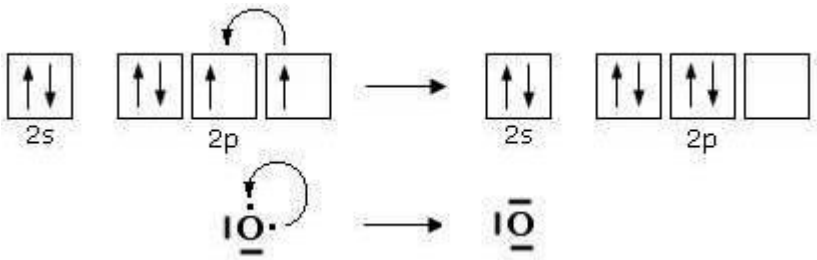
Ibridazione

Legame di coordinazione (o dativo)

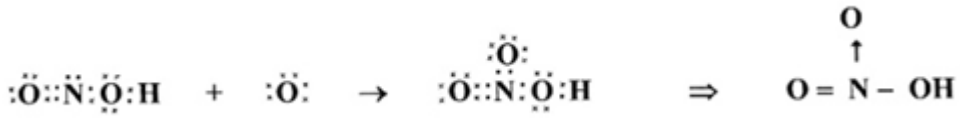
- Legame di tipo σ
- datore (lone pair) + accettore (orbitale vuoto energeticamente adatto)

Meccanismo

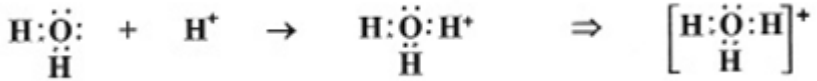
- Ossigeno: $1s^2 2s^2 2p^4$



- acido nitrico dall'acido nitroso (O accettore)



- ione idronio (O donatore)



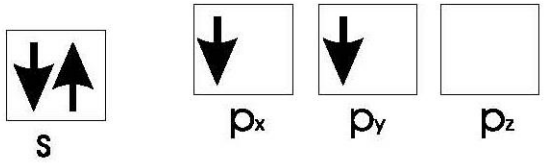
- Meccanismo (promozione)

Manganese [Ar] $3d^5\ 4s^2$

- $3d^5\ 4s^2$ Mn^{2+}
- $3d^3\ 4s^2\ 4p^2$ Mn^{4+}
- $3d^0\ 4s^2\ 4p^5$ Mn^{-}
- $3d^1\ 4s^2\ 4p^4$ Mn^{2-}

