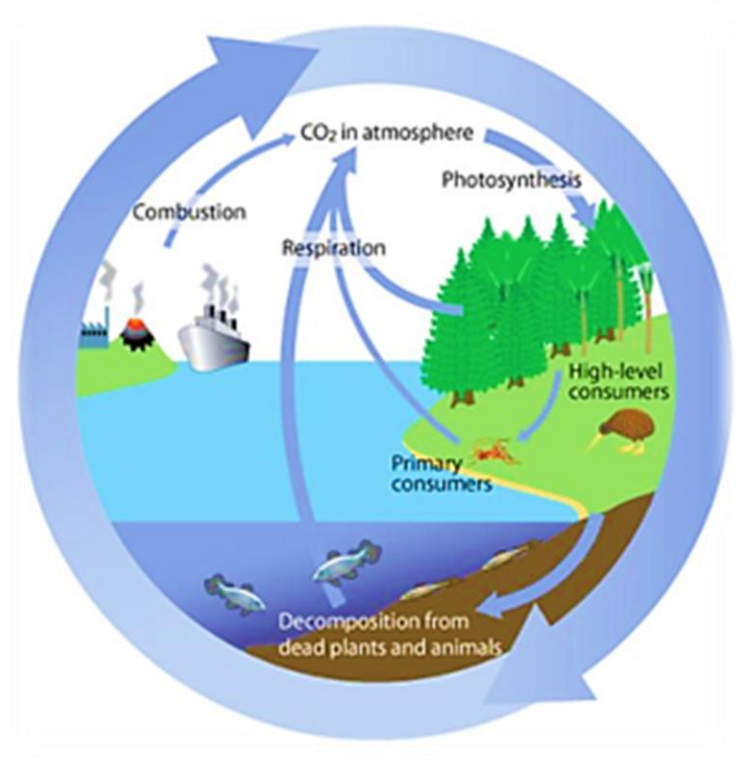
INTRODUCCION A LA QUIMICA ORGÁNICA

[CARBONO, HIBRIDACIÓN Y ENLACES]



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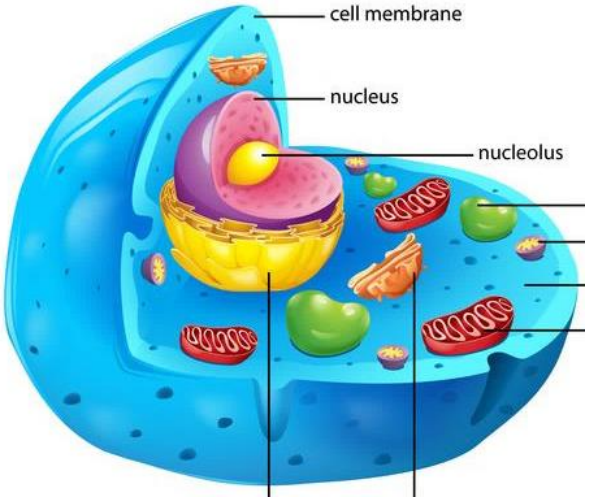
Universidad de Chile

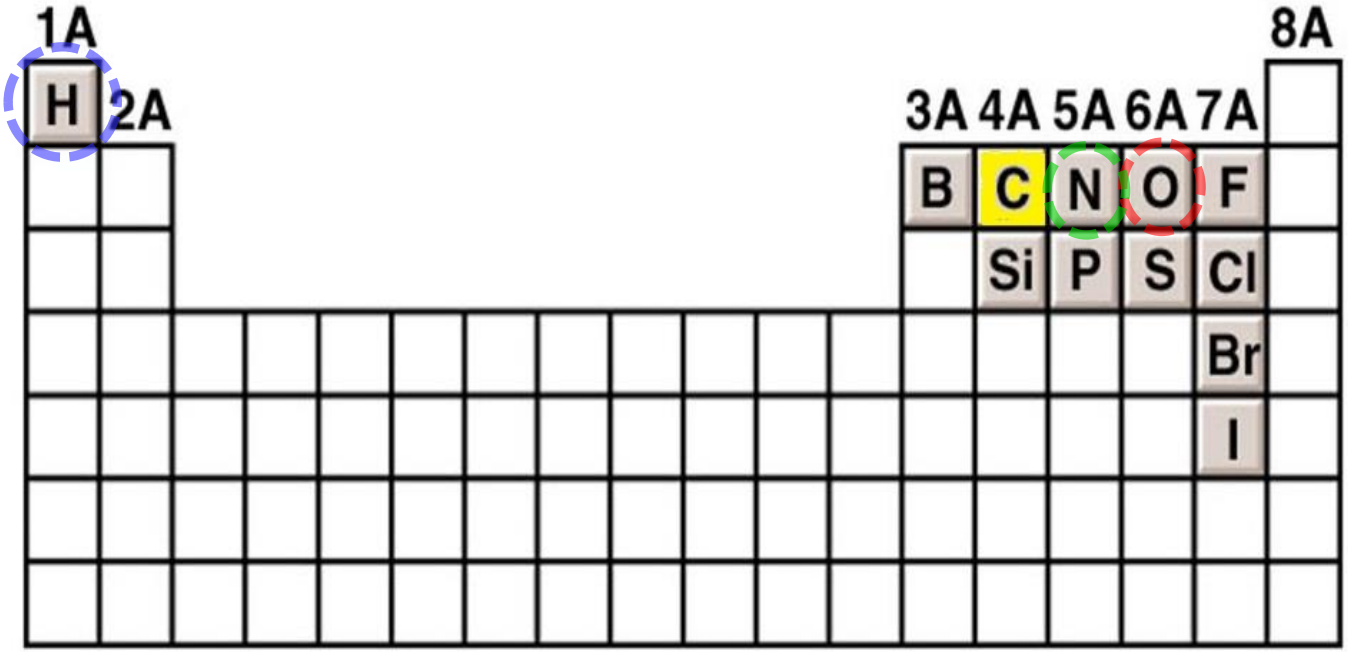
Introducción

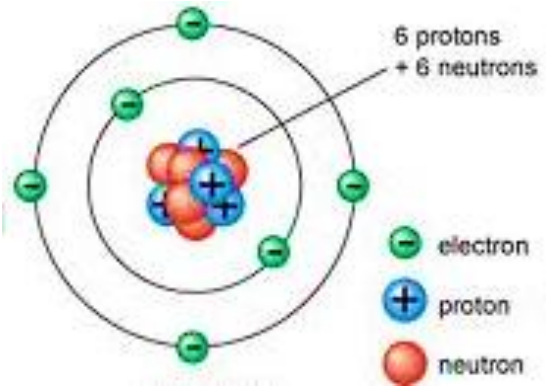
- La ***química orgánica*** estudia los compuestos de carbono (C)
- C el principal componente de las ***moléculas orgánicas***
- Presentes naturalmente en ***seres vivos*** como constituyentes y como fuentes de energía.
- ~13 millones de compuestos orgánicos (100 mil inorgánicos)

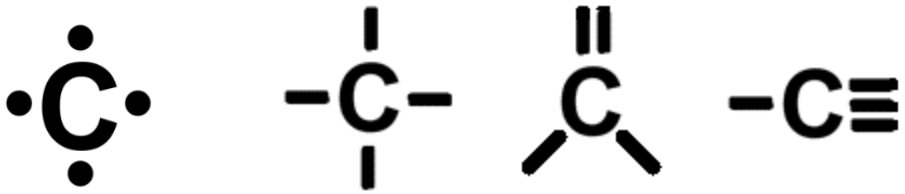


- Los compuestos orgánicos estan presentes en
  - Alimentos (carbohidratos, grasas y proteinas)
  - Combustibles (carbon, gas, petroleo)
  - Plásticos (PVC, polietileno, Teflon)
  - Fibras naturales y sintéticas
  - Fármacos
  - Higiene y cosmética
  - Colorantes y pinturas
  - Agroquímicos

