

## La forma delle molecole e gli orbitali “ibridi”.

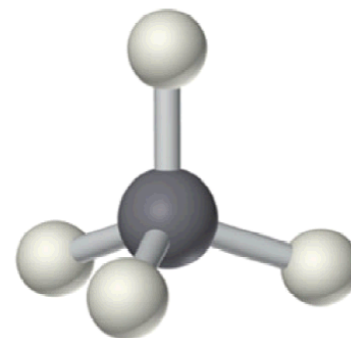
Se nel metano i quattro atomi di idrogeno fossero legati

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




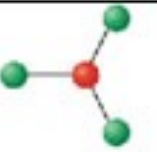
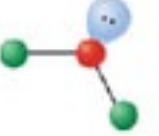


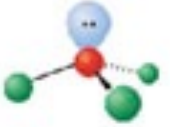




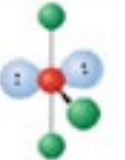
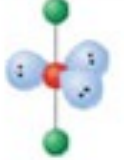



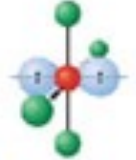
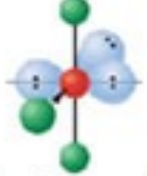
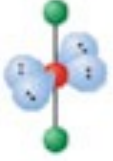
$90^\circ$  ,  $90^\circ$  ,  $90^\circ$  ,  $135^\circ$  .

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 ( $\text{CH}_4$ )



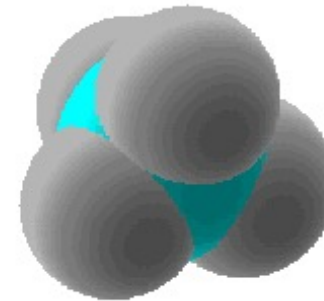
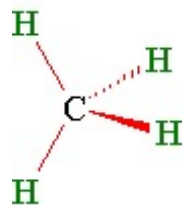
Methane,  $\text{CH}_4$

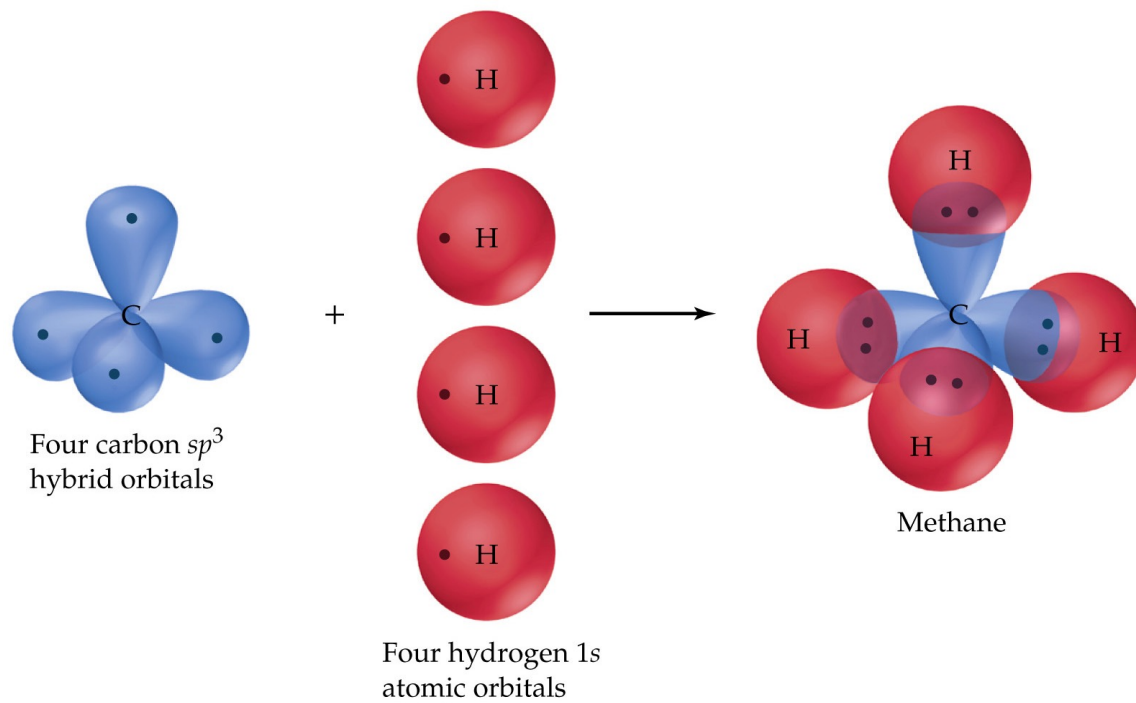
Number of Electron Dense Areas	Electron-Pair Geometry	Molecular Geometry				
		No Lone Pairs	1 lone Pair	2 lone Pairs	3 lone Pairs	4 lone Pairs
2 	Linear	 Linear				
3 	Trigonal planar	 Trigonal planar	 Bent			
4 	Tetrahedral	 Tetrahedral	 Trigonal pyramidal	 Bent		
5 	Trigonal bipyramidal	 Trigonal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

