

La forma delle molecole e gli orbitali “ibridi”.

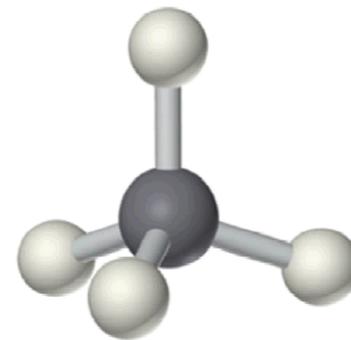
Se nel metano i quattro atomi di idrogeno fossero legati

Con 3 orbitali p ed un orbitale s, la geometria sarebbe:

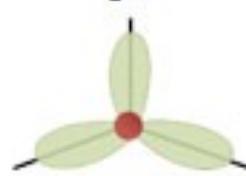
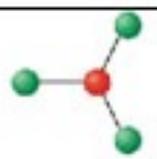
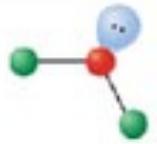
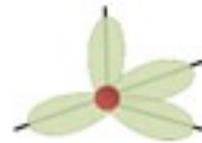
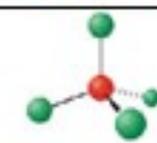
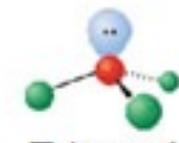
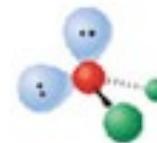
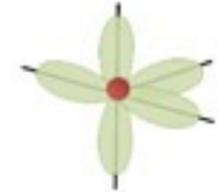
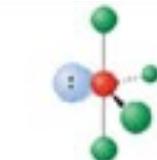
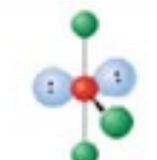
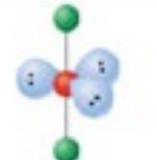
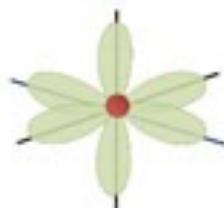
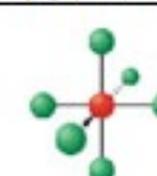
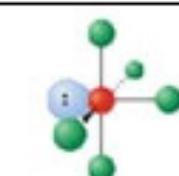
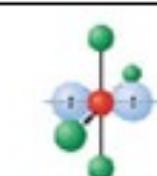
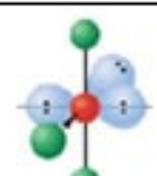
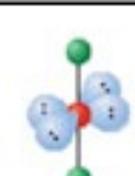
90° , 90° , 90° , 135° .

Il modello VESPR (valence electron-shell pair repulsion) spiega che per avere la massima distanza tra coppie di e^- , gli orbitali si ricombinano con una nuova geometria raggiungendo un minimo energetico.

Metano (CH_4)



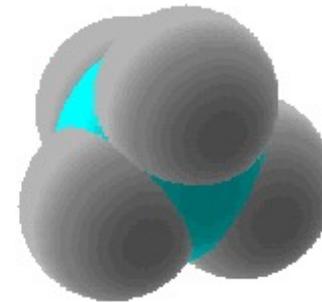
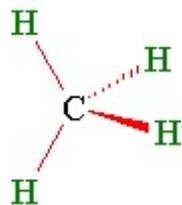
Methane, CH_4

