Ibridizzazione (o ibridazione)

$$\psi_i = a_i\,\psi(s) + b_i\,\psi(p_x) + c_i\,\psi(p_y) + d_i\,\psi(p_z)$$

$$\psi_1 = a_1\,\psi(s) + b_1\,\psi(p_x) + c_1\,\psi(p_y) + d_1\,\psi(p_z)$$
$$\psi_2 = a_2\,\psi(s) + b_2\,\psi(p_x) + c_2\,\psi(p_y) + d_2\,\psi(p_z)$$
$$\psi_3 = a_3\,\psi(s) + b_3\,\psi(p_x) + c_3\,\psi(p_y) + d_3\,\psi(p_z)$$
$$\psi_4 = a_4\,\psi(s) + b_4\,\psi(p_x) + c_4\,\psi(p_y) + d_4\,\psi(p_z)$$

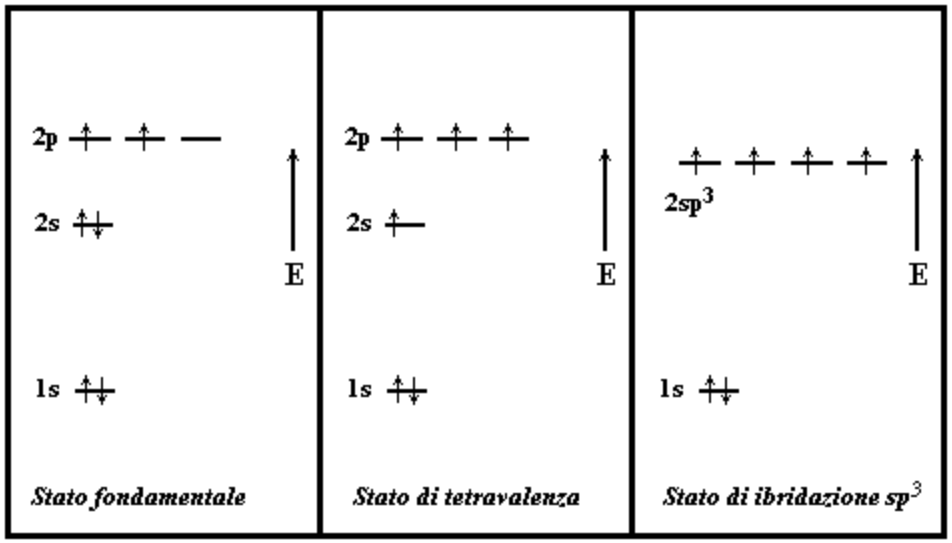
$$\psi(s) = f(r)$$
$$\psi(p_x) = f(r)\,3^{1/2}\,\mathrm{sen}\vartheta\,\cos\varphi$$
$$\psi(p_y) = f(r)\,3^{1/2}\,\mathrm{sen}\vartheta\,\mathrm{sen}\varphi$$
$$\psi(p_z) = f(r)\,3^{1/2}\,\cos\vartheta$$