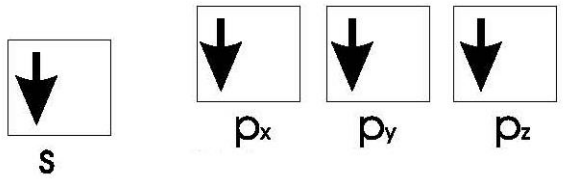
Carbonio

[He] $2s^2\ 2p^2$

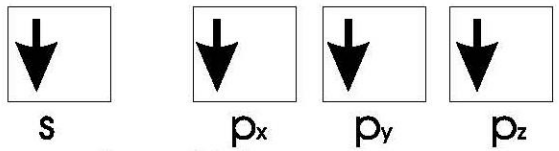


2 legami covalenti

PROMOZIONE



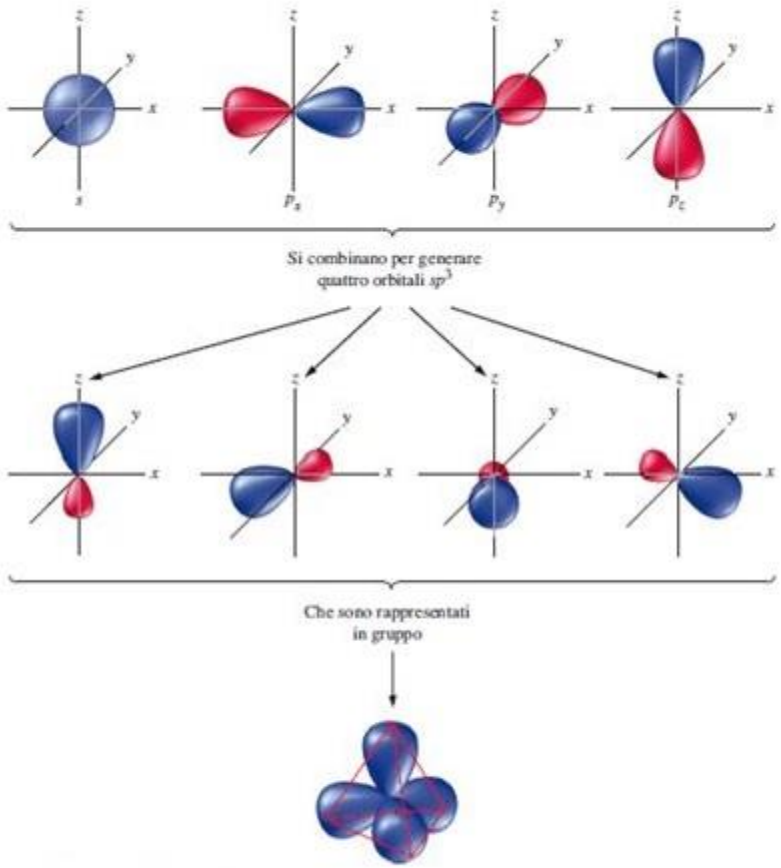
IBRIDAZIONE

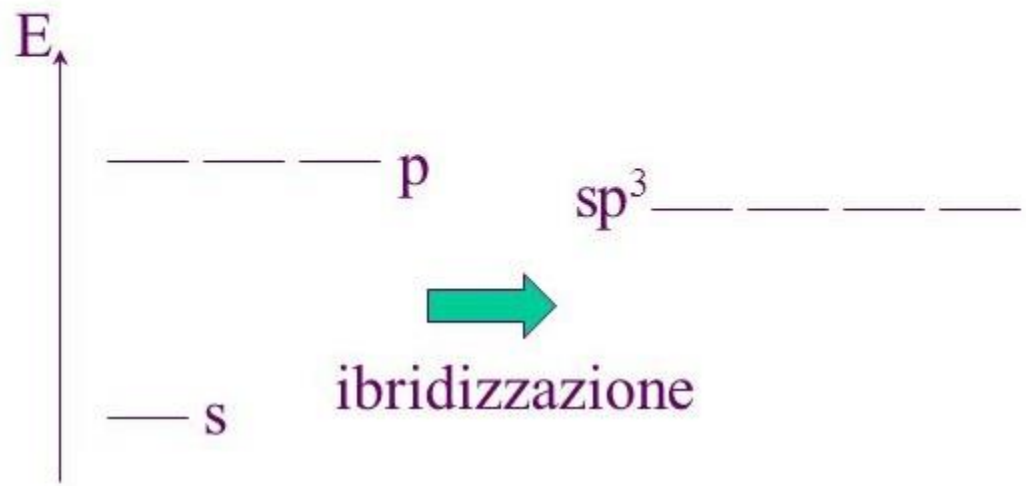


4 legami covalenti

Ibridazione sp^3

1 orbitale s + 3 orbitali p → 4 orbitali identici

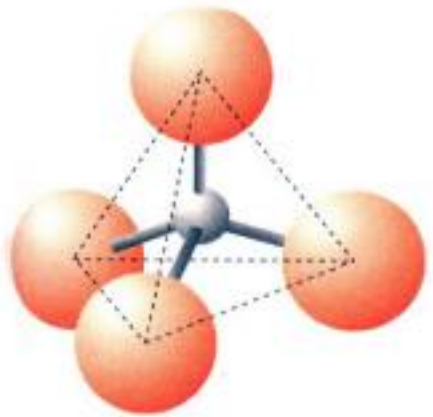




Ogni orbitale ibrido ha il 25% di carattere *s* e il 75% di carattere *p*

n° orbitali ibridi = n° orbitali atomici di partenza

geometria ottimizzata → maggiore concentrazione carica → legami + forti



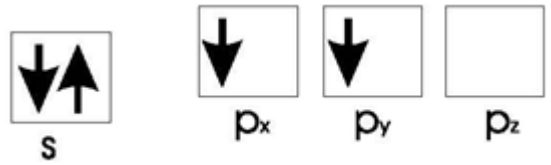
l'angolo tra gli orbitali è di 109° circa