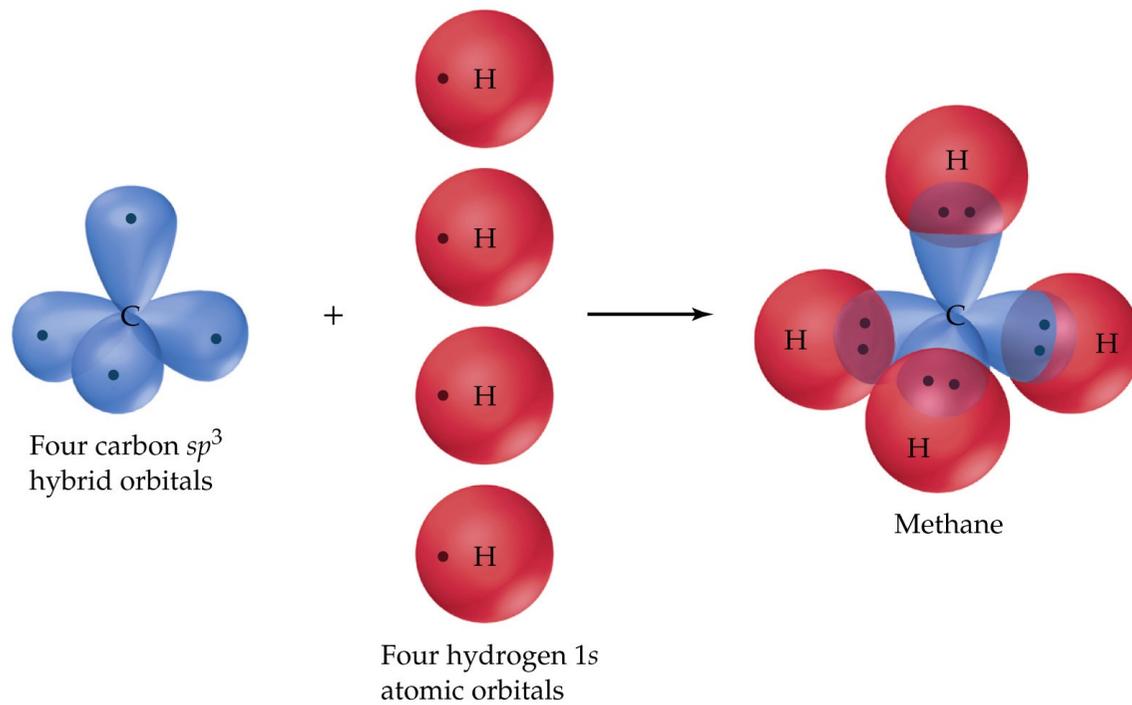
Number of Electron Dense Areas	Electron-Pair Geometry	Molecular Geometry				
		No Lone Pairs	1 lone Pair	2 lone Pairs	3 lone Pairs	4 lone Pairs
2 	Linear	 Linear				
3 	Trigonal planar	 Trigonal planar	 Bent			
4 	Tetrahedral	 Tetrahedral	 Trigonal pyramidal	 Bent		
5 	Trigonal bipyramidal	 Trigonal bipyramidal	 Sawhorse	 T-shaped	 Linear	
6 	Octahedral	 Octahedral	 Square pyramidal	 Square planar	 T-shaped	 Linear

Ricombinando 1 orbitale s e 3 orbitali p: sp^3

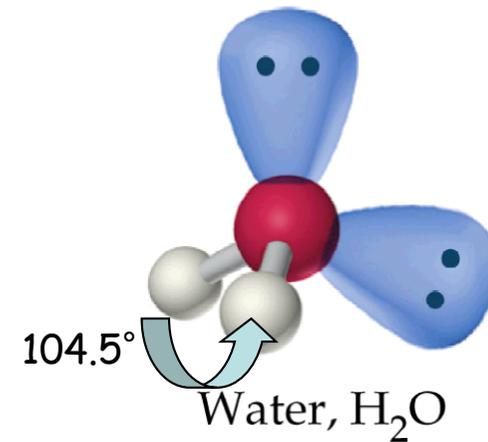
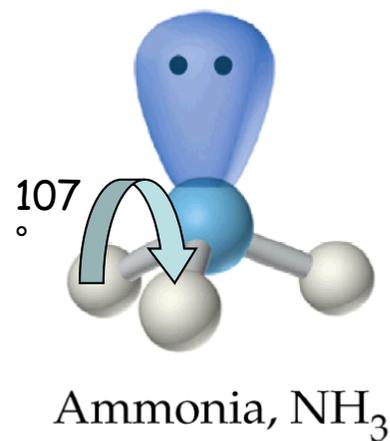
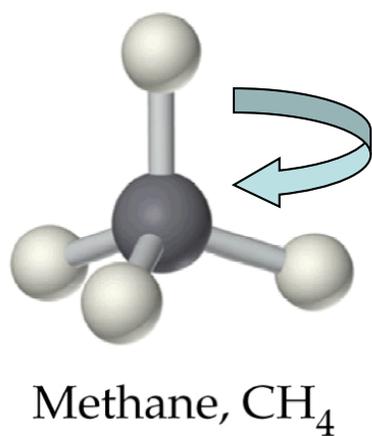


