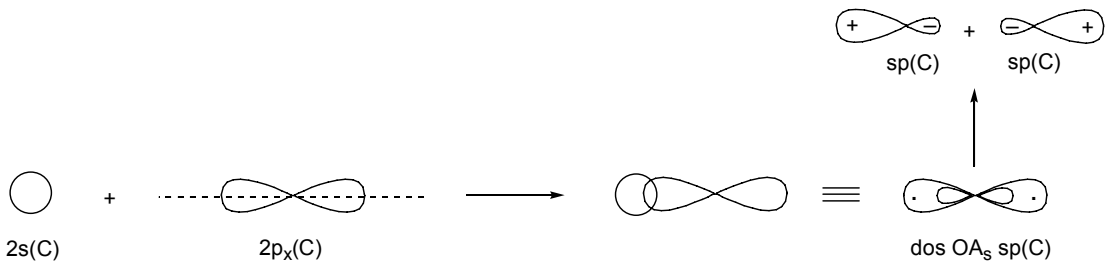
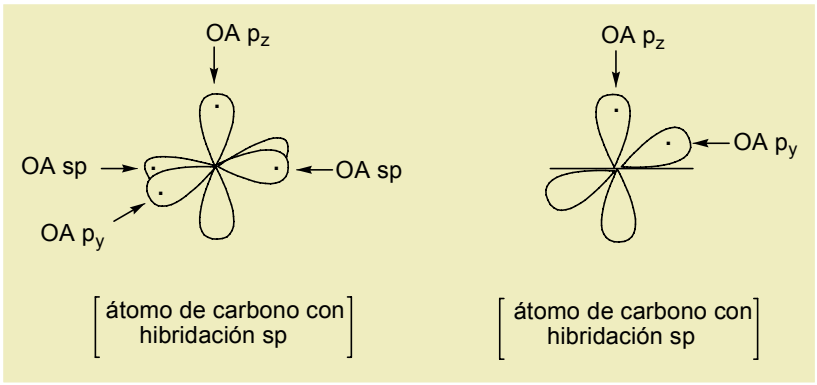
ESTRUCTURA ELECTRÓNICA DE LAS MOLÉCULAS ORGÁNICAS

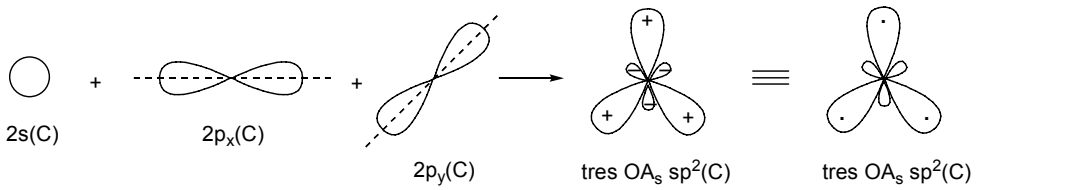
ORBITALES ATÓMICOS HÍBRIDOS LOCALIZADOS DEL CARBONO

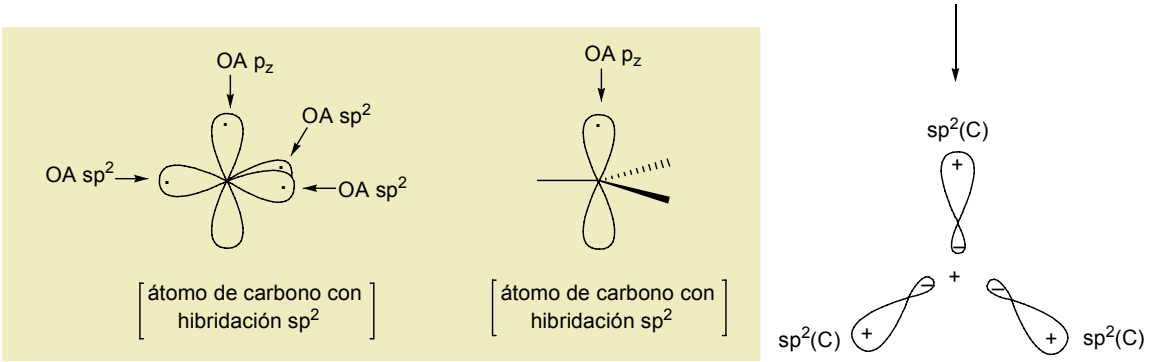
***HIBRIDACIÓN** sp: Los híbridos sp se obtienen por combinación lineal de un OA 2s y un OA 2p de carbono*



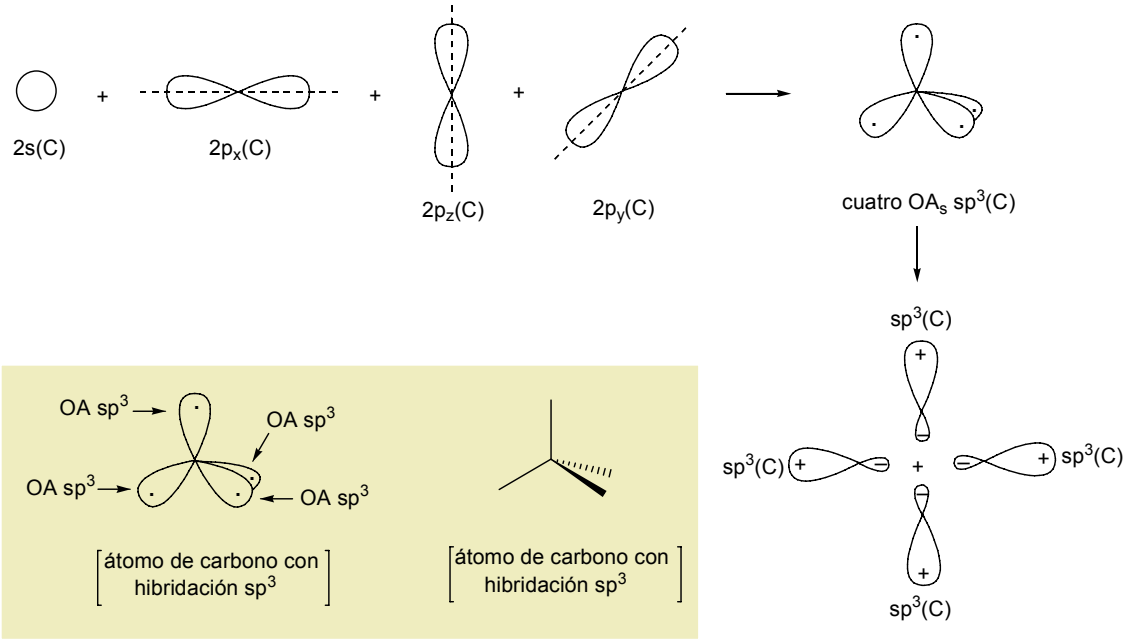


***HIBRIDACIÓN** sp^2: Los híbridos sp^2 se obtienen por combinación lineal de un OA 2s y dos OAs 2p de carbono*





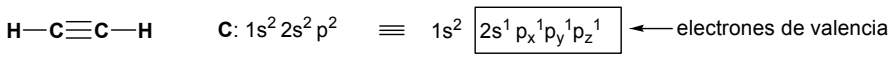
HIBRIDACIÓN *sp^3: Los híbridos sp^3 se obtienen por combinación lineal de un OA 2s y tres OAs 2p de carbono*



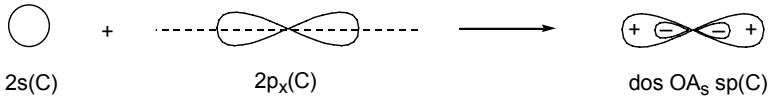
ORBITALES MOLECULARES LOCALIZADOS

Los OMs localizados se obtienen por combinación lineal de OAs localizados (OAs híbridos) entre sí o por combinación lineal de OAs localizados con otros OAs (p.e. un OA 1s del átomo de hidrógeno)

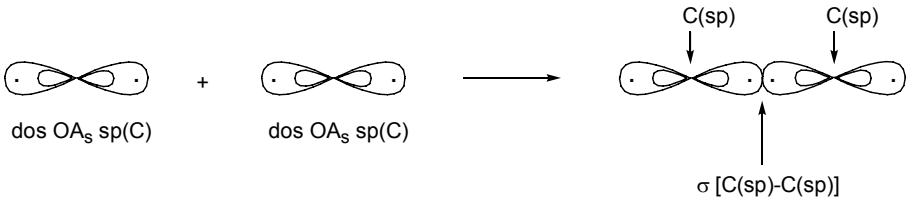
ORBITALES MOLECULARES LOCALIZADOS DEL ACETILENO



