

# VSEPR

$$N^{\circ} \text{sterico} = N^{\circ} G' + N^{\circ} \text{..} \quad \text{NON CONTANO I LEGAMI } \pi$$

atomo centrale A; sostituenti X, doppietti E

$N^{\circ} \text{sterico}$

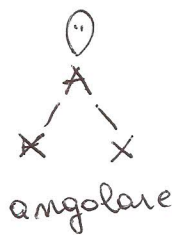
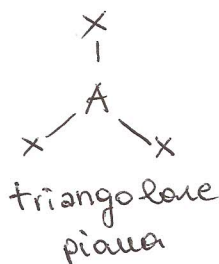
ibridazione

2



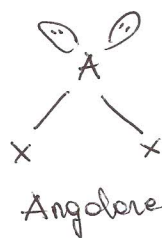
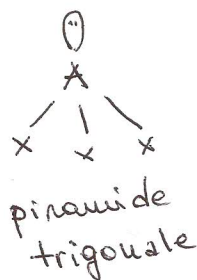
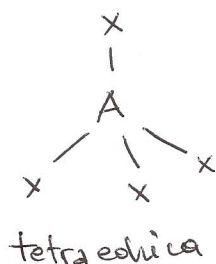
$sp$

3



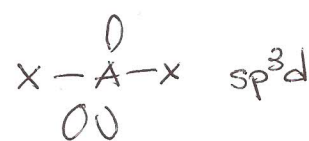
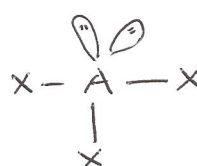
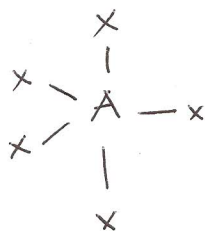
$sp^2$

4



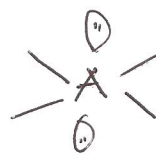
$sp^3$

5



lineare

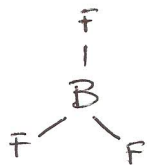
6



$sp^3d^2$

CO  $sp$

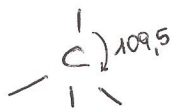
BF<sub>3</sub>  $sp^2$



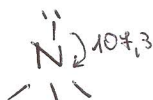
SO<sub>2</sub>  $sp^2$



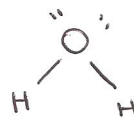
CH<sub>4</sub>  $sp^3$



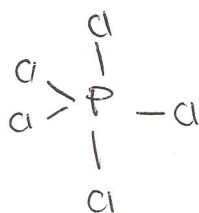
NH<sub>3</sub>



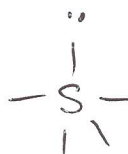
H<sub>2</sub>O



PCl<sub>5</sub> ( $sp^3d$ )

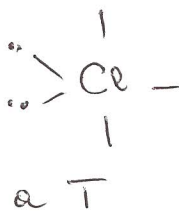


(SF<sub>4</sub>)

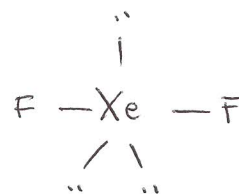


trigonal bipyramide

CeF<sub>3</sub>



XeF<sub>2</sub>



lineare

( $sp^3d^2$ )