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

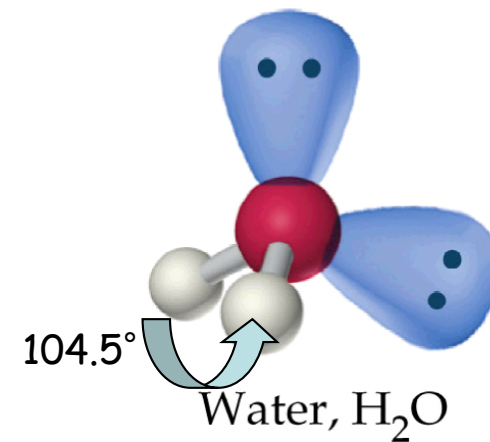
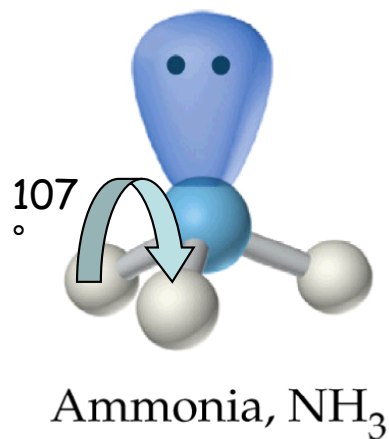
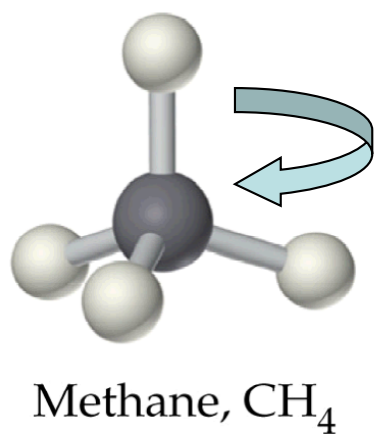


4 orbitali di uguale energia a geometria tetraedrica





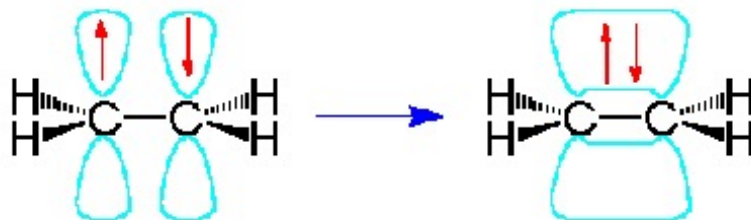
Gli orbitali che contengono un “lone pair” distorcono la geometria (e sono disponibili per legami dativi).