repulsione tra gli orbitali → zone dense di carica negativa

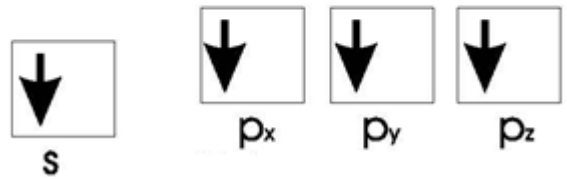
condizione di massima stabilità

Ibridazione sp^2

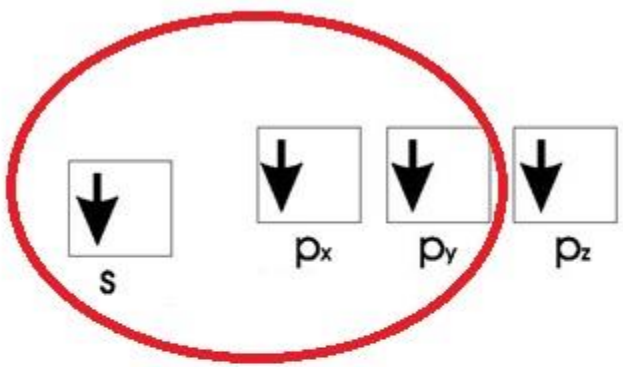
[He] $2s^2\ 2p^2$

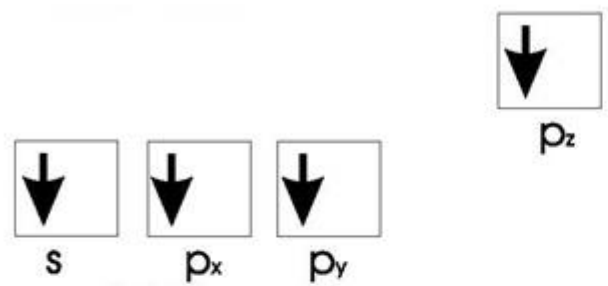


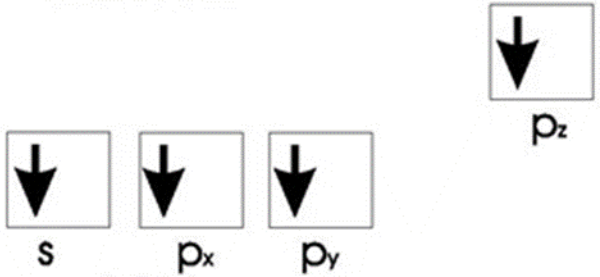
PROMOZIONE



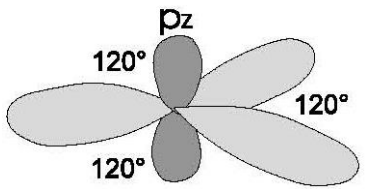
IBRIDAZIONE







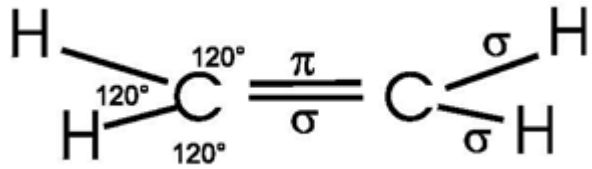
1 orbitale s + 2 orbitali p → 3 orbitali identici



