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DE CHILE

Fundamentos de Química Orgánica
Capítulo 2: “El enlace en moléculas orgánicas”

Susan Lühr

Fundamentos de Química Orgánica

Unidad 1
NOMENCLATURA
(nombres)

Unidad 2
CONTRUCCIÓN
(enlaces, ángulos)

Unidad 3
ARQUITECTURA 3D
(estereoquímica)

COMPUESTOS ORGÁNICOS

Unidad 4
COMPORTAMIENTO
(reactividad: alcanos, cicloalcanos)

Unidad 5
REACTIVIDAD
(halogenados)

Unidad 6
REACTIVIDAD
(alquenos y alquinos)

Unidad 7
REACTIVIDAD
(aromáticos)

Unidad 8
RECONOCIMIENTO-CARACTERIZACIÓN
(MS, IR, RMN ^{1}H, ^{13}C)

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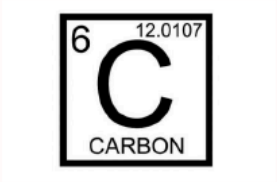
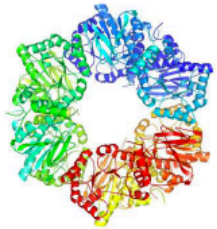
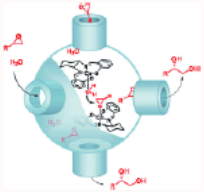
Introducción







Una de las importancias de la química orgánica es que esta ciencia se relaciona con diversas áreas.

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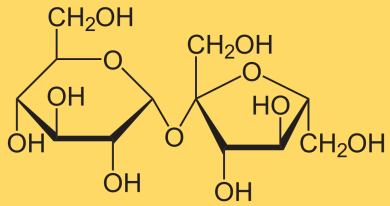
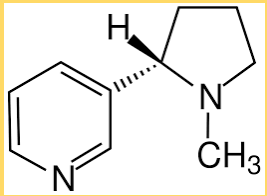
Introducción

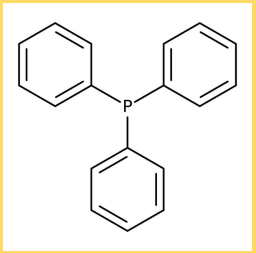
Principales átomos que constituyen la moléculas orgánicas.

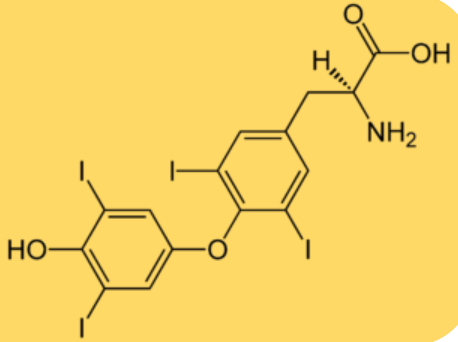
Group 1A												3A	4A	5A	6A	7A	8A
H	2A																He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															

Ejemplos:









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Estructura del átomo

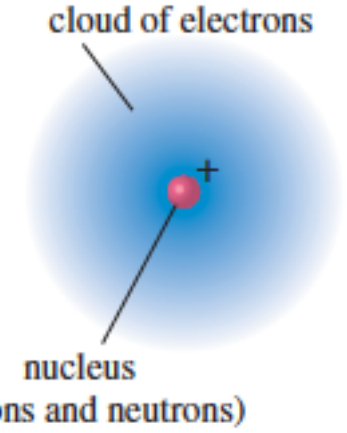
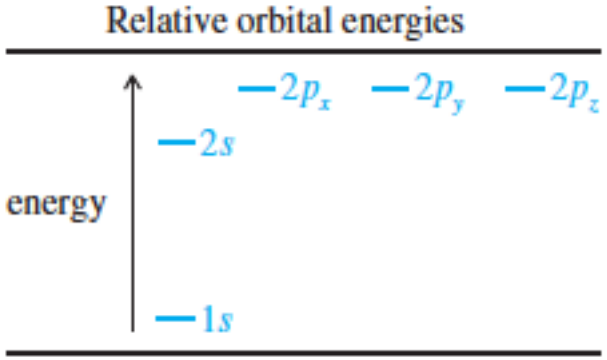


FIGURE 1-1
Basic atomic structure. An atom has a dense, positively charged nucleus surrounded by a cloud of electrons.

Los átomos están compuestos
Por protones, neutrones y electrones.
Número atómico: número de protones en el núcleo.



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Estructura del átomo - electrones

Werner Heisenberg
1933

Los electrones forman enlaces y determinan la estructura de las moléculas. Estos se comportan como partículas, pero principalmente como ondas (se explica mejor su comportamiento).

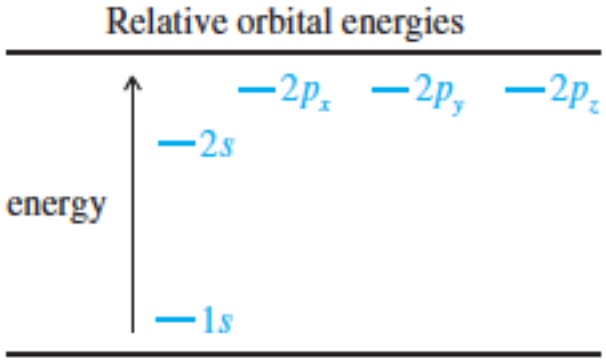
Dónde se encuentran los electrones?

Se encuentran en orbitales alrededor del núcleo.

Principio de Heisenberg: Nunca podemos determinar dónde se encuentra el electrón, pero si podemos determinar la densidad electrónica, que es la posibilidad de encontrar al electrón en una parte específica del orbital.

Orbital atómico: zona o espacio geométrico con un cierto estado de energía, donde es probable definir la distribución de la densidad electrónica, es decir encontrar electrones. (Definido por una Función matemática "Schrödinger") Ψ (n, l, m, s).

Los electrones se agrupan en capas a diferentes distancias del núcleo.



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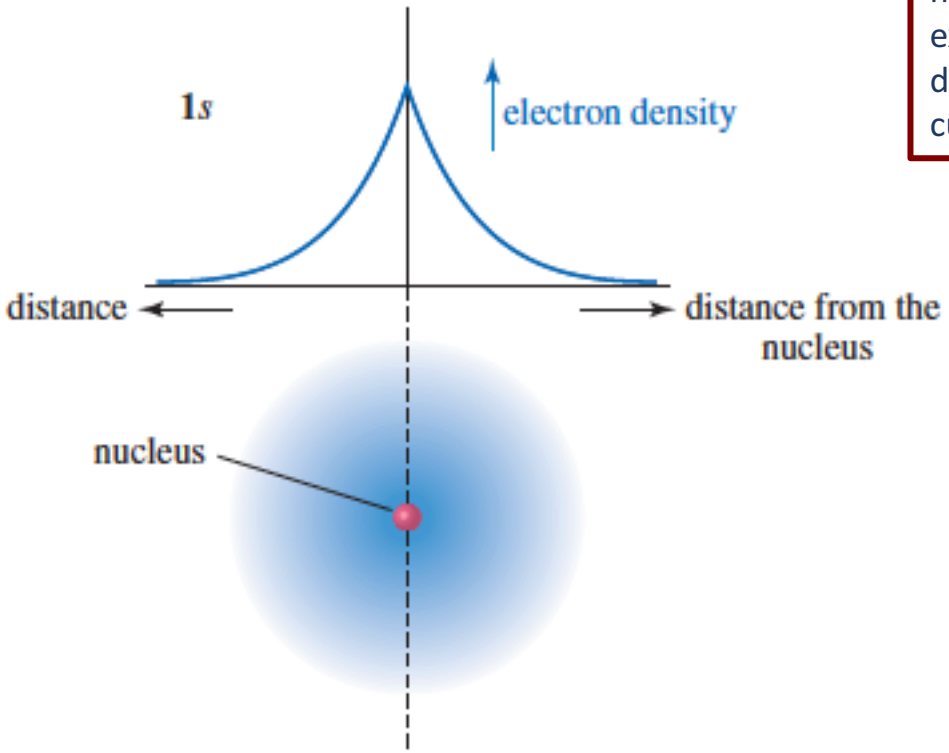
Estructura del átomo



La densidad electrónica se encuentra mayormente cerca del núcleo y decae exponencialmente al aumentar la distancia de este desde el núcleo hacia cualquier dirección.

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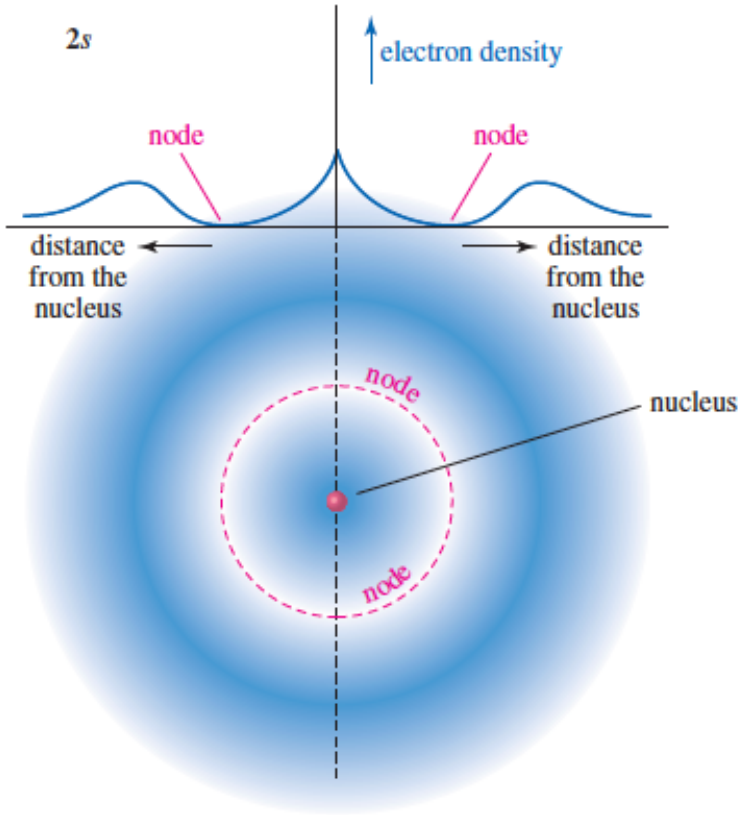
Estructura del átomo



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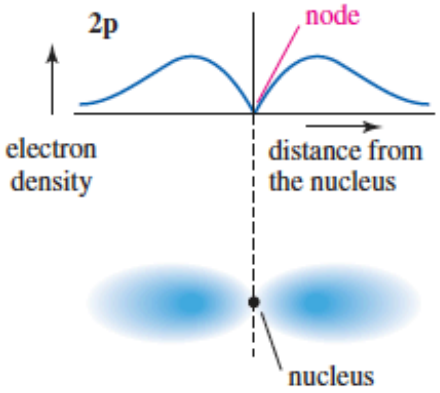
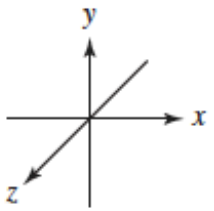
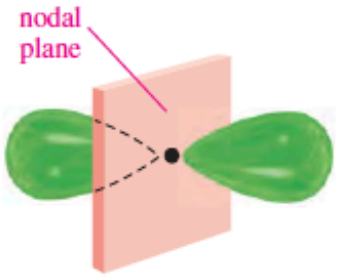
Estructura del átomo

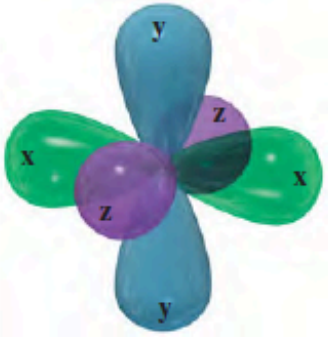




directions of axes
(z comes out toward us)



the $2p_x$ orbital



the $2p_x$, $2p_y$, and $2p_z$ orbitals superimposed at 90° angles

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¿Cómo se forman los enlaces?