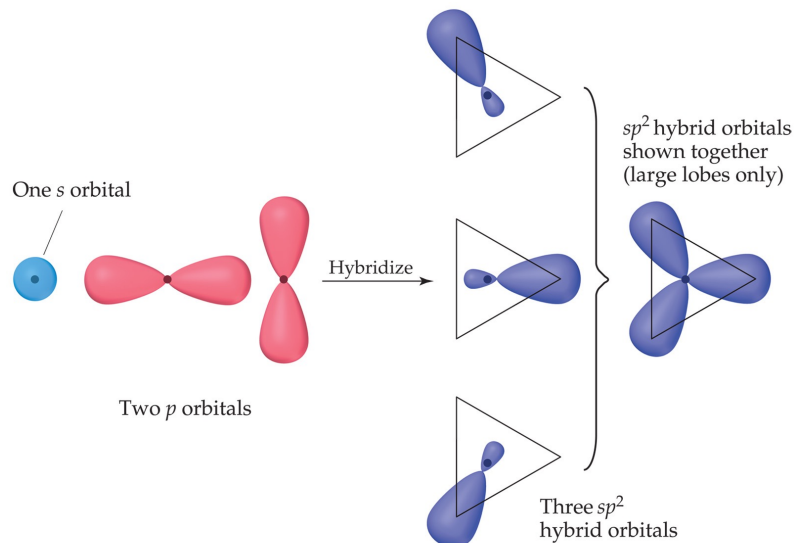
## Ricombinando 1 orbitale s e 2 orbitali p: $sp^2$