4 orbitali di uguale energia a geometria tetraedrica





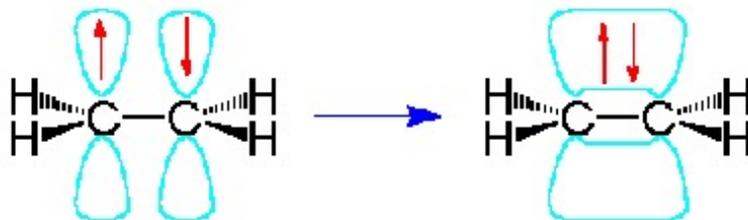
Gli orbitali che contengono un “lone pair” distorcono la geometria (e sono disponibili per legami dativi).



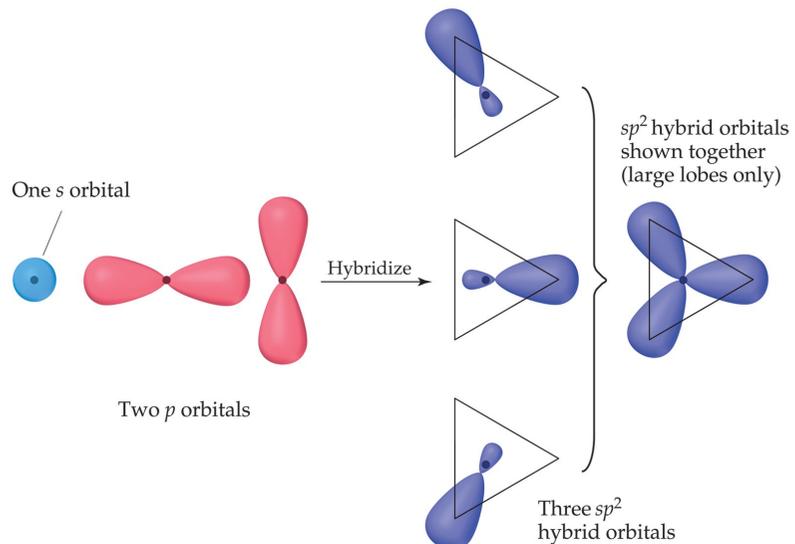
Ricombinando 1 orbitale s e 2 orbitali p: sp^2



3 orbitali di uguale energia a geometria trigonale + 1 orbitale p.