$$\int \psi_i^2\,dV = 1$$

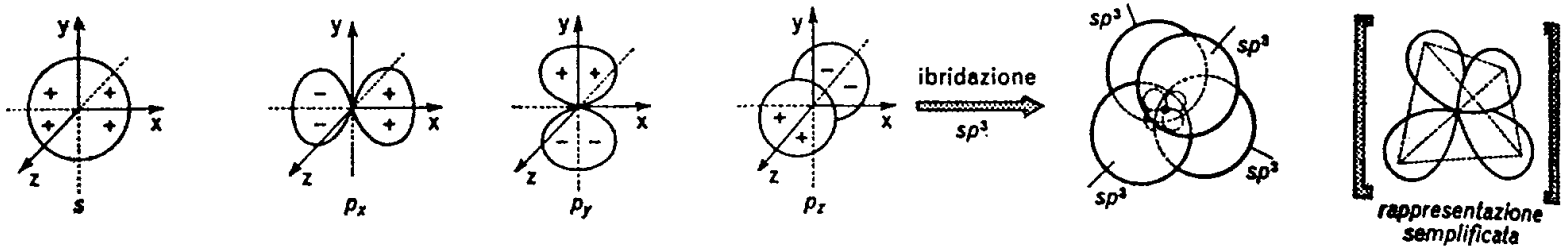
i = 1, 2, 3, 4

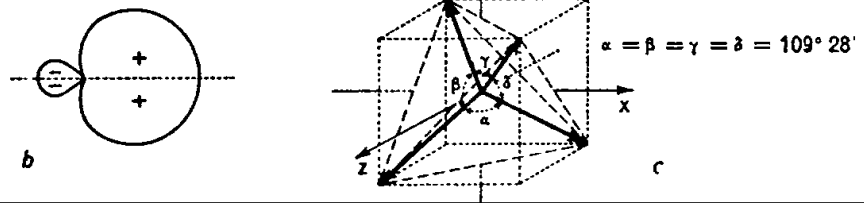
$$a_i^2 + b_i^2 + c_i^2 + d_i^2 = 1$$

Ibridizzazione sp^3 dell'atomo di C

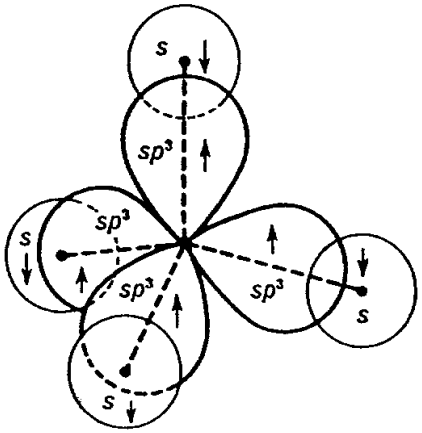


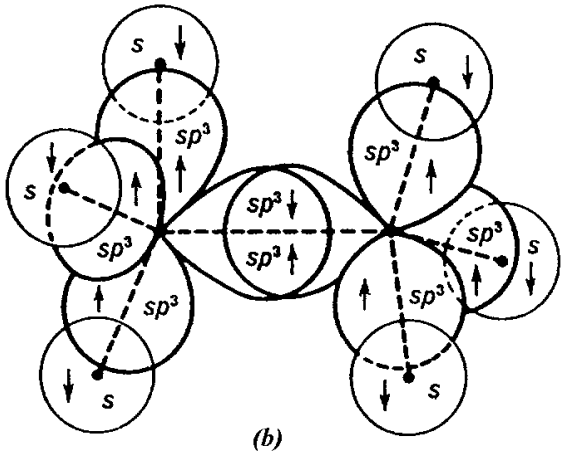
a





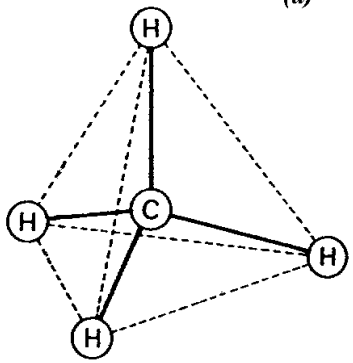
Idrocarburi ALCANI C_nH_{2n+2}

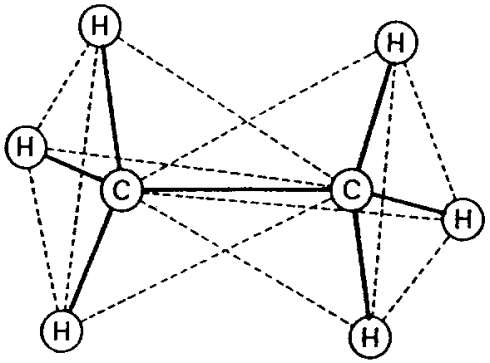




(a) *(b)*

Le molecole del metano (a) e dell'etano (b)