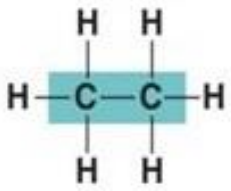
Importancia del carbono

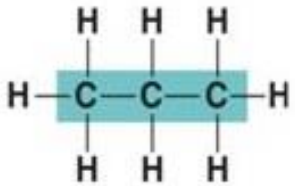


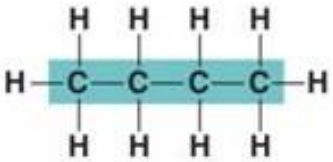


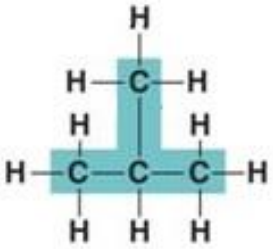


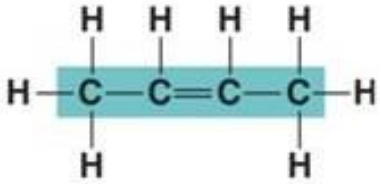
Versatilidad del carbono

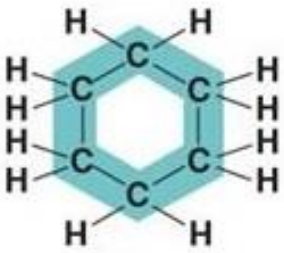


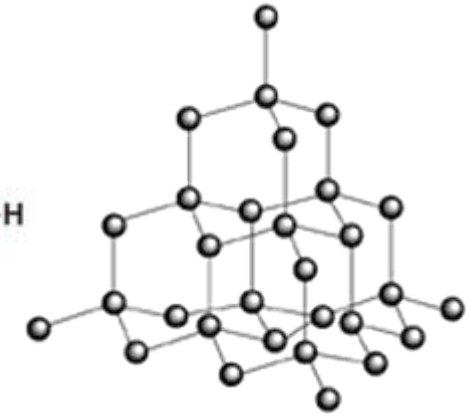




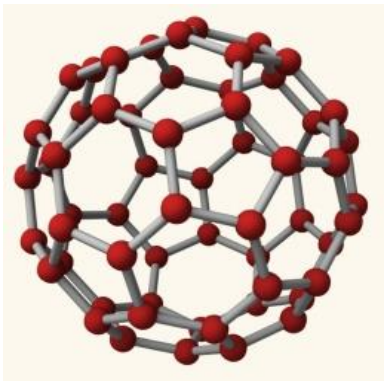




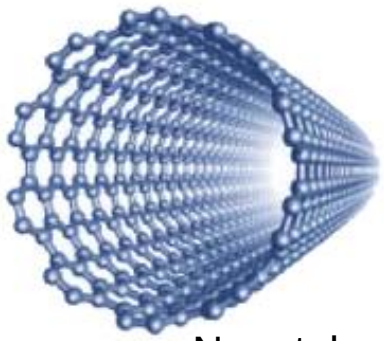




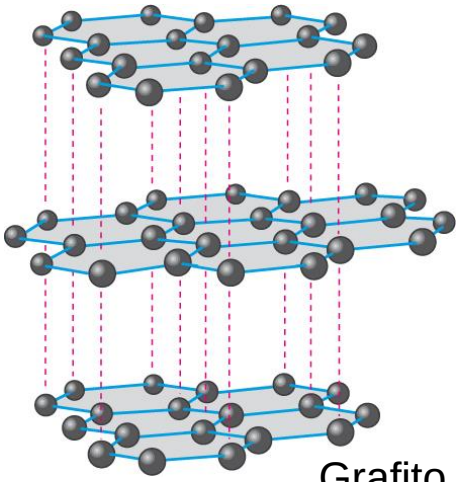
Diamante



Fullereno C-60



Nanotubos C_n

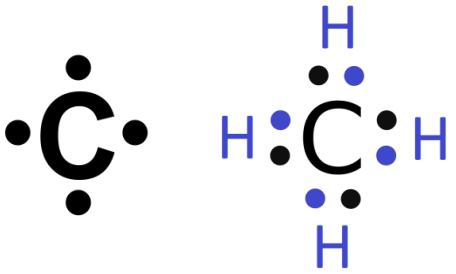


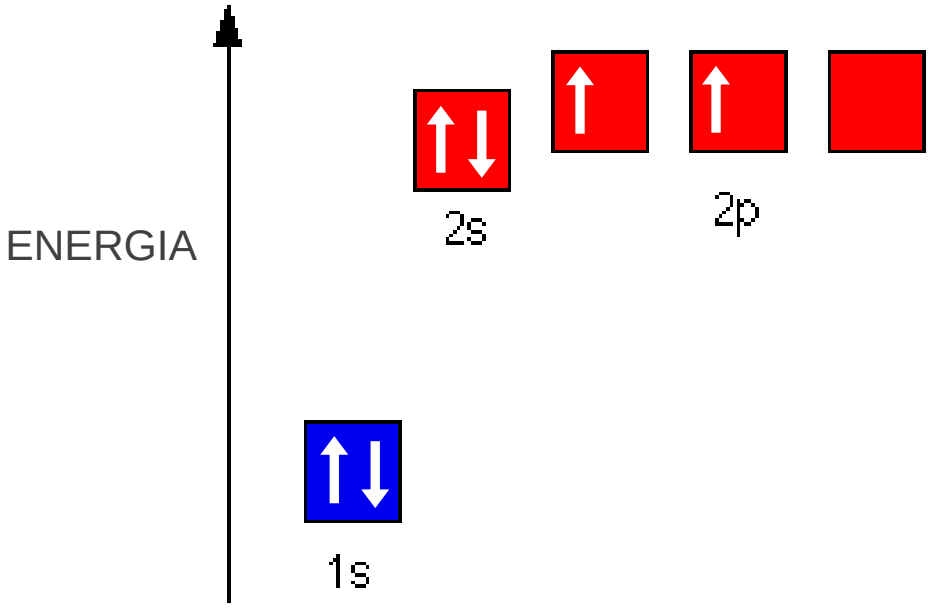
Grafito

Configuración electrónica del carbono

C (Z=6)

$1s^2\ 2s^2\ 2p^2$





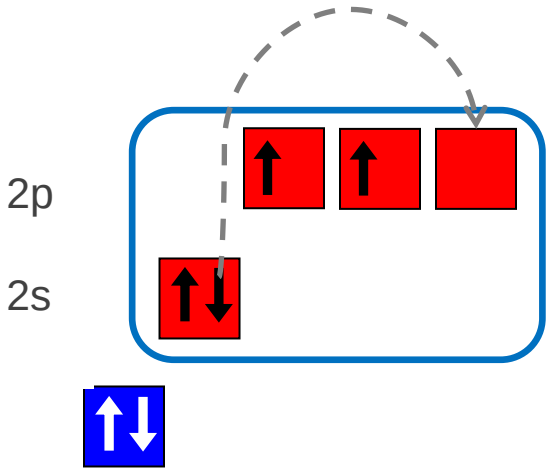
El C posee 4 electrones de valencia y por lo tanto puede formar 4 enlaces… ¿Cómo se concilia esto con la configuración electrónica del C?

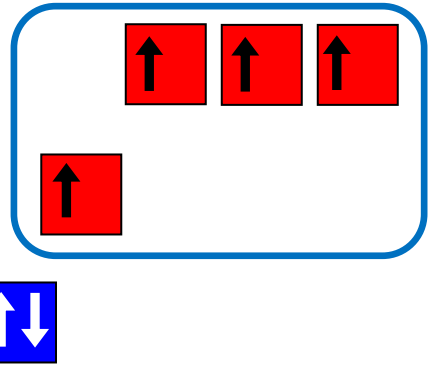
C (Z=6) $1s^2$ $2s^2$ $2p^2$

$1s^2$ $2s^2$ $2p_x^1$ $2p_y^1$ $2p_z$

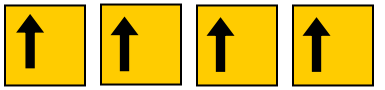
$1s^2$ $2s^1$ $2p_x^1$ $2p_y^1$ $2p_z^1$