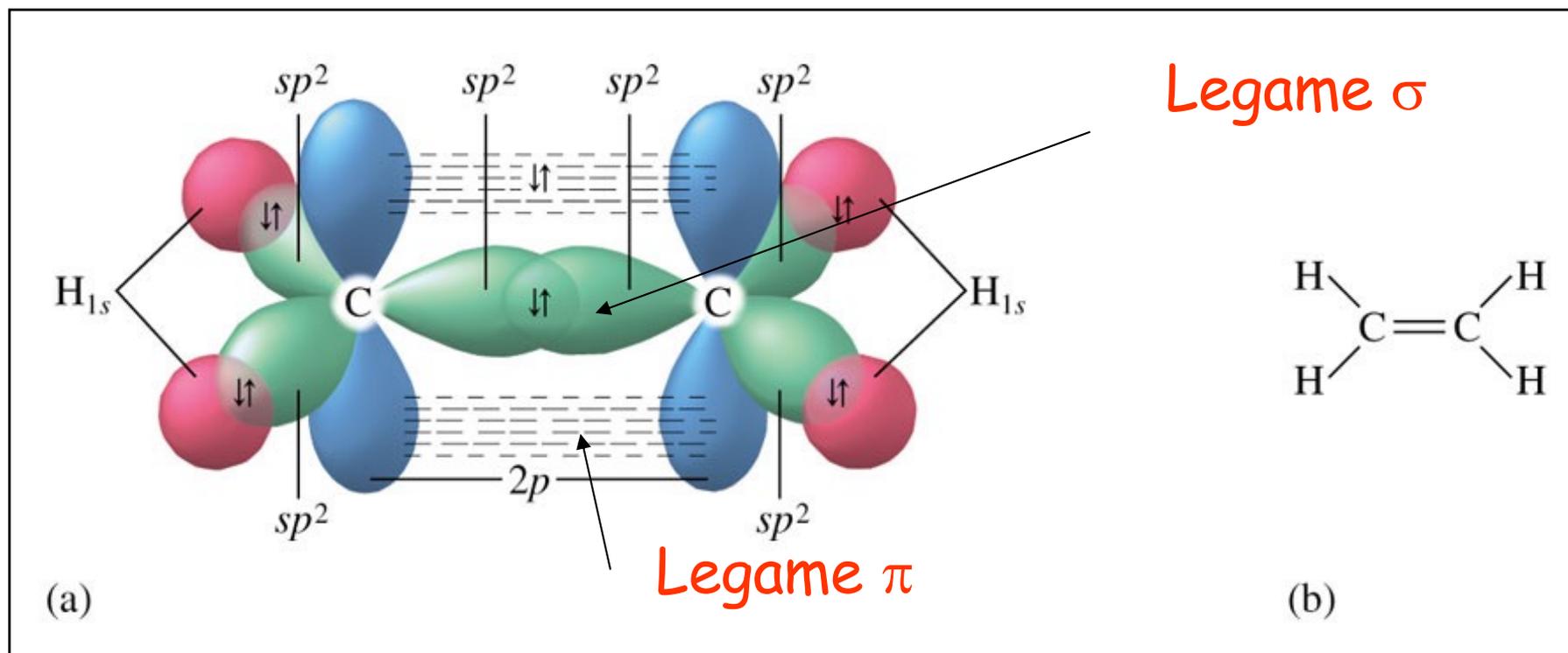


Esempio: etene



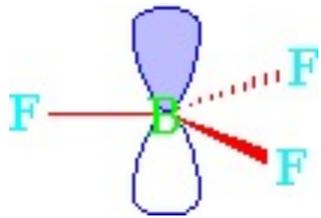
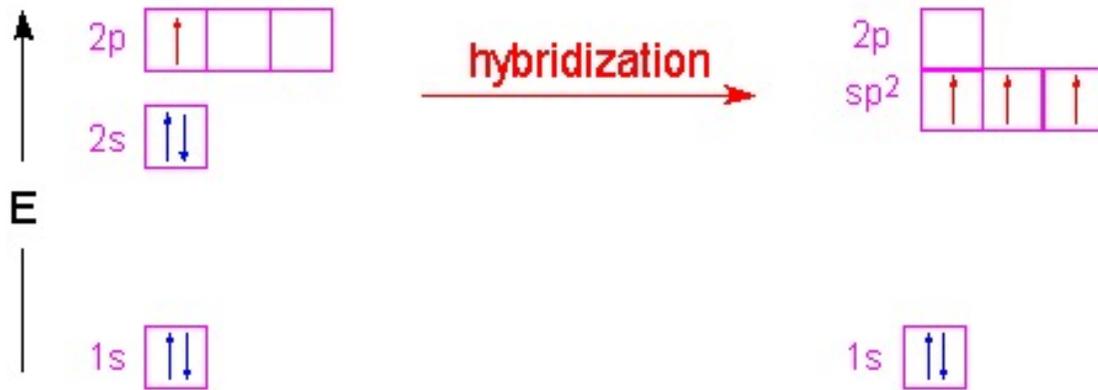
Sp^2 : geometria trigonale planare
(120°)

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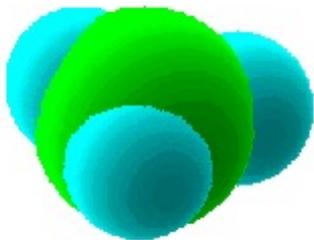