n = 3 C_3H_8 Propano

n = 4 C_4H_{10} Butano

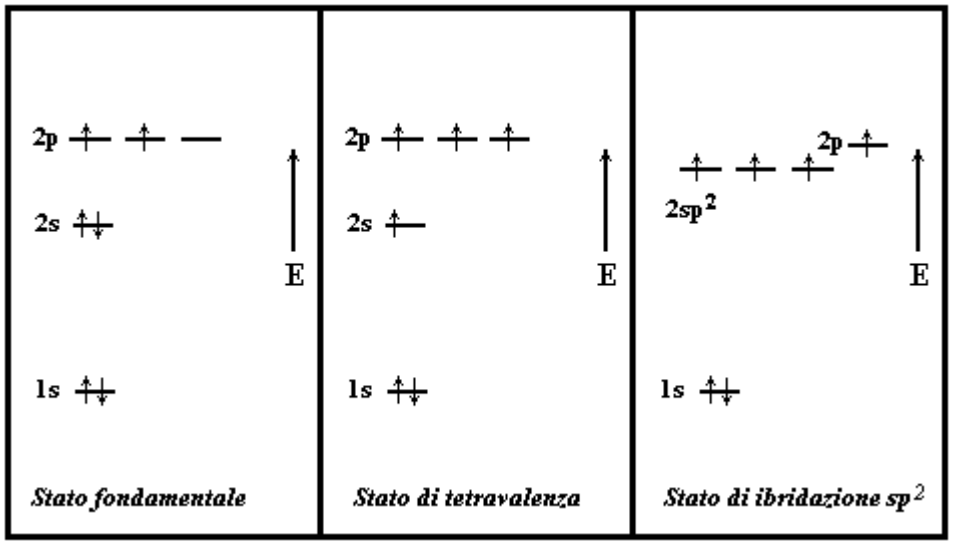
n = 5 C_5H_{12} Pentano

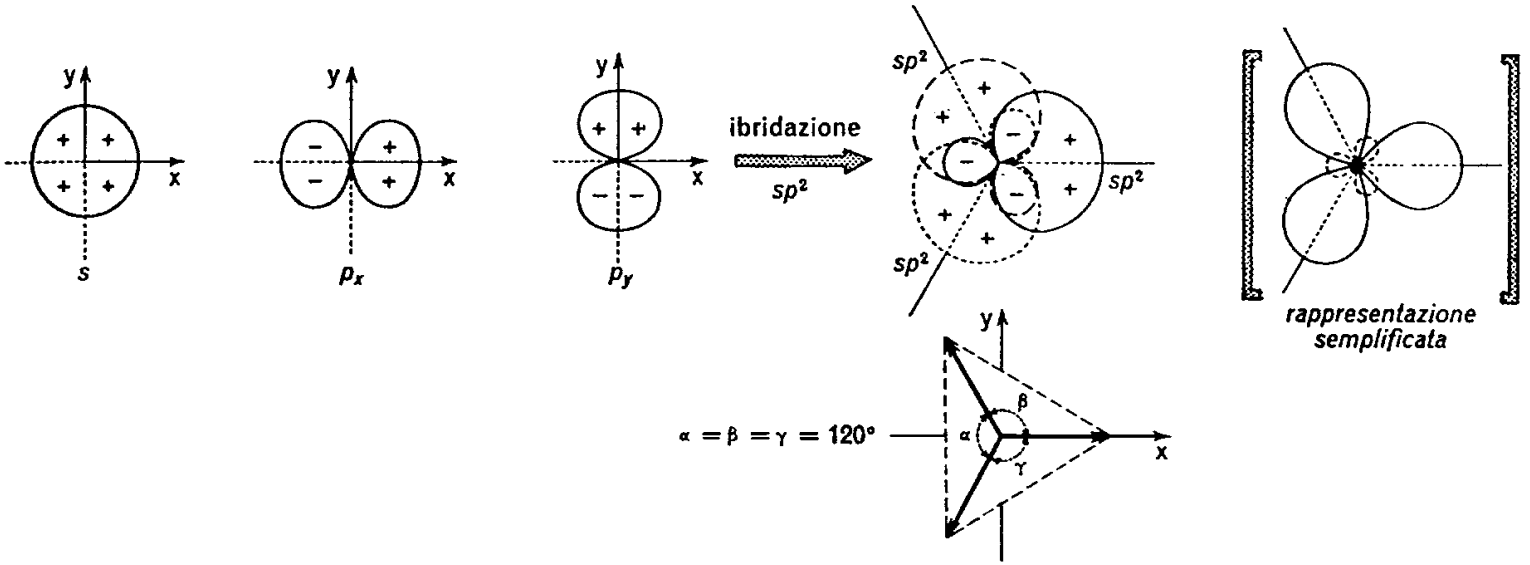
n = 6 C_6H_{14} Esano

n = 7 C_7H_{16} Eptano

n = 8 C_8H_{18} Ottano

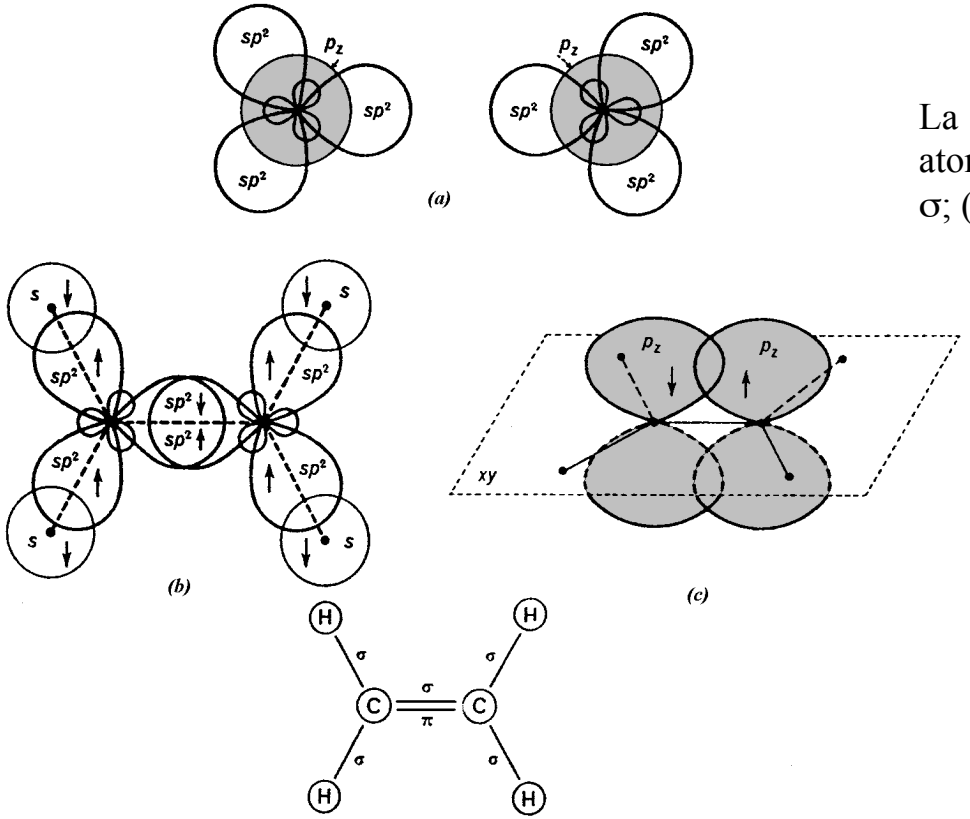
Ibridizzazione sp^2 dell'atomo di C





Idrocarburi ALCHENI

$$C_nH_{2n}$$



La molecola dell'etilene C_2H_4: (a)orbitali dei due atomi di carbonio partecipanti ai legami; (b) legame σ; (c) legame π.