1 Formación de dos OAs híbridos sp de carbono:

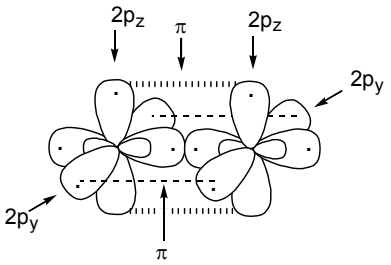


2 Formación de un OM localizado σ[C(sp)-C(sp)] por combinación lineal de dos OAs híbridos sp de C:



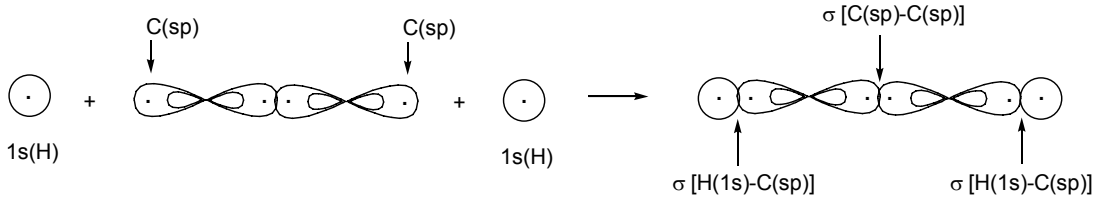
La combinación lineal de dos OAs p, empleando el eje de simetria de ambos (interacción frontal), da lugar a orbitales moleculares σ (enlace σ)

3 Formación de dos OMs localizados π por combinación lineal de dos OAs (p_y ,p_z) de C:

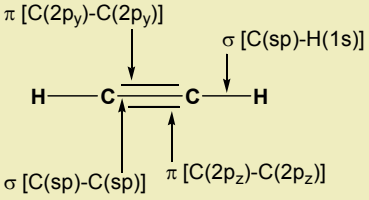


La combinación lineal de dos OAs p, de forma paralela (interacción lateral), da lugar a orbitales moleculares π (enlace π)

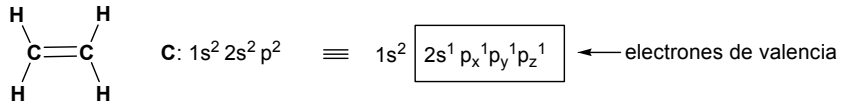
4 Formación de dos OMs σ por combinación lineal de un OA híbrido localizado sp del C y un OA 1s del H:



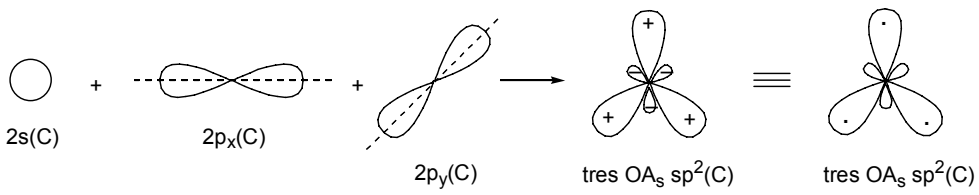
ORBITALES MOLECULARES LOCALIZADOS DEL ACETILENO



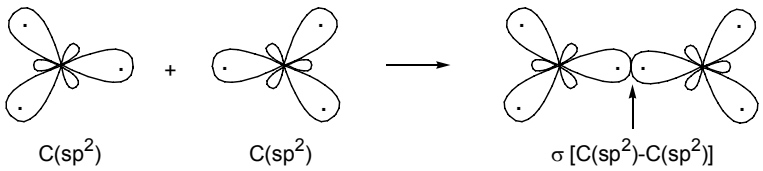
ORBITALES MOLECULARES LOCALIZADOS DEL ETILENO



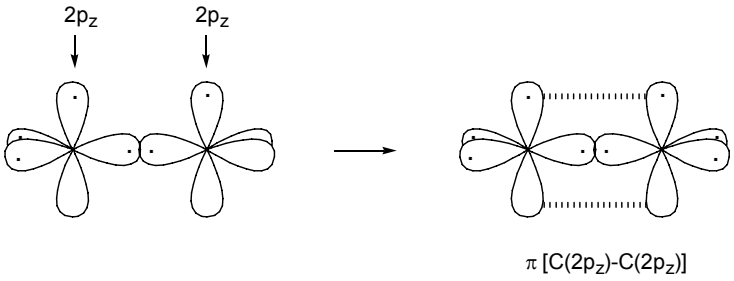
Formación de tres OAs híbridos sp^2 de carbono:



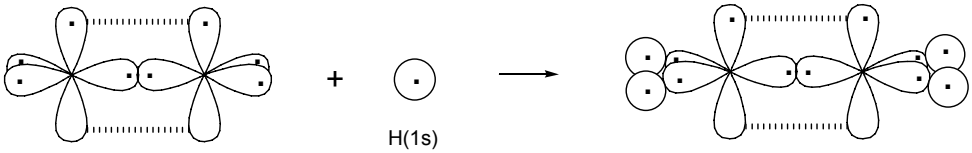
2 Formación de un OM localizado $\sigma[C(sp^2)\text{-}C(sp^2)]$ por combinación lineal de dos OAs híbridos sp^2 de C:



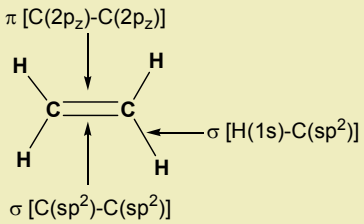
3 Formación de un OM localizado $\pi[C(p_z)\text{-}C(p_z)]$ por combinación lineal de OAs p_z del C:



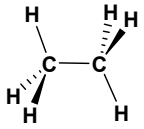
Formación de cuatro OMs localizados $\sigma[C(sp^2)\text{-}H(1s)]$ por combinación lineal de híbridos $C(sp^2)$ e H(1s):



ORBITALES MOLECULARES LOCALIZADOS DEL ETILENO

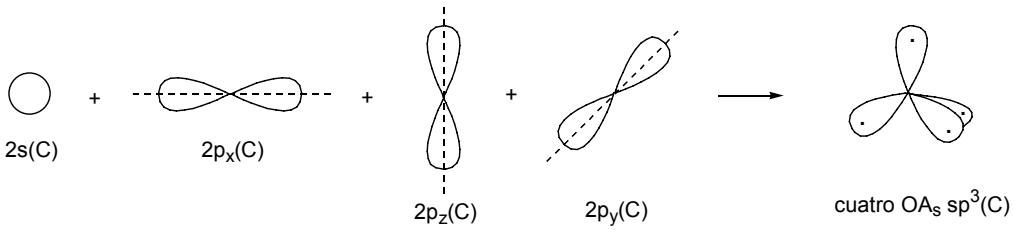


ORBITALES MOLECULARES LOCALIZADOS DEL ETANO

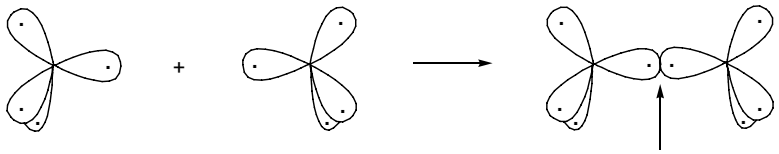


C: $1s^2\ 2s^2\ p^2$ ≡ $1s^2$ $\boxed{2s^1\ p_x{}^1 p_y{}^1 p_z{}^1}$ ← electrones de valencia

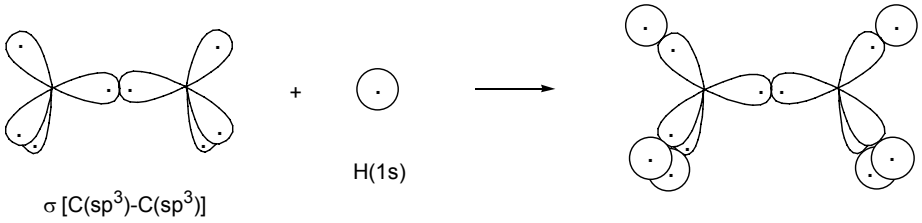
1 Formación de cuatro OAs híbridos sp^3 de C:



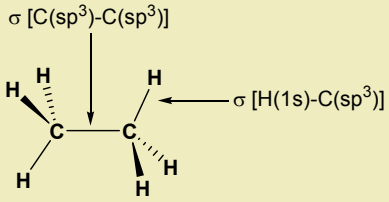
2 Formación de un OM localizado σ[C(sp^3)-C(sp^3)] por combinación lineal de dos OAs híbridos sp^3 de C:



3 Formación de seis OMs localizados σ[C(sp^3)-H(1s)] por combinación lineal de híbridos C(sp^3) e H(1s):



ORBITALES MOLECULARES LOCALIZADOS DEL ETANO

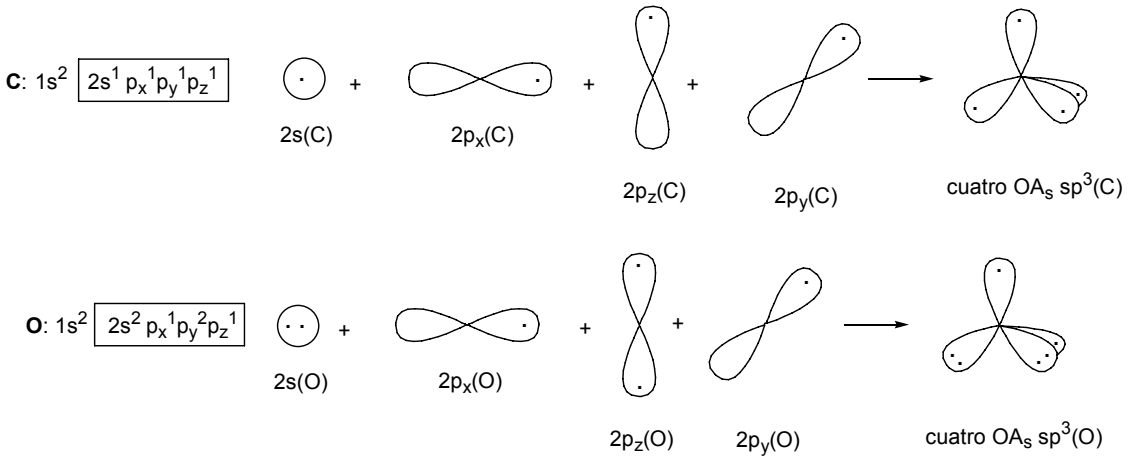


TIPOS DE HIBRIDACIÓN Y GEOMETRÍA MOLECULAR

átomo	híbrido	tipo de enlace	geometría	grupo funcional
C($2s^1px^1py^1pz^1$)	sp	σ [C(sp)-C(sp)]	—C—C—	—C≡C— (alquinos)
	sp^2	σ [C(sp^2)-C(sp^2)]		(alquenos)
	sp^3	σ [C(sp^3)-C(sp^3)]		(alcanos)
O($2s^1px^1py^2pz^1$)	sp^3	σ [C(sp^3)-O(sp^3)]		(alcoholes, éteres)
	sp^2	σ [C(sp^2)-O(sp^2)]		(aldehidos, cetonas)
N($2s^2px^1py^1pz^1$)	sp^3	σ [C(sp^3)-N(sp^3)]		(aminas)
	sp	σ [C(sp)-N(sp)]	—C—N	—C≡N: (nitrilos)

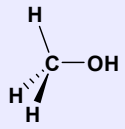
ESTRUCTURA ELECTRÓNICA DE GRUPOS FUNCIONALES

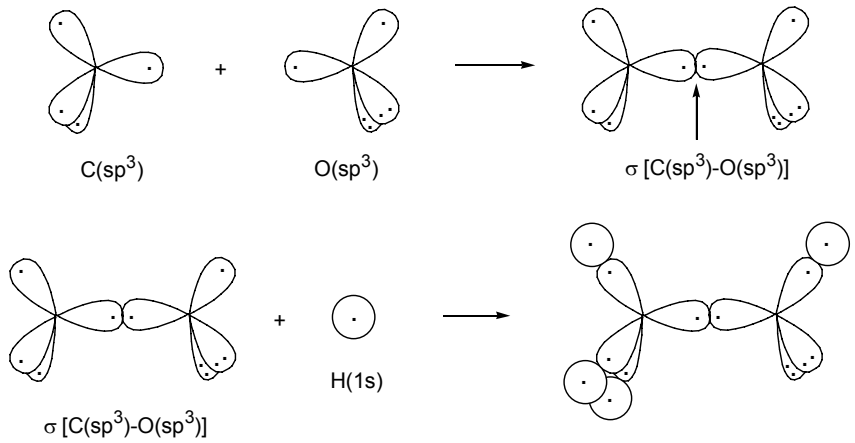
ALCOHOLES Y ÉTERES



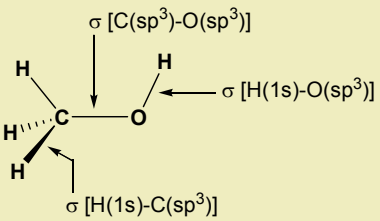
Orbitales moleculares localizados del metanol

Metanol:



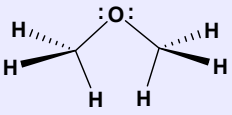


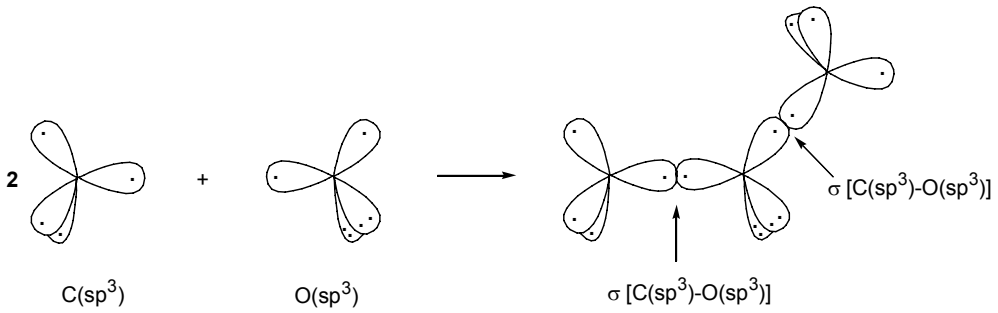
ORBITALES MOLECULARES LOCALIZADOS DEL METANOL