Il doppio legame non può ruotare

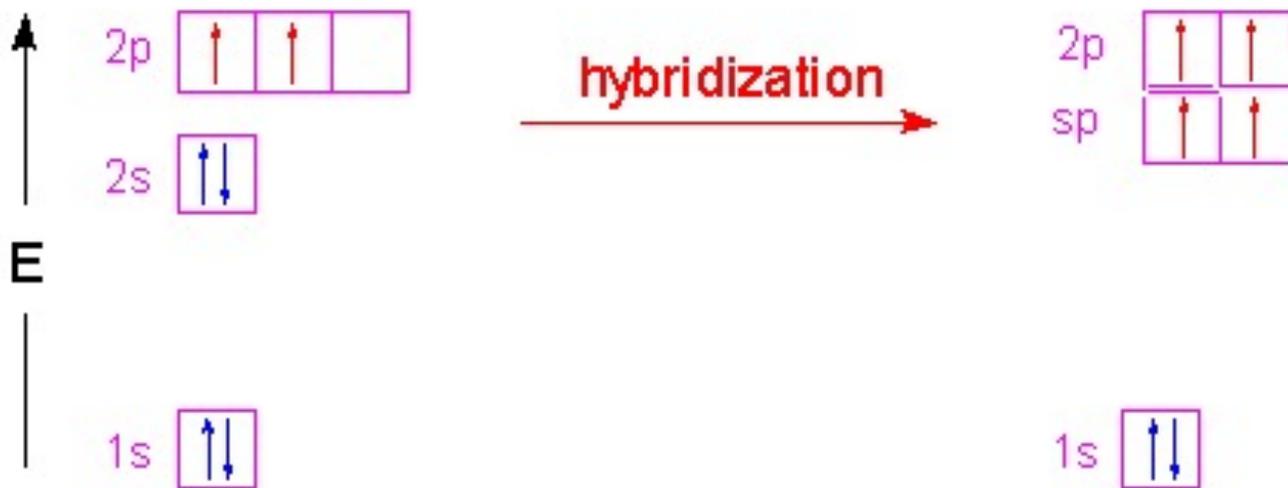
Nel BF_3 (apparente eccezione alla regola dell'ottetto):



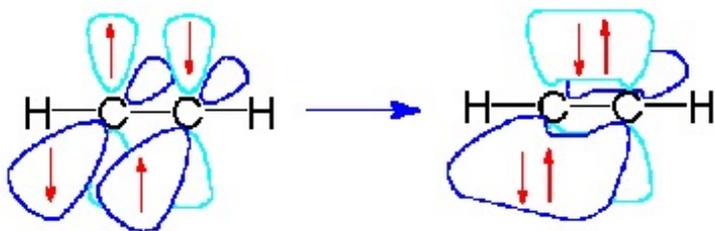
Rimane un orbitale vuoto p + 3 orbitali sp^2 .