$1s^2$ $2sp^1$ $2sp^1$ $2sp^1$ $2sp^1$

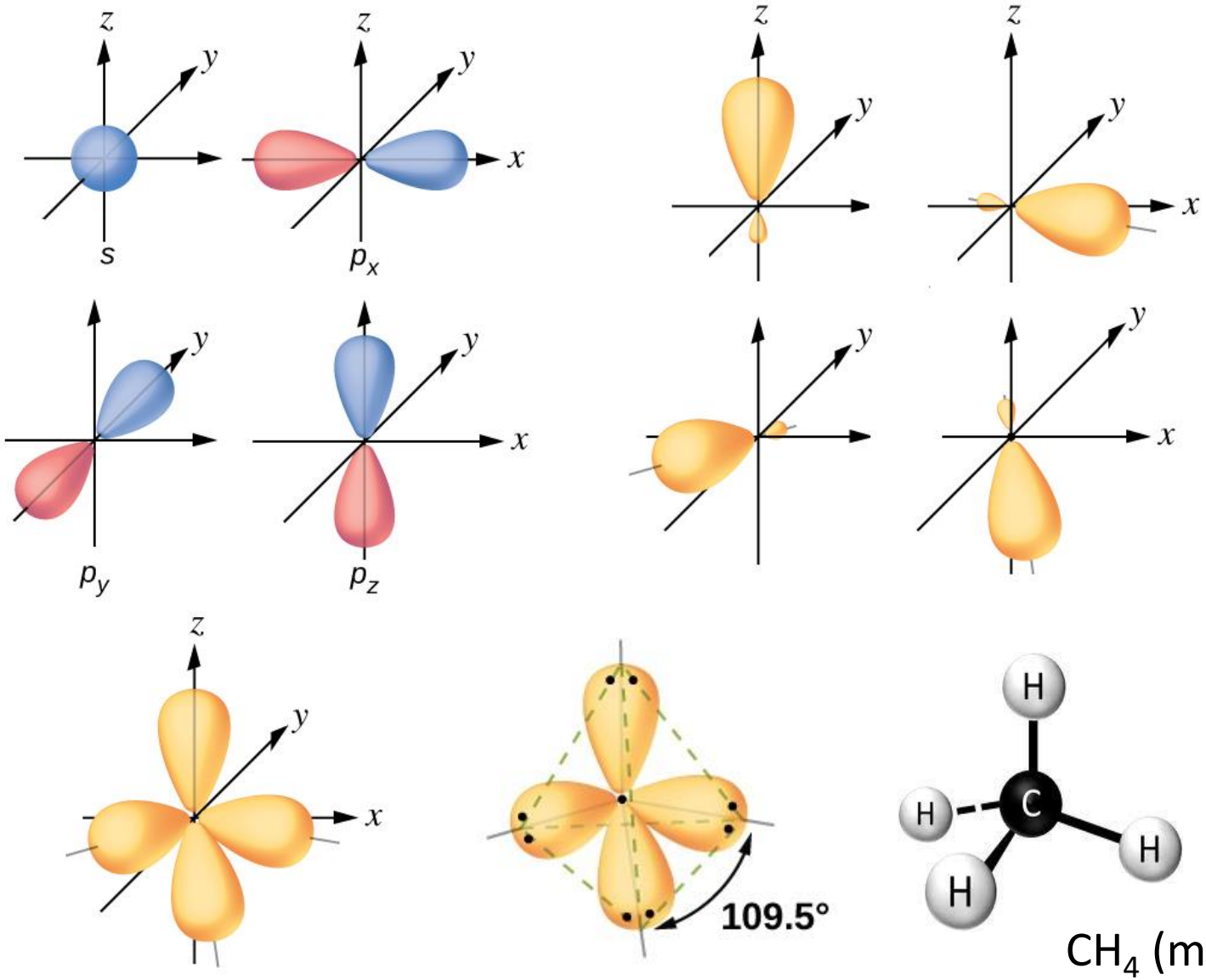




Se forman 4 orbitales "hibridos" *sp3*



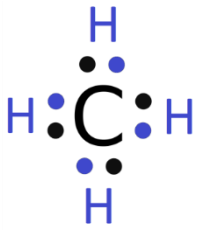
Hibridación SP3

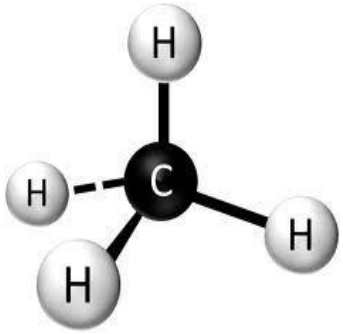


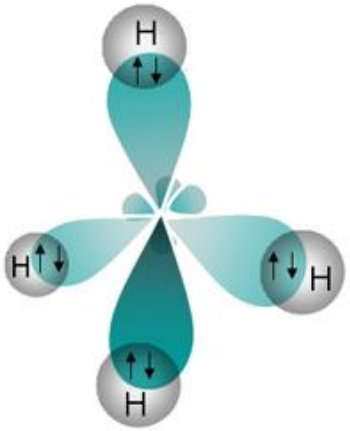
CH_4 (metano)

http://philschatz.com/chemistry-book/contents/m51057.html

Hibridación SP3 / Enlaces sigma

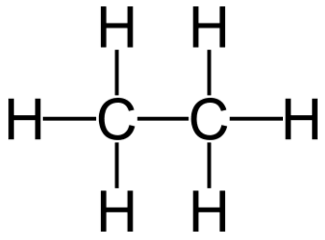


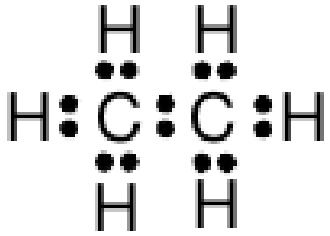


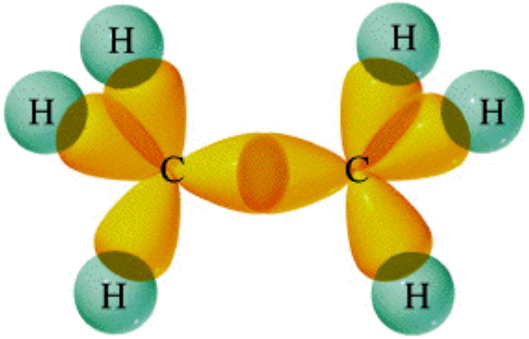


Se forma sólo un tipo de enlace sigma (σ) entre:

- orbital s del H
- orbital sp3 del C





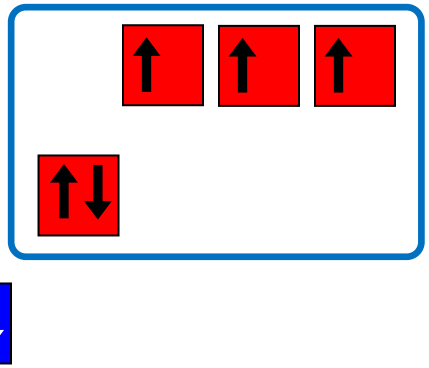


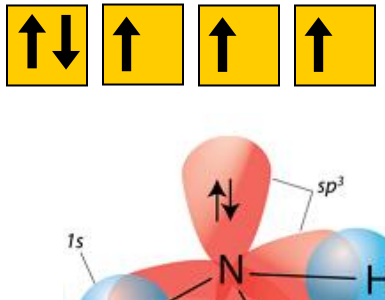
En el etano se forman dos tipos de enlace sigma (σ):

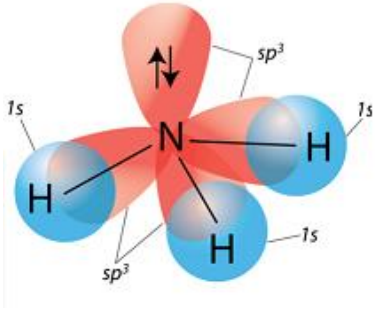
- orbital s del H / orbital sp3 del C
- orbitales sp3 de ambos carbonos

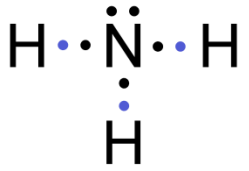
Hibridación SP3 / Nitrógeno y Oxígeno

N (Z=7) $1s^2$ $2s^2$ $2p^3$



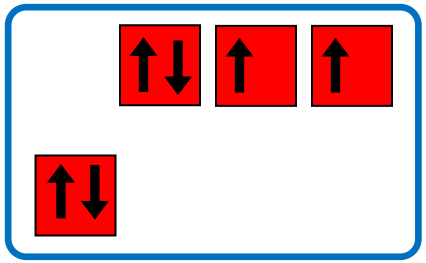


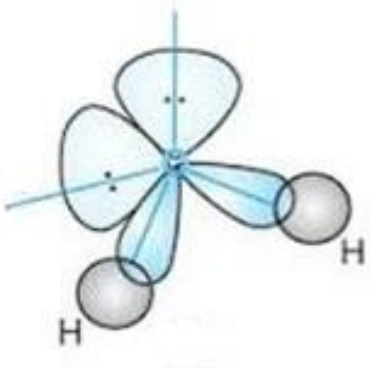


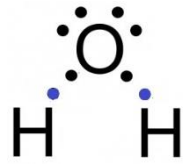


NH_3 (amoníaco)

O (Z=8) $1s^2$ $2s^2$ $2p^4$

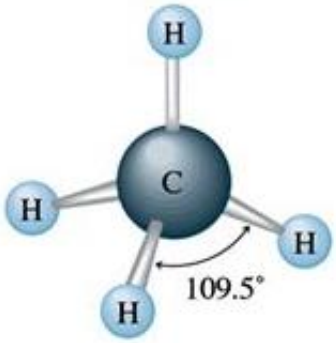
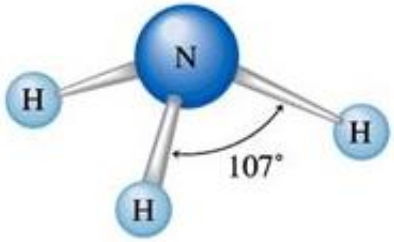
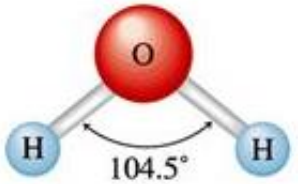






