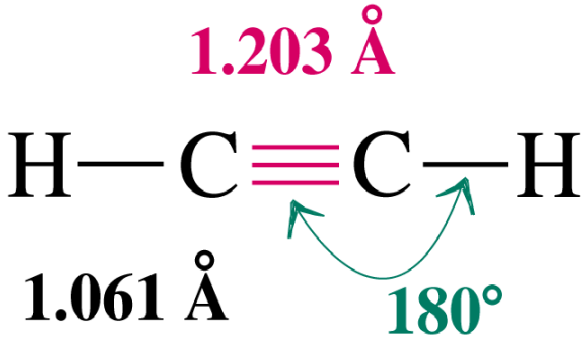
Grupos Alquenila

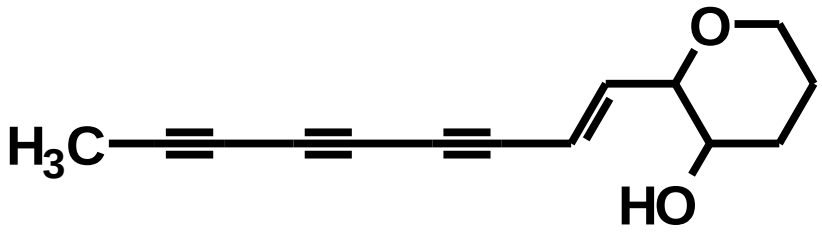
Grupos Alquenila	Nomes Comuns	Exemplos
$CH_2=$	metileno	 metilenociclohexano
$CH_2=CH-$	vinila	$CH_2=CHCl$ cloreto de vinila
$CH_2=CHCH_2-$	alila	$CH_2=CHCH_2Cl$ cloreto de alila

Ácidos graxos insaturados (PUFAs - poly-unsaturated fatty acids) mais comuns (múltiplos de C2)

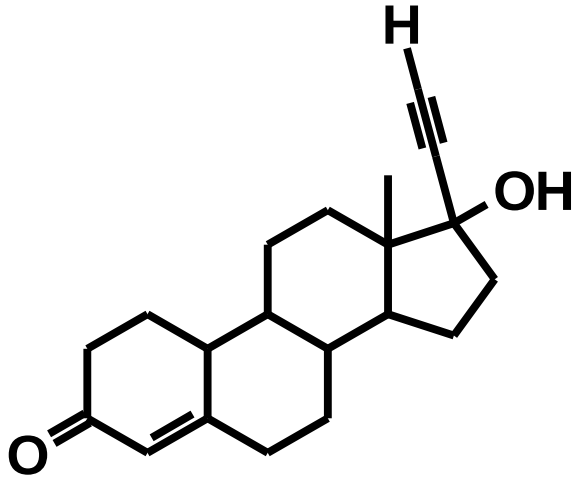
esqueleto carbônico	Estrutura	Nome comum	Ponto de fusão
16:1(Δ^{9})	$CH_3(CH_2)_5{=}CH(CH_2)_7CO_2H$	ácido palmitoleico	-0,5
18:1(Δ^{9})	$CH_3(CH_2)_7{=}CH(CH_2)_7CO_2H$	ácido oleico	13,4
18:2($\Delta^{9,12}$)	$CH_3(CH_2)_4{=}CHCH_2CH{=}CH(CH_2)_7CO_2H$	ácido α–linolênico	-5
18:3($\Delta^{9,12,15}$)	$CH_3CH_2CH{=}CHCH_2CH{=}CHCH_2CH{=}CH(CH_2)_7CO_2H$	ácido linolênico	-11
20:4($\Delta^{5,8,11,14}$)		ácido araquidônico	-49,5