Ricombinando 1 orbitale s e 1 orbitale p: sp

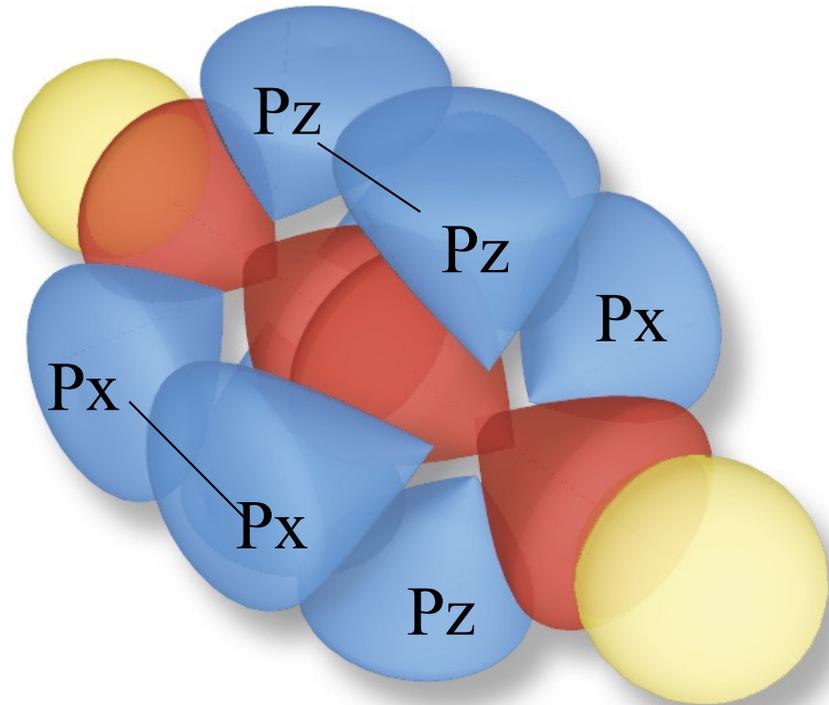


2 orbitali di uguale energia a geometria lineare + 2 orbitali p.



Esempio: etino

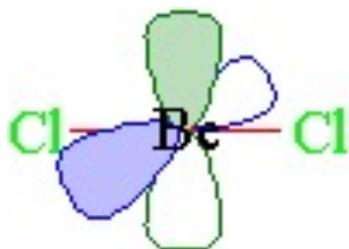
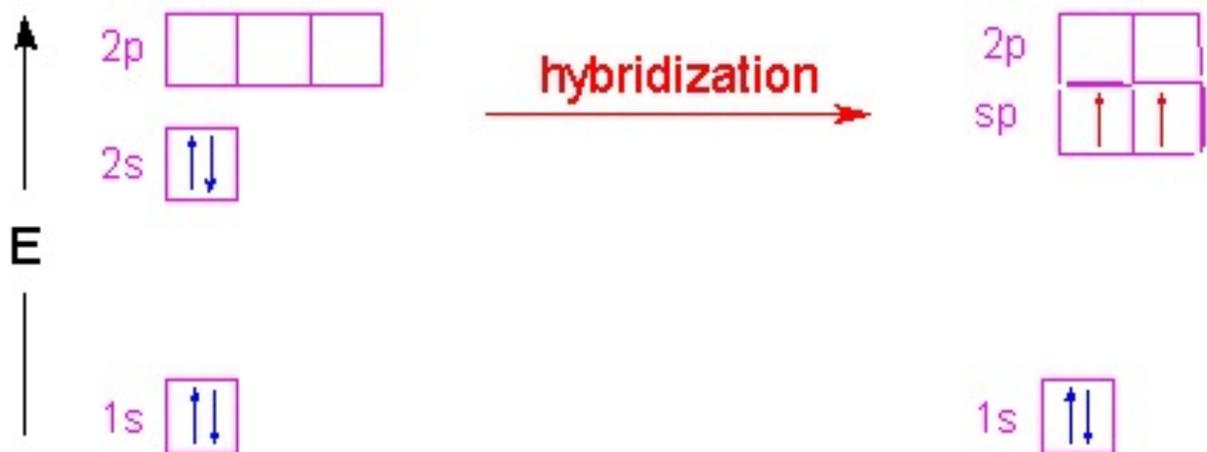
Sp: geometria lineare
(180°)



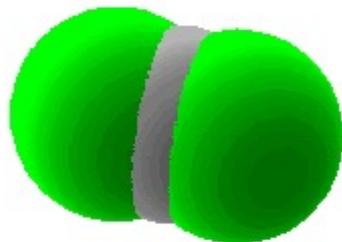
Etino

Il triplo legame non può ruotare

Nel BeCl_2 (apparente eccezione alla regola dell'ottetto):

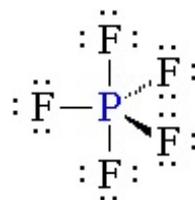
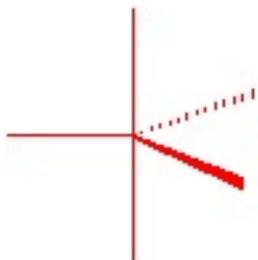


Rimangono 2 orbitali vuoti p + 2 orbitali sp .