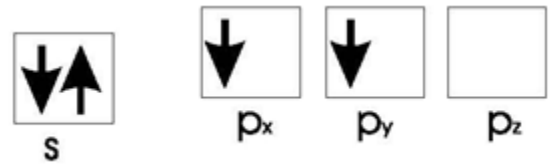
angoli di 120°

orbitale p_z perpendicolare al piano individuato dai tre orbitali

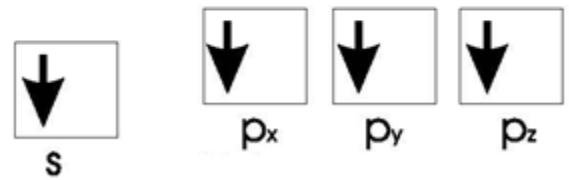
CH_2CH_2



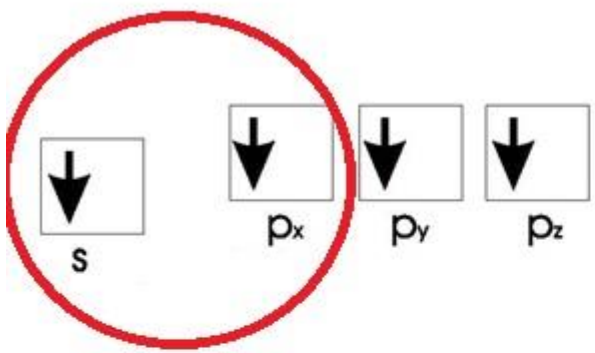
Ibridazione sp

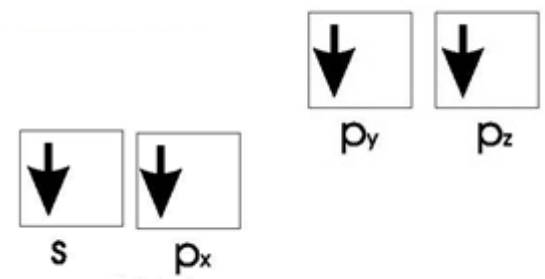


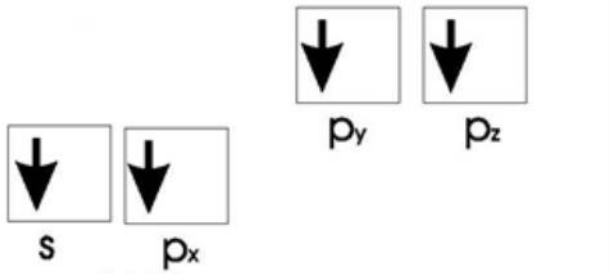
PROMOZIONE

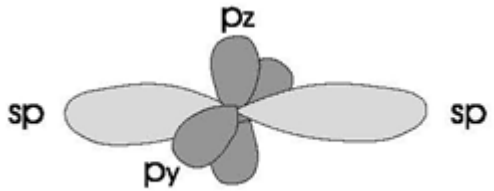


IBRIDAZIONE







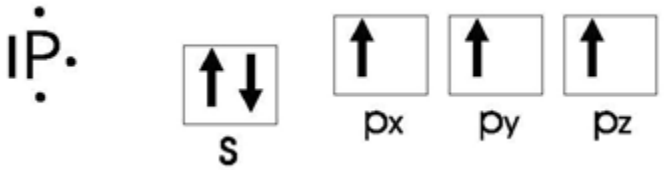


2 orbitali sp che giacciono su di una retta formando angoli di 180°

2 orbitali non ibridati p_y e p_z a 90° tra loro e rispetto ai due orbitali sp

Ibridazione sp^3d

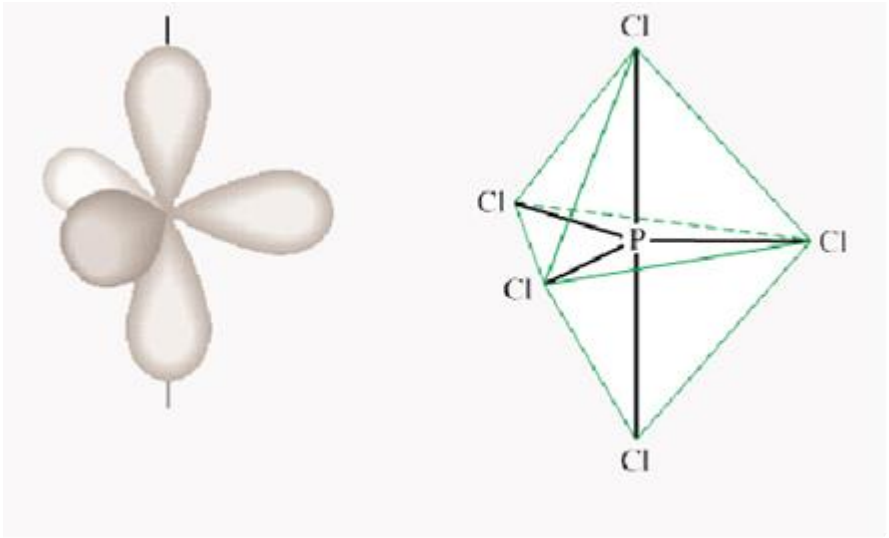
- Fosforo $3s^2\ 3p^3$