Regla del octeto

Enlace covalente

Enlace iónico

Estructura de Lewis

Electrones de valencia

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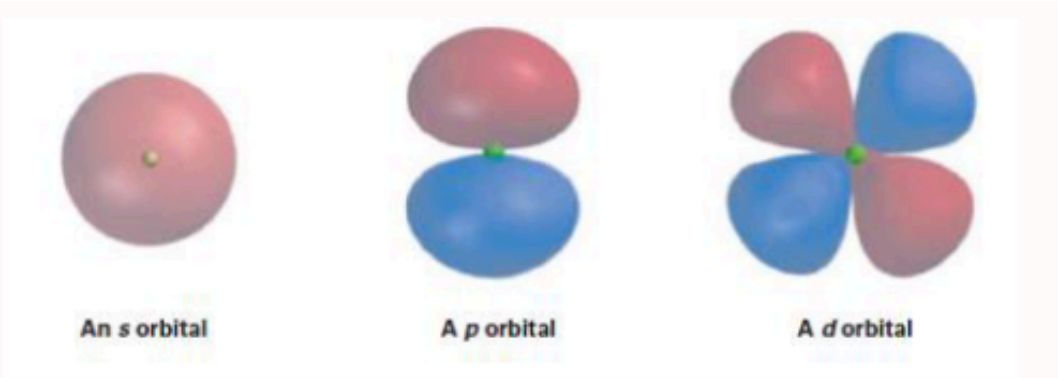
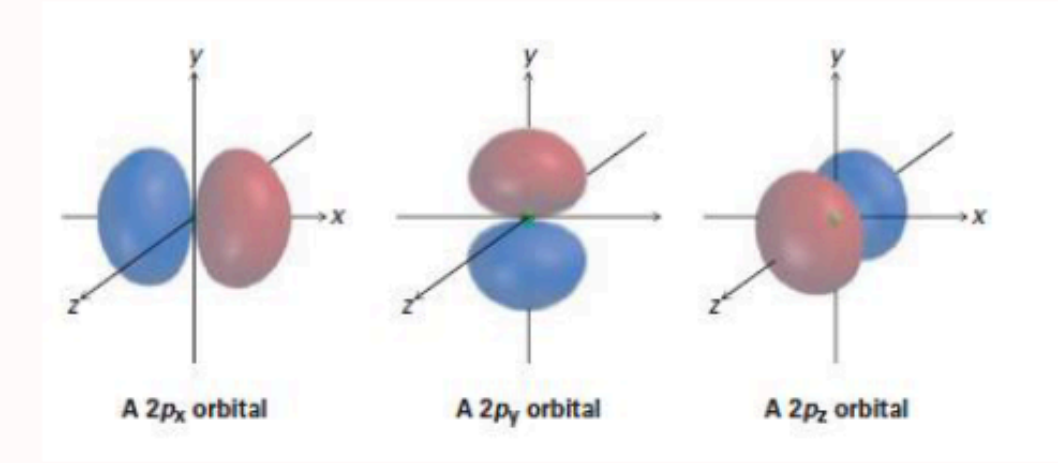
¿Cómo se forman los enlaces? Orbitales atómicos





Orbital atómico: zona o espacio geométrico donde es probable encontrar electrones. (Función matemática) Ψ (n, l, m, s)

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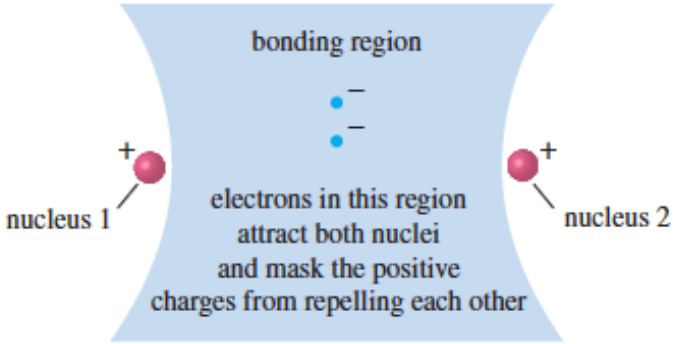
Combinación de orbitales atómicos

Combinación lineal de Orbitales moleculares (CLOA): es el proceso por el cual se suman y restan funciones de onda dando como resultados nuevas funciones de onda características de los nuevos orbitales formados, por medio de su combinación y traslape.

Número de orbitales iniciales es igual al número de orbitales nuevos formados.

Orbitales moleculares: se generan cuando interactúan orbitales de átomos diferentes (interacciones de enlace o de antienlace).
Orbitales moleculares híbridos: se generan cuando interactúan orbitales de átomos iguales (geometría de los enlaces).



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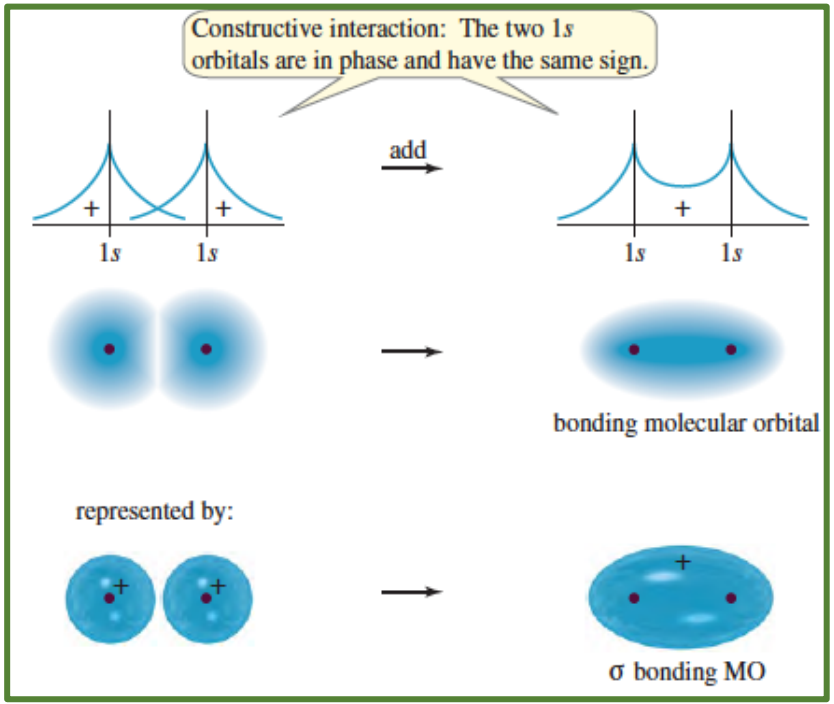
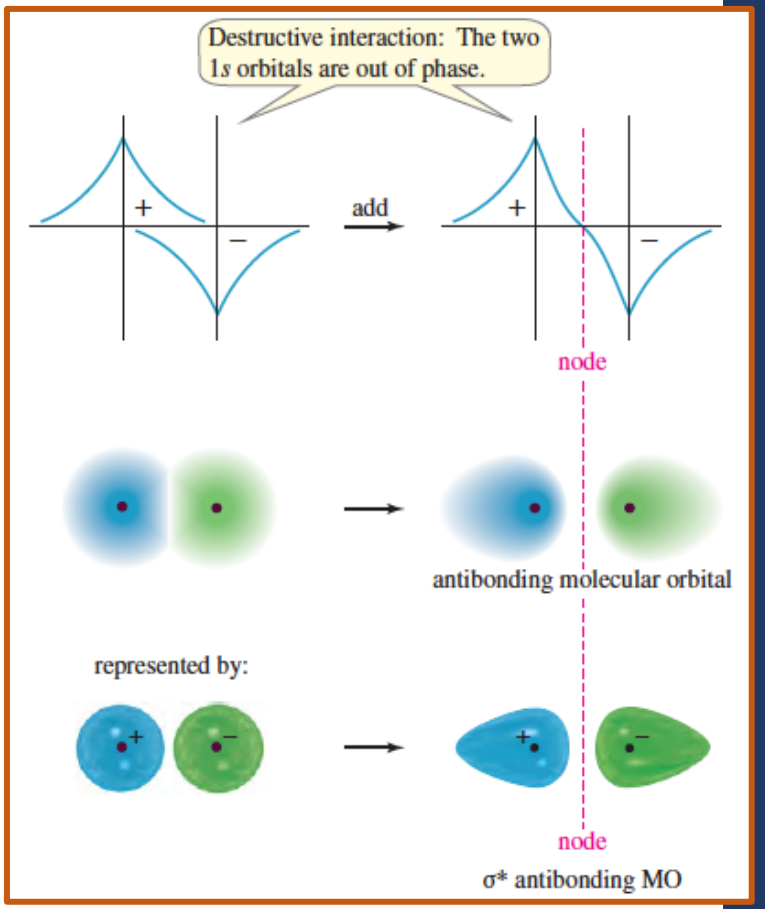
Enlace Sigma – H-H

Las funciones de onda 1s se: suman (refuerzan) **constructivamente** o se cancelan **destructivamente** en el lugar donde se traslapan.



Fn en fase de igual signo en región internuclear.