n = 3 C_3H_6 Propene

n = 4 C_4H_8 Butene

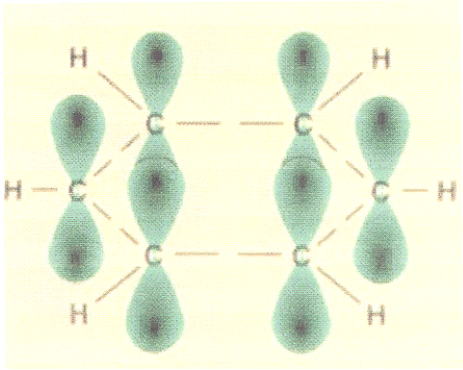
n = 5 C_5H_{10} Pentene

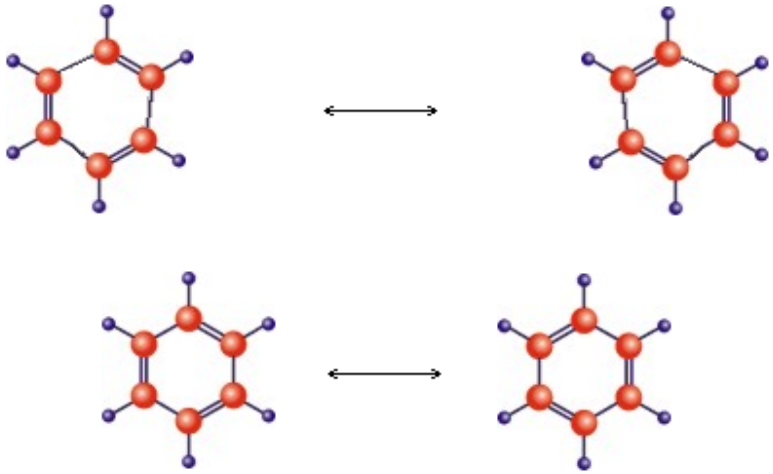
n = 6 C_6H_{12} Esene

n = 7 C_7H_{14} Eptene

n = 8 C_8H_{16} Ottene

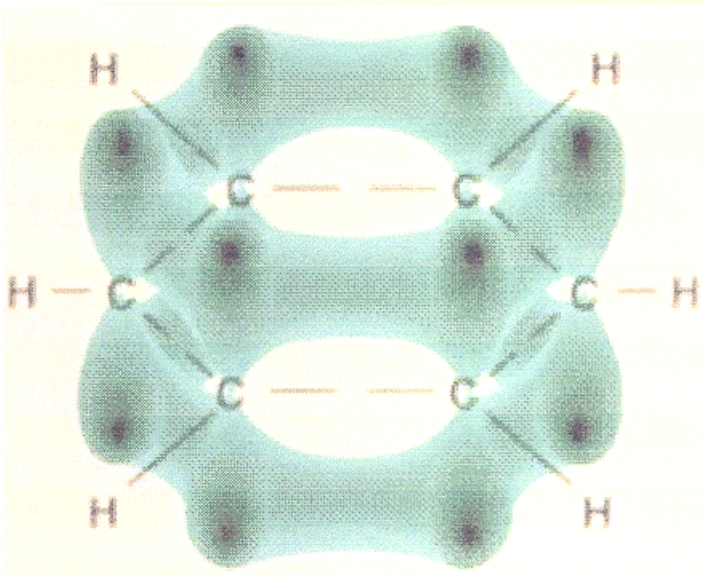
Il benzene C_6H_6



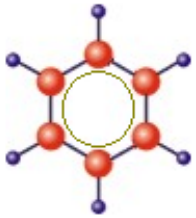


Formule limite di kekulé

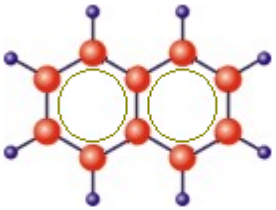
Composti aromatici: il numero di elettroni p di atomi di C adiacenti deve soddisfare la formula $4n+2$



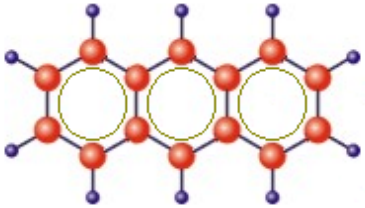
Composti aromatici: il numero di elettroni p di atomi di C adiacenti deve soddisfare la formula $4n+2$