SF<sub>6</sub>



BrF<sub>5</sub>



XeF<sub>4</sub>

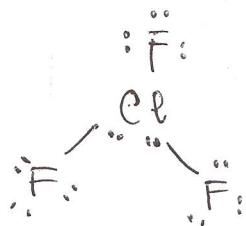


quadrata  
planare

## $\text{ClF}_3$

$$\text{u}^\circ \text{ elettroni} = 7 + 3 \cdot 7 = 28$$

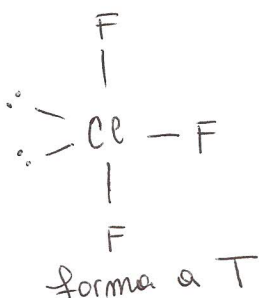
$$\text{coppie} = 14$$



$$CF_{\text{Cl}} = 7 - 4 - \frac{1}{2} \cdot 6 = 0 \quad \text{ok}$$

$$CF_{\text{F}} = 7 - 6 - \frac{1}{2} \cdot 2 = 0$$

$$m = 3 + 2 = 5 \rightarrow sp^3d \text{ (bipiramide trigonale)}$$

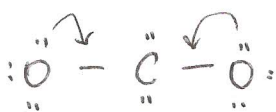


# VSEPR

x

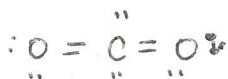
## $\text{CO}_2$

$$\text{u}^\circ \text{ elettroni} = 4 + 2 \cdot 6 = 16 \rightarrow 8 \text{ coppie}$$



$$CF_{\text{O}} = 6 - 6 - \frac{1}{2} \cdot 2 = -1$$

$$CF_{\text{C}} = 4 - 0 - \frac{1}{2} \cdot 2 = +2$$



$$CF_{\text{O}} = 6 - 4 - \frac{1}{2} \cdot 4 = 0$$

ok

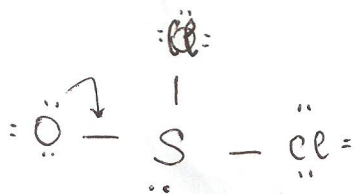
$$CF_{\text{C}} = 4 - 0 - \frac{1}{2} \cdot 8 = 0$$

$$\Rightarrow \text{numero sterico} = \frac{6}{2} + 0 = 2 \Rightarrow sp \quad \text{lineare}$$

# SOCl<sub>2</sub>

$$n^{\circ} \text{ elettroni} = 6 + 6 + 2 \cdot 7 = 26$$

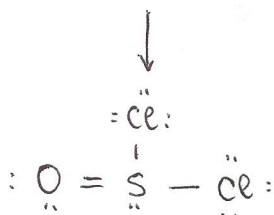
$$\text{coppie} = 13$$



$$CF_S = 6 - 2 - \frac{1}{2} \cdot 6 = 1$$

$$CF_O = 6 - 6 - \frac{1}{2} \cdot 2 = -1$$

$$CF_{Cl} = 7 - 6 - \frac{1}{2} \cdot 2 = 0$$

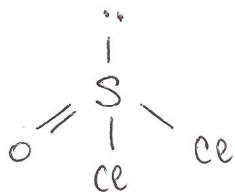


$$CF_S = 6 - 2 - \frac{1}{2} \cdot 8 = 0$$

$$CF_O = 6 - 4 - \frac{1}{2} \cdot 4 = 0$$

$$CF_{Cl} = 0$$

$$n \text{ sterico} = \frac{6}{3} + 1 = 4 \Rightarrow sp^3 \text{ (tetraedica)}$$



oppure

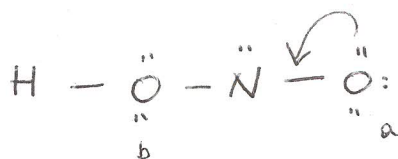


piramide trigonale



$$u^\circ \text{ elettroni} : 1 + 5 + 2 \cdot 6 = 18$$

$$u^\circ \text{ coppie} : 9 \text{ di cui } 3 \text{ per legami } \sigma$$



$$CF_N = 5 - 2 - \frac{1}{2} \cdot 4 = 1$$

$$CF_{O_a} = 6 - 6 - \frac{1}{2} \cdot 2 = -1$$

$$CF_{O_b} = 6 - 4 - \frac{1}{2} \cdot 4 = 0$$

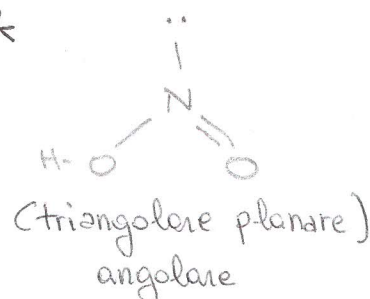
$$CF_H = 1 - 0 - \frac{1}{2} \cdot 2 = 0$$