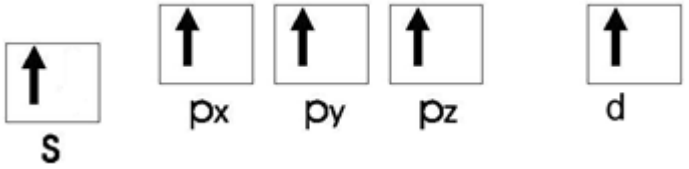
- PCl_3

Ibridazione orbitali **d** e/o **f**

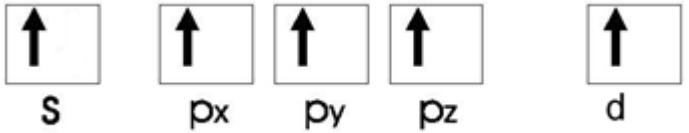
- il fosforo promuove un elettrone **3s** in un orbitale **3d** vuoto
- effettua una *ibridazione* ***sp^3d***
- condivide i 5 elettroni spaiati così ottenuti



PROMOZIONE

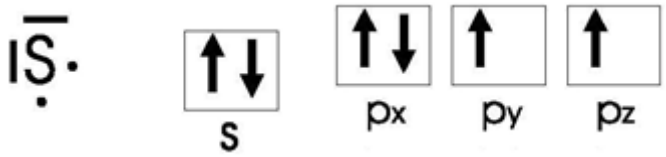


IBRIDAZIONE

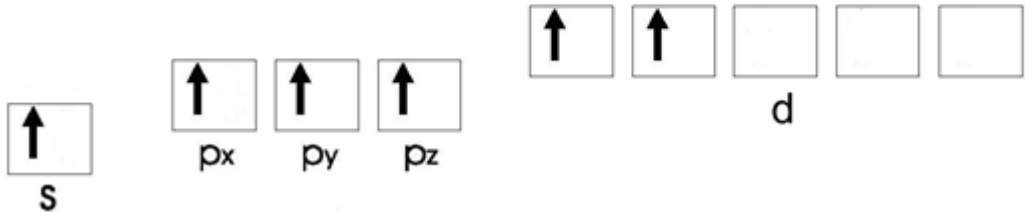


Ibridazione sp^3d^2

- Zolfo $3s^2\ 3p^4$



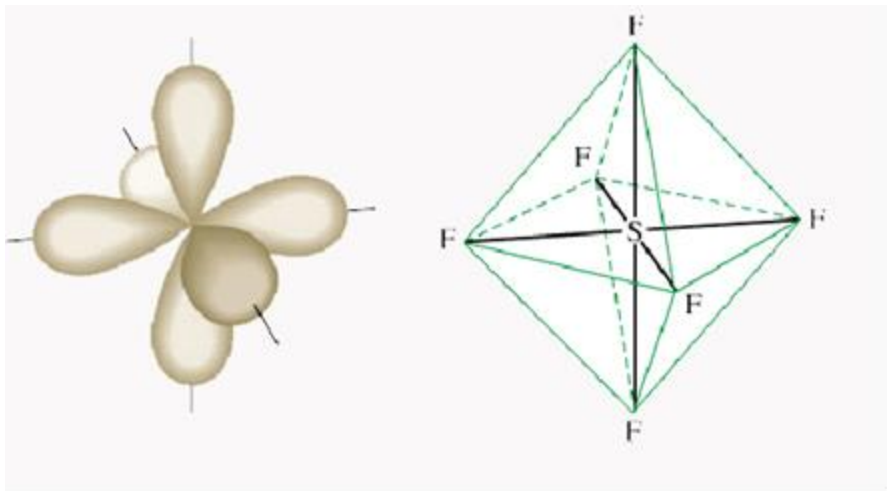
PROMOZIONE



IBRIDAZIONE

- Lo zolfo promuove un elettrone **3s** e un elettrone **$3p_x$** in due orbitali **3d** vuoti
- effettua una *ibridazione* ***sp^3d^2***
- condivide i 6 elettroni spaiati così ottenuti