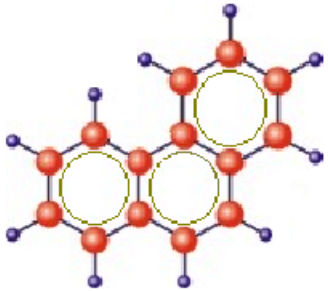
Benzene



Naftalina



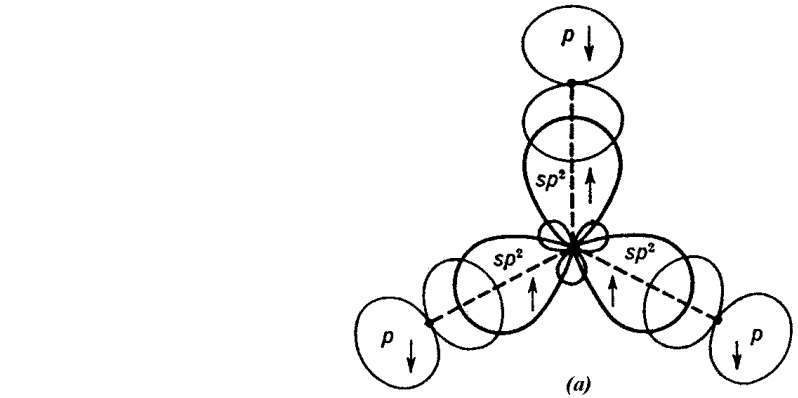
Antracene

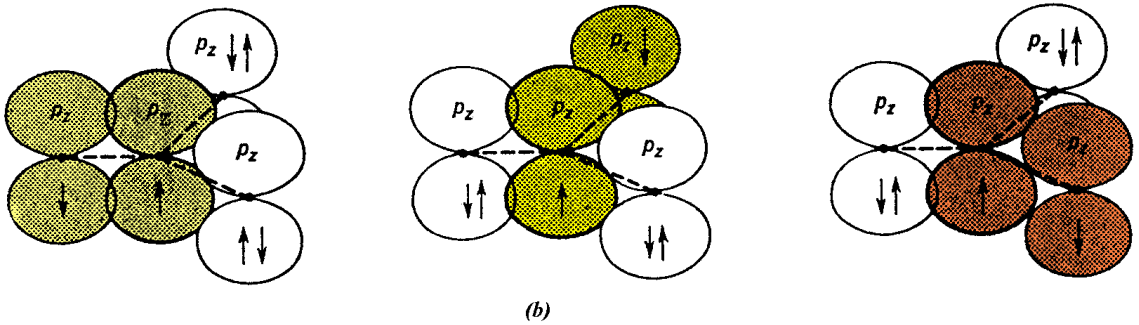


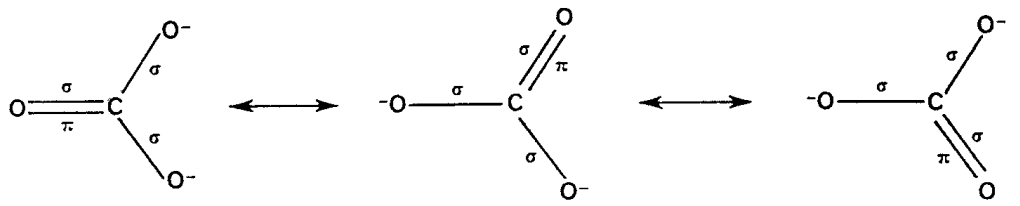
Fenantrane

Esempio di ibridizzazione sp^2.