ALCINOS



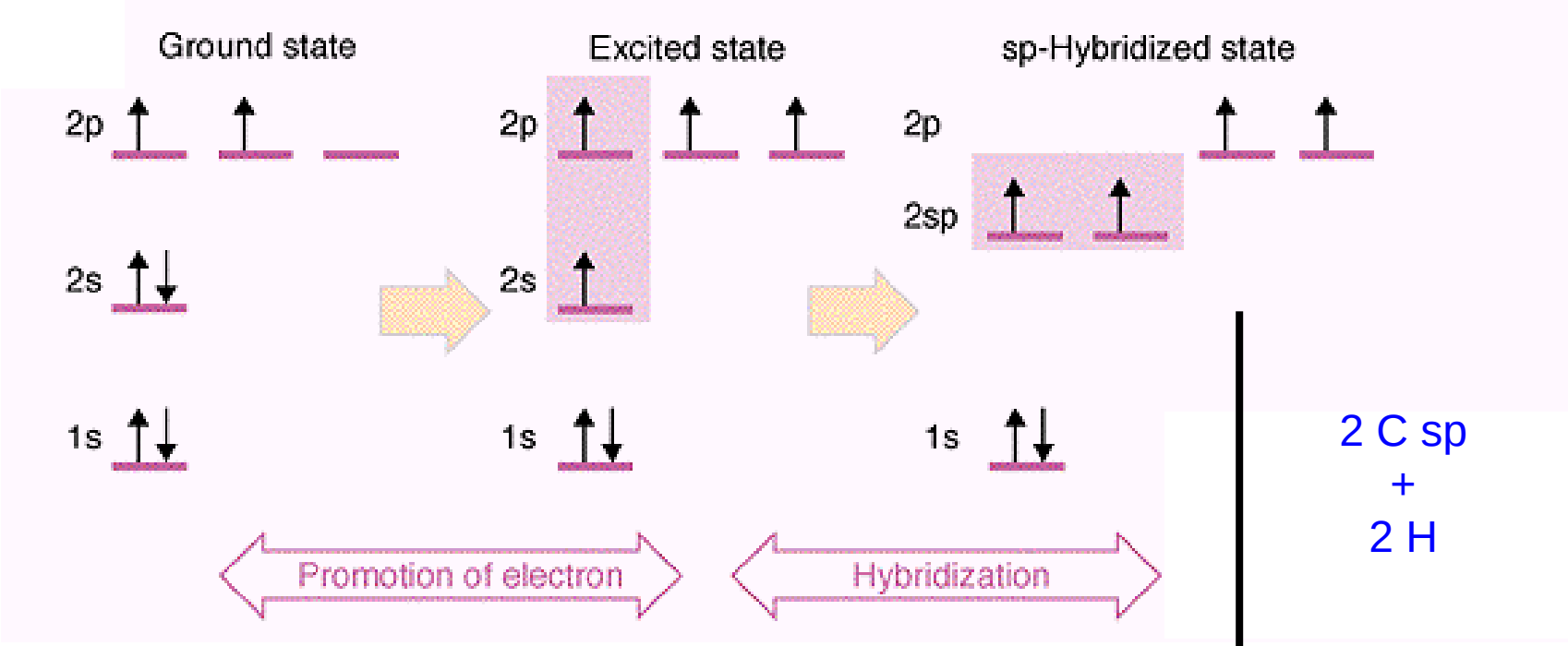


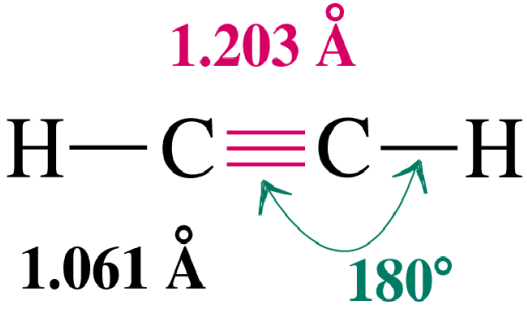
Ichthyothereol: a polyyne that occurs in plants in the genus Ichthyothere and is highly toxic to fish.