H_2O (agua)

Hibridación SP3 y geometría

	Metano	*Amoníaco*	*Agua*
			
Electronica	**tetrahédrica**	**tetrahédrica**	**tetrahedrica**
Molecular	**tetrahédrica**	**trigonal-piramidal**	**angular**

sp3 con é enlazantes

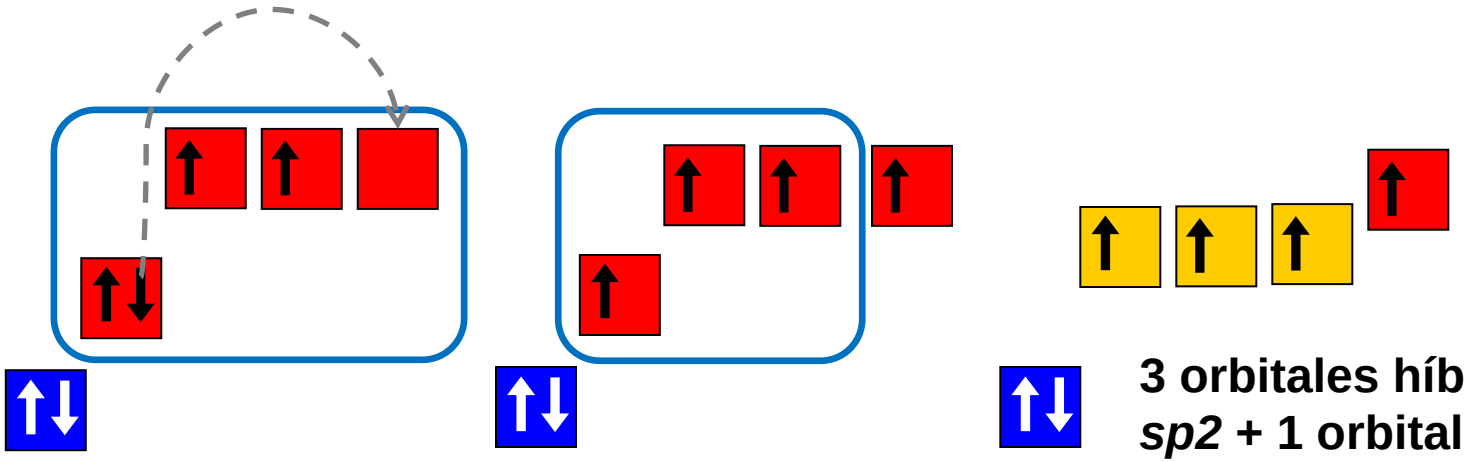
sp3 con par de é libres

C (Z=6) $1s^2$ $2s^2$ $2p^2$

$1s^2$ $2s^2$ $2p_x^1$ $2p_y^1$ $2p_z$

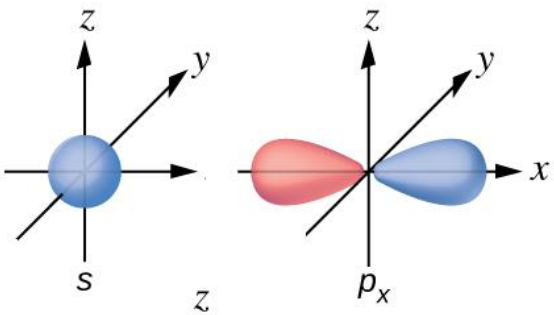
$1s^2$ $2s^1$ $2p_x^1$ $2p_y^1$ $2p_z^1$

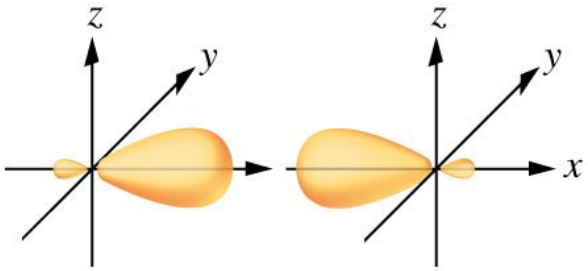
$1s^2$ $2sp^1$ $2sp^1$ $2sp^1$ $2p_z^1$

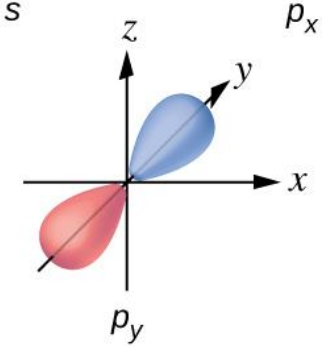


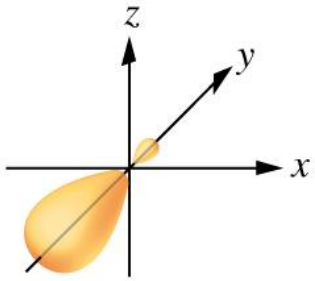
3 orbitales híbridos *sp2* + 1 orbital p

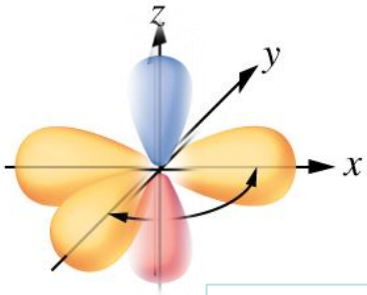
Hibridación SP2

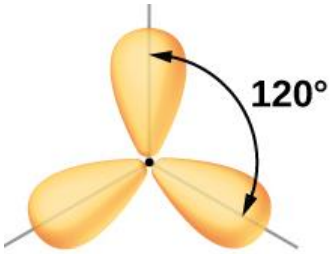




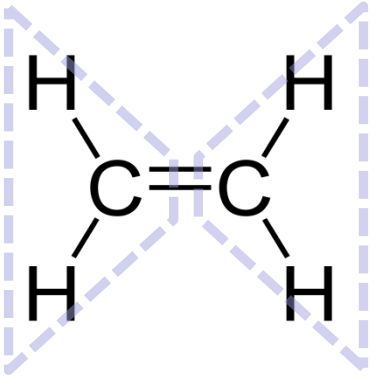








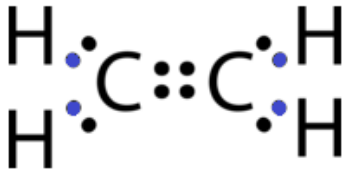
$CH_2{=}CH_2$ (eteno)

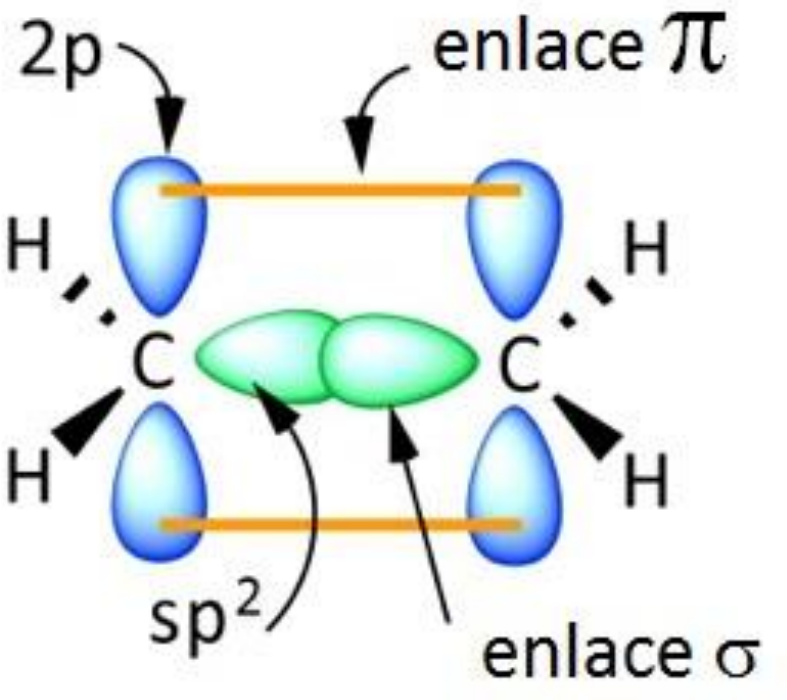


- Los 3 orbitales hibridos sp^2 ocupan el mismo plano, mientras que el orbital p libre es perpendicular a dicho plano. → ***la geometria de los carbonos sp2 es TRIGONAL PLANA***