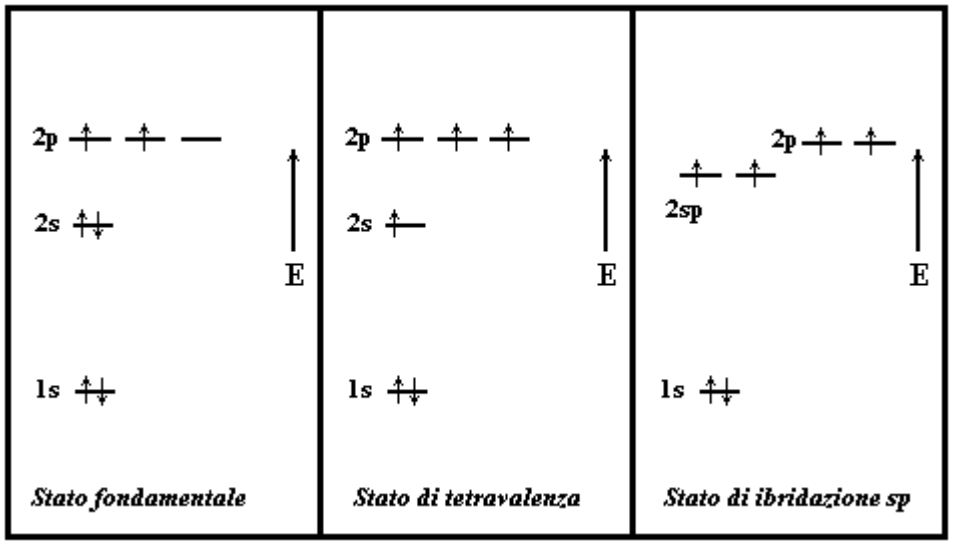
Lo ione carbonato $[CO_3^{2-}]$

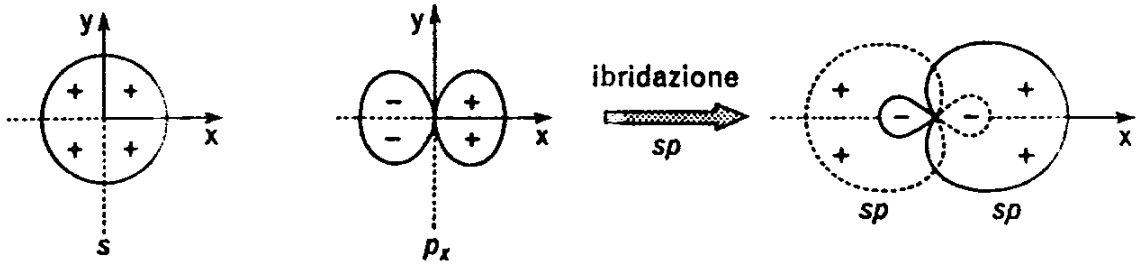






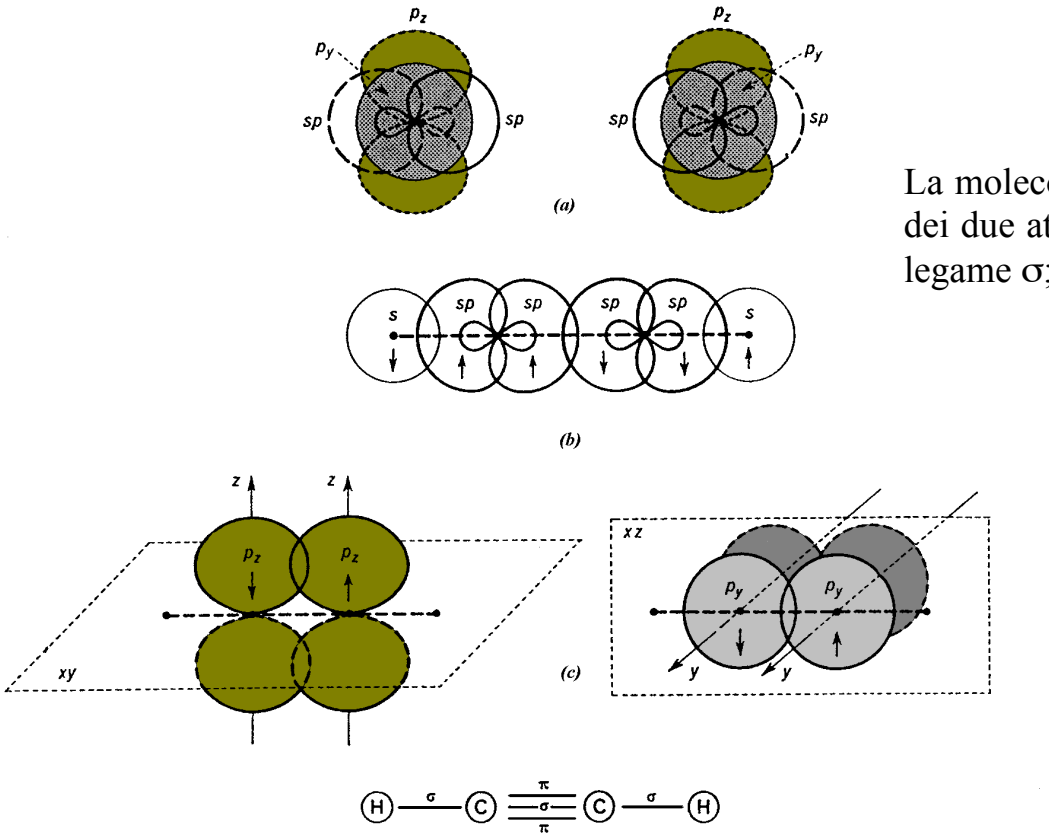
Ibridizzazione sp dell'atomo di C





Idrocarburi ALCHINI

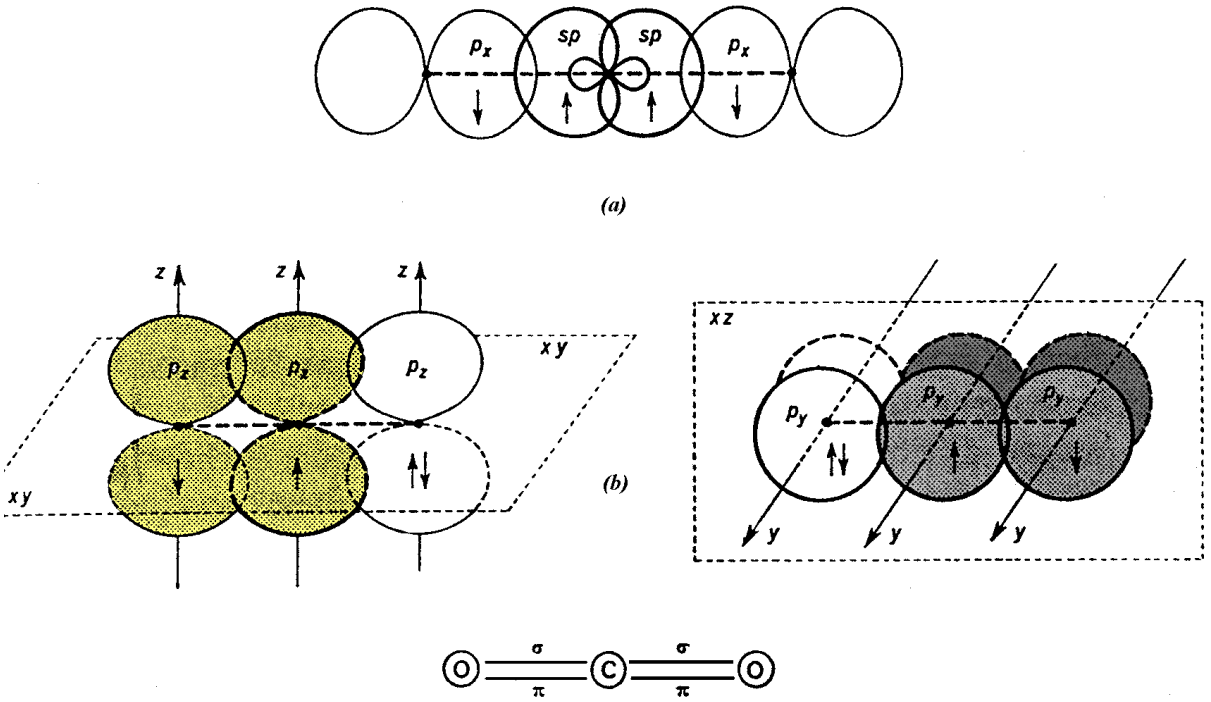
$$C_nH_{2n-2}$$



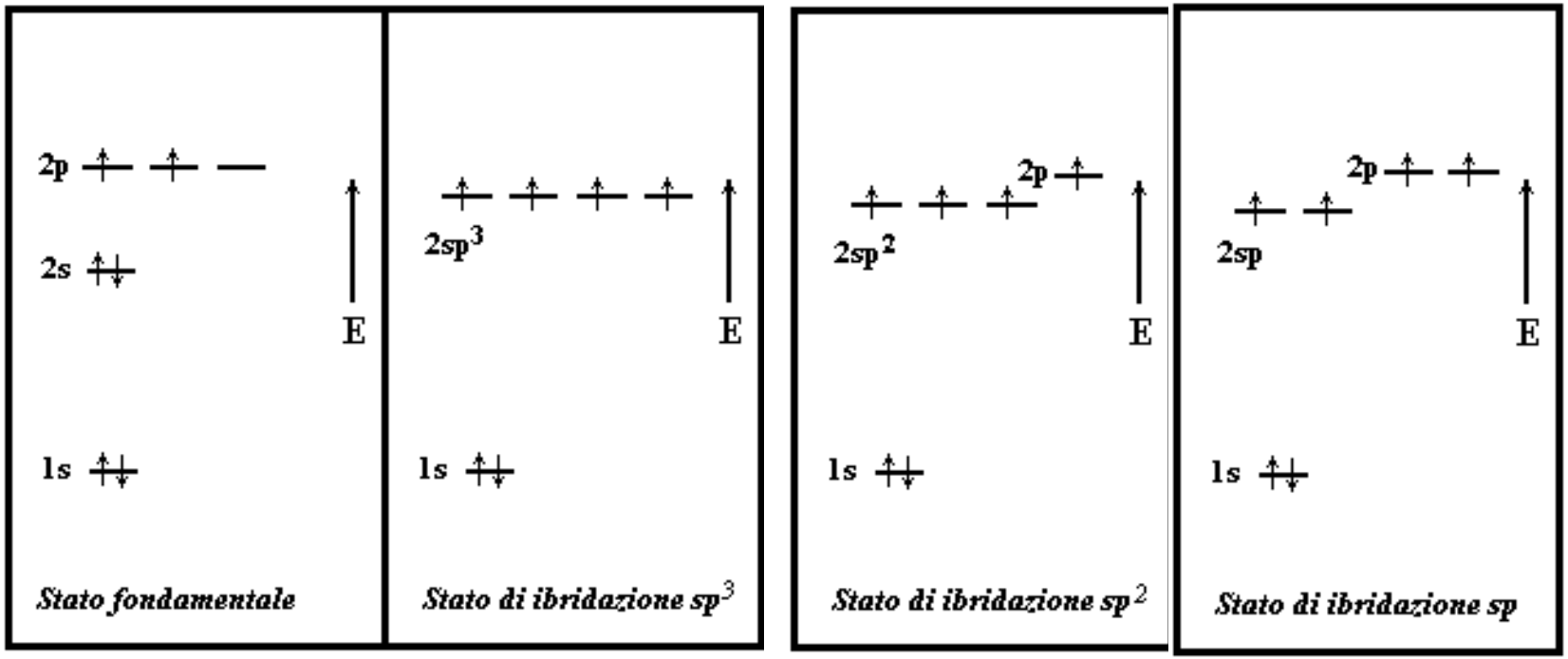
La molecola dell'acetilene o etino C_2H_2: (a) orbitali dei due atomi di carbonio partecipanti ai legami; (b) legame σ; (c) legame π.

n = 3	C_3H_4	Propino	n = 6	C_6H_{10}	Esino