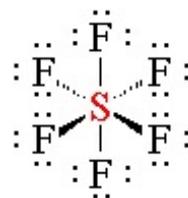
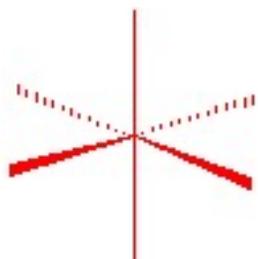
Altre eccezioni alla regola dell'ottetto: sp^3d e sp^3d^2

sp^3d

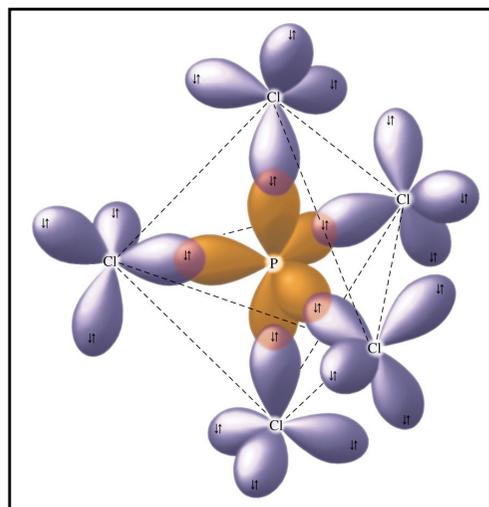


3 Angoli 120° + 2 ortogonali

sp^3d^2

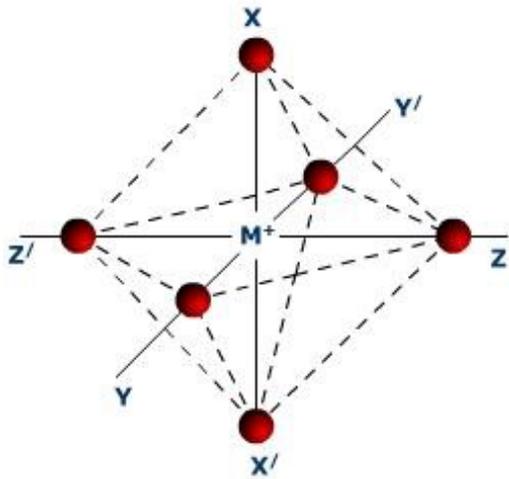


4 Angoli 90° + 2 ortogonali

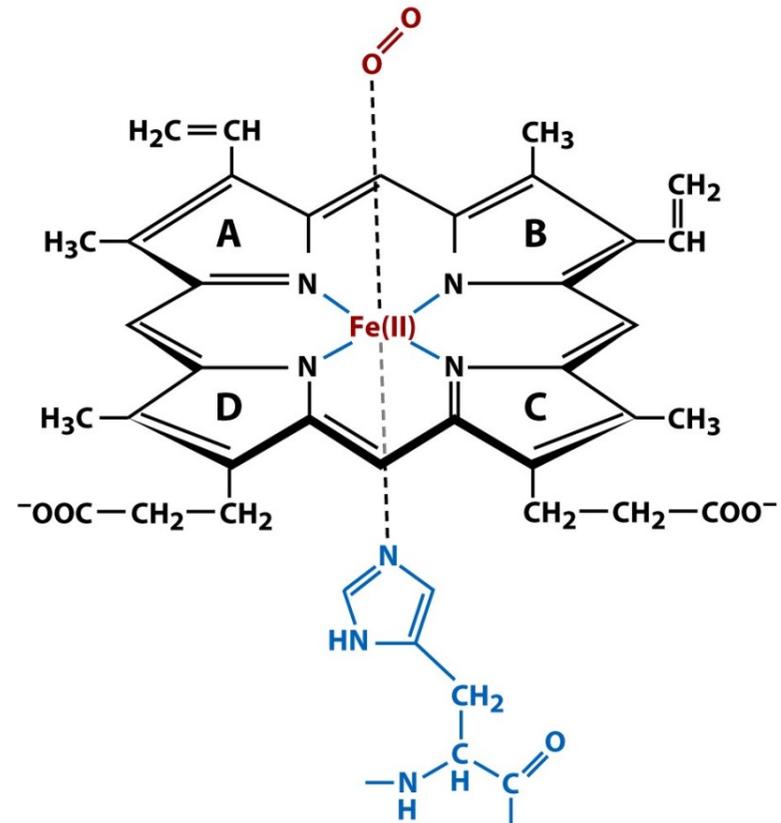


PCl_5

Coordinazione ottaedrica di metalli



L'eme nella mioglobina e nell'emoglobina.