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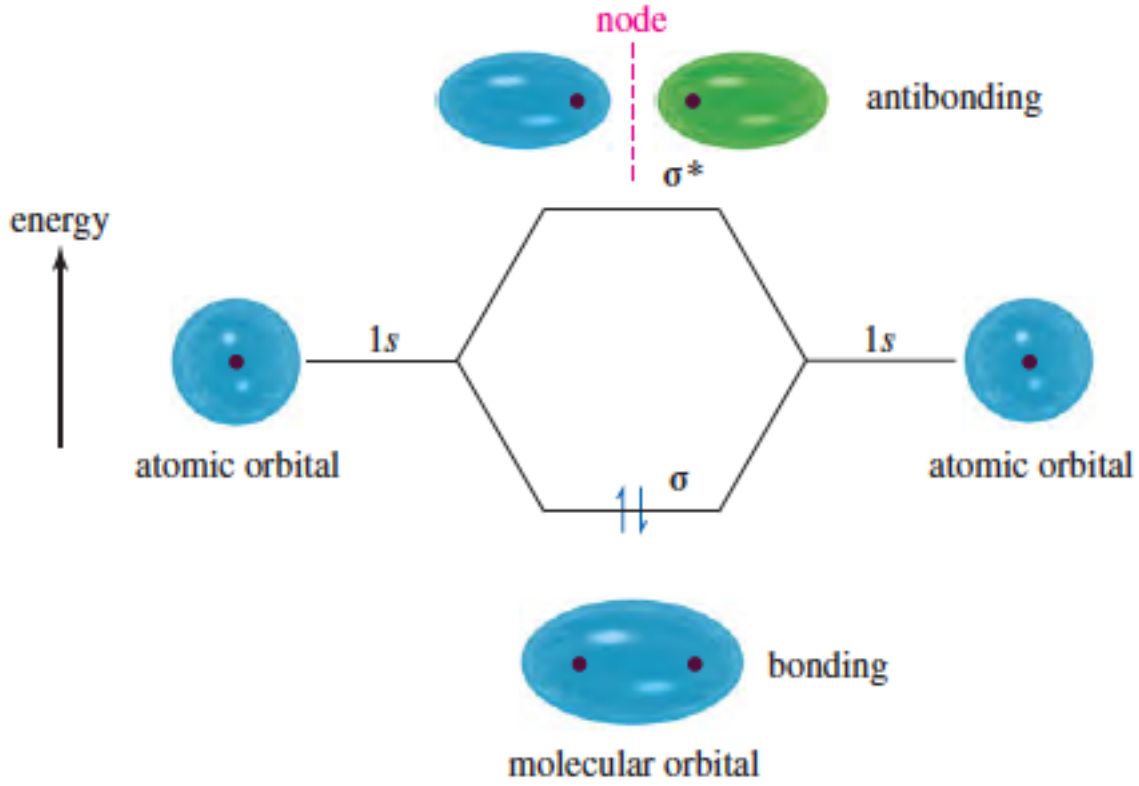
Enlace Sigma – H-H



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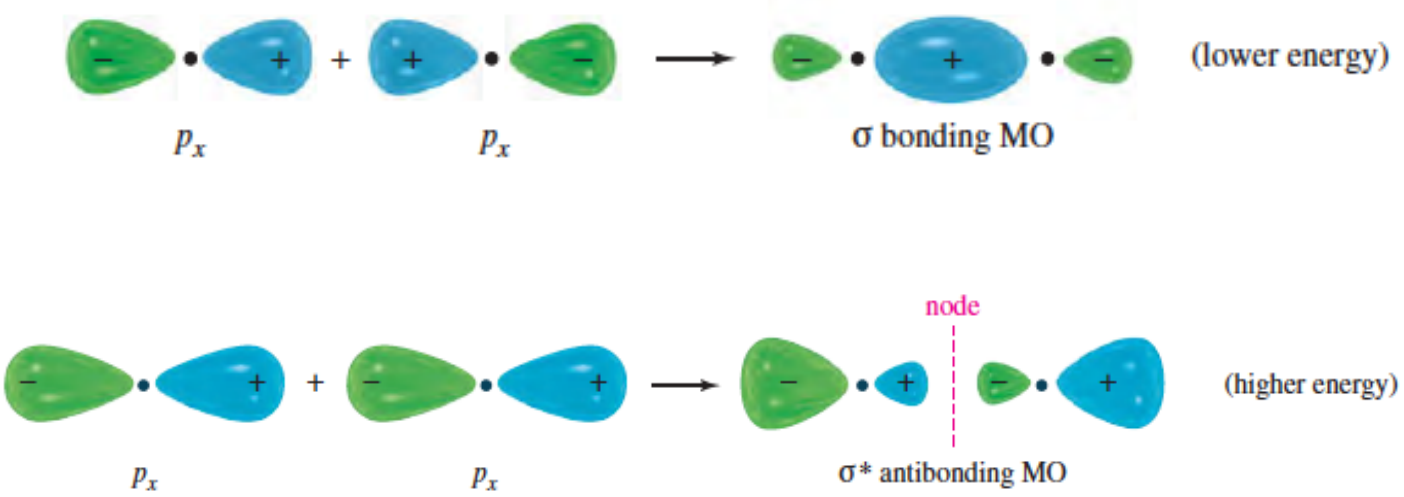
Enlace Sigma – dos orbitales p



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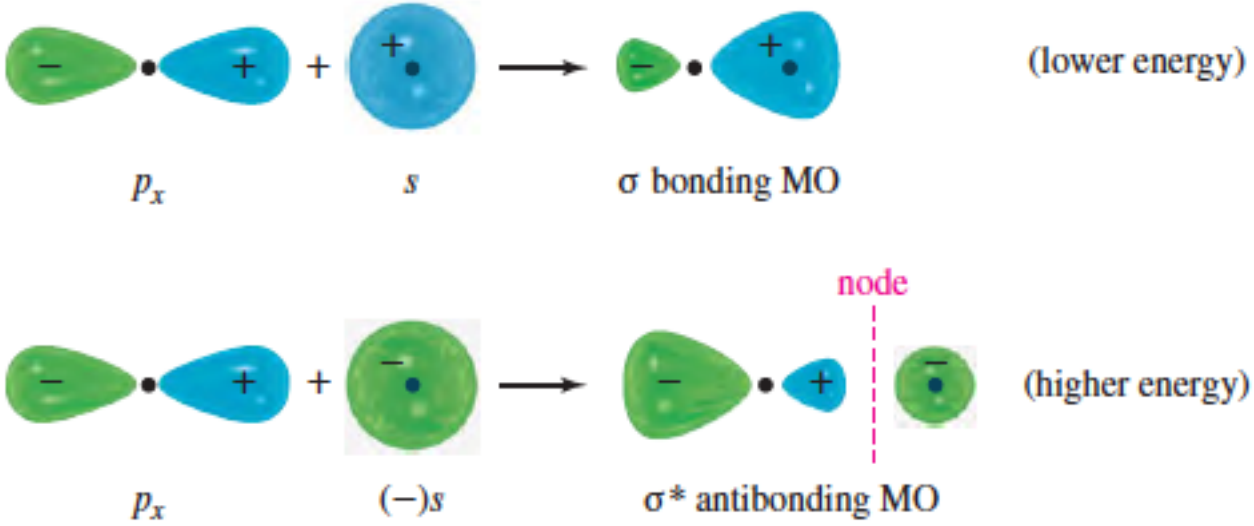
Enlace Sigma – orbital p + s



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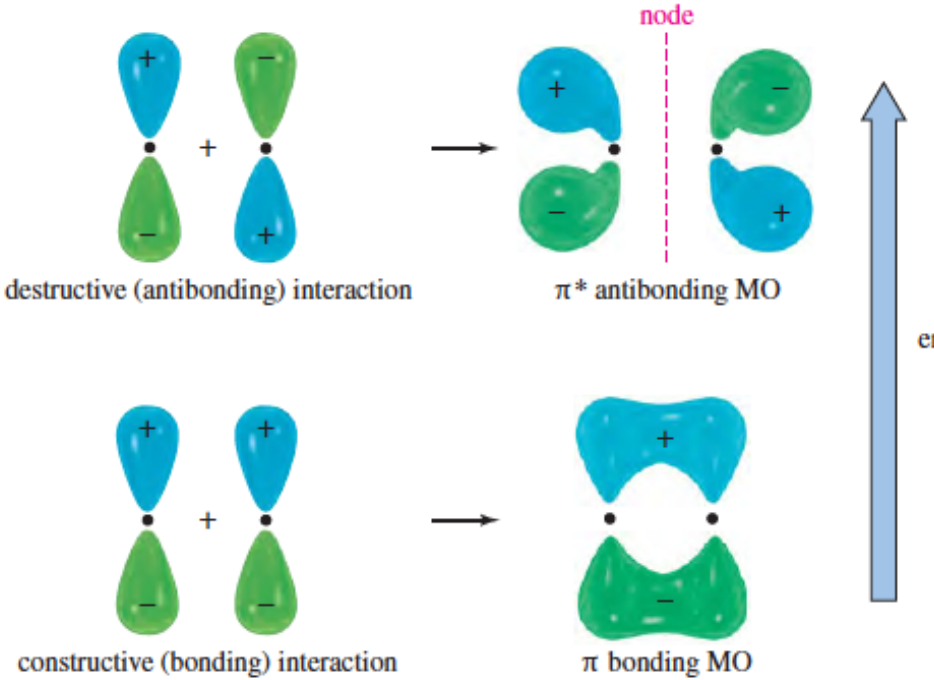
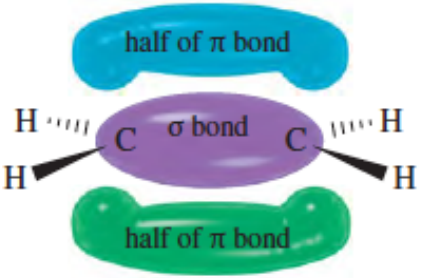
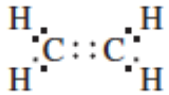
Enlace pi







Lewis structure of ethylene

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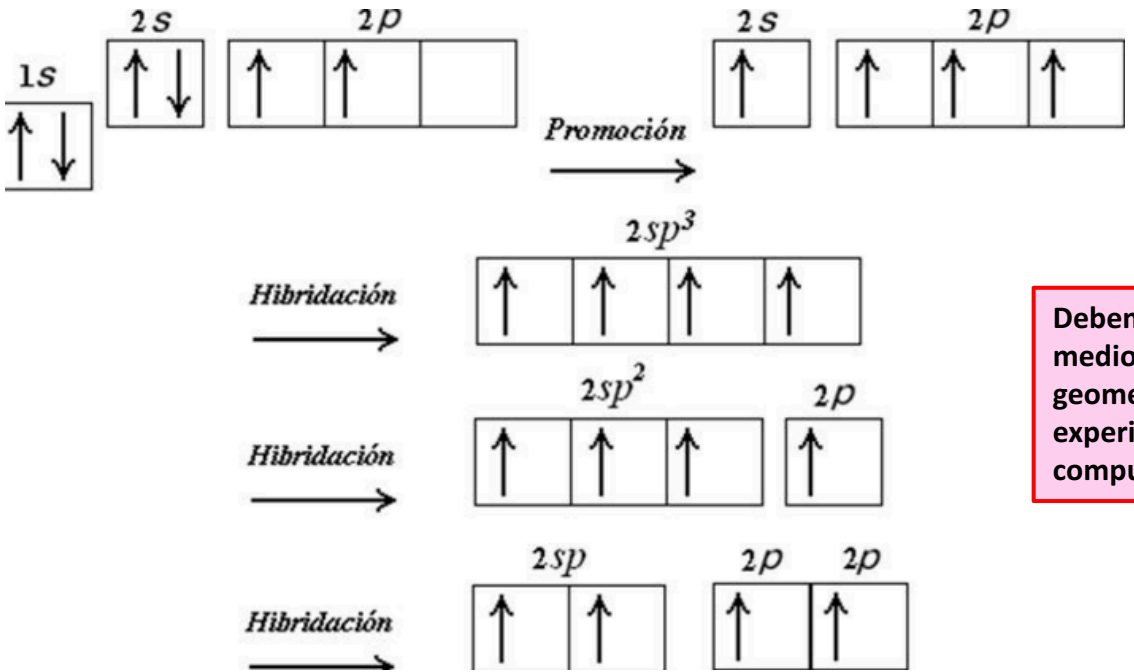
Hibridación orbitales atómicos del carbono

La hibridación surge de la combinación matemática de los diferentes orbitales atómicos para justificar la formación de enlaces y sus propiedades. **Combinación lineal de Orbitales moleculares (CLOA)**

Configuración electrónica C



Debemos dar respuestas por medio de teorías a las geometrías que se conocen experimentalmente de los compuestos orgánicos.