SF_6



Valence-Shell Electron-Pairs Repulsion (VSEPR)

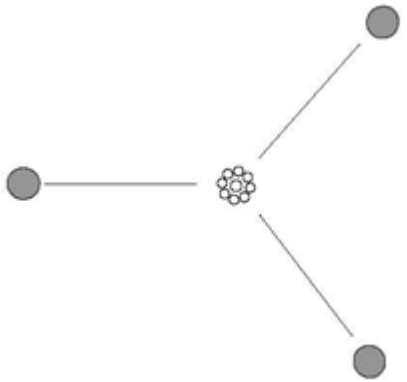
repulsione tra doppietti elettronici dello strato di valenza

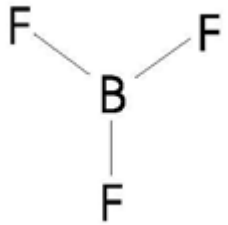
- i legami sono composti da coppie di elettroni
- gli elettroni sono particelle cariche negativamente
- le cariche di segno uguale si respingono
- i sistemi tendono ad un minimo di energia

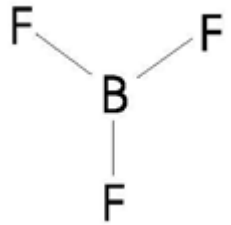
geometria che minimizza le repulsioni → minimizza l'energia

CO_2	O = C = O
BeF_2	F – Be – F
HCN	H – C ≡ N
CaH_2	H – Ca – H

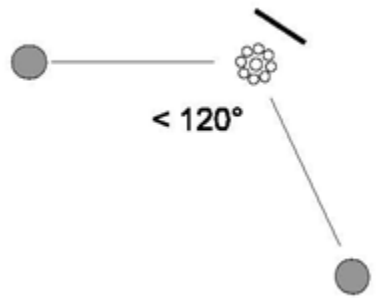
BF_3



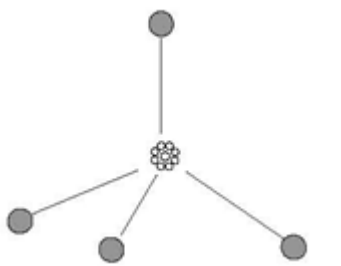




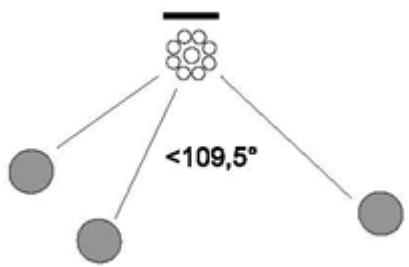
se al posto di un legame un doppietto di elettroni non legati?

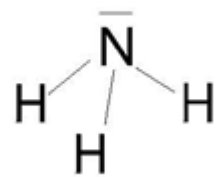


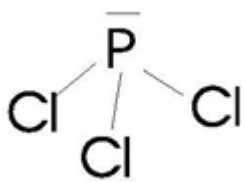
CH_4



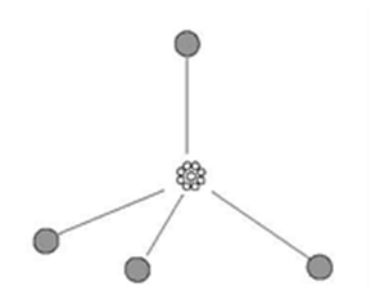
se al posto di un legame un doppietto di elettroni non legati?