n = 4	C_4H_6	Butino	n = 7	C_7H_{12}	Eptino
n = 5	C_5H_8	Pentino	n = 8	C_8H_{14}	Ottino

La molecola del diossido di carbonio CO_2



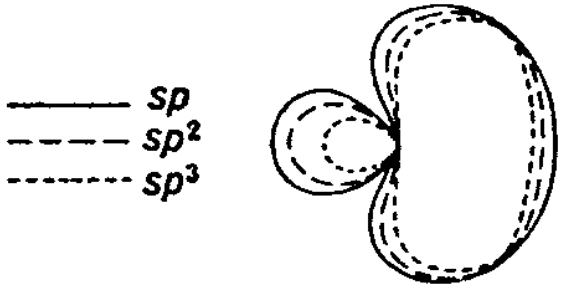
(a) Legame σ ; (b) legame π



$s < sp < sp^2 < sp^3 < p$

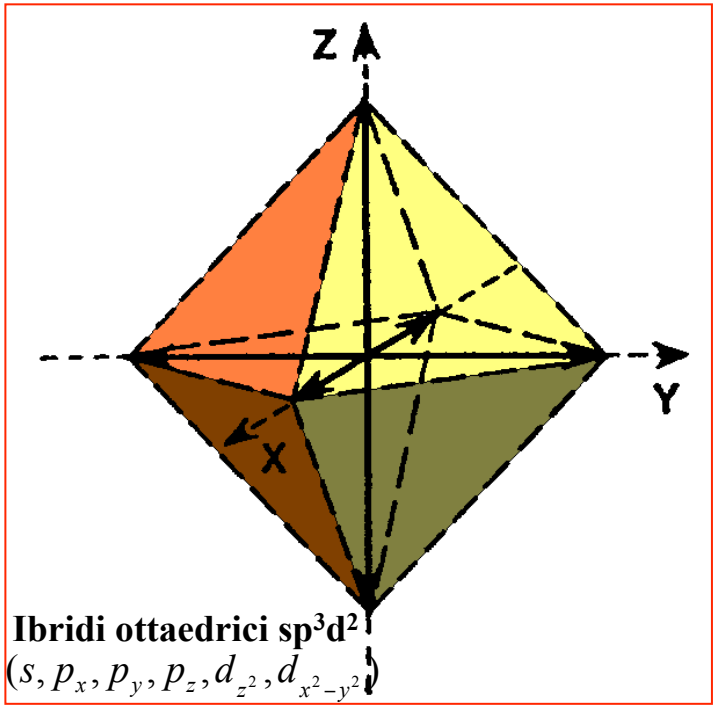
energia più bassa

energia più alta



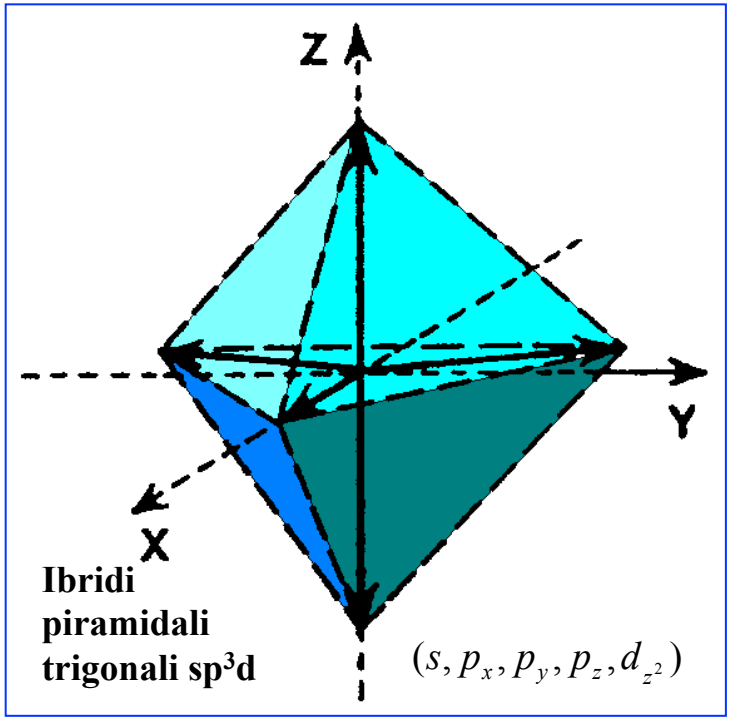
contorni rappresentativi degli orbitali ibridi sp^3, sp^2, sp dell'atomo di carbonio [$\psi^2 = 0{,}01$]