Orbitali vuoti disponibili per legami di coordinazione: Metalli di Transizione

Ibridi di risonanza

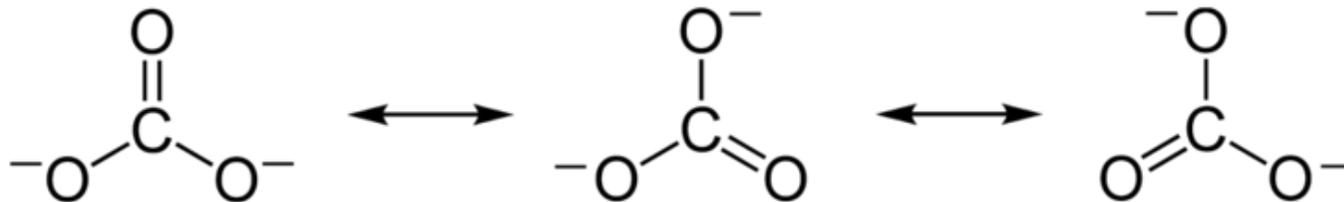


Lo ione carbonato: $\text{H}_2\text{CO}_3 + 2\text{H}_2\text{O} \rightleftharpoons \text{CO}_3^{2-} + 2\text{H}_3\text{O}^+$

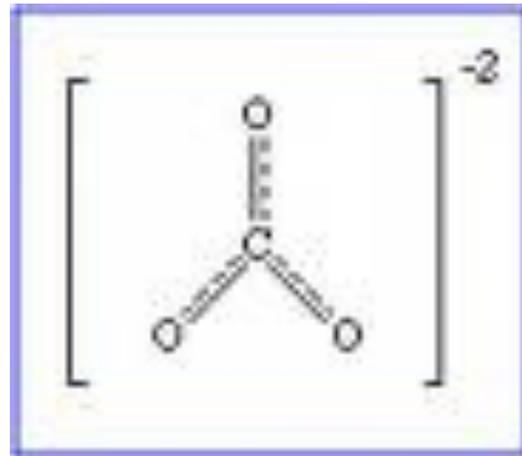
Dovrebbe avere un legame doppio e due singoli, ma

- hanno lunghezza uguale
- inoltre lo ione è più stabile di quanto dovrebbe.

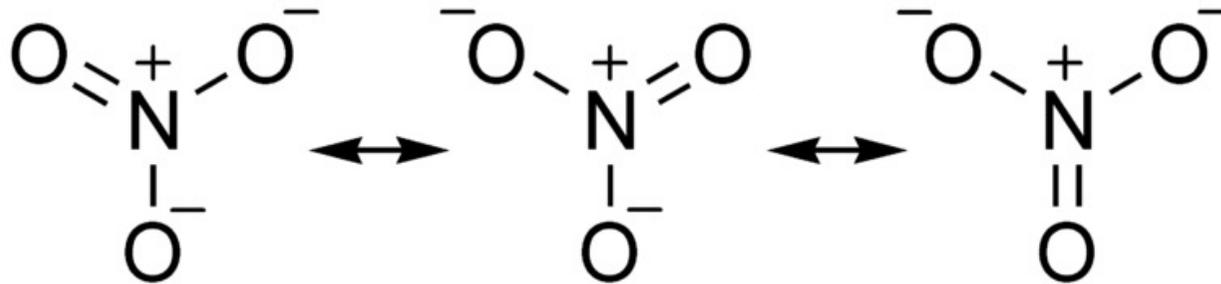
Sono presenti strutture di risonanza.



Ovvero la struttura non è rappresentabile con delle strutture di Lewis, ma gli elettroni del **doppio legame** sono **delocalizzati** sulla molecola.



Questo avviene anche in altri casi, es.:



Ione nitrato, deriva dalla dissociazione dell' **acido nitrico**.

...ed in molti composti del carbonio.