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Hibridación sp^3

Combinación de 1 orbital s y 3 orbitales p, dando 4 orbitales híbridos sp^3.

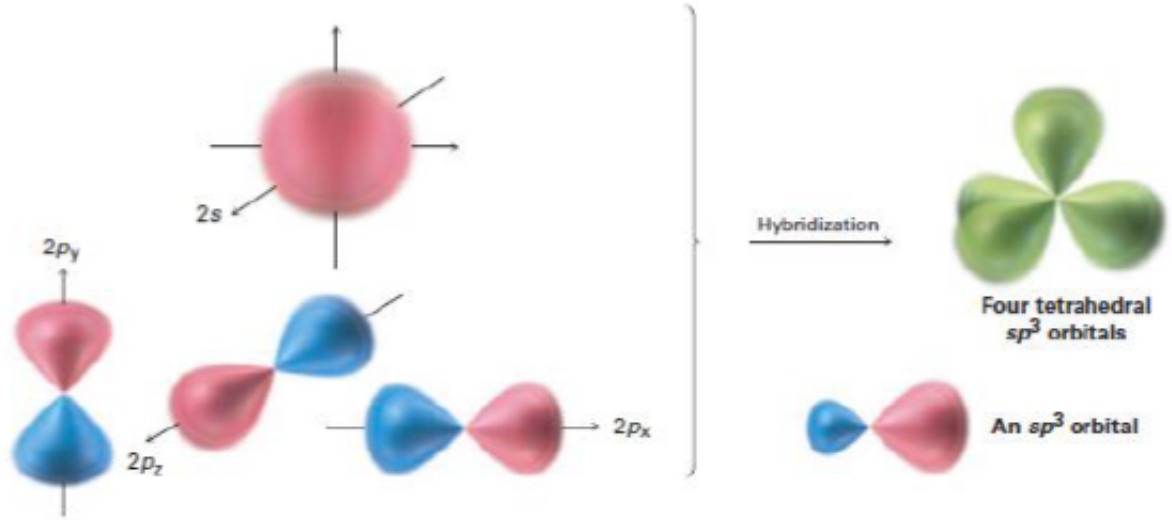

Figure 1.10 Four sp^3 hybrid orbitals, oriented to the corners of a regular tetrahedron, are formed by combination of an *s* orbital and three *p* orbitals (red/blue). The sp^3 hybrids have two lobes and are unsymmetrical about the nucleus, giving them a directionality and allowing them to form strong bonds when they overlap an orbital from another atom.

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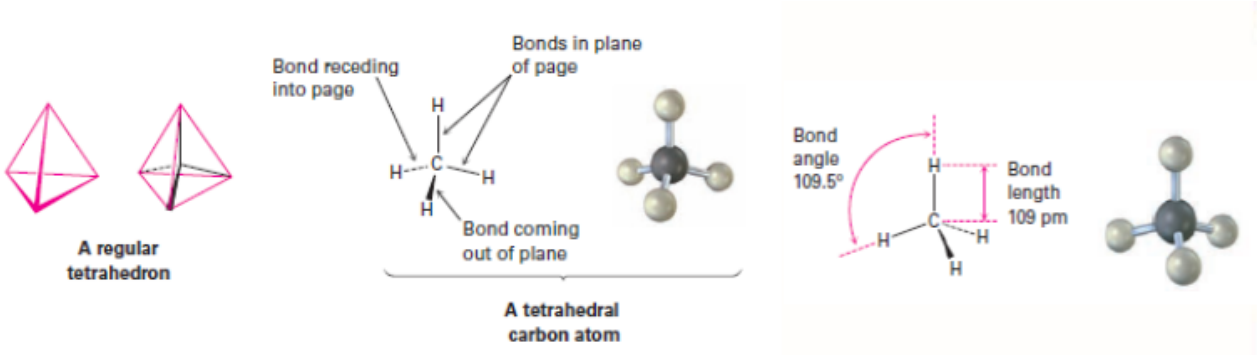
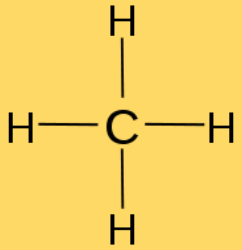
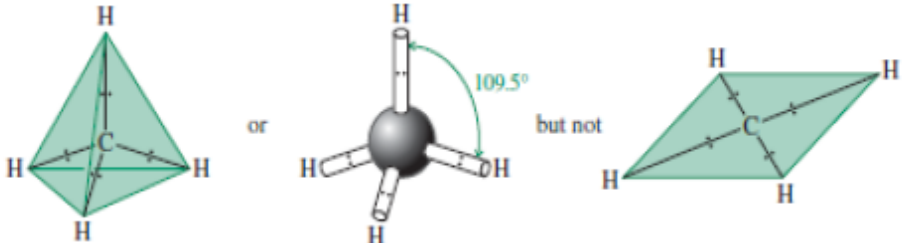
Hibridación sp^3 - Metano

Combinación de 1 orbital s y 3 orbitales p, dando 4 orbitales híbridos sp^3.

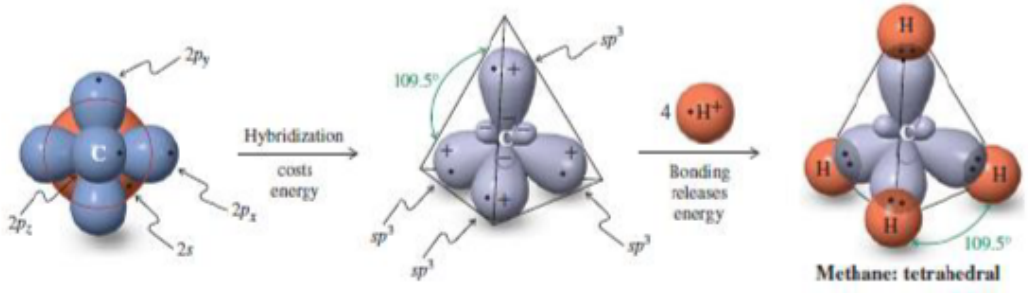


Estructura de Lewis
Metano





Según la **Teoría de Repulsión de electrones de la capa de valencia** las moléculas orgánicas adoptan diferentes geometrías.



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Hibridación sp^3 - Etano

Combinación de 1 orbital s y 3 orbitales p, dando 4 orbitales híbridos sp^3.

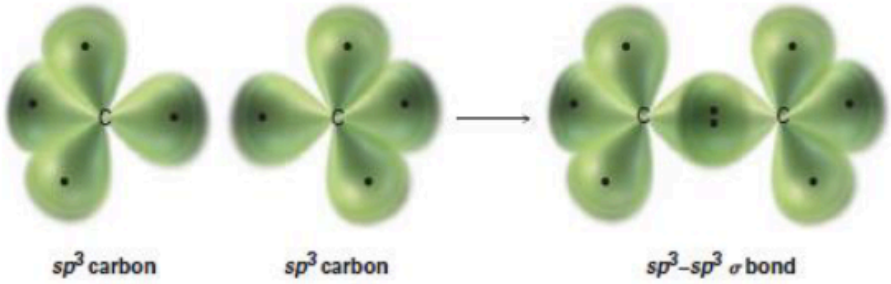
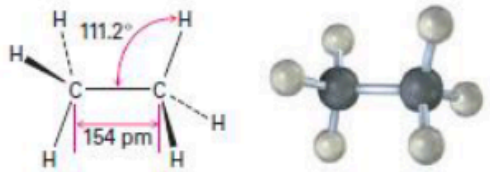
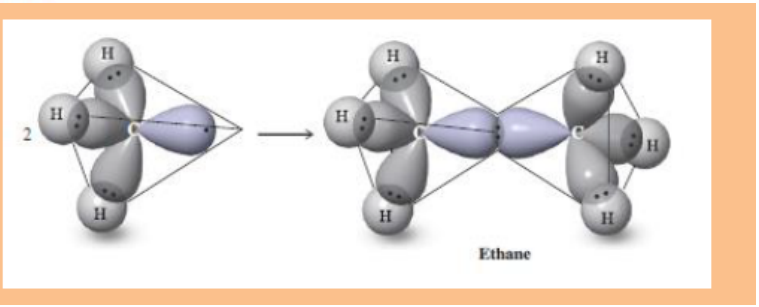


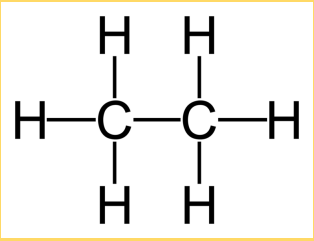
Figure 1.12 The structure of ethane. The carbon–carbon bond is formed by σ overlap of sp^3 hybrid orbitals. For clarity, the smaller lobes of the sp^3 hybrid orbitals are not shown.



Ethane



Estructura de Lewis
Etano



Según la **Teoría de Repulsión de electrones de la capa de valencia** las moléculas orgánicas adoptan diferentes geometrías.