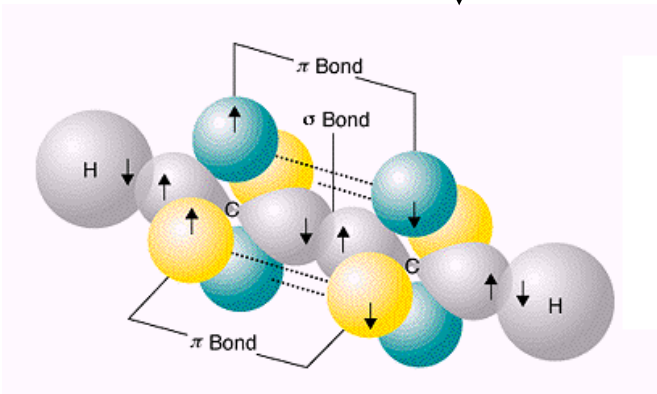


Ethinylestradiol: is an estrogen widely used in birth control pills in combination with Progestins.

Obtaining sp-hybridized carbon atoms







Alkynes - Nomenclature

- Alkynes are named in the same general way that alkenes are named.

- In the IUPAC system, change the –*ane* ending of the parent alkane name to the suffix –*yne*.

- Choose the longest continuous chain that contains both atoms of the triple bond and number the chain to give the triple bond the lower number.

Índice de deficiência de hidrogênio

MM 82 Compatível com C_6H_{10}

Se fosse saturado seria C_6H_{14} (CnH_2n+2)

4H de diferença = 2 H_2 (duas deficiências)

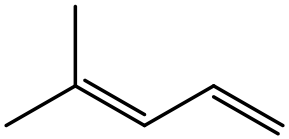
IDH= nC+1 – nH/2 + nN/2

P.ex. C_6H_{10} **IDH= 6+1 – 10/2= 7-5= 2**

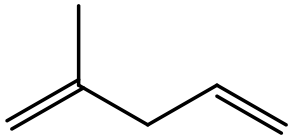
Índice de deficiência de hidrogênio

MM 82 Compatível com C_6H_{10}

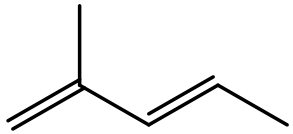
Quais estruturas seriam possíveis?



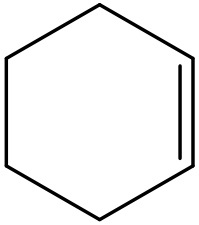
4-methylpenta-1,3-diene



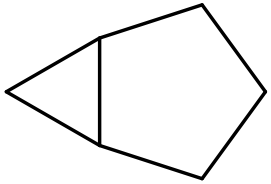
2-methylpenta-1,4-diene



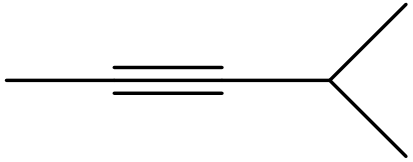
(*E*)-2-methylpenta-1,3-diene



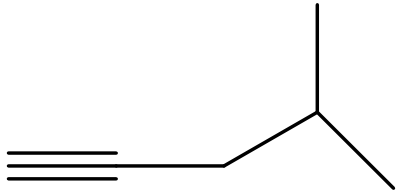
cyclohexene



bicyclo[3.1.0]hexane



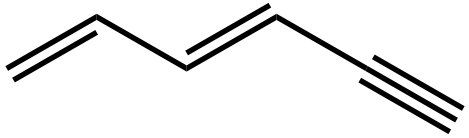
4-methylpent-2-yne



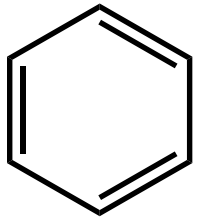
4-methylpent-1-yne

Possíveis estruturas para C_6H_6 ?

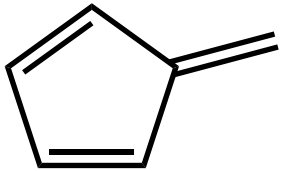
IDH = 4



(*E*)-hexa-1,3-dien-5-yne



benzene



fulvene

IDH= 1 pode ser uma dupla ou um anel

IDH para C_6H_5Br ? (= C_6H_6)

X (F, Cl, Br e I) são monovalentes

IDH para C_6H_6O ? (= C_6H_6)

Oxigênio é divalente