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

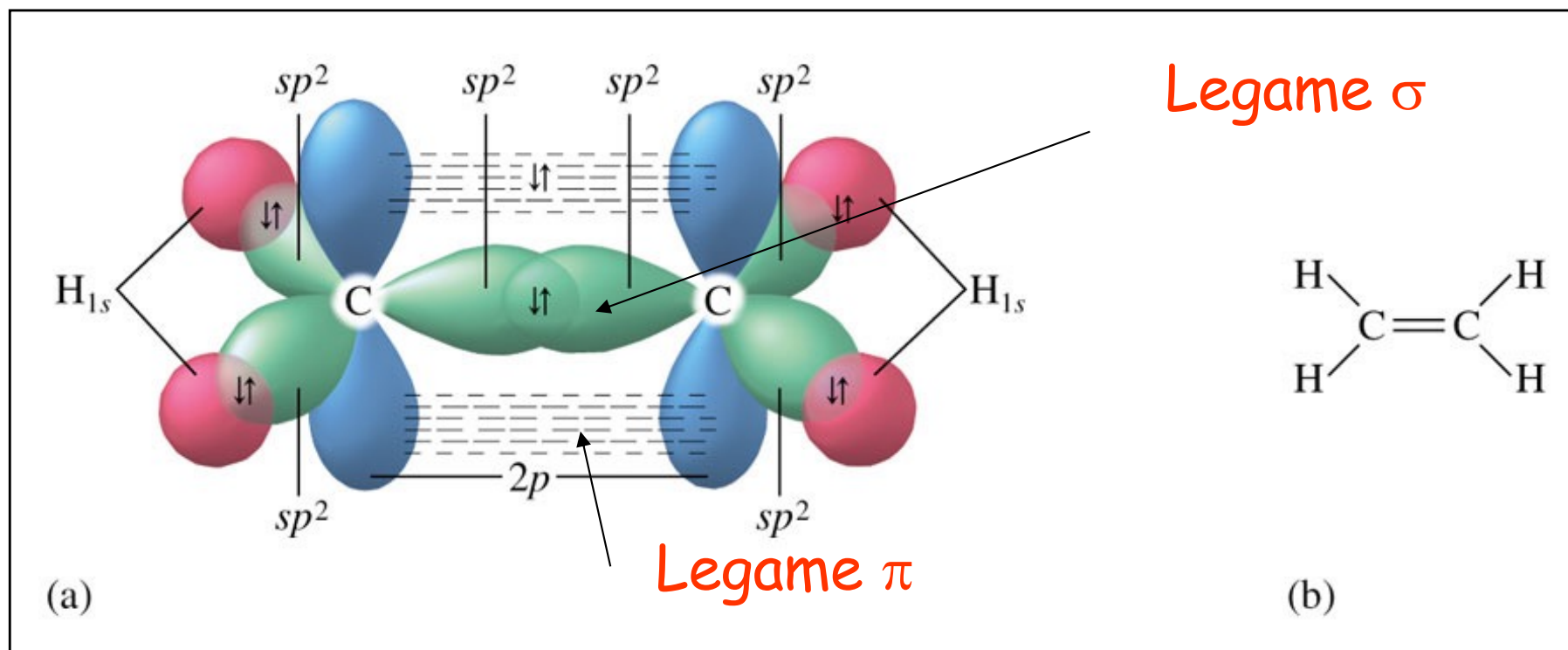


Esempio: etene



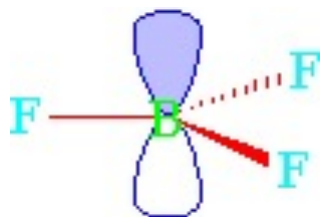
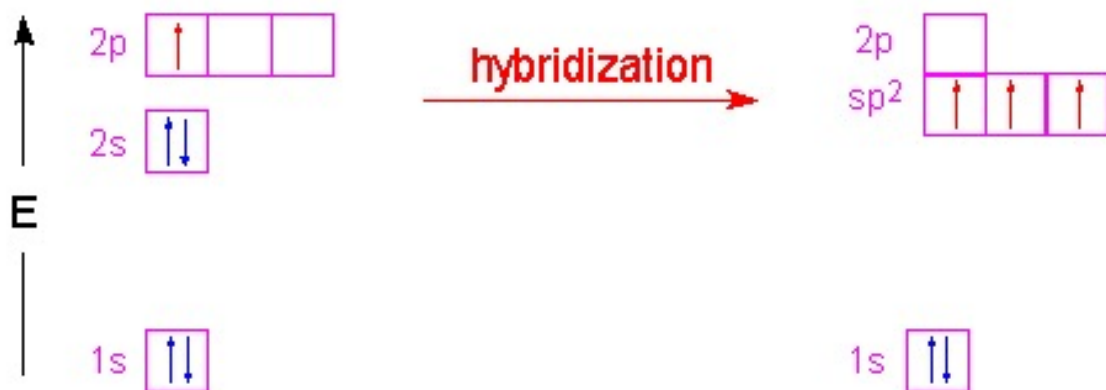
$Sp^2$ : geometria trigonale planare  
( $120^\circ$ )

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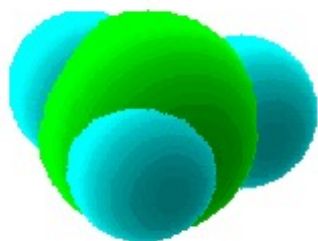


Il doppio legame non può ruotare

Nel  $\text{BF}_3$  (apparente eccezione alla regola dell'ottetto):



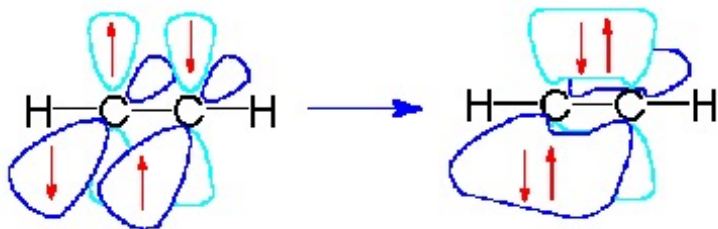
Rimane un orbitale vuoto p + 3 orbitali  $sp^2$ .



## Ricombinando 1 orbitale s e 1 orbitale p: sp



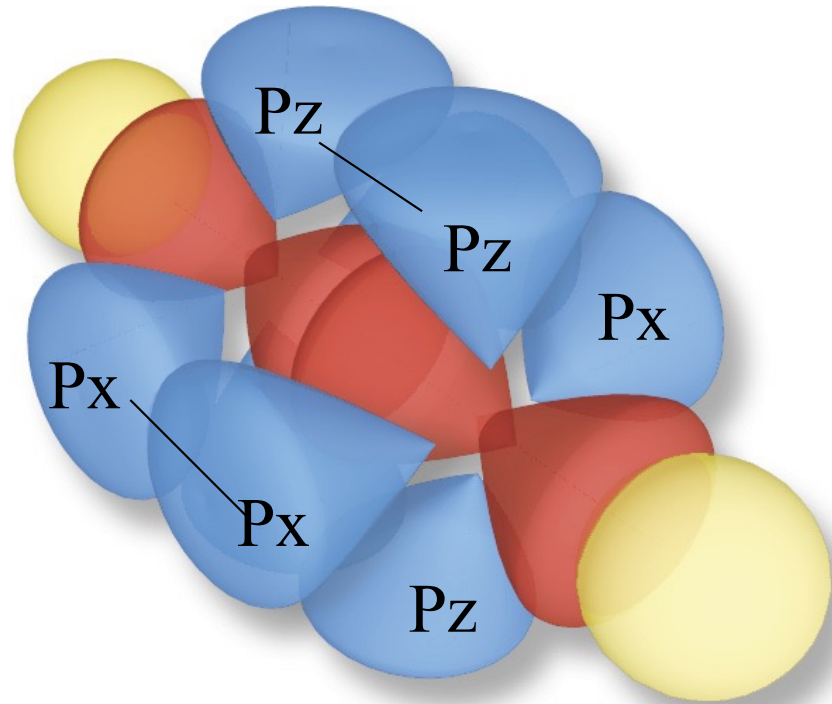
2 orbitali di uguale energia a geometria lineare + 2 orbitali p.