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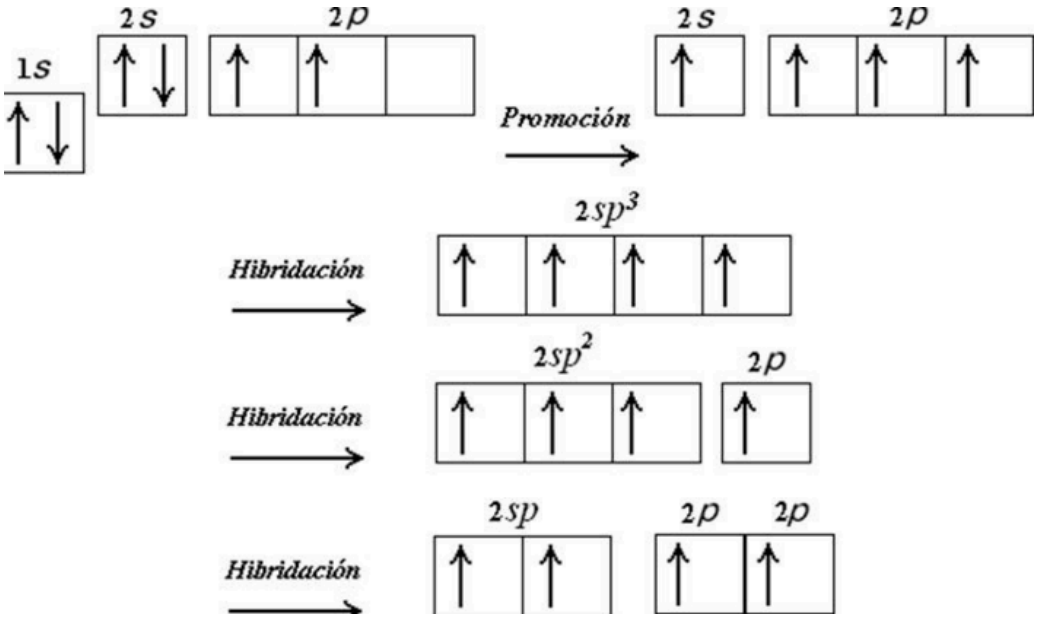
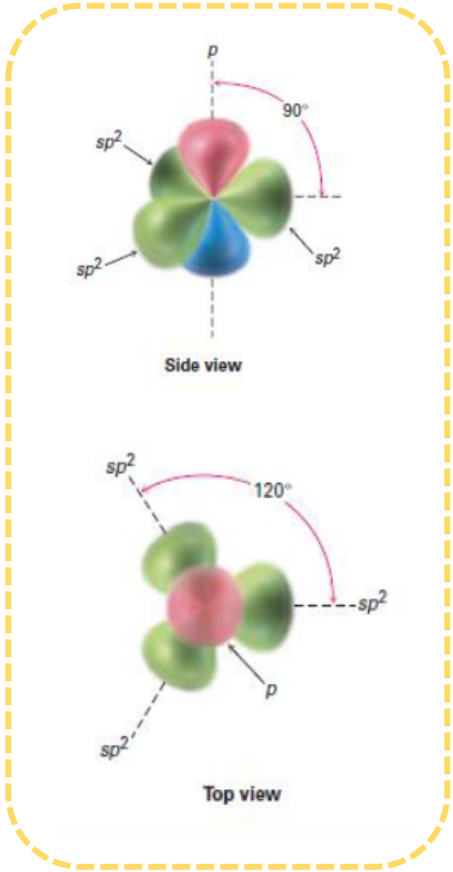
Hibridación sp^2

Combinación de 1 orbital s y 2 orbitales p, dando 3 orbitales híbridos sp^2 y un orbital p libre.





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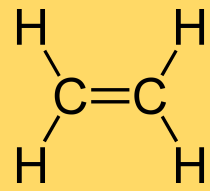
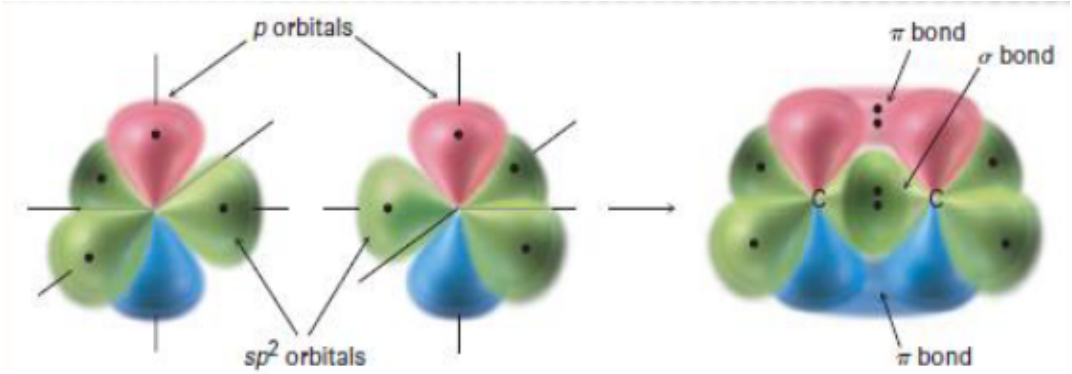
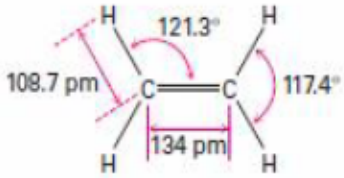
Hibridación sp^2 – Eteno

Combinación de 1 orbital s y 2 orbitales p, dando 3 orbitales híbridos sp^2 y un orbital p libre.

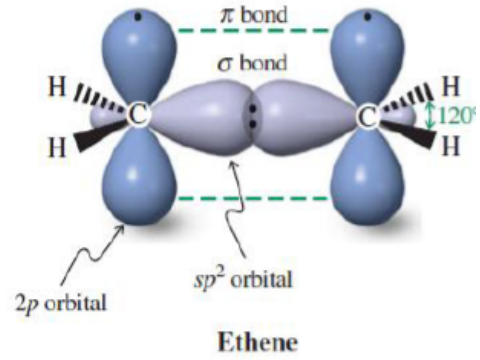
Estructura de Lewis
Eteno







Solapamiento de 2 **orbitales sp^2 forman el enlace sigma** y los orbitales p libres forman el **enlace pi**.



Ethene

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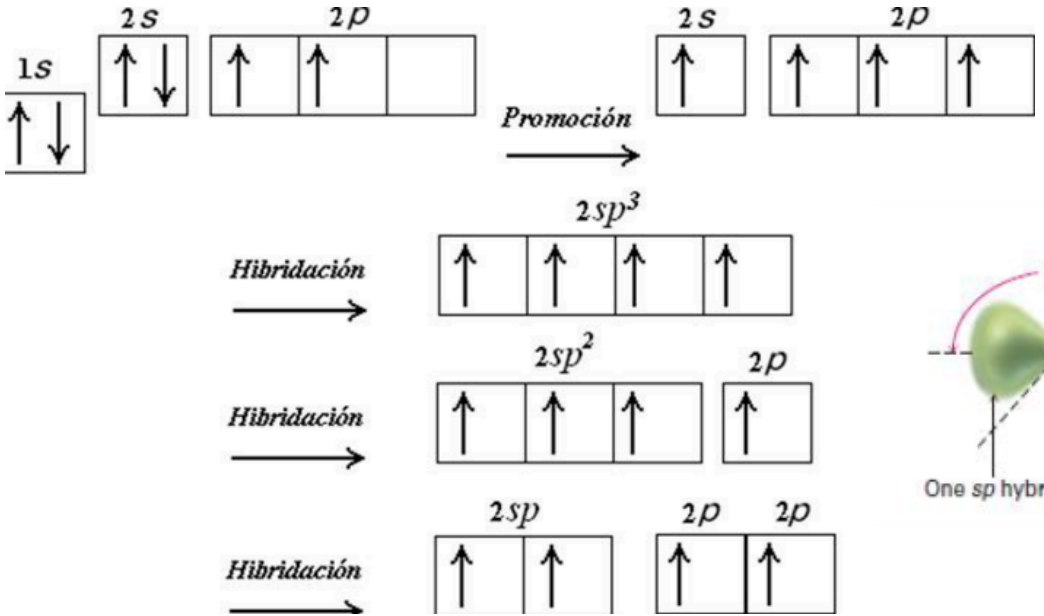
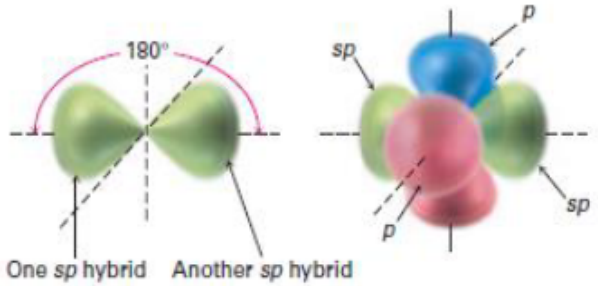
Hibridación sp

Combinación de 1 orbital s y 1 orbital p, dando 2 orbitales híbridos sp y 2 orbitales libres p.





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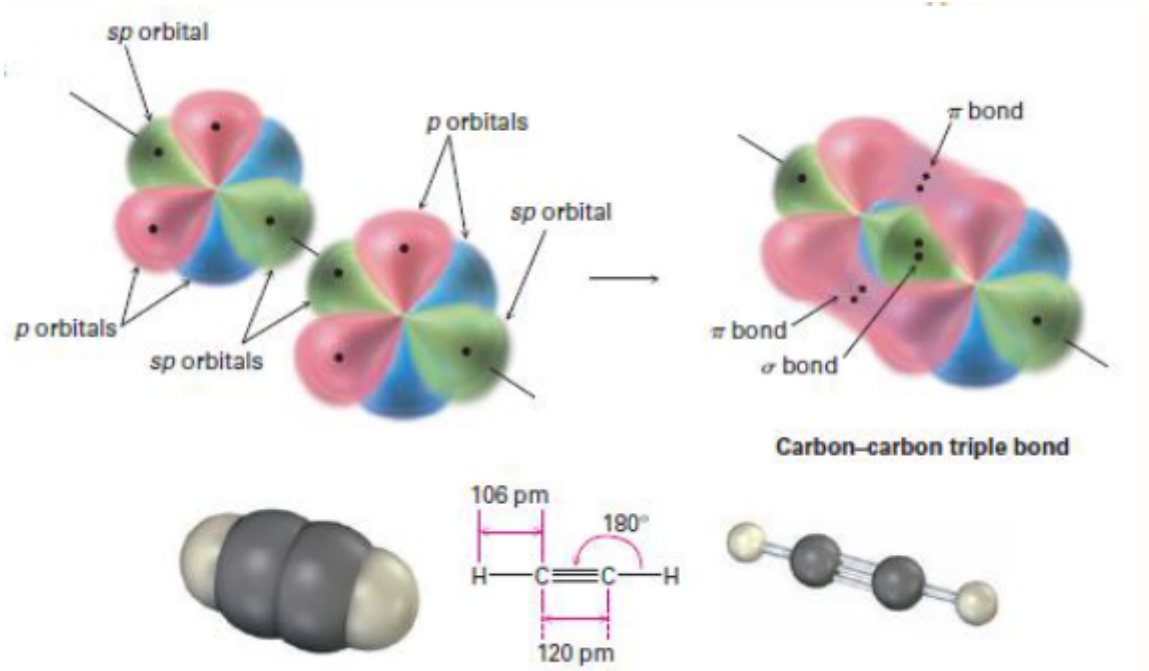
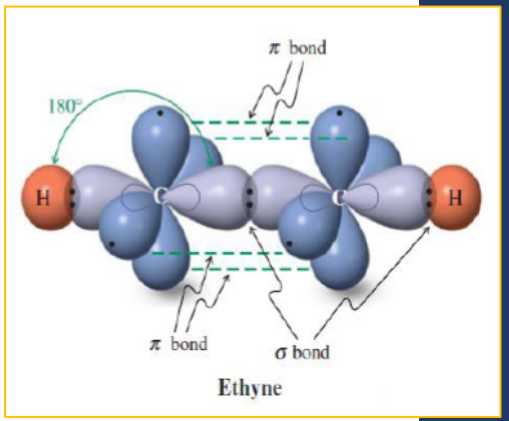
Hibridación sp – Etino (acetileno)

Combinación de 1 orbital s y 1 orbital p, dando 2 orbitales híbridos sp y 2 orbitales libres p.