$$CF_N = 5 - 2 - \frac{1}{2} \cdot 6 = 0$$

$$CF_{O_a} = 6 - 4 - \frac{1}{2} \cdot 4 = 0 \quad \text{Ok}$$

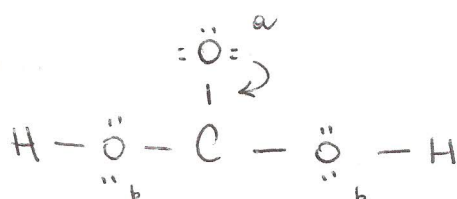
$$u_s = \frac{6 + \cdot\cdot}{2 + 1} = 3 \Rightarrow sp^2$$



$$u^\circ \text{ elettroni} = 2 + 4 + 3 \cdot 6 = 24$$

$$u^\circ \text{ coppie} = 12$$

$$u^\circ \text{ coppie "esterne"} = 12 - 5 = 7$$

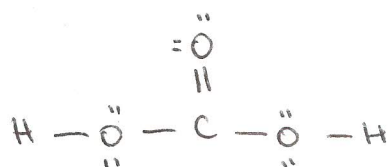


$$CF_C = 4 - 0 - \frac{1}{2} \cdot 6 = 1$$

$$CF_{O_a} = 6 - 6 - \frac{1}{2} \cdot 2 = -1$$

$$CF_{O_b} = 6 - 4 - \frac{1}{2} \cdot 2 = 0$$

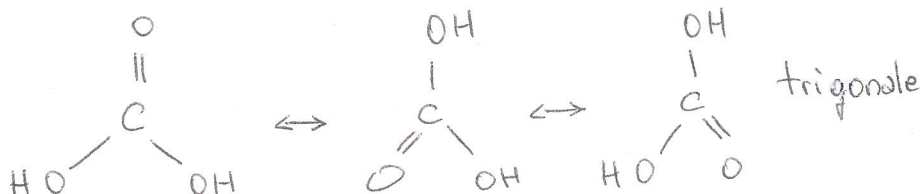
$$CF_H = 1 - 0 - \frac{1}{2} \cdot 2 = 0$$



$$CF_C = 4 - 0 - \frac{1}{2} \cdot 8 = 0$$

$$CF_{O_a} = 6 - 4 - \frac{1}{2} \cdot 4 = 0 \quad \text{Ok}$$

$$u_s = \frac{6 + \cdot\cdot}{3 + 0} = 3 \Rightarrow sp^2$$

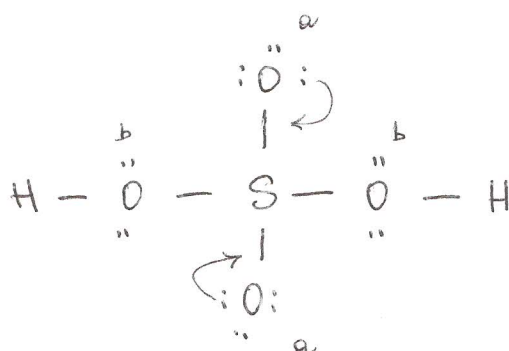




# STRUTTURE DI LEWIS  
# VSEPR

$$n^{\circ} \text{ elettroni} = 2 + 6 + 4 \cdot 6 = 32 e^{-}$$

$$n^{\circ} \text{ coppie} = 16 \text{ coppie}$$



l'idrogeno e' sempre periferico

Nel distribuire le coppie  
restante (16 - 6 = 10 coppie)

fra gli atomi esterni NON  
CONSIDERO L'IDROGENO che ha  
già raggiunto la stabilità e