Hibridación SP2

$CH_2=CH_2$ (eteno)





Se forman 5 enlaces sigma (σ)

- Entre 2 orbitales sp2 de ambos carbonos

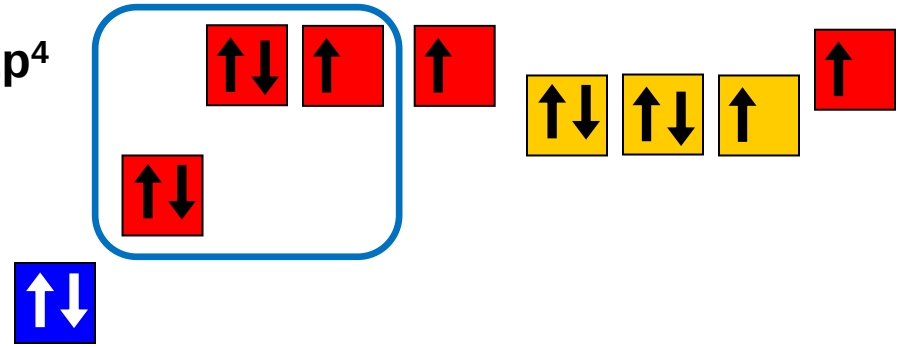
- Entre un orbital sp2 del carbono y el orbital s del hidrógeno.

Se forma un enlace pi (π)

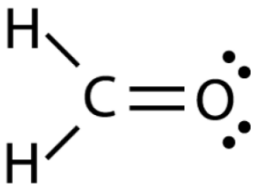
- Entre orbitales p libres que no participaron en la hibridación *sp2*.

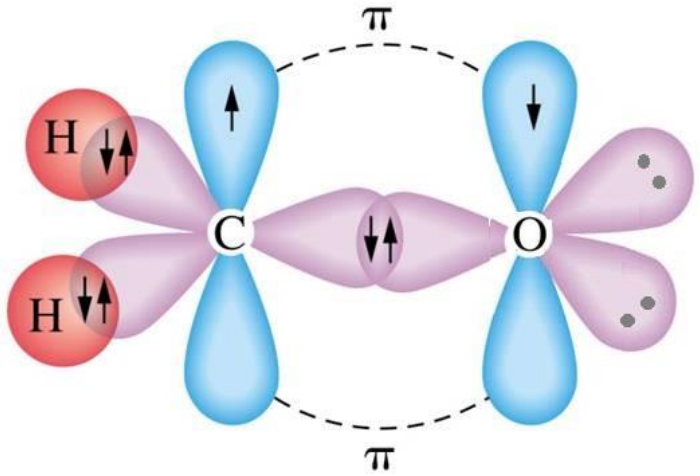
Hibridación SP2 - Oxígeno

O (Z=8) $1s^2$ $2s^2$ $2p^4$



HCHO
(formaldehido
o metanal)





- Los 2 pares de electrones no apareados del O ocupan 2 orbitales hibridos ***sp2***.
- Se forma un enlace pi (π) entre orbitales p libres del O y del C, que no fueron utilizados para formar los orbitales hibridos sp2 del C y del O..

Resumen – hibridación de orbitales

	N° de átomos unidos a cada carbono		
	4 (3H+1C)	*3 (2H+1C)*	*2 (1H+1C)*
Molécula representativa	CH_3CH_3	$CH_2=CH_2$	$CH\equiv CH$
Hibridación	sp3	sp2	sp
Geometría	tetrahédrica	trigonal	lineal
> enlace	109,5°	120°	180°
Tipos de enlace (C)	4 simples	2 simples + 1 doble	1 simple + 1 triple
Orbitales moleculares	**7 σ (6 CH +1 CC)**	**5 σ (4 CH + 1 CC) 1 π**	**3 σ (2 CH + 1 CC) 2 π**
Longitud enlace C-C	1,54 A°	1,34 A°	1,20 A°
Energía enlace C-C	347 kJ	611 kJ	837 kJ

HIDROCARBUROS ALIFÁTICOS I

ALCANOS

Ulises Urzúa

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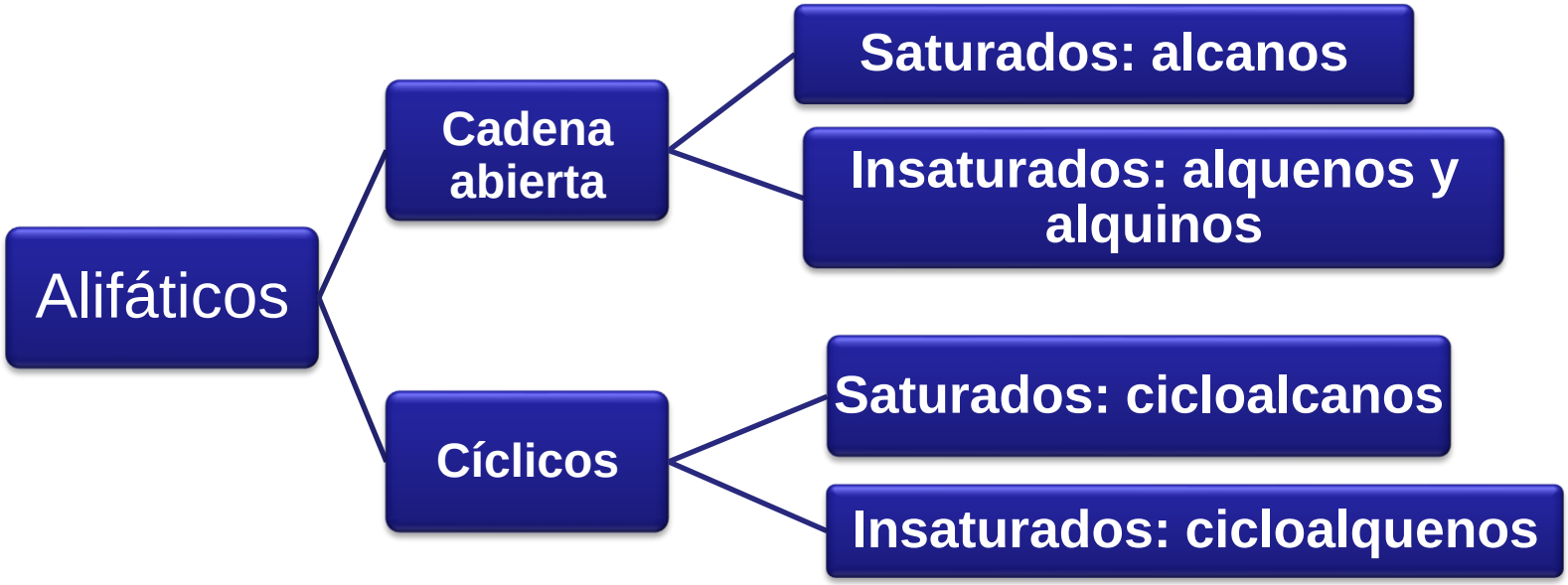
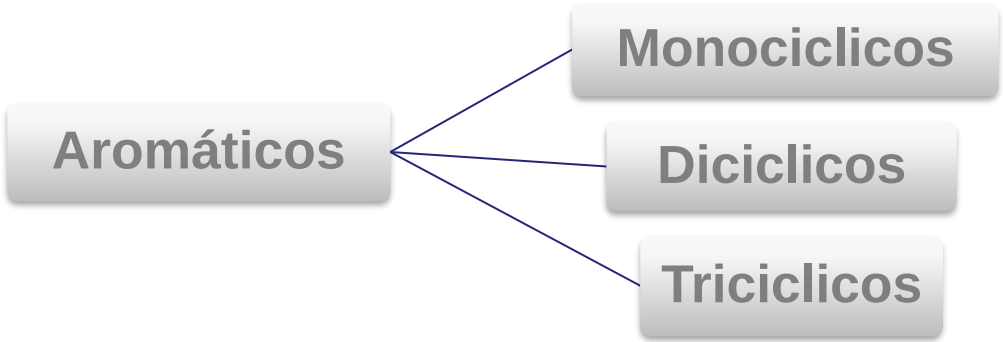
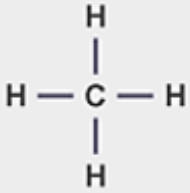
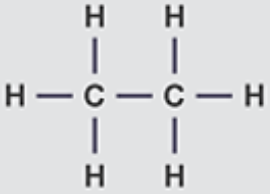
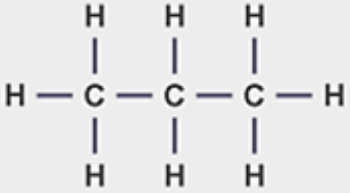
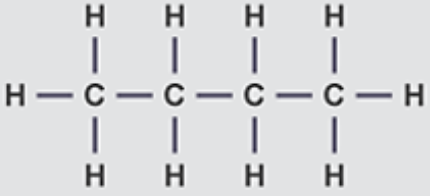
Universidad de Chile