Estructura de Lewis
Etino

$$H{-}C{\equiv}C{-}H$$





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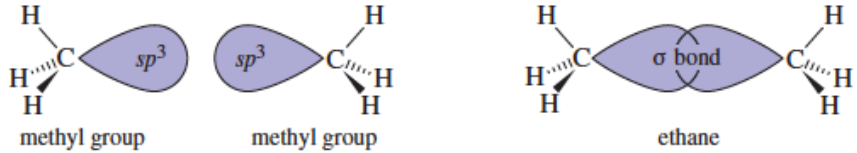
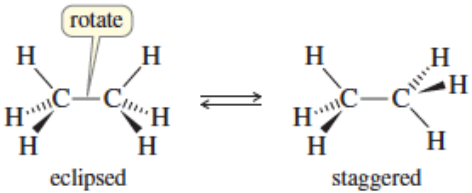
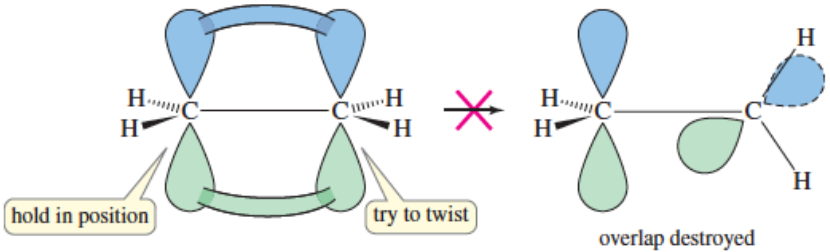
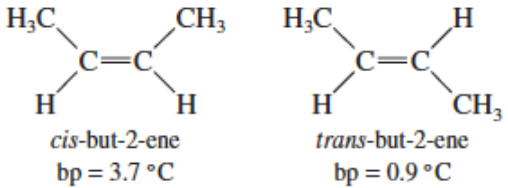
Rotación de enlace









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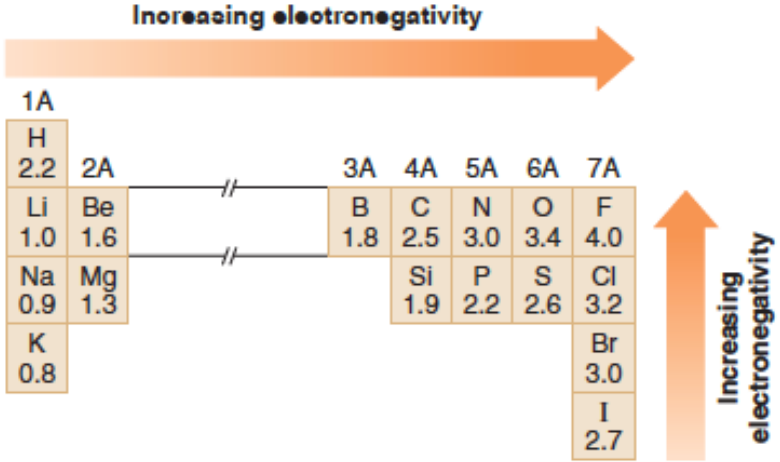
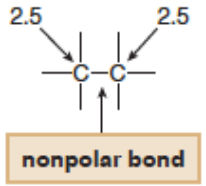
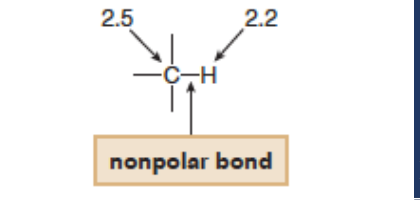
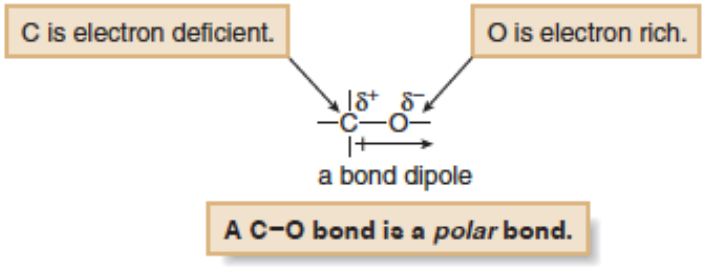
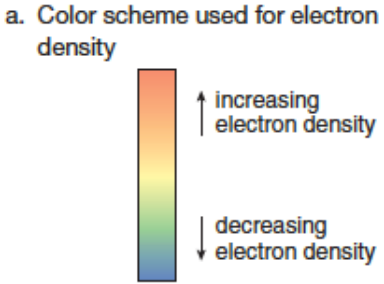
Electronegatividad

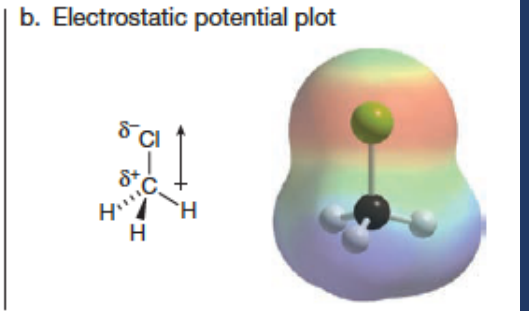




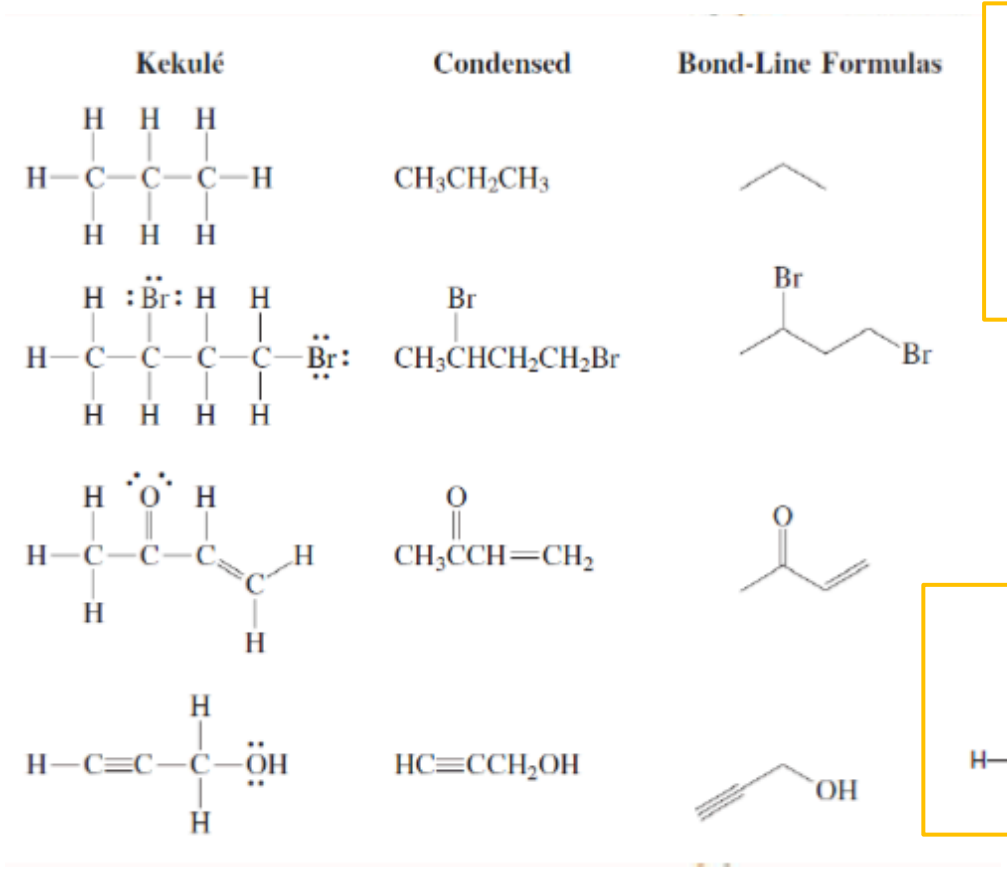


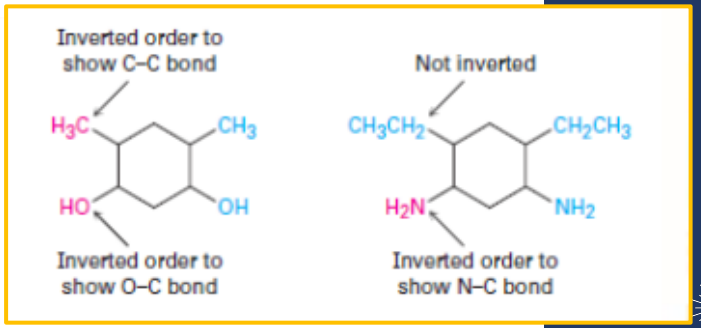


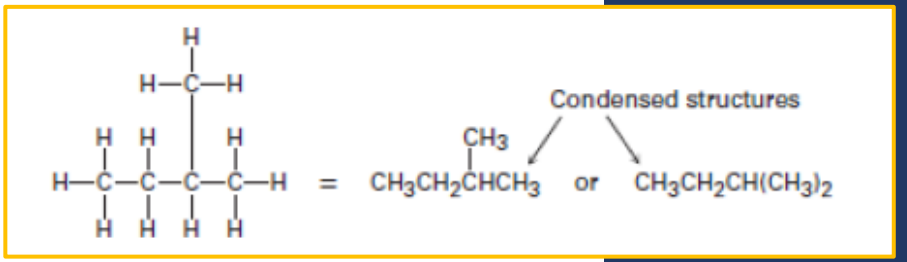




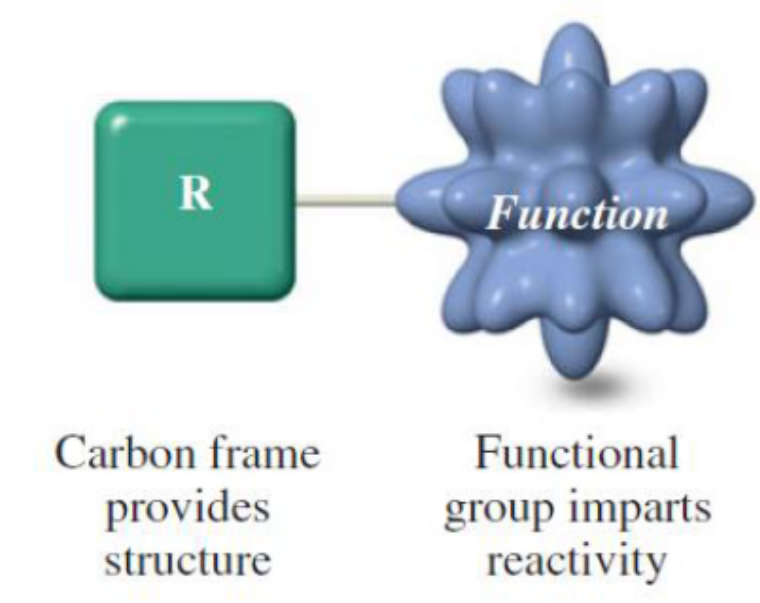
¿Cómo dibujar los compuestos orgánicos?