Esempio: etino



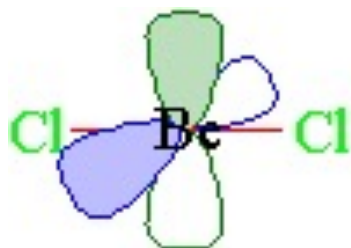
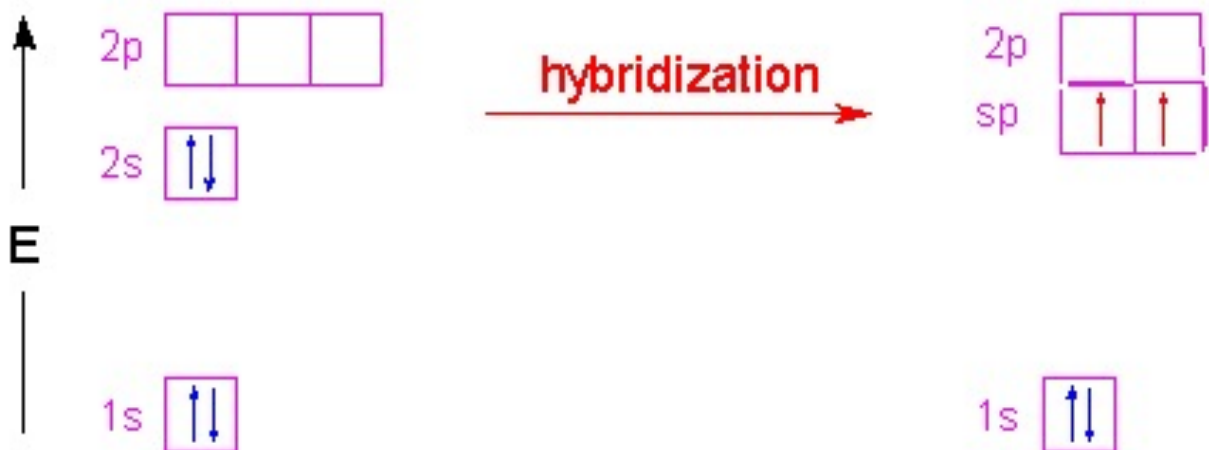
Sp: geometria lineare  
( $180^\circ$ )



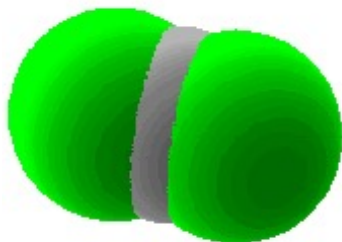
Etino

Il triplo legame non può ruotare

Nel  $\text{BeCl}_2$  (apparente eccezione alla regola dell'ottetto):

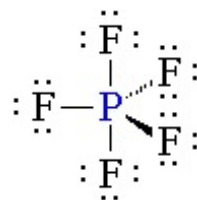
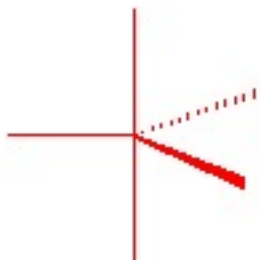


Rimangono 2 orbitali vuoti  $p$  + 2 orbitali  $sp$ .