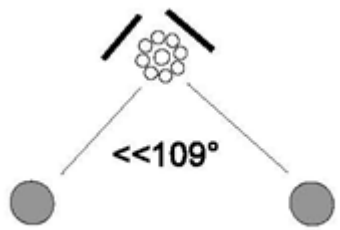


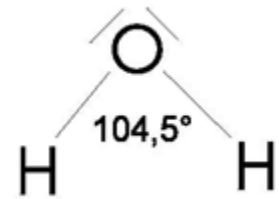


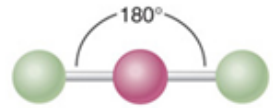
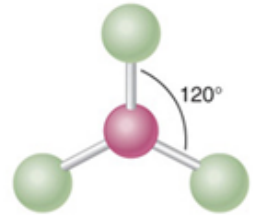
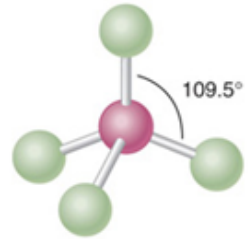
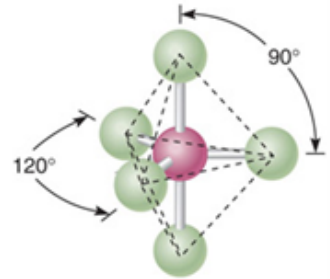
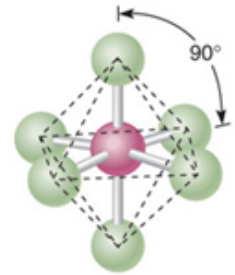


se al posto di un legame due doppietti di elettroni non legati?

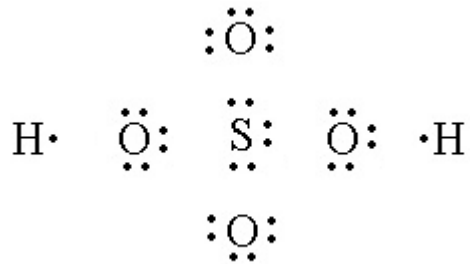




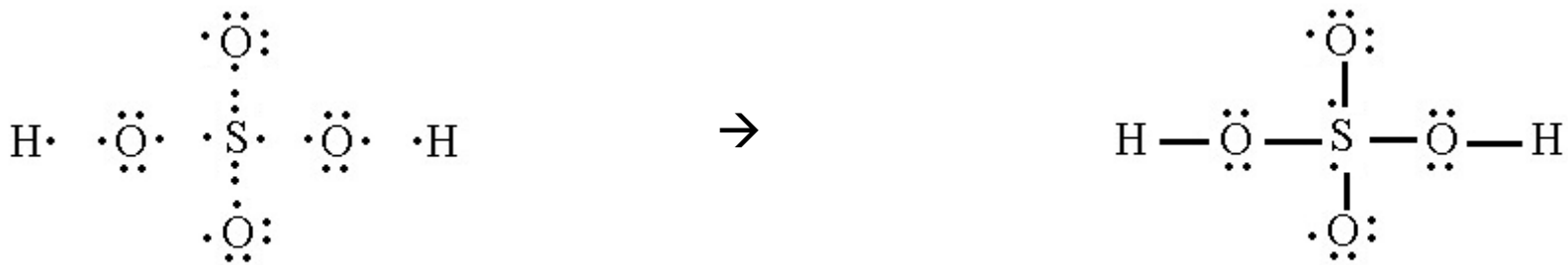


Specie tipiche	Orientazione delle coppie elettroniche	Angoli di legame previsti	Esempio	Modello ball & stick
AX_2	Lineare	180°	BeF_2	
AX_3	Trigonale planare	120°	BF_3	
AX_4	Tetraedro	109.5°	CH_4	
AX_5	Bipiramide trigonale	90° 120° 180°	PF_5	
AX_6	Ottaedro	90° 180°	SF_6	

- Nelle strutture di Lewis l'atomo di H è sempre terminale (legato ad un solo atomo)
- Nei composti poliatomici, in genere, l'atomo centrale è quello a più bassa elettronegatività
- Si disegna, tenendo conto dei precedenti due criteri, la struttura di Lewis della molecola

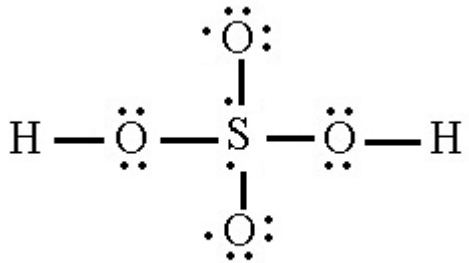


- Si sistemano per primi (a coppie) gli elettroni di legame



- Si verifica il completamento dell’ottetto degli atomi legati a quello centrale (doppietto nel caso di H)

- Se avanzano elettroni si collocano sull'atomo centrale



- Se l'atomo centrale ha più di 8 elettroni attorno a sé, si formano doppi o tripli legami in modo da annullare quante più cariche formali è possibile