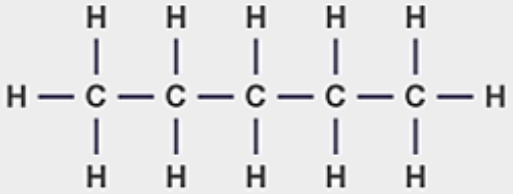
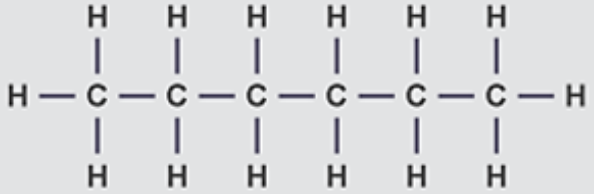
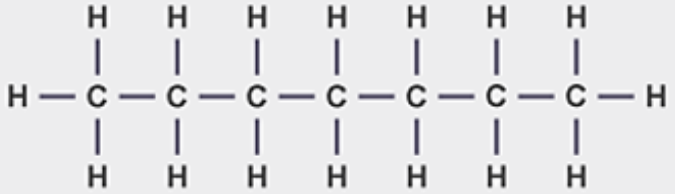
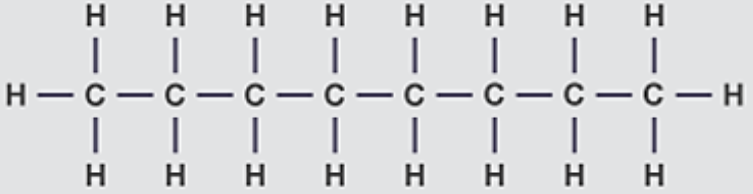
Hidrocarburos alifáticos



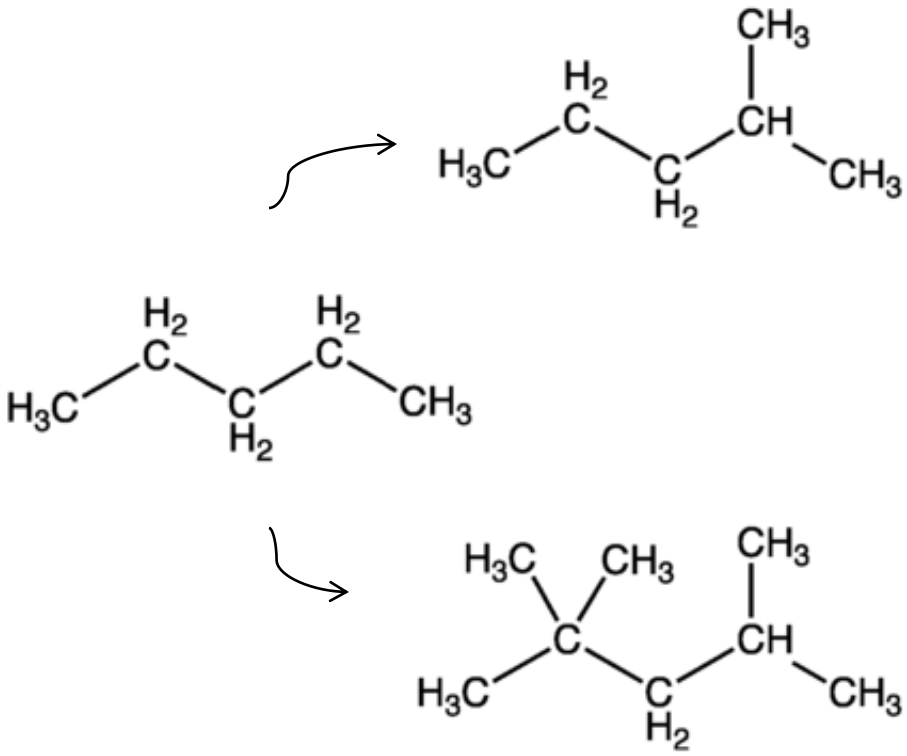


A. Alcanos de cadena contínua ($C_n H_{2n+2}$)

Molecular formula	Full structural formula
CH_4 Metano	
C_2H_6 Etano	
C_3H_8 Propano	
C_4H_{10} Butano	

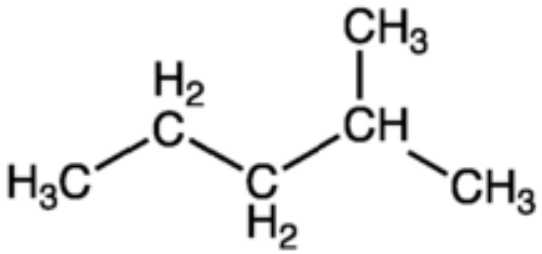
Molecular formula	Full structural formula
C_5H_{12} Pentano	
C_6H_{14} Hexano	
C_7H_{16} Heptano	
C_8H_{18} Octano	

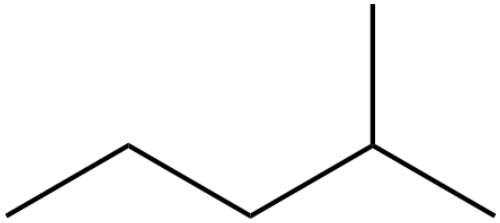
B. Alcanos de cadena ramificada:
Un hidrógeno unido a un carbono “interno” de la cadena, es reemplazado por un carbono o una cadena corta de carbonos

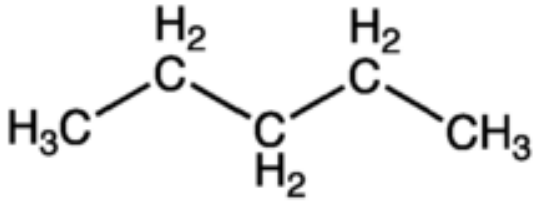


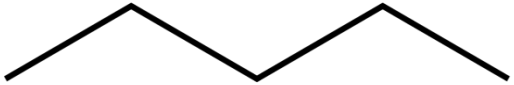
#C	formula	nombre
1	$-CH_3$	metil
2	$-CH_2CH_3$	etil
3	$-CH_2CH_2CH_3$	propil
4	$-CH_2(CH_2)_2CH_3$	butil
5	$-CH_2(CH_2)_3CH_3$	pentil

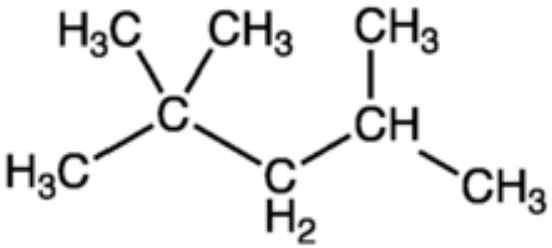
C. Alcanos lineales y ramificados: formula estructural condensada

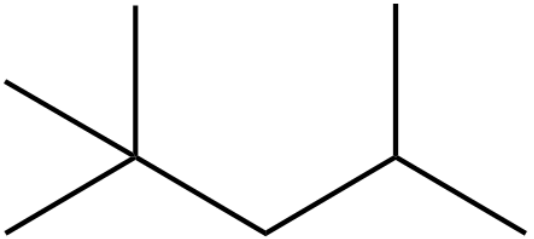






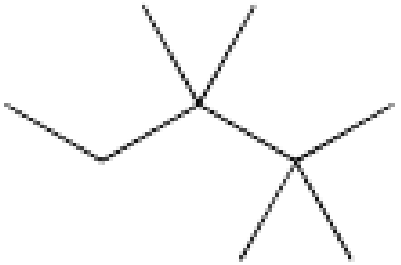




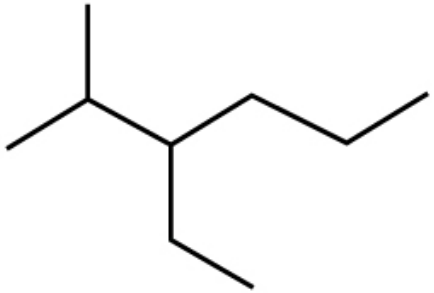


D. Alcanos ramificados: nociones de nomenclatura

a) Identificar cadena hidrocarbonada de mayor longitud
b) Identificar grupos alquilo sustituyentes
c) Asignar posiciones de grupos alquilo de tal forma que *la suma de ellas sea la menor posible* – considerar prioridad alfabética