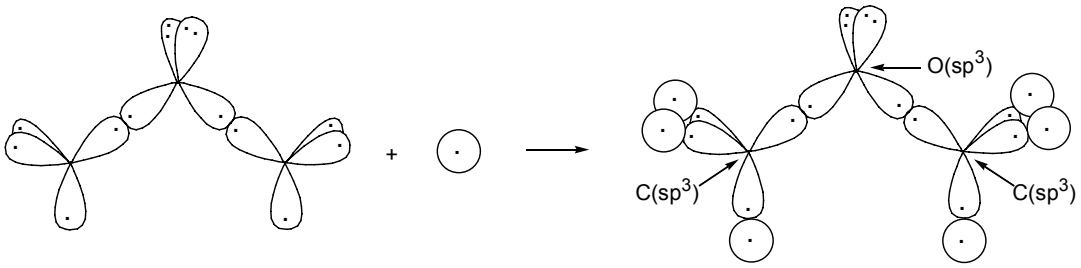


Orbitales moleculares localizados del dimetil éter

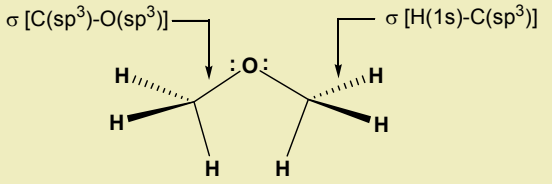
Dimetil éter: $CH_3—\ddot{O}—CH_3$



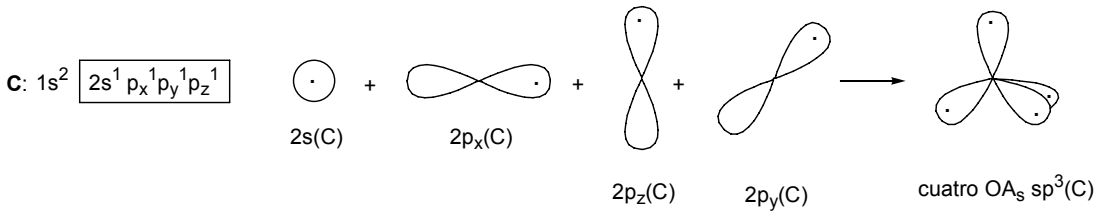


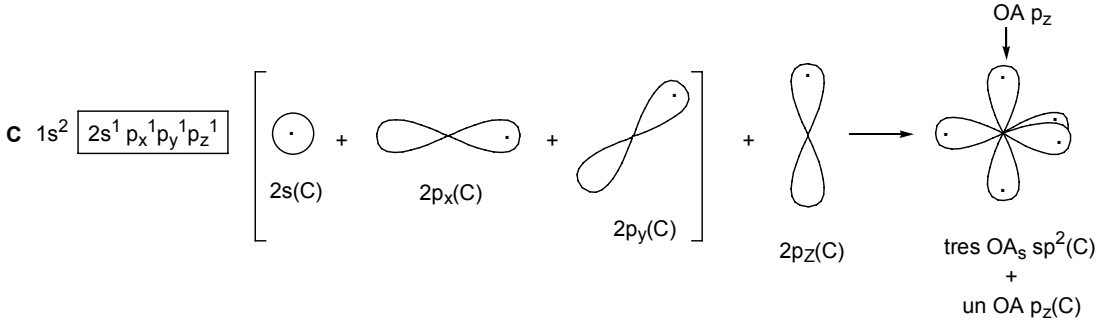


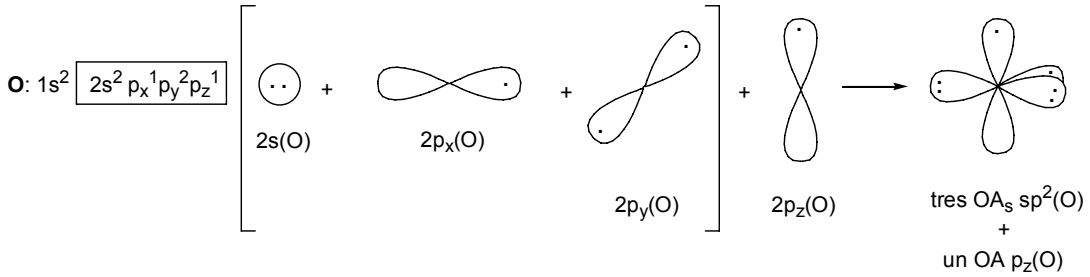
ORBITALES MOLECULARES LOCALIZADOS DEL DIMETIL ÉTER



ALDEHIDOS Y CETONAS

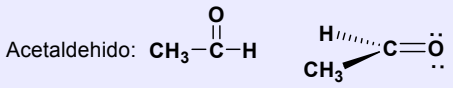


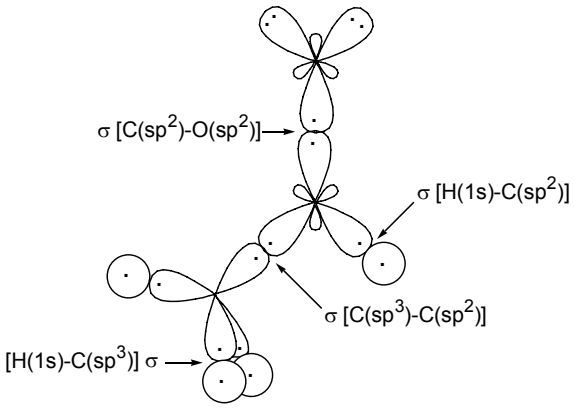


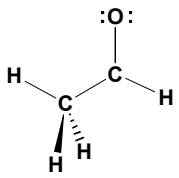


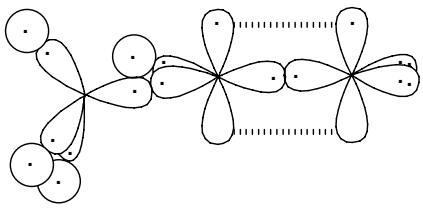
Con el fin de no complicar los dibujos, primero aparece un diagrama con el esqueleto de enlaces σ, y después otro con los enlaces π.

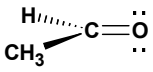
Orbitales moleculares localizados del acetaldehido

Acetaldehido: 

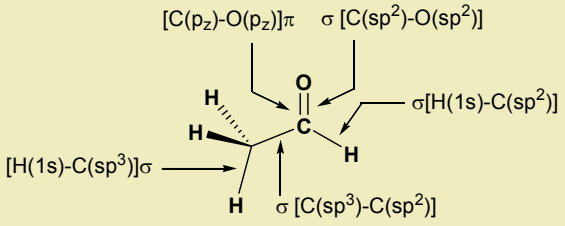




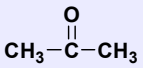
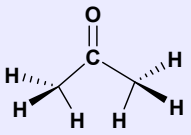


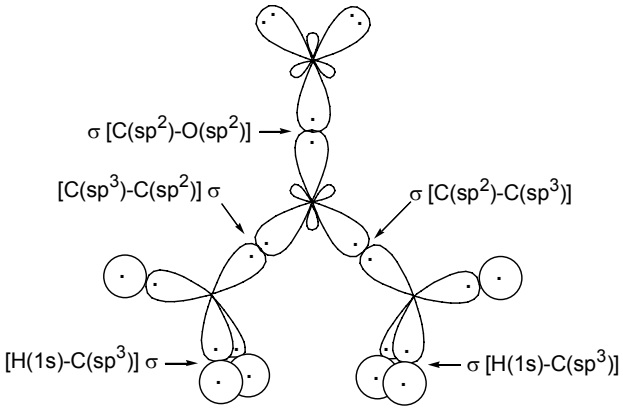


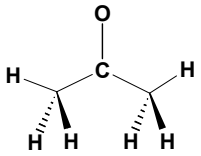
ORBITALES MOLECULARES LOCALIZADOS DEL ACETALDEHIDO

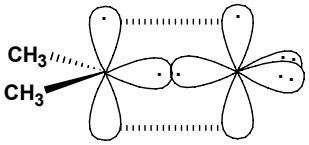


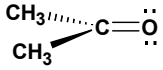
Orbitales moleculares localizados de la dimetilcetona

Dimetilcetona:  