Grupos funcionales



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Introducción: electronegatividad

H 2.1																He
Li 1.0	Be 1.6											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.9	Ni 1.9	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe
Cs 0.7	Ba 0.9	La 1.0	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.9	Bi 1.9	Po 2.0	At 2.1	Rn

Figure 2.2 Electronegativity values and trends. Electronegativity generally increases from left to right across the periodic table and decreases from top to bottom. The values are on an arbitrary scale, with F = 4.0 and Cs = 0.7. Elements in red are the most electronegative, those in yellow are medium, and those in green are the least electronegative.

Enlaces polares existen debido a la diferencia de electronegatividad entre los átomos que los conforman

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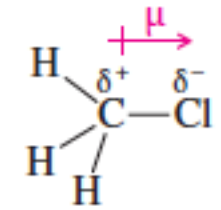
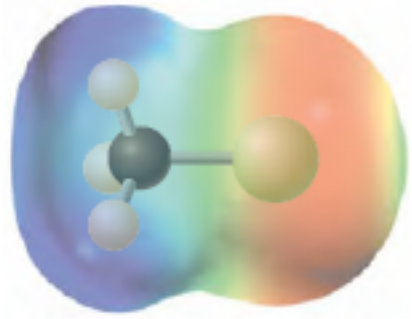
Polaridad



chloromethane


chloromethane

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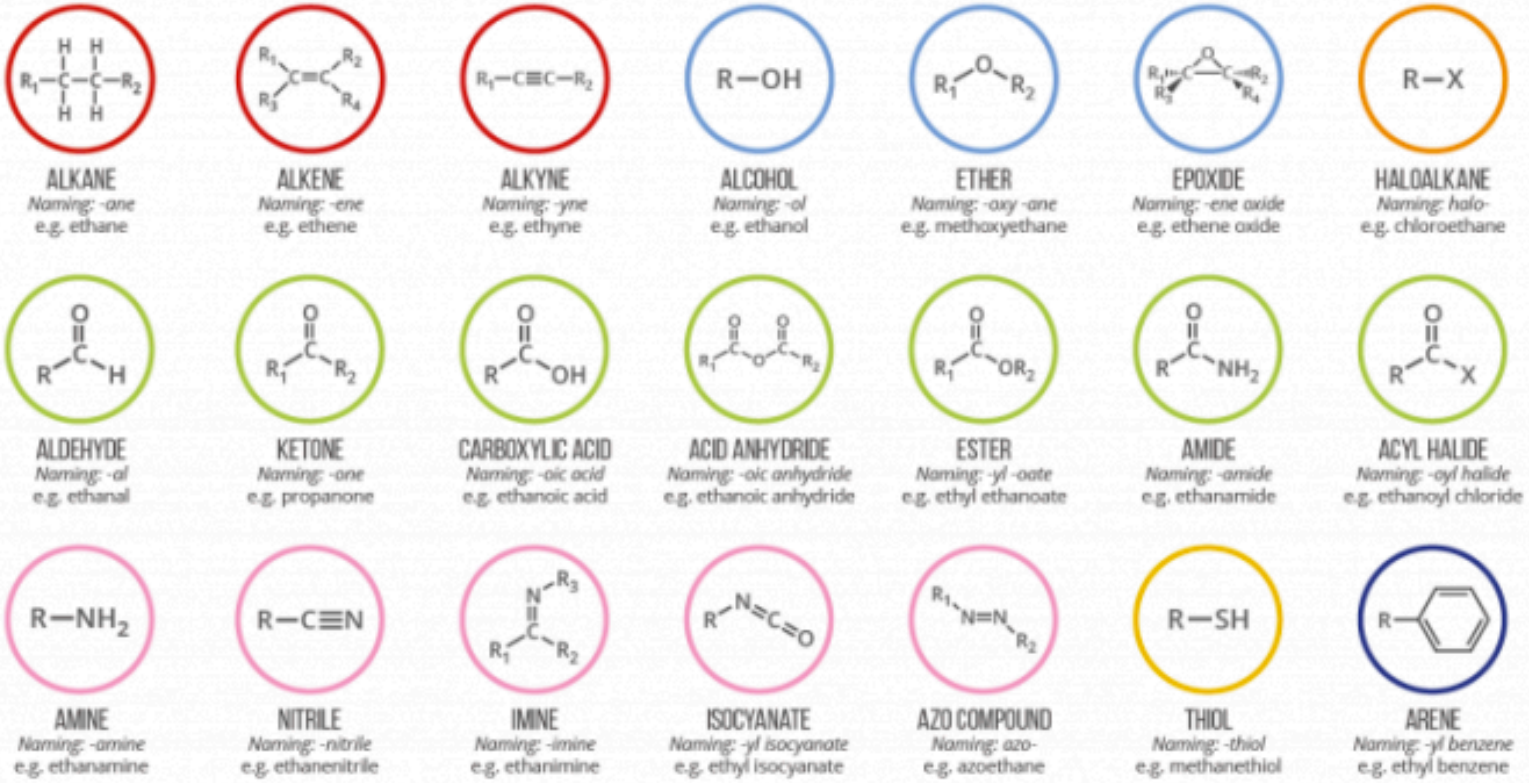
FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

FUNCTIONAL GROUPS ARE GROUPS OF ATOMS IN ORGANIC MOLECULES THAT ARE RESPONSIBLE FOR THE CHARACTERISTIC CHEMICAL REACTIONS OF THOSE MOLECULES. IN THE GENERAL FORMULAE SHOWN BELOW FOR EACH FUNCTIONAL GROUP, 'R' REPRESENTS THE REST OF THE MOLECULE, AND 'X' REPRESENTS ANY HALOGEN ATOM.

HYDROCARBONS | SIMPLE OXYGEN HETEROATOMICS | HALOGEN HETEROATOMICS | CARBONYL COMPOUNDS | NITROGEN-BASED | SULFUR-BASED | AROMATIC



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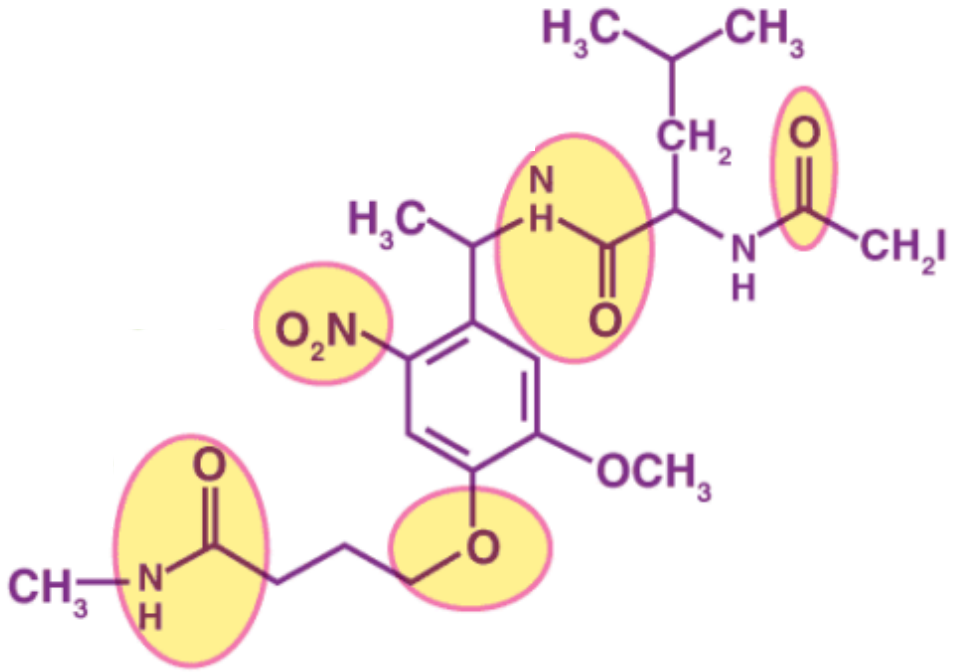
Grupos funcionales



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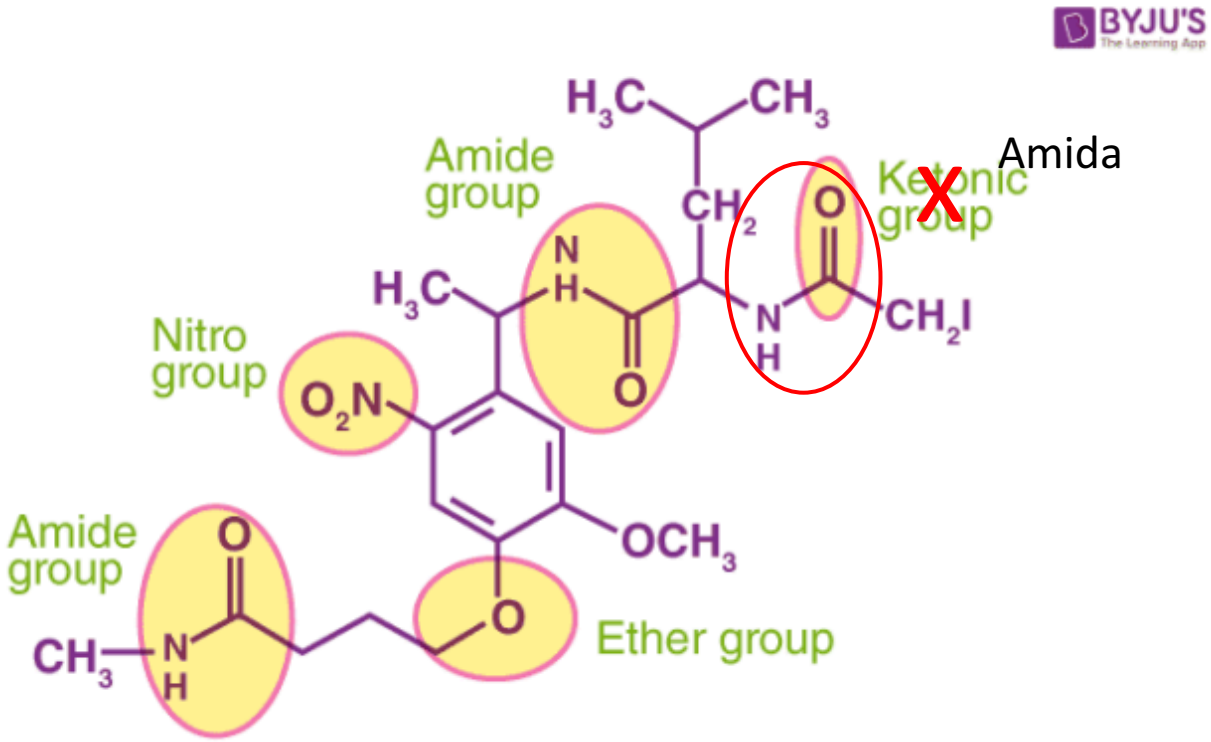
Grupos funcionales



Amida

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Ejercicios

Draw a Lewis structure for methanol, a compound with molecular formula CH_4O.