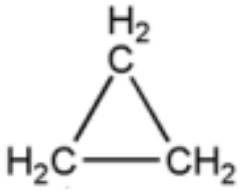
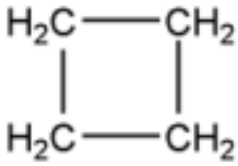
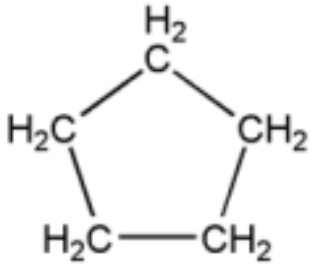
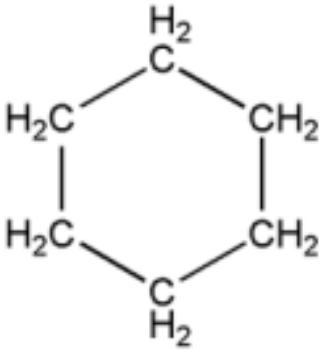
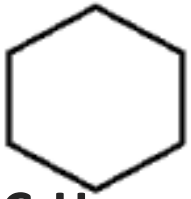


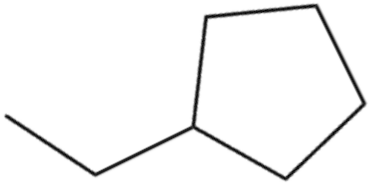
2,2,3,3-tetrametilpentano
no 3,3,4,4-tetrametil

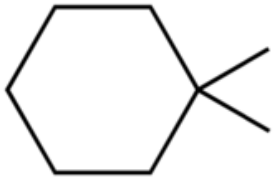


3-etil-2-metilhexano
no 4-etil-5-metil

Cicloalcanos

ciclopropano	ciclobutano	ciclopentano	ciclohexano
			
			
C_3H_6	C_4H_8	C_5H_{10}	C_6H_{12}





$$2\ C_nH_{2n+2} + (3n+1)\ O_2 \rightarrow 2n\ CO_2 + (2n+2)\ H_2O + \text{calor}$$

$$C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O + \text{calor}$$

ENTALPIAS DE COMBUSTION [kcal(kJ)/mol], 25°C

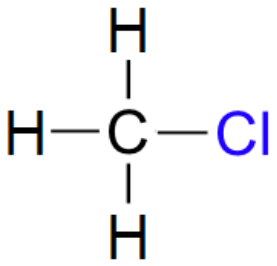
Compound (state)	Name	ΔH°_{comb}
CH_4 (gas)	Methane	−212.8 (−890.4)
C_2H_6 (gas)	Ethane	−372.8 (−1559.8)
$CH_3CH_2CH_3$ (gas)	Propane	−530.6 (−2220.0)
$CH_3(CH_2)_2CH_3$ (gas)	Butane	−687.4 (−2876.1)
$(CH_3)_3CH$ (gas)	2-Methylpropane	−685.4 (−2867.7)
$CH_3(CH_2)_3CH_3$ (gas)	Pentane	−845.2 (−3536.3)
$CH_3(CH_2)_3CH_3$ (liquid)	Pentane	−838.8 (−3509.5)
$CH_3(CH_2)_4CH_3$ (liquid)	Hexane	−995.0 (−4163.1)
 (liquid)	Cyclohexane	−936.9 (−3920.0)

B.1 Alcanos de cadena contínua – T° fusión y ebullición

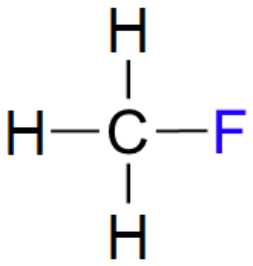
Compuesto	# C	Formula	T fusión (°C)	T ebullición (°C)
Metano	1	CH_4	-182.5	-161.5
Etano	2	C_2H_6	-183.2	-88.6
Propano	3	C_3H_8	-187.7	-42.1
Butano	4	C_4H_{10}	-138.3	-0.5
Pentano	5	C_5H_{12}	-129.7	36.1
Hexano	6	C_6H_{14}	-95.3	68.7
Heptano	7	C_7H_{16}	-90.6	98.4
Octano	8	C_8H_{18}	-56.8	125.7
Nonano	9	C_9H_{20}	-53.6	150.8
Decano	10	$C_{10}H_{22}$	-29.7	174.0