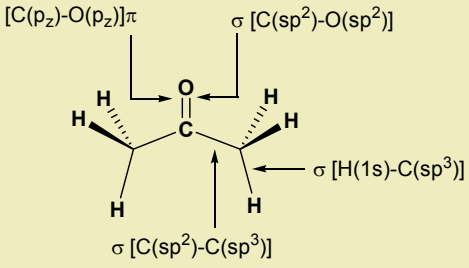




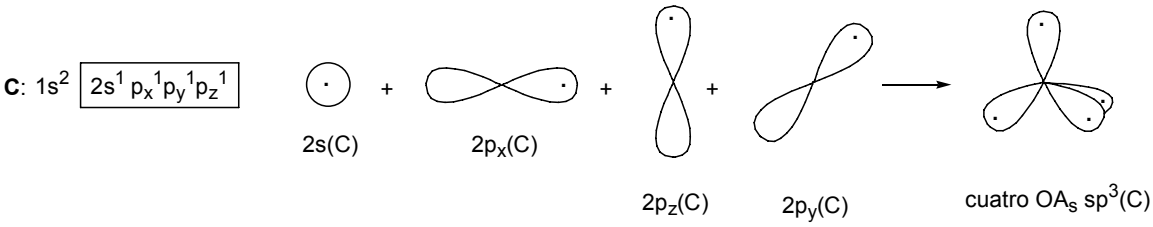


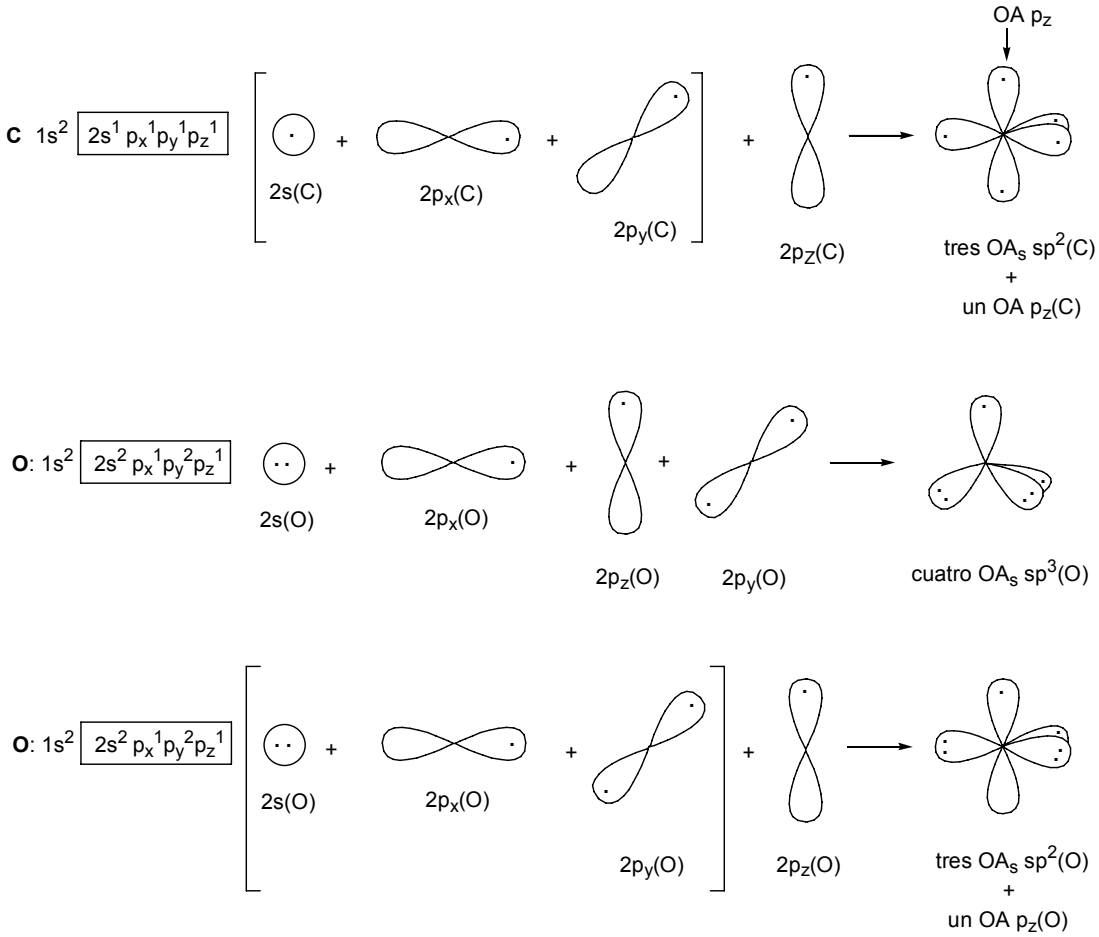


ORBITALES MOLECULARES LOCALIZADOS DE LA DIMETILCETONA



ÁCIDOS CARBOXÍLICOS

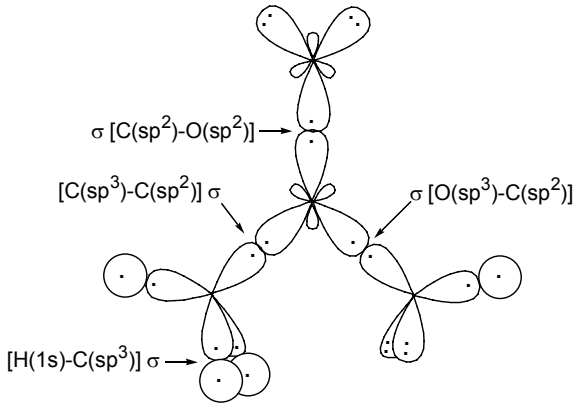


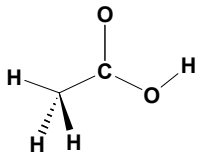


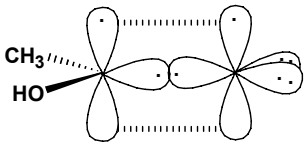
Con el fin de no complicar los dibujos, primero aparece un diagrama con el esqueleto de enlaces σ, y después otro con los enlaces π.

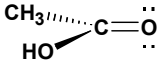
Orbitales moleculares localizados del ácido acético

Ácido acético: $CH_3-C(=O)-OH$

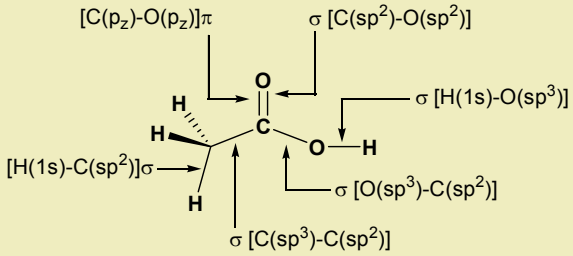








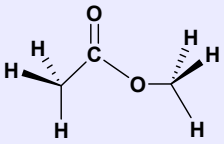
ORBITALES MOLECULARES LOCALIZADOS DEL ÁCIDO ACÉTICO

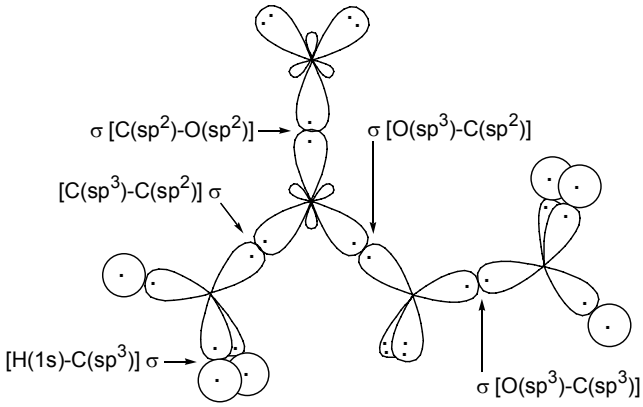


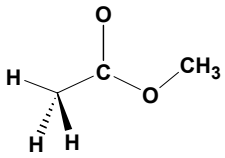
ÉSTERES

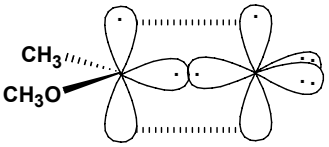
Orbitales moleculares localizados del acetato de metilo

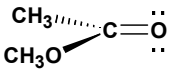
Acetato de metilo: $CH_3-C(=O)-OCH_3$



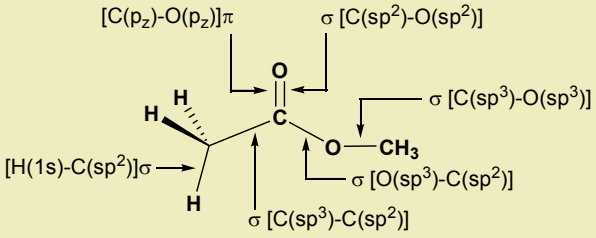






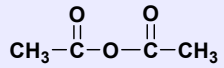


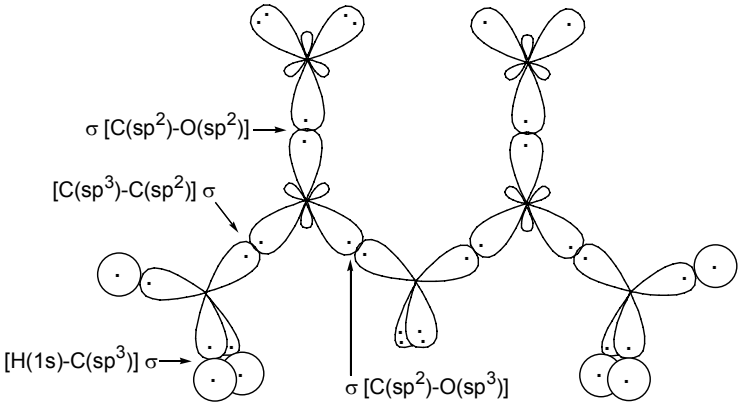
ORBITALES MOLECULARES LOCALIZADOS DEL ACETATO DE METILO

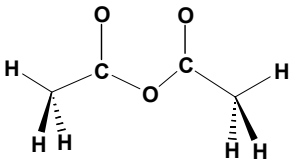


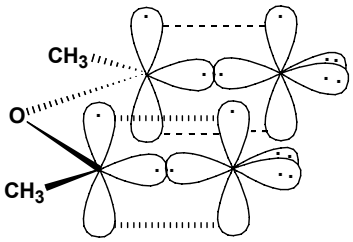
ANHIDRIDOS DE ÁCIDOS

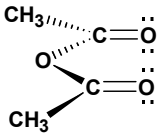
Orbitales moleculares localizados del anhidrido acético

Anhidrido acético: 

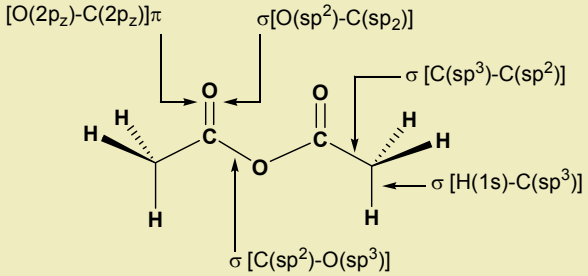






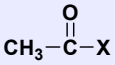


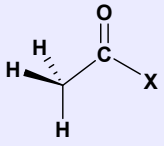
ORBITALES MOLECULARES LOCALIZADOS DEL ANHIDRIDO ACÉTICO