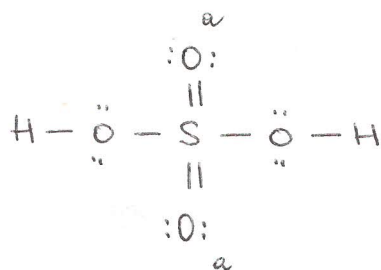
comunque non può accettare  
altri elettroni. Inizio la distribuzione  
degli O senza idrogeno perché sono  
quelli con meno elettroni

$$CF_H = 1 - 0 - \frac{1}{2} \cdot 2 = 0 \quad \text{ok}$$

$$CF_S = 6 - 0 - \frac{1}{2} \cdot 8 = +2$$

$$CF_{O_a} = 6 - 6 - \frac{1}{2} \cdot 2 = -1$$

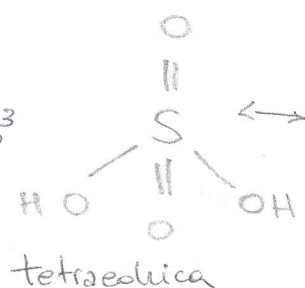
$$CF_{O_b} = 6 - 4 - \frac{1}{2} \cdot 4 = 0 \quad \text{ok}$$



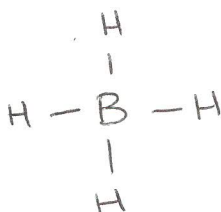
$$CF_S = 6 - 0 - \frac{1}{2} \cdot 12 = 0$$

$$CF_{O_a} = 6 - 4 - \frac{1}{2} \cdot 4 = 0$$

$$M_S = 6 + 0 = 6 \rightarrow sp^3$$



$$n^{\circ} \text{ coppie} = \frac{3 + 4 + 1}{2} = 4 \text{ coppie}$$

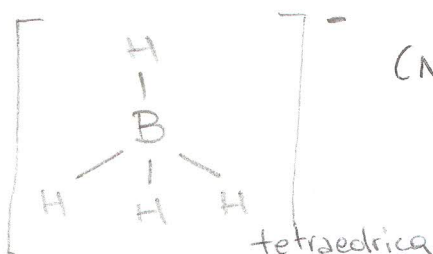


$$CF_H = 1 - 0 - \frac{1}{2} \cdot 2 = 0$$

$$CF_B = 3 - 0 - \frac{1}{2} \cdot 8 = -1 \leftarrow \text{e' negativa e pari alla carica dello ione considerato}$$

=> la struttura e' corretta!

$$M_S = 4 + 0 = 4 \quad sp^3$$

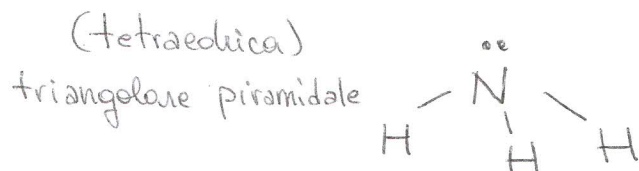


(Notare che il boro ha raggiunto l'ottetto)

# # STRUTTURE DI LEWIS # VSEPR



$$\text{u}^\circ \text{ coppie} = \frac{5+3}{2} = 4 e^-$$



$$CF_N = 5 - 2 - \frac{1}{2} \cdot 6 = 0$$

$$CF_F = 1 - \frac{1}{2} \cdot 2 = 0$$

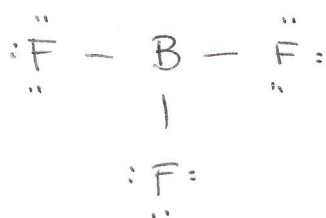
$$m_s = \frac{5}{2} + \frac{1}{2} = 3 \rightarrow sp^3$$

l'ultima coppia da sistemare  
non può stare sugli atomi  
esterni dato che ci sono solo  
idrogeni che non sono in grado  
di ospitarli.

VIETATO CONSIDERARE LA  
POSSIBILITA' DI UN DOPPIO LEGAME  
CHE COINVOLGA UN ATOMO DI  
IDROGENO !!!



$$\text{u}^\circ \text{ coppie} = \frac{3+3 \cdot 7}{2} = \frac{24}{2} e^- = 12 \text{ coppie}$$