***Ejercicio**: Grafique PM versus T fusión y versus T ebullición*

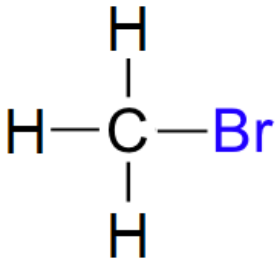
clorometano



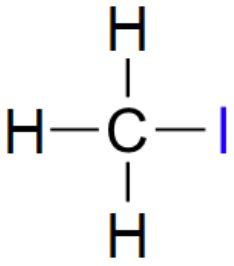
fluorometano

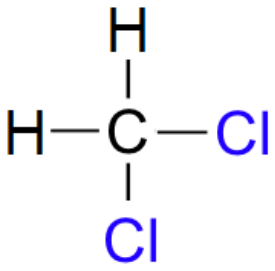


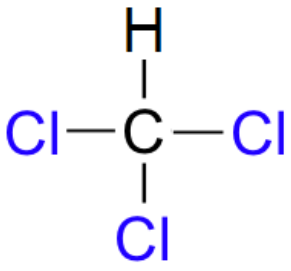
bromometano

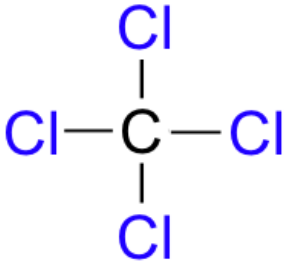


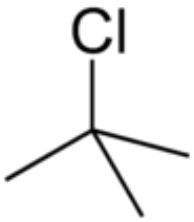
iodometano

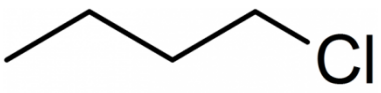


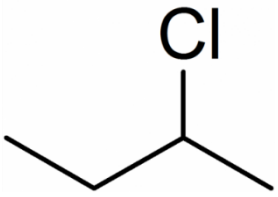


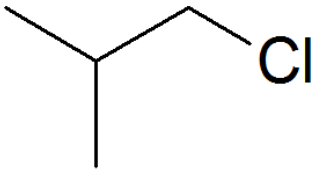


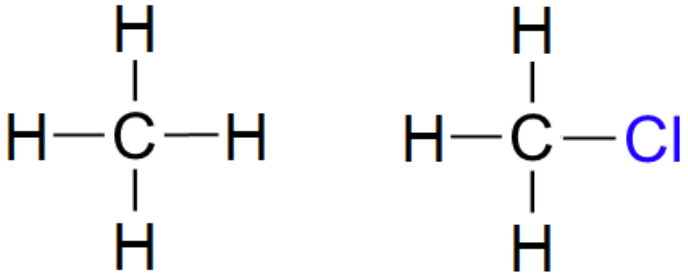




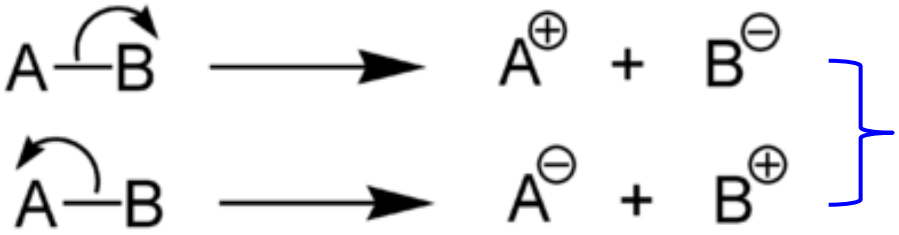






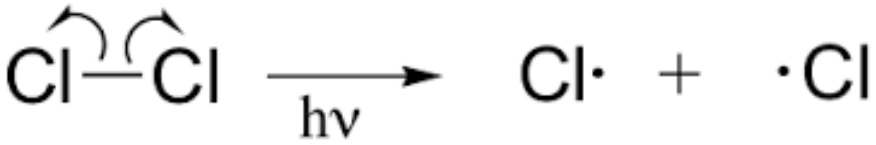


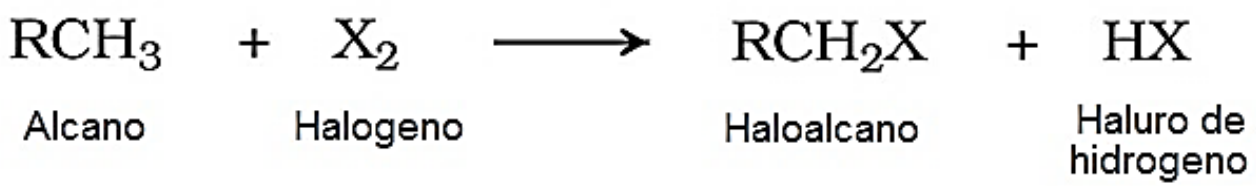
Sustitución por radicales libres



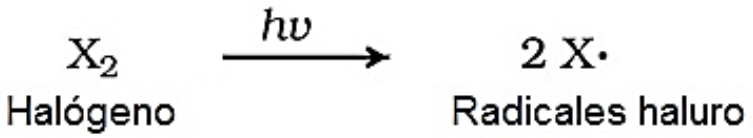
heterólisis

homólisis



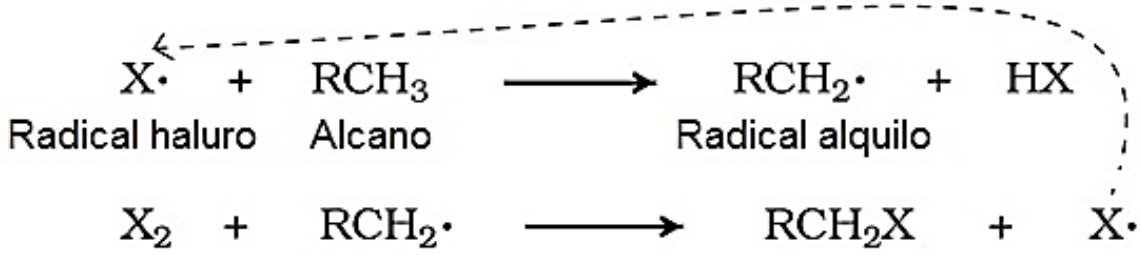


Iniciación



ΔH°= +58 kcal/mol

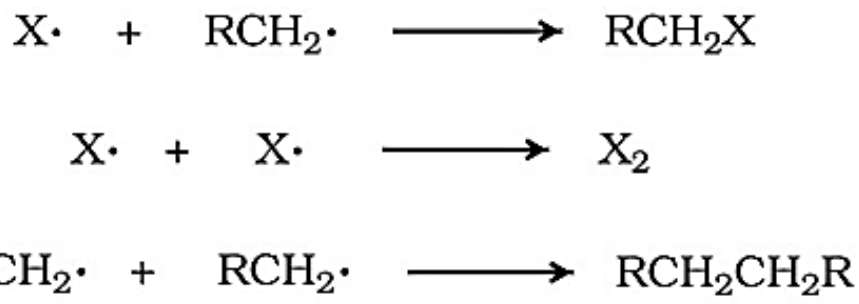
Propagación



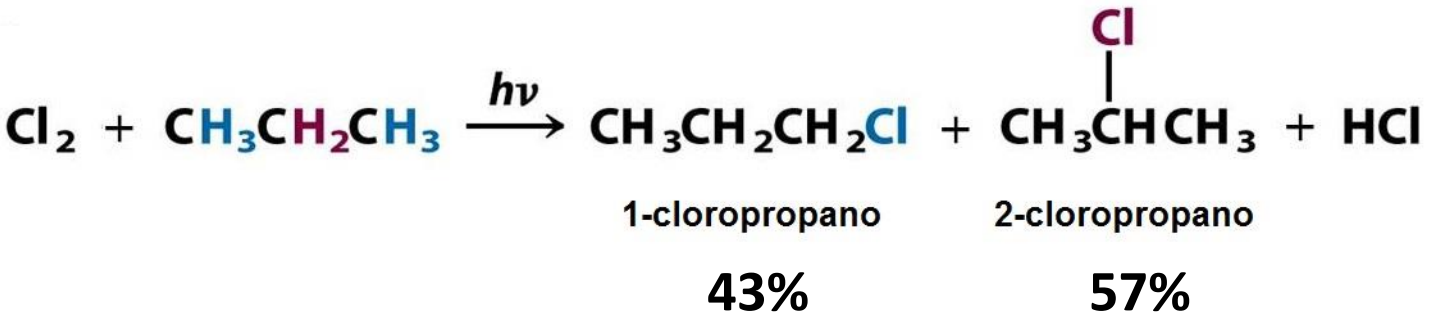
ΔH°= +2

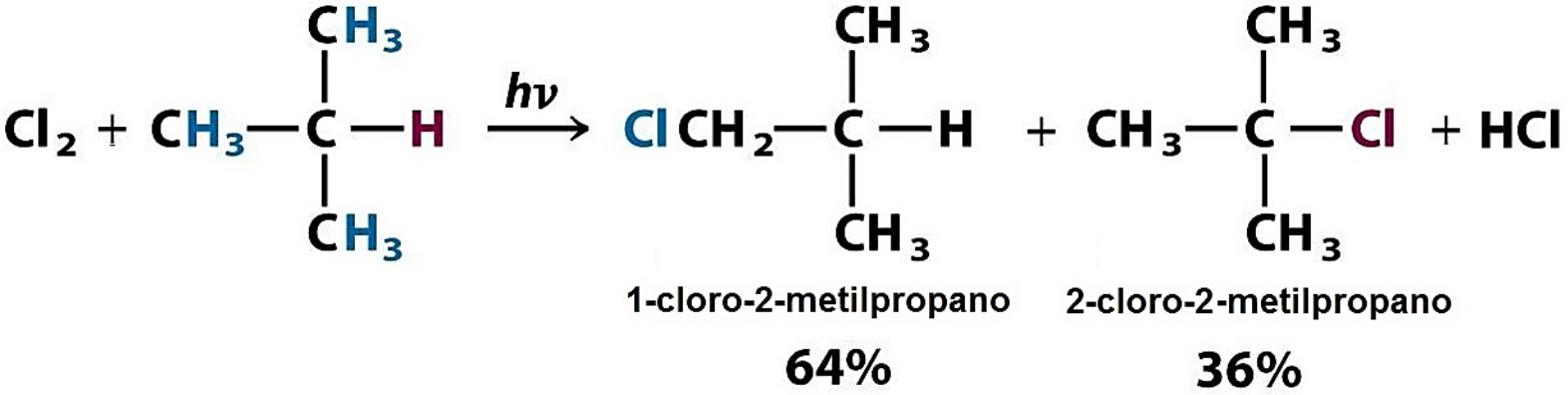
ΔH°= -27

Terminación

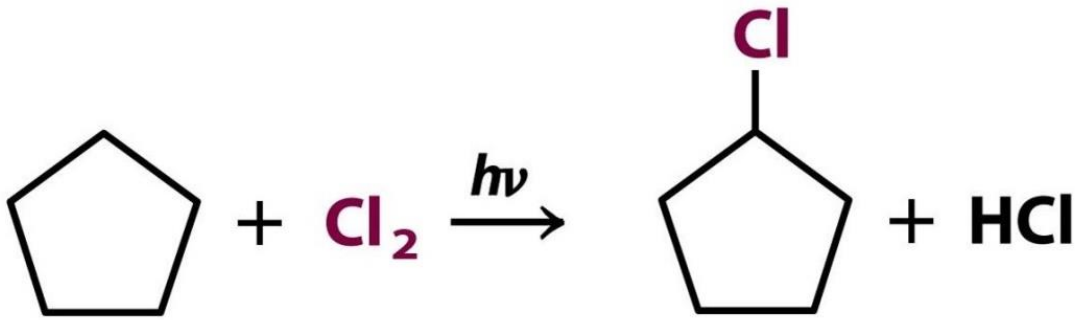


Halogenación – más de un producto

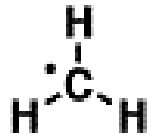
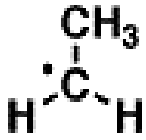
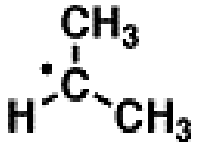
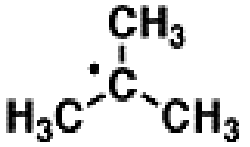




Halogenación – estabilidad de radicales



Ciclopentano — Clorociclopentano 92.7%

Metilo		Primario		Secundario		Terciario
	<		<		<	
– estable						+ estable

- Reacción en la que un nucleófilo reemplaza a un “grupo saliente” (X), por ej. en un haloalcano.
- Cuando X sale, se “lleva” ambos electrones del enlace R–X.
- Permite la síntesis de un alcohol a partir de un haloalcano.

$$OH^- + CH_3Cl \rightarrow CH_3OH + Cl^-$$

Bibliografía

Bailey & Bailey, 5a Ed 1998
Vollhardt-Schore, 5a Ed 2007
Schmid, 1ª Ed, 1996

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