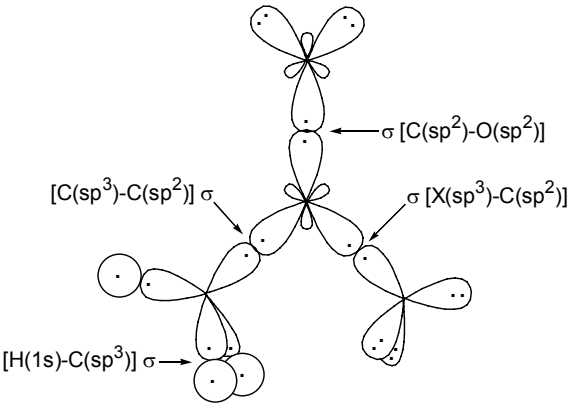


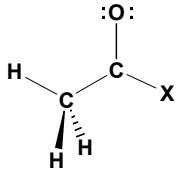
HALUROS DE ÁCIDOS

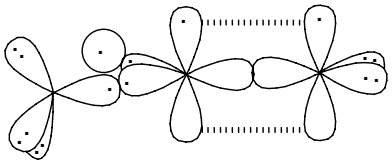
Orbitales moleculares localizados de un haluro de acetilo

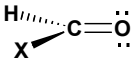
Haluro de acetilo: 



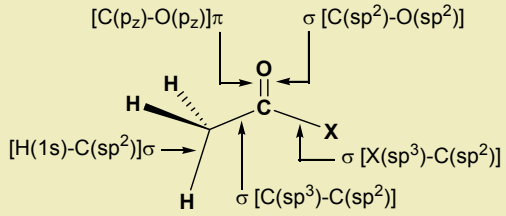








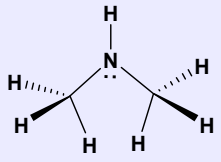
ORBITALES MOLECULARES LOCALIZADOS DE UN HALURO DE ÁCIDO

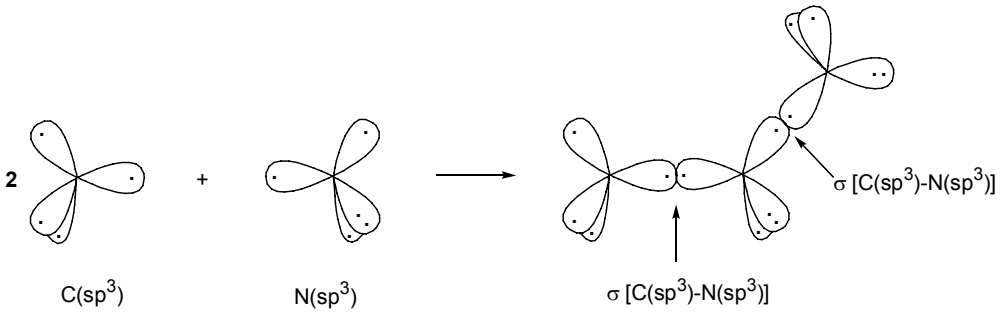


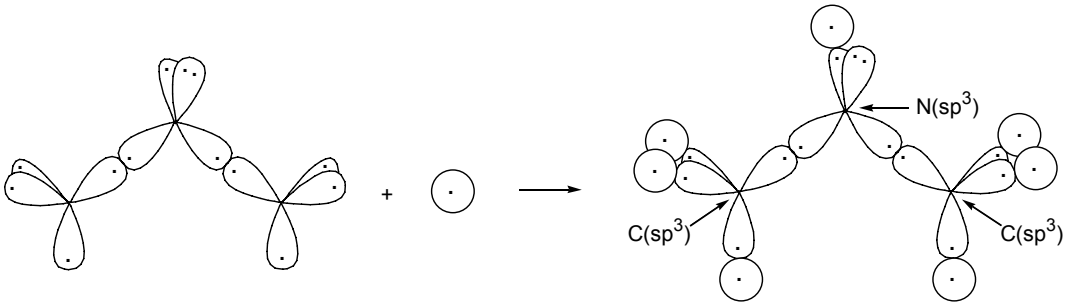
AMINAS

Orbitales moleculares localizados de la dimetilamina

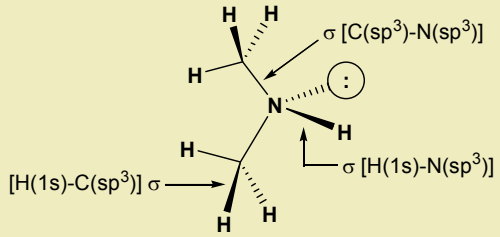
Dimetilamina: $CH_3-\underset{\cdot\cdot}{\overset{H}{N}}-CH_3$







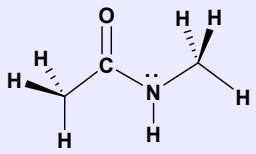
ORBITALES MOLECULARES LOCALIZADOS DE LA DIMETILAMINA

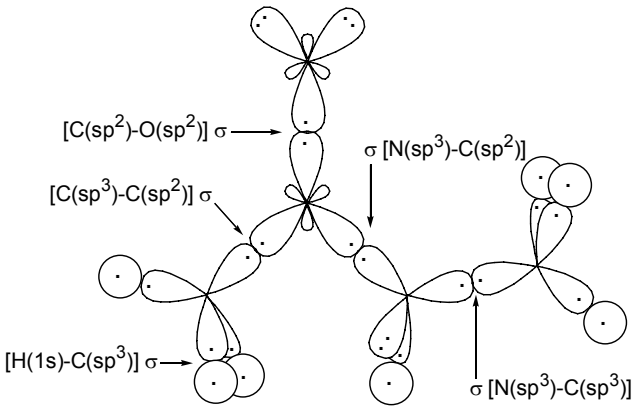


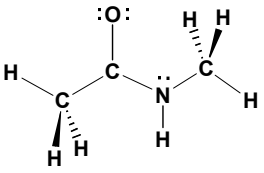
AMIDAS

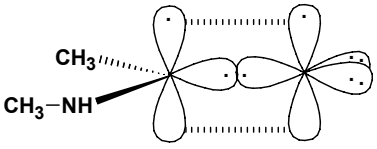
Orbitales moleculares localizados de la N-metilacetamida

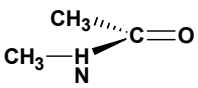
N-Metilacetamida: $CH_3-C(=O)-NH-CH_3$



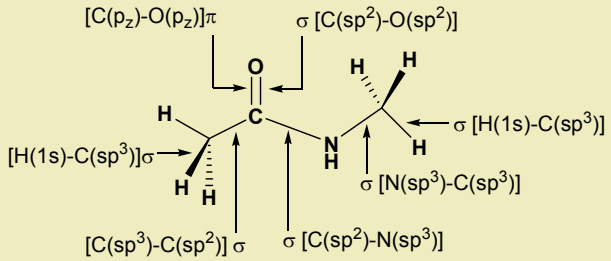








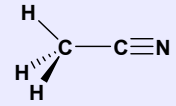
ORBITALES MOLECULARES LOCALIZADOS DE LA N-METILACETAMIDA

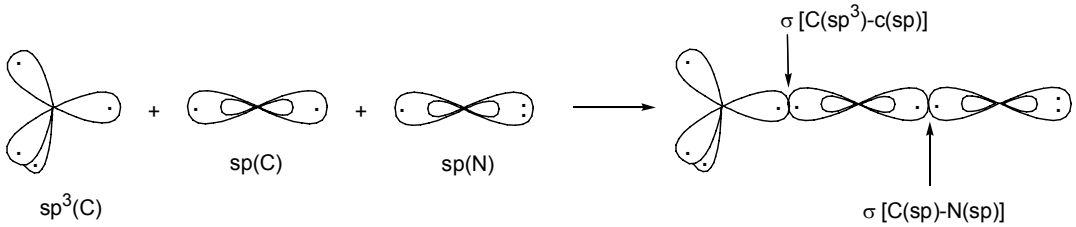


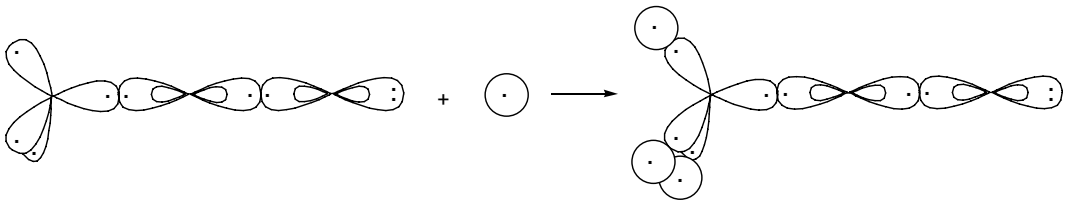
NITRILOS

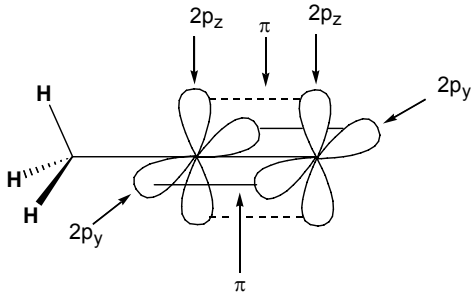
Orbitales moleculares localizados del etanonitrilo