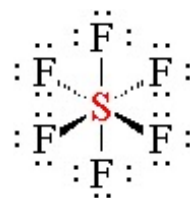
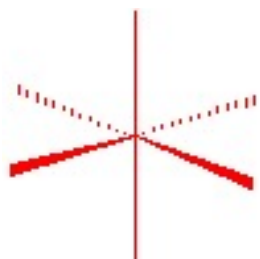
# Altre eccezioni alla regola dell'ottetto: $sp^3d$ e $sp^3d^2$

$sp^3d$

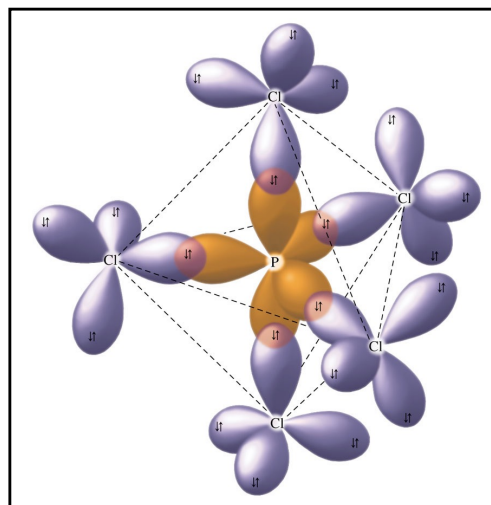


3 Angoli  $120^\circ$  + 2 ortogonali

$sp^3d^2$

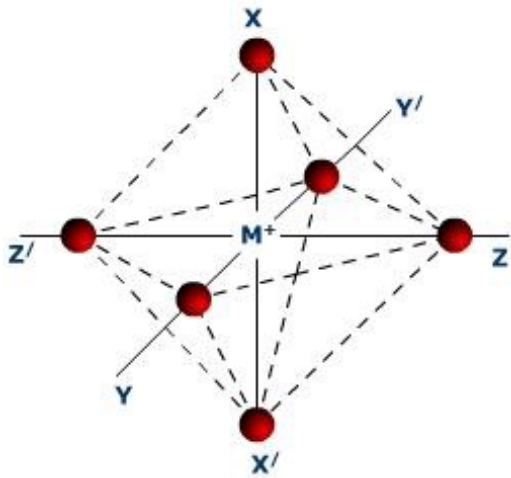


4 Angoli  $90^\circ$  + 2 ortogonali

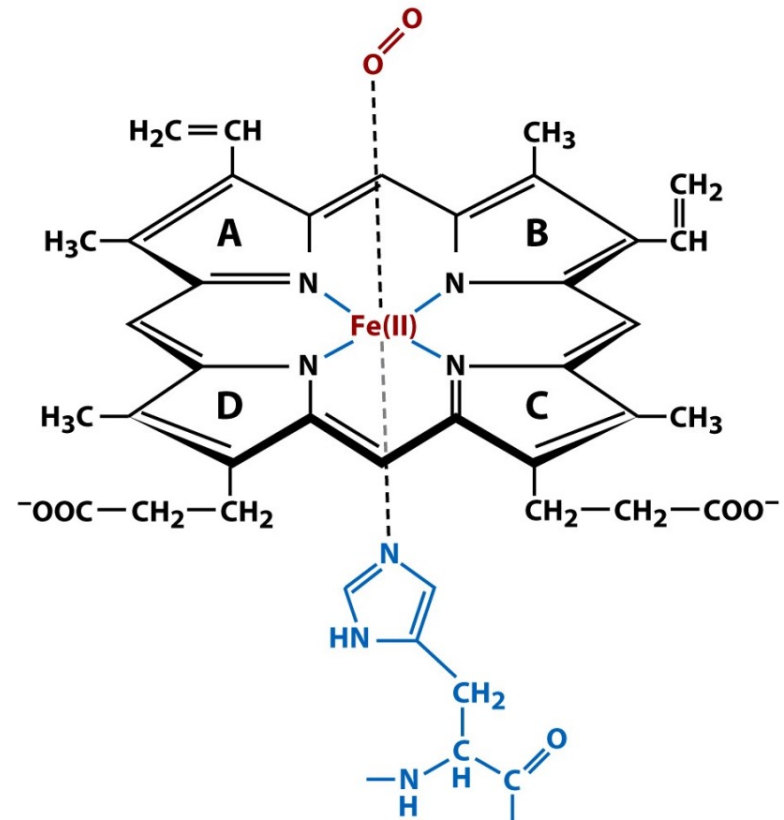


$PCl_5$

# Coordinazione ottaedrica di metalli



L'eme nella mioglobina e nell'emoglobina.



