Strutture di Lewis.

1) **Disegnare la molecola o lo ione poliatomico con gli atomi legati *mediante legami singoli*.**

2) **Sommare il numero di elettroni di valenza su ciascun atomo nella molecola per trovare il numero totale degli elettroni di valenza. Se la molecola è carica (cioè se è uno ione poliatomico) sommare un elettrone per ogni carica negativa o sottrarre un elettrone per ciascuna carica positiva. *Dividere gli elettroni di valenza totale per due*, per ottenere i doppietti elettronici.**

3) **Sottrarre il numero di doppietti che occorrono per *formare legami singoli tra gli atomi e usare i rimanenti per completare l'ottetto intorno a ciascun atomo*, eccetto l'idrogeno. Se vi sono doppietti insufficienti per completare tutti gli ottetti, completare prima quelli degli atomi più elettronegativi. *Quindi assegnare le cariche formali*.**

4) **Se qualche atomo ha ancora l'ottetto incompleto, convertire i doppietti non leganti in leganti. In altre parole, *usare i doppietti non leganti per formare doppi e tripli legami finché ciascun atomo ha un ottetto*. Quindi riassegnare le cariche formali.**

5) **Se la regola 4 crea cariche formali addizionali, usare la struttura data dalla regola 3.**

6) **Se l'atomo centrale proviene dal periodo 3 o da periodi più avanti, la regola dell'ottetto non si applica. Formare legami addizionali multipli per allontanare il maggior numero possibile di cariche formali.**

Teoria VSEPR

Valence Shell Electron Pair Repulsion

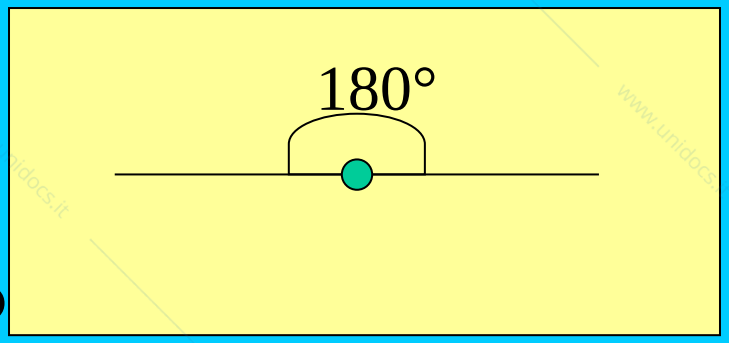
Teoria della repulsione delle coppie di elettroni del guscio di valenza

La disposizione geometrica dei legami intorno a un atomo in una molecola dipende dal numero totale di coppie di elettroni nel guscio di valenza di un atomo, comprese sia le coppie leganti che quelle non leganti.

Numero Sterico

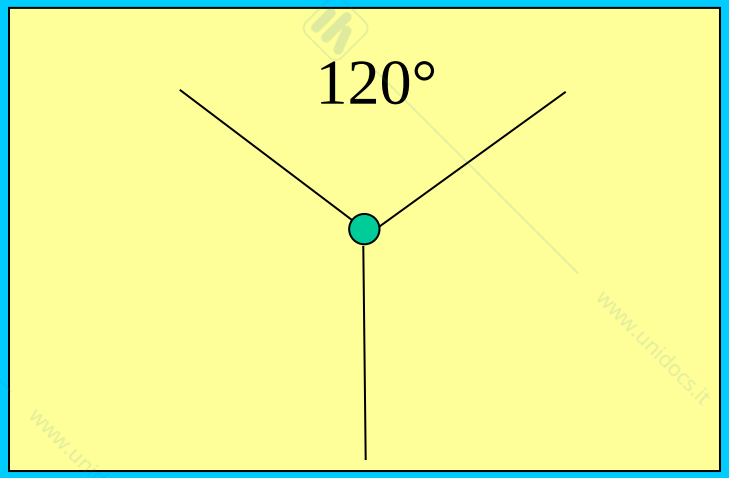
NS = n° atomi legati + doppietti solitari

NS = 2



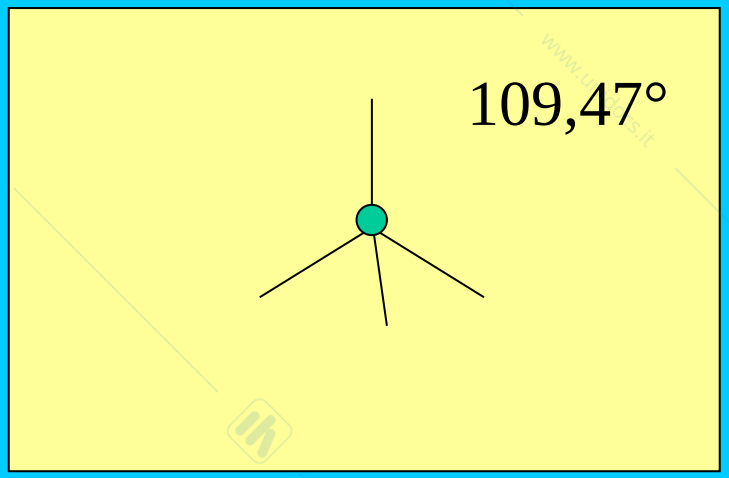
Ibridizzazione dell'atomo centrale: sp

NS = 3



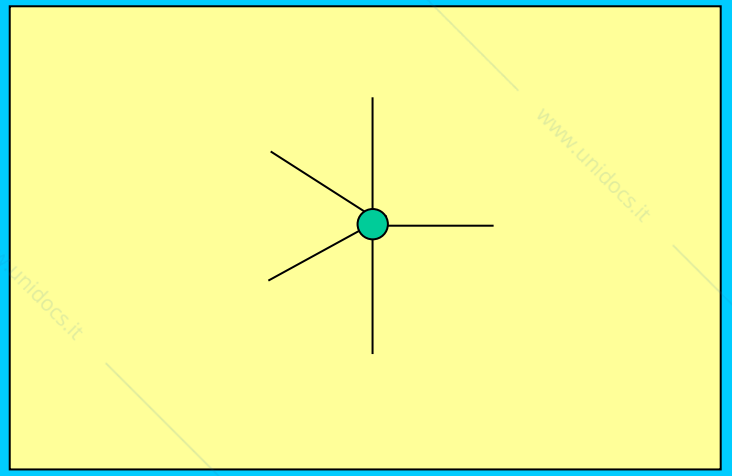
Ibridizzazione dell'atomo centrale: sp^2

NS = 4



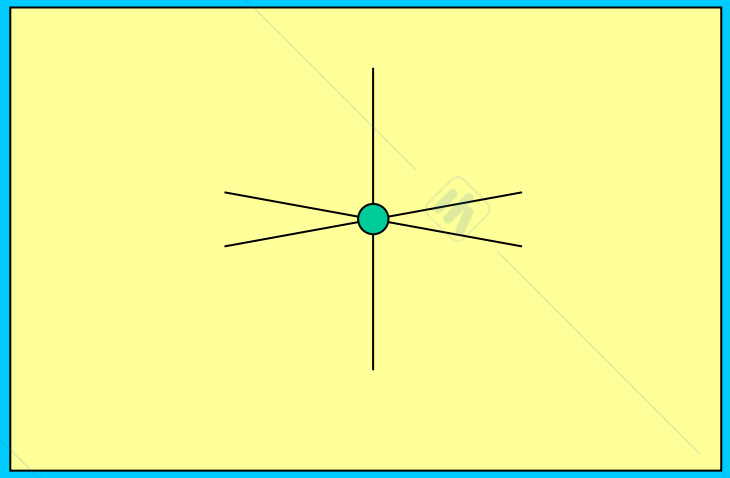
Ibridizzazione dell'atomo centrale: sp^3

NS = 5



Ibridizzazione dell'atomo centrale: sp^3d

NS = 6



Ibridizzazione dell'atomo centrale: sp^3d^2

Si definisce dipolo elettrico un sistema costituito da due cariche elettriche puntiformi q, dello stesso valore ma di segno contrario, vincolate tra loro ad una distanza d.

Il momento dipolare μ è dato dal prodotto della carica per la distanza

$$\mu = q \cdot d$$

Una molecola possiede un momento dipolare μ, quando *il baricentro delle cariche positive e quello delle cariche negative non coincidono*.

Le molecole che presentano un momento dipolare diverso da zero si dicono polari, mentre quelle che non hanno un momento dipolare sono apolari.

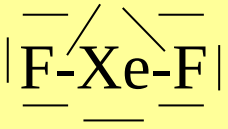
XeF_2

elettroni di valenza

F 7 x 2 +

Xe 8

22



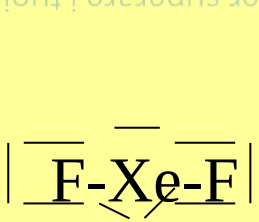
Doppietti =22 : 2 = 11

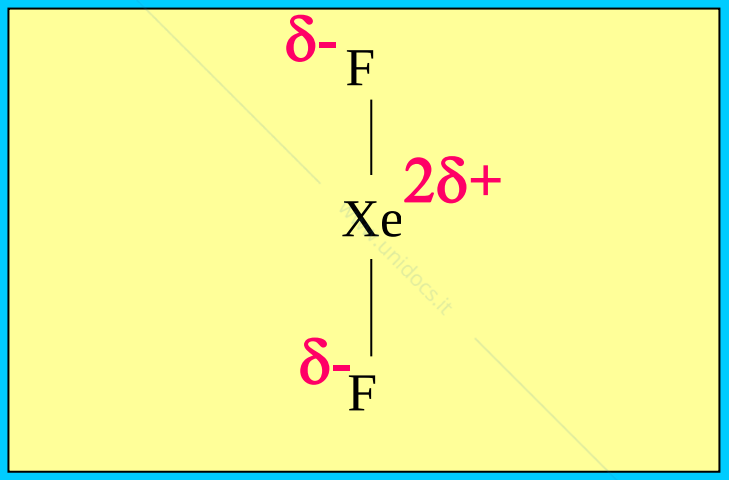
C.F. fluoro = 7 – 6 –1 = 0

C.F. xenon = 8 – 6 –2 = 0

XeF_2

NS = 5

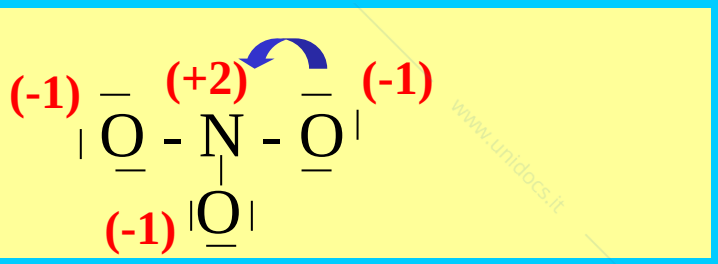




molecola lineare

molecola apolare

NO_3^-



elettroni di valenza

O 6 x 3 +

N 5 +

1 (car. negat.)

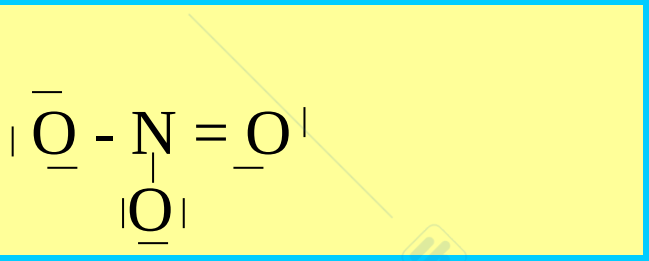
24

C.F. azoto = 5 – 0 –3 = +2

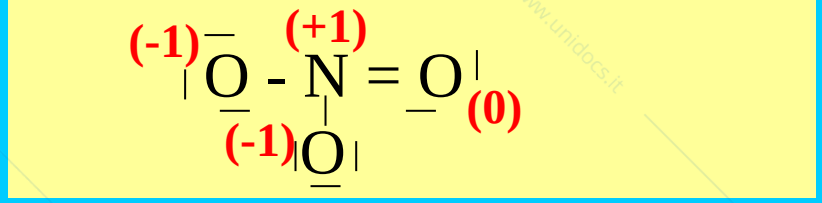
C.F. ossigeno = 6 – 6 –1 = -1

Doppietti = 24 : 2 = 12

L'azoto non ha l'ottetto completo (applicare la regola 4)



NO_3^-



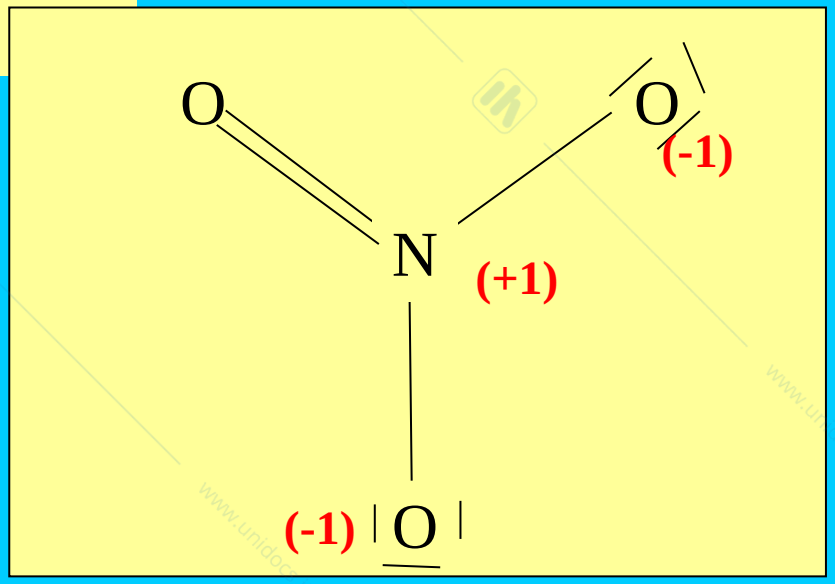
C.F. azoto = 5 – 0 –4 = +1

C.F. ossigeno = 6 – 4 –2 = 0

C.F. ossigeno = 6 – 6 –1 = -1

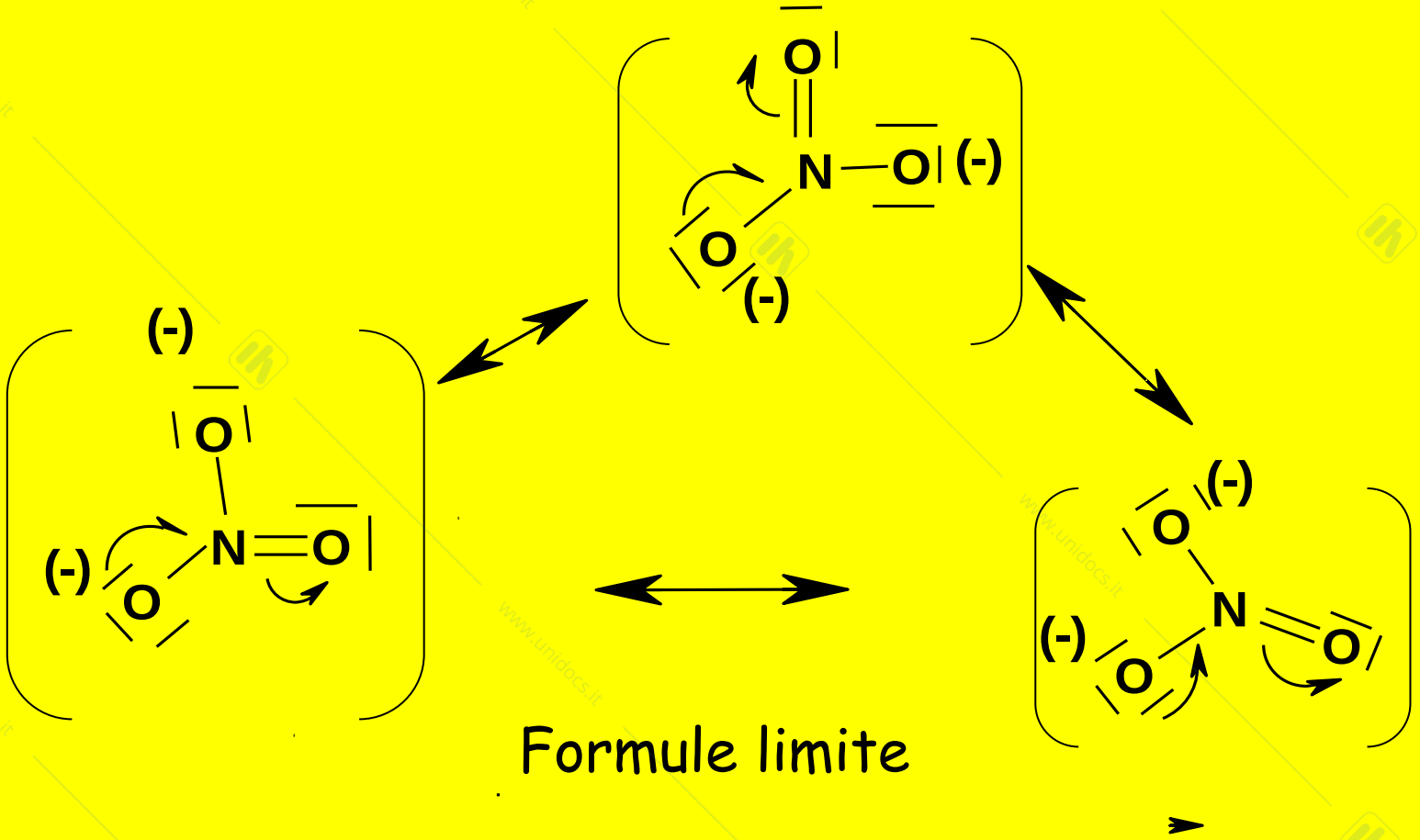
L'azoto appartiene al *secondo periodo*, di conseguenza non può avere più di 8 elettroni, quindi non possiamo minimizzare ulteriormente la C.F.

NS = 3
Ibridizzazione dell'azoto
sp^2



Geometria: triangolare

Risonanza(mesomeria): la molecola è più stabile quando gli elettroni sono delocalizzati



NO_3^-

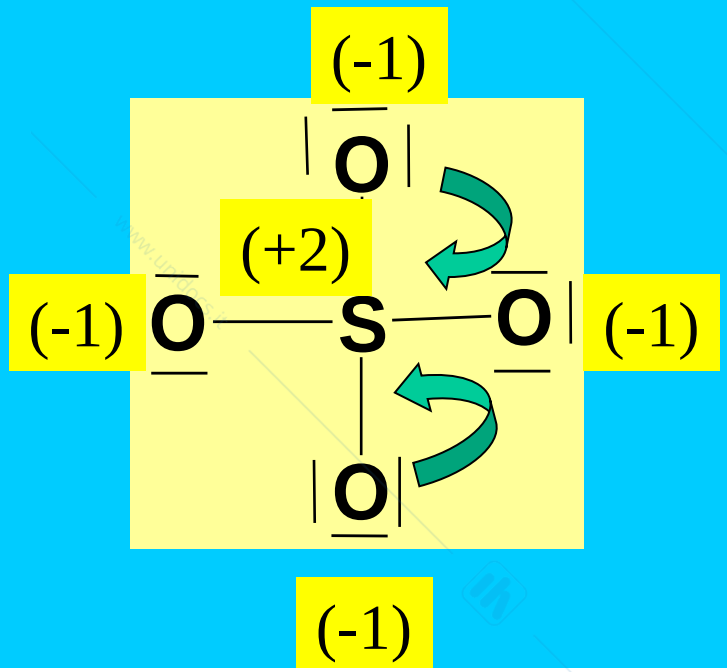
SO_4^{2-}

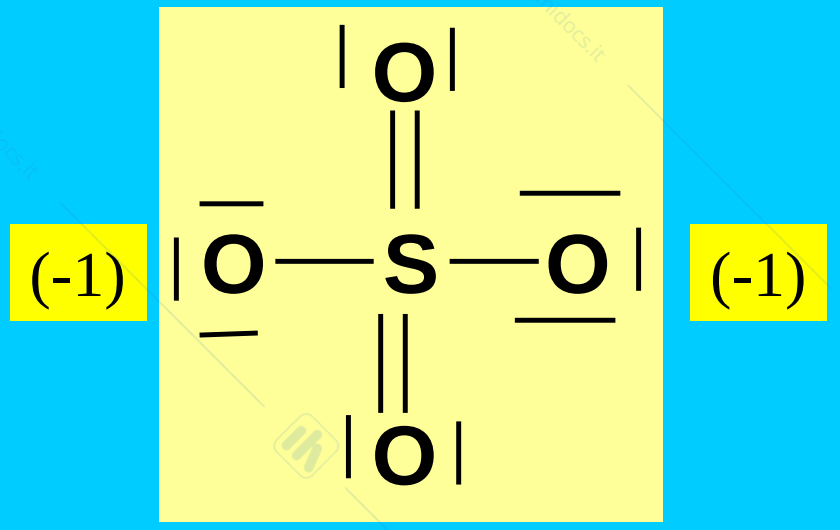
elettroni di valenza

O	6 x 4 = 24+
S	6 +
-	2
	32

Possiamo ancora minimizzare le CF poiché lo S appartiene al terzo periodo, orbitali d disponibili (espansione del guscio di valenza).

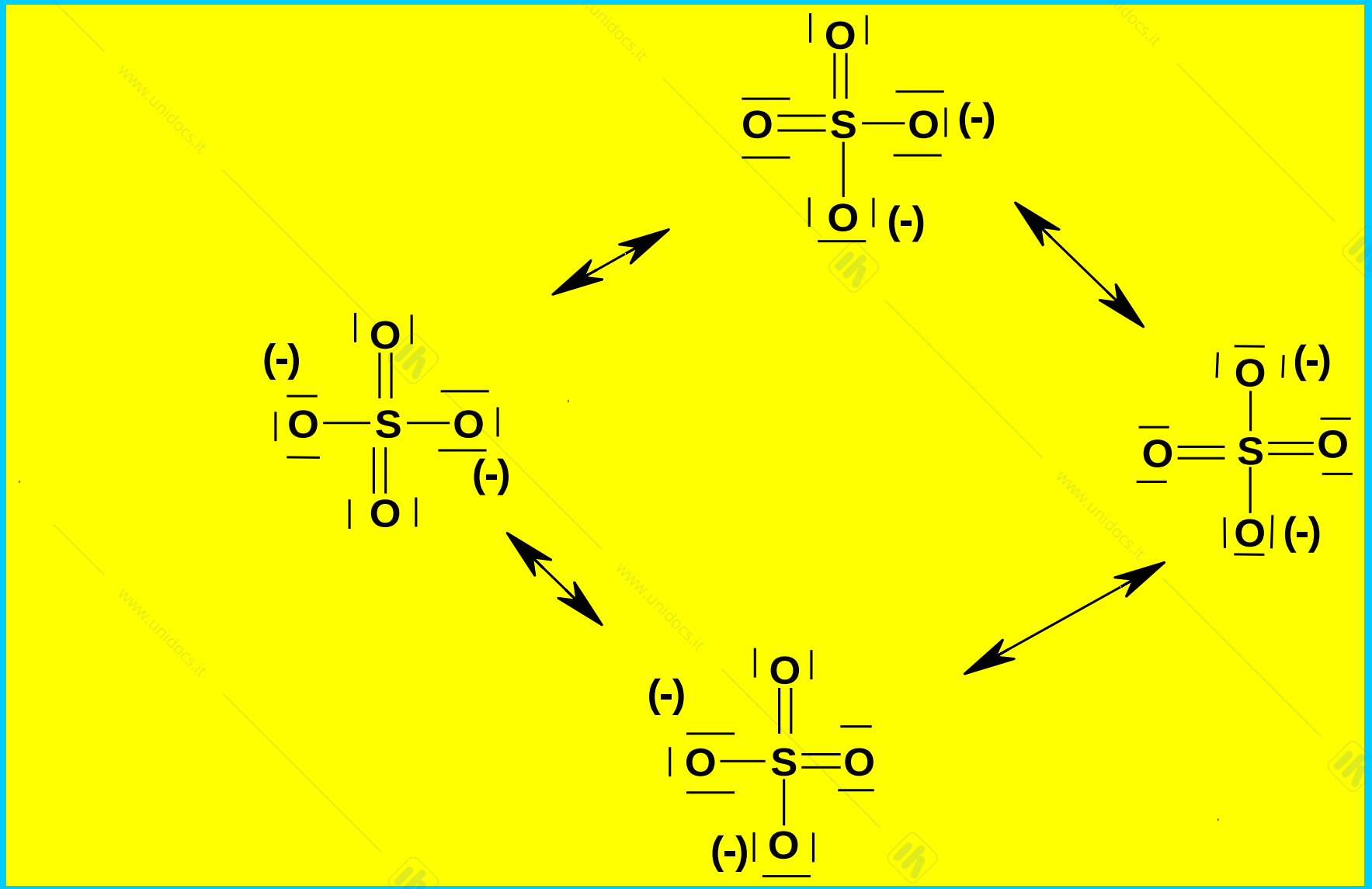
Doppietti = 32 : 2 = 16





SO_4^{2-}

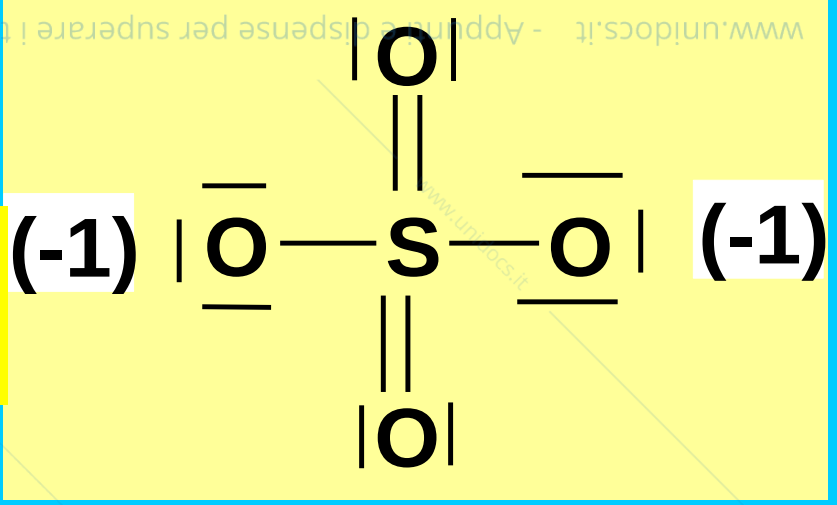
Risonanza

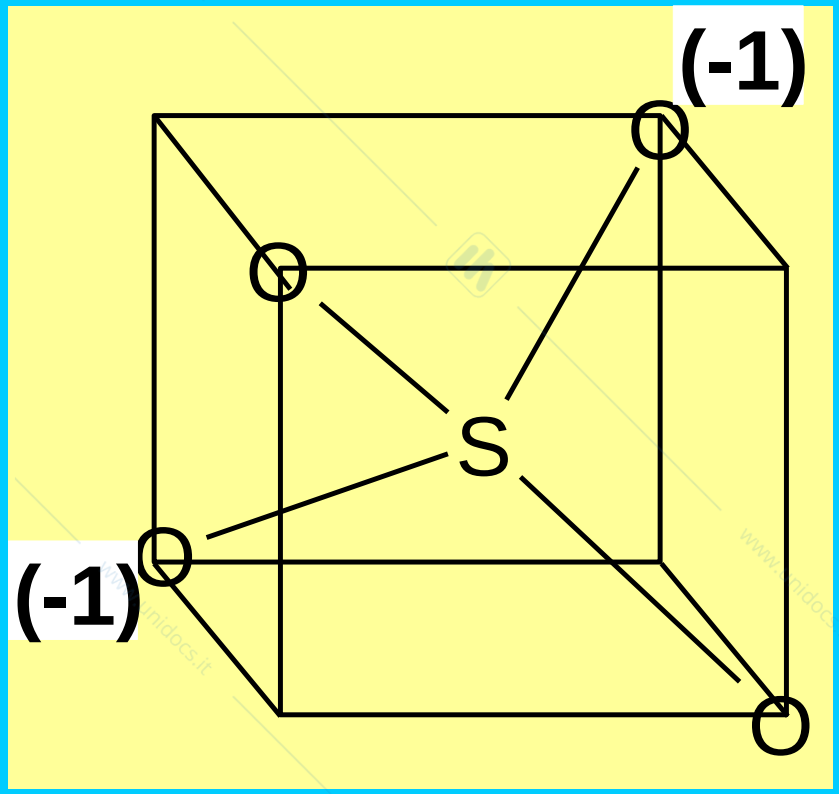


SO_4^{2-}