Ejercicios

Draw a Lewis structure for methanol, a compound with molecular formula CH_4O.

Step [1]
Arrange the atoms.

H
H C O H
H

- four atoms around C
- two atoms around O

Step [2]
Count the electrons.

1 C × 4 e^- = 4 e^-
1 O × 6 e^- = 6 e^-
4 H × 1 e^- = 4 e^-
14 e^- total

Step [3]
Add the bonds and lone pairs.

Add bonds first... ...then lone pairs.

only 10 electrons used

In Step [3], placing bonds between all atoms uses only 10 electrons, and the O atom does not yet have a complete octet. To complete the structure, give the O atom two nonbonded electron pairs. This uses all 14 electrons, giving every H two electrons and every second-row element eight. We have now drawn a valid Lewis structure.

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What orbitals are used to form each of the C – C and C – H bonds in $CH_3CH_2CH_3$ (propane)? How many σ bonds are present in this molecule?

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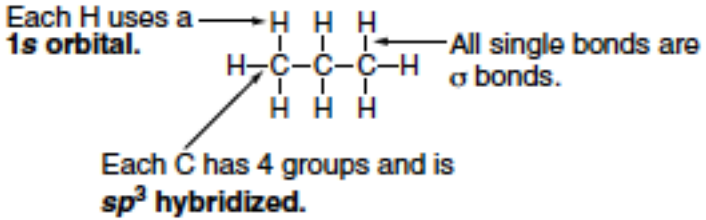
What orbitals are used to form each of the C – C and C – H bonds in $CH_3CH_2CH_3$ (propane)? How many σ bonds are present in this molecule?



Each C–C bond is Csp^3–Csp^3.
Each C–H bond is Csp^3–H1s.

Total of 10 σ bonds.

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What orbitals are used to form each bond in methanol, CH_3OH?

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What orbitals are used to form each bond in methanol, CH_3OH?

- All C–H bonds are formed from C_{sp^3}–H_{1s}.
- The C–O bond is formed from C_{sp^3}–O_{sp^3}.
- The O–H bond is formed from O_{sp^3}–H_{1s}.

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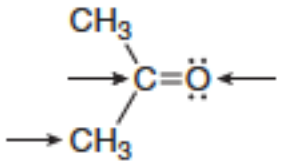
Answer each question for the molecule acetone, drawn below:



acetone

a. Determine the hybridization of the indicated atoms.
b. What orbitals are used to form the C–O double bond?
c. In what type of orbital does each lone pair reside?

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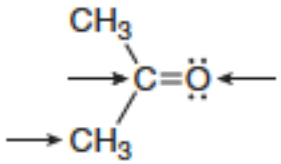
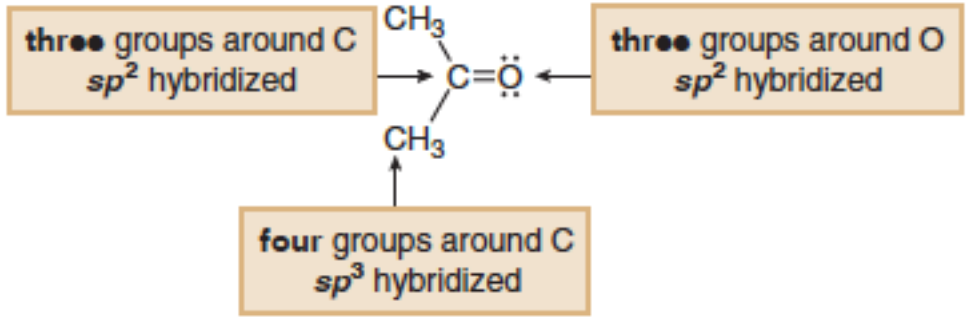
Answer each question for the molecule acetone, drawn below:



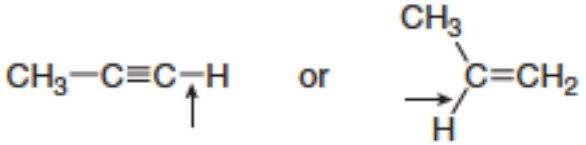
acetone

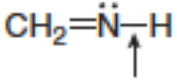
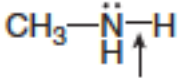
a. Determine the hybridization of the indicated atoms.
b. What orbitals are used to form the C–O double bond?
c. In what type of orbital does each lone pair reside?

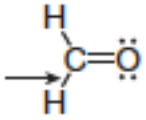
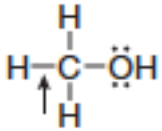
a.



Which of the indicated bonds in each pair of compounds is shorter?

a.  or

c.  or 

b.  or 

Which of the indicated bonds in each pair of compounds is shorter?

a. $CH_3-C\equiv C-H$ or $CH_3-C(CH_3)=CH_2$ (H)

c. $CH_2=\ddot{N}-H$ or $CH_3-\ddot{N}(H)-H$

b. $H-C(=O)-H$ or $H-C(-H)-OH$

Bond length and bond strength are inversely related: **longer bonds are weaker bonds**. Single bonds are weaker and longer than double bonds, which are weaker and longer than triple bonds. Increasing percent *s*-character increases bond strength and decreases bond length.

a. $CH_3-C\equiv C-H$ or $CH_3-C(CH_3)=CH_2$ (H)

C_{sp}–H1*s*
50% *s*-character
shorter bond

C_{sp^2}–H1*s*
33% *s*-character

c. $CH_2=\ddot{N}-H$ or $CH_3-\ddot{N}(H)-H$

N_{sp^2}–H1*s*
33% *s*-character
shorter bond

N_{sp^3}–H1*s*
25% *s*-character

b. $H-C(=O)-H$ or $H-C(-H)-OH$

C_{sp^2}–H1*s*
33% *s*-character
shorter bond

C_{sp^3}–H1*s*
25% *s*-character

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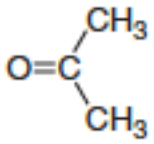
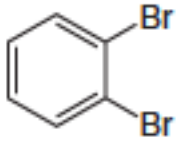
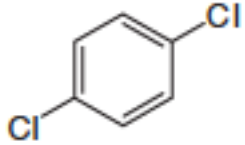
Label the polar bonds in each molecule. Indicate the direction of the net dipole (if there is one).

a. $CHBr_3$
b. $CH_3CH_2OCH_2CH_3$
c. CBr_4

d. 

e. 

f. 

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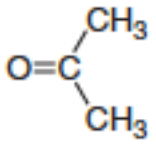
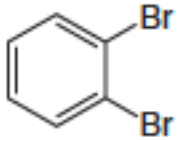
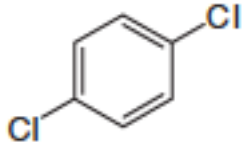
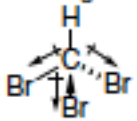
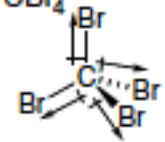
a. $CHBr_3$
b. $CH_3CH_2OCH_2CH_3$
c. CBr_4

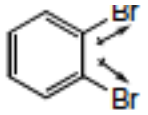
d. 

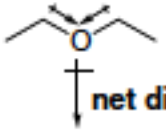
e. 

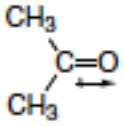
f. 

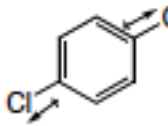
a. $CHBr_3$  net dipole

c. CBr_4  no net dipole

e.  net dipole

b. $CH_3CH_2OCH_2CH_3$  net dipole

d.  net dipole

f.  no net dipole

Ketene, $CH_2=C=O$, is an unusual organic molecule that has a single carbon atom doubly bonded to two different atoms. Determine the hybridization of both C atoms and the O in ketene. Then, draw a diagram showing what orbitals are used to form each bond (similar to Figures 1.12 and 1.13).

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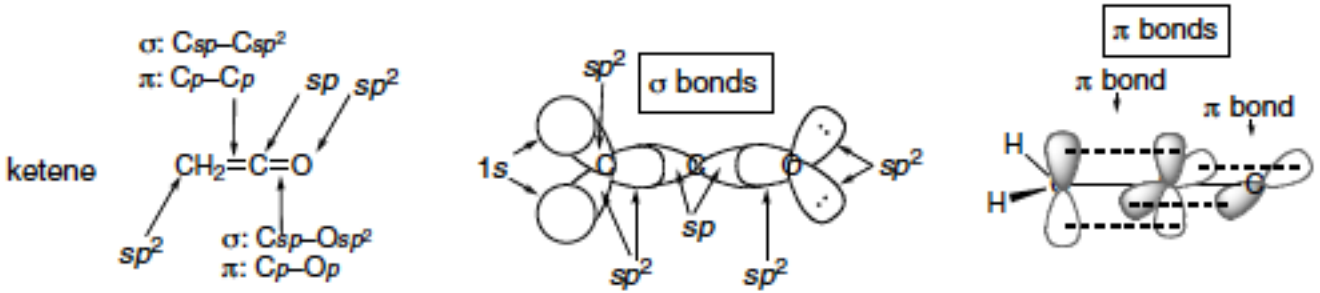
Ketene, $CH_2=C=O$, is an unusual organic molecule that has a single carbon atom doubly bonded to two different atoms. Determine the hybridization of both C atoms and the O in ketene. Then, draw a diagram showing what orbitals are used to form each bond (similar to Figures 1.12 and 1.13).



[For clarity, only the large bonding lobes of the hybrid orbitals are drawn.]