Etanonitrilo: $CH_3-C\equiv N:$

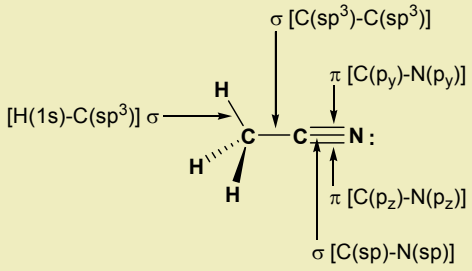




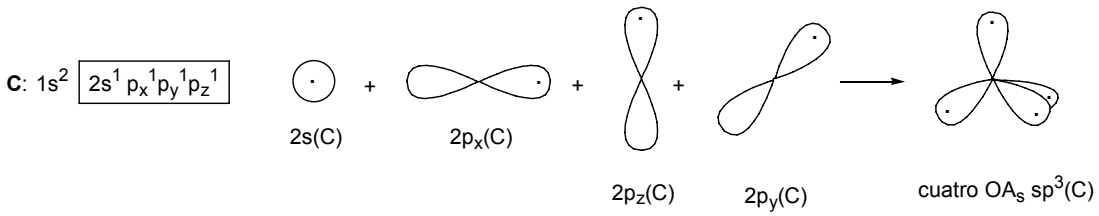


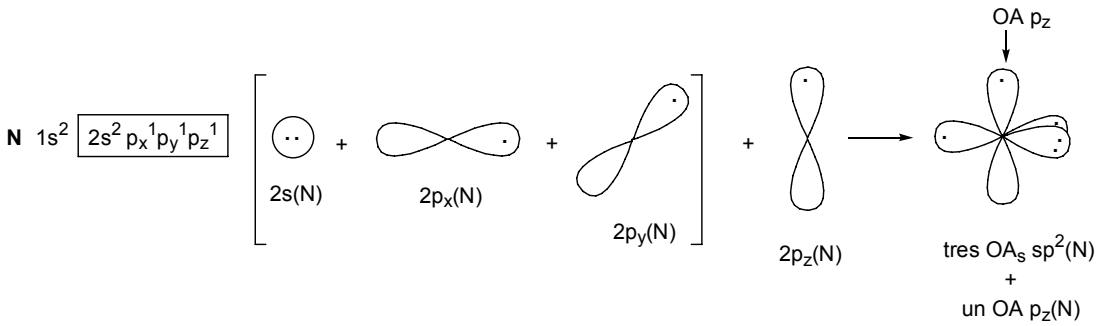


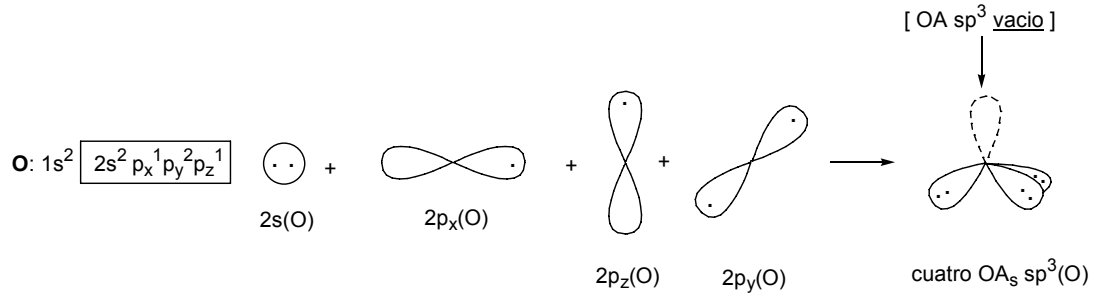
ORBITALES MOLECULARES LOCALIZADOS DEL ACETONITRILO

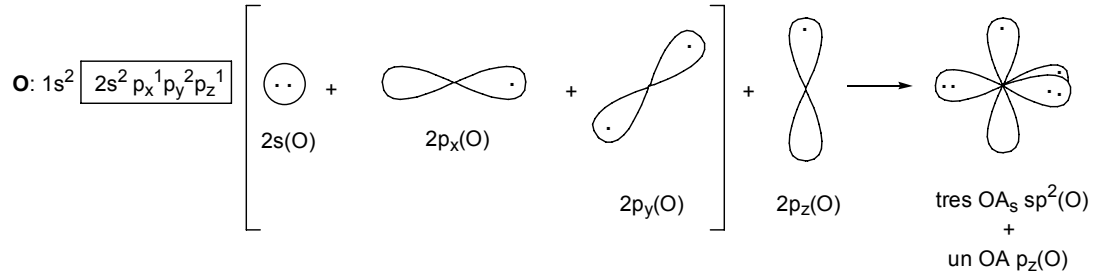


NITRODERIVADOS



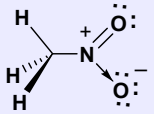


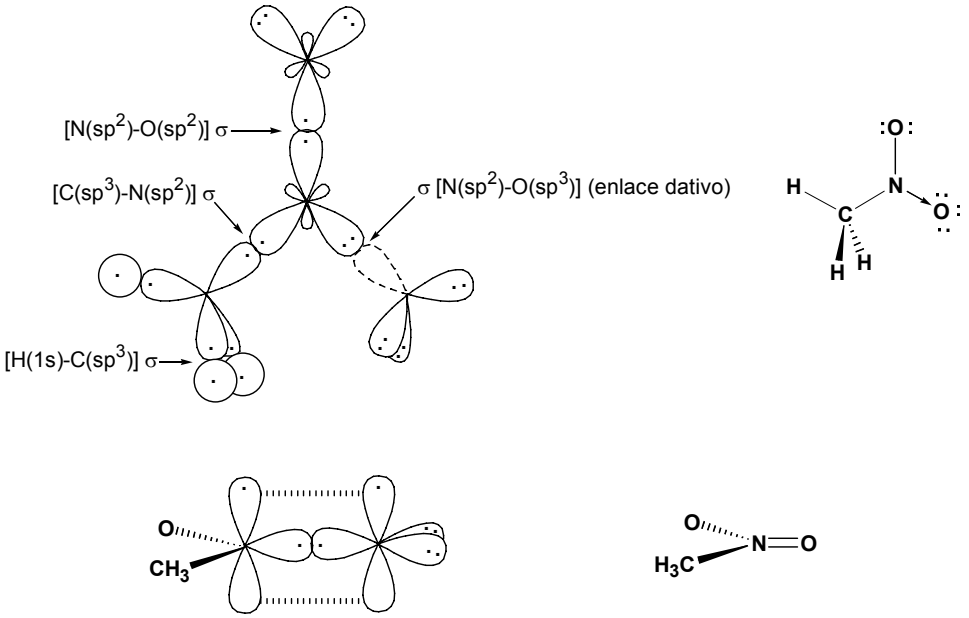




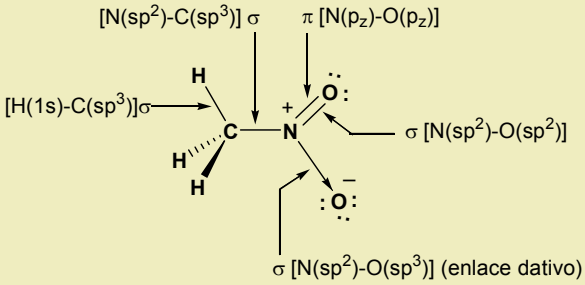
Orbitales moleculares localizados del nitrometano

Nitrometano: CH_3-NO_2





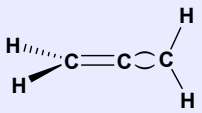
ORBITALES MOLECULARES LOCALIZADOS DEL NITROMETANO

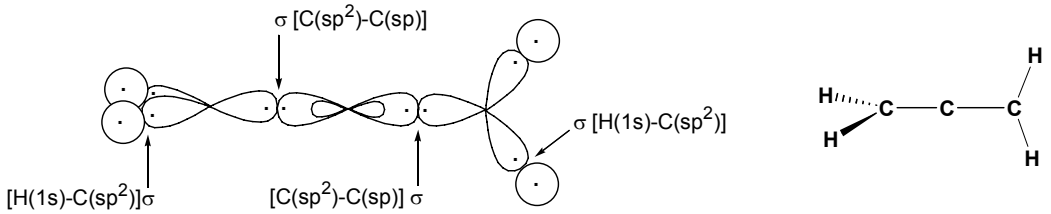


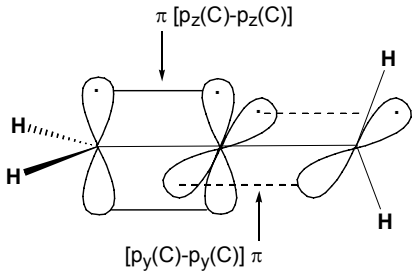
CUMULENOS

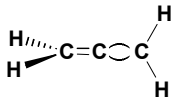
Orbitales moleculares localizados del 1,2-propadieno