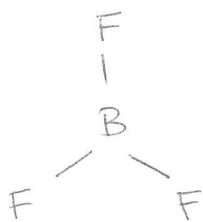
$$CF_B = 3 - 0 - \frac{1}{2} \cdot 6 = 0$$

$$CF_F = 7 - 6 - \frac{1}{2} \cdot 2 = 0$$

Nota → il B non ha raggiunto l'ottetto  
ma la sua carica formale è zero

⚠ Questo è un caso particolare  
da ricordare per il quale la  
teoria di Lewis non è esatta

$$m_s = \frac{6}{2} + \frac{0}{2} = sp^2$$

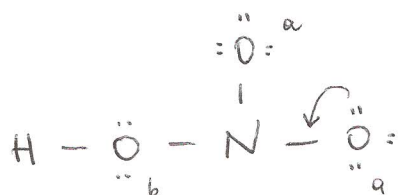


trigonale planare



$\text{HNO}_3$ 

no coppie = 12 di cui 4 per legami  $\sigma$

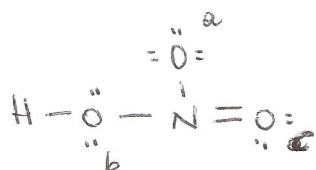


$$CF_N = 5 - 0 - \frac{1}{2} \cdot 6 = +2$$

$$ff_{O_a} = 6 - 6 - \frac{1}{2} \cdot 2 = -1$$

$$CF_0 = 6 - 4 - \frac{1}{2} \cdot 4 = 0$$

$$CF_H = 1 - 0 - \frac{1}{2} \cdot 2 = 0$$



$$CF_N = 5 - 0 - \frac{1}{2} \cdot 8 = +1$$

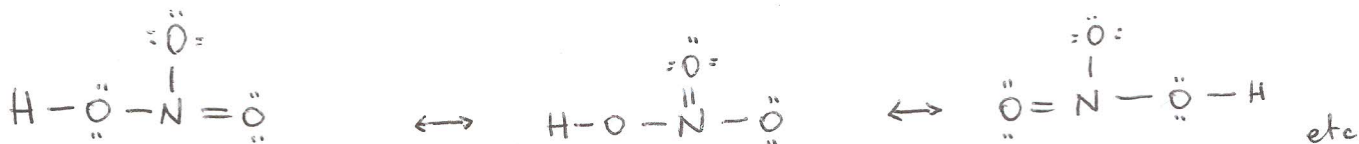
$$CF_{0c} = 6 - 4 - \frac{1}{2} \cdot 4 = 0$$

$$CF_{0A} = -1$$

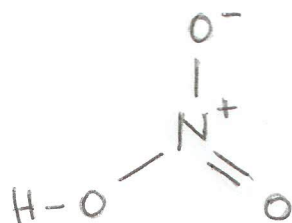
$$C_{F_{ob}} = 0$$

$$CF_H = 0$$

⚠ Per annullare la carica formale su N dovrei formare un altro doppio legame fra  $O_a$  e N, MA l'azoto è un elemento del 2° periodo che non ha la possibilità di espandere l'ottetto (che ha già raggiunto con questa struttura)  $\Rightarrow$  devo concludere che questa è la migliore struttura possibile.



$$u_s = \frac{6 + 0}{3 + 0} = 3 \rightarrow sp^2$$



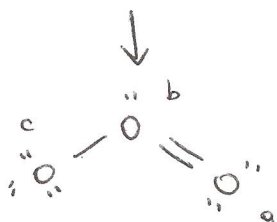
Assegno la carica negativa a O  
e la carica positiva a N sulla  
base della rispettiva carica formale



$O_3$ 

$$n^{\circ} \text{ elettroni} = 3 \cdot 6 = 18$$

$$n^{\circ} \text{ coppie} = 9$$



$$CF_{O_a} = 6 - 4 - \frac{1}{2} \cdot 2 = 0$$

$$CF_{O_b} = 6 - 2 - \frac{1}{2} \cdot 6 = +1$$

$$CF_{O_c} = 6 - 6 - \frac{1}{2} \cdot 2 = -1$$

Dato che l'ossigeno non può espandere l'ottetto questa è la miglior struttura che posso ipotizzare



(triangolare piana)  
angolare

$$us = \frac{6 + \dots}{2 + 1} = 3 \quad sp^2$$