Orbitali vuoti disponibili per legami di coordinazione: Metalli di Transizione

## Ibridi di risonanza



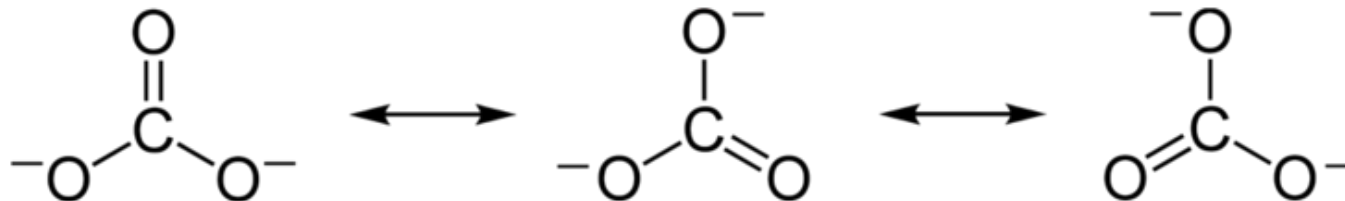
Lo ione carbonato:  $\text{H}_2\text{CO}_3 + 2\text{H}_2\text{O} \rightleftharpoons \text{CO}_3^{2-} + 2\text{H}_3\text{O}^+$

Dovrebbe avere un legame doppio e due singoli, ma

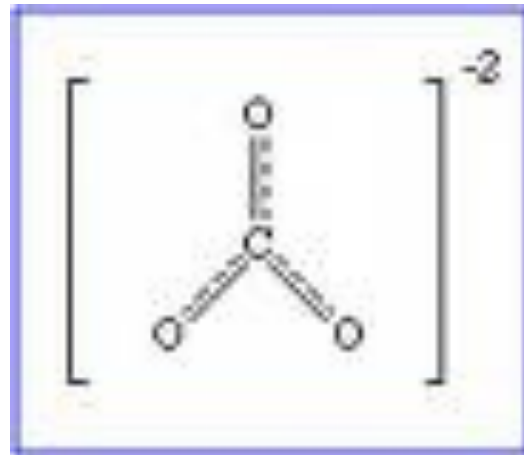
- hanno lunghezza uguale

- inoltre lo ione è più stabile di quanto dovrebbe.

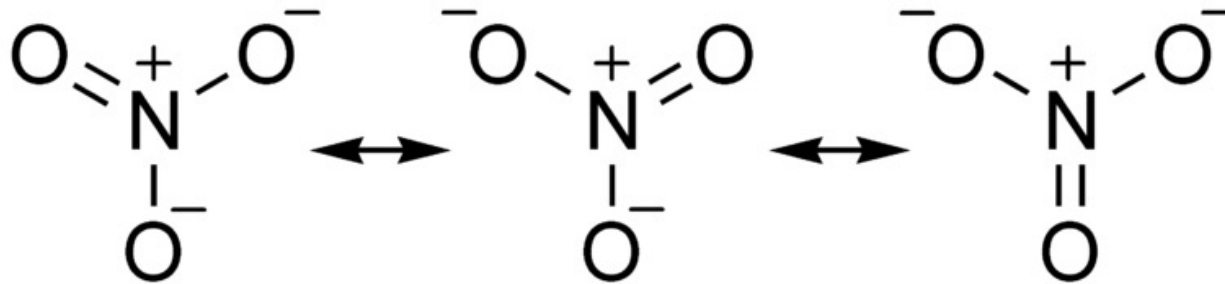
**Sono presenti strutture di risonanza.**



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.