1,2-Propadieno: $H_2C{=}C{=}CH_2$

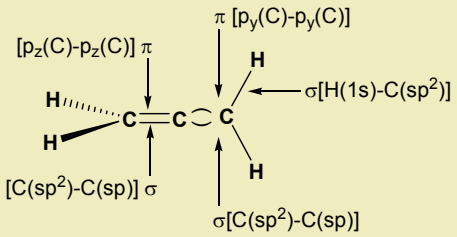






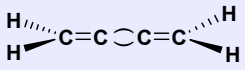


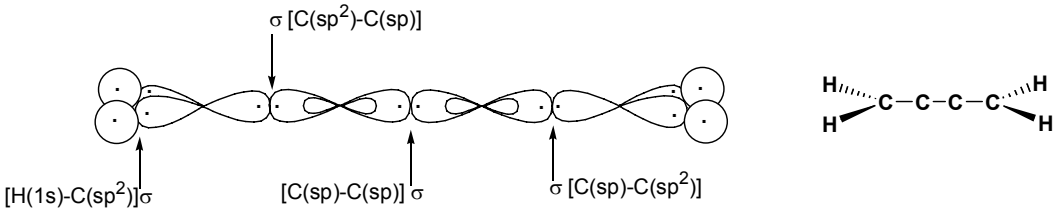
ORBITALES MOLECULARES LOCALIZADOS DEL 1,2-PROPADIENO

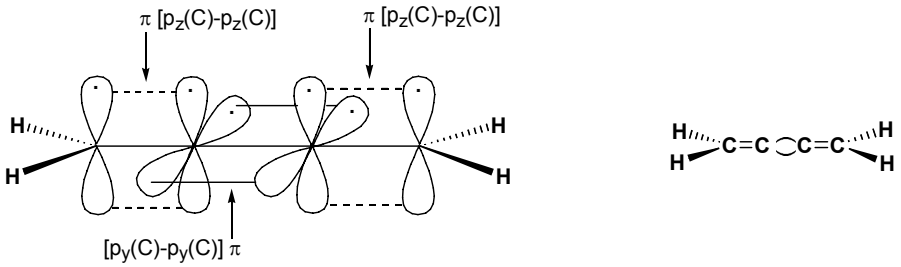


Orbitales moleculares localizados del 1,2,3-butatrieno

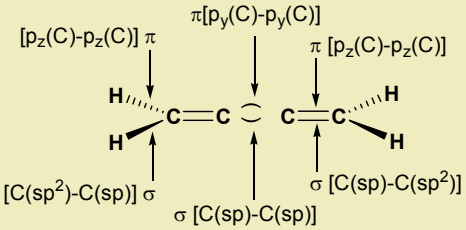
1,2,3-Butatrieno: $H_2C{=}C{=}C{=}CH_2$







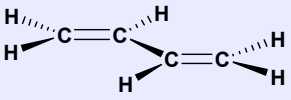
ORBITALES MOLECULARES LOCALIZADOS DEL 1,2,3-BUTATRIENO

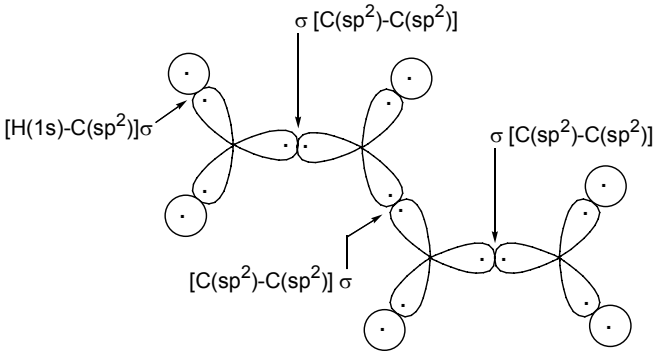


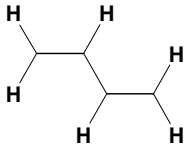
POLIOLEFINAS CONJUGADAS

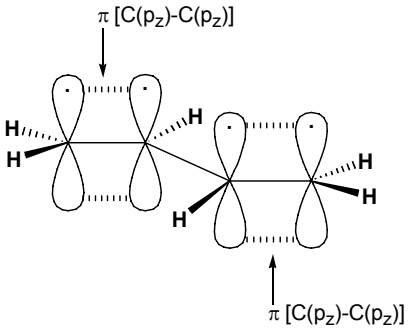
Orbitales moleculares localizados del1,3-butadieno

1,3-Butadieno: $CH_2{=}CH{-}CH{=}CH_2$

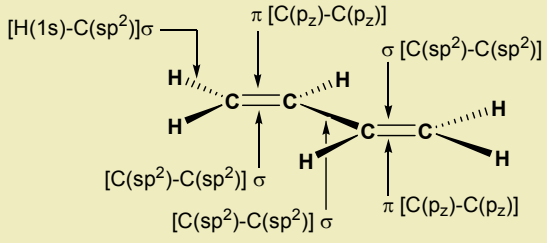






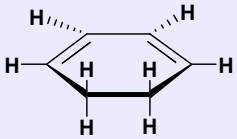


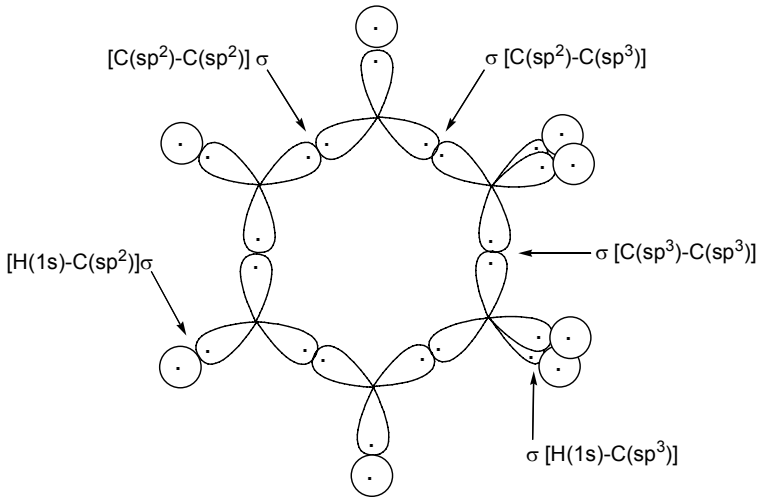
ORBITALES MOLECULARES LOCALIZADOS DEL 1,3-BUTADIENO

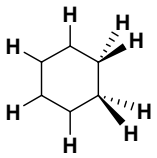


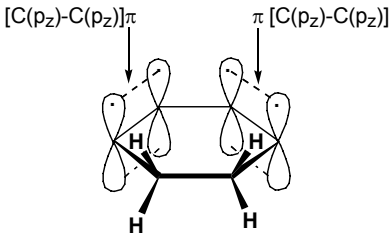
Orbitales moleculares localizados del 1,3-ciclohexadieno

1,3-Ciclohexadieno:

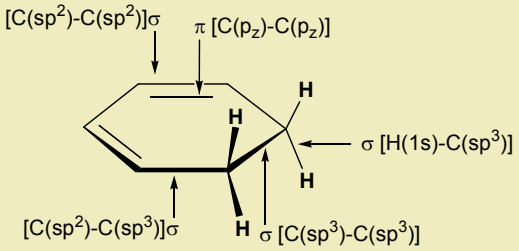








ORBITALES MOLECULARES LOCALIZADOS DEL 1,3-CICLOHEXADIENO



EL MODELO DE ENLACE DESLOCALIZADO

ADVERTENCIA IMPORTANTE

La flecha de doble sentido ⟷ se utiliza cuando una molécula no puede representarse de forma inequívoca con un sólo dibujo. Las distintas formas de dibujarla reciben el nombre de estructuras resonantes, y se relacionan entre sí mediante dicho símbolo.

Las **estructuras resonantes** se utilizan para dibujar las moléculas que aparecen en los tres apartados siguientes.

APARTADO 1

Radicales, cationes y aniones de **moléculas acíclicas y cíclicas con dobles enlaces conjugados**, y número impar de átomos de carbono (alilo, pentadienilo, bencilo, etc.) Esta clase de moléculas reciben el nombre de **hidrocarburos alternantes impares** (ver más adelante, p. 114)