Altri tipi di ibridizzazione



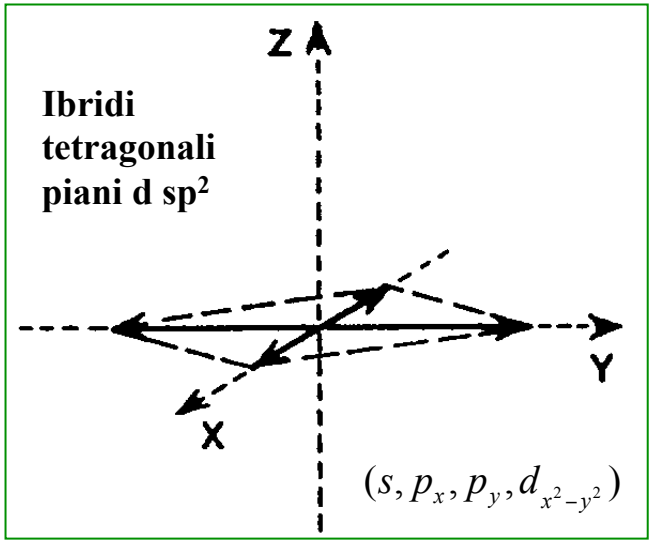
Ibridi ottaedrici sp^3d^2

$(s, p_x, p_y, p_z, d_{z^2}, d_{x^2-y^2})$



Ibridi piramidali trigonali sp^3d

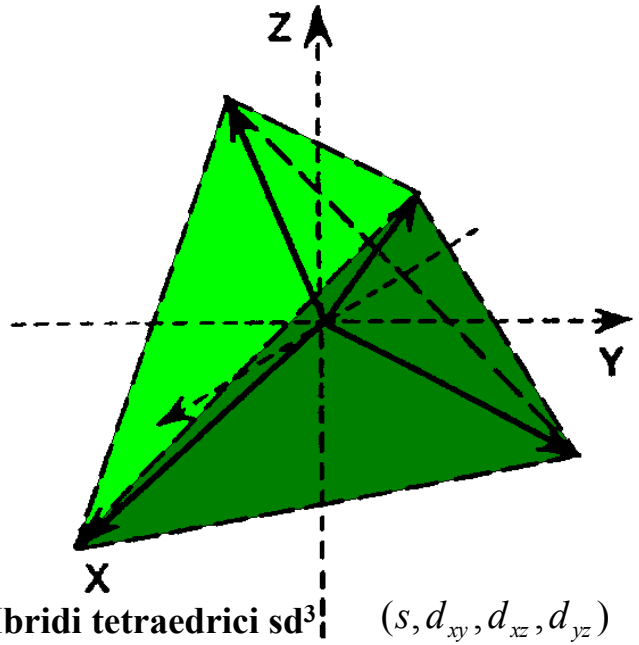
$(s, p_x, p_y, p_z, d_{z^2})$



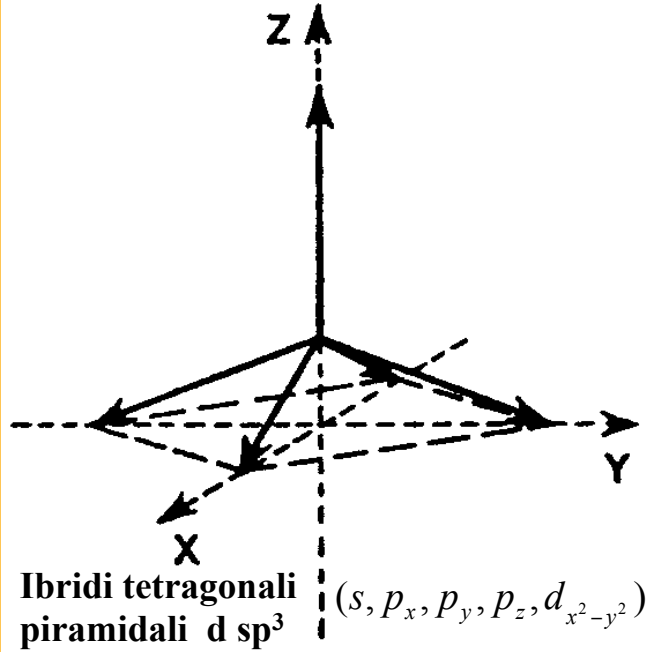
Ibridi tetragonali piani d sp^2

$(s, p_x, p_y, d_{x^2-y^2})$

Altri tipi di ibridizzazione



Ibridi tetraedrici sd³ $(s, d_{xy}, d_{xz}, d_{yz})$



Ibridi tetragonali piramidali d sp³ $(s, p_x, p_y, p_z, d_{x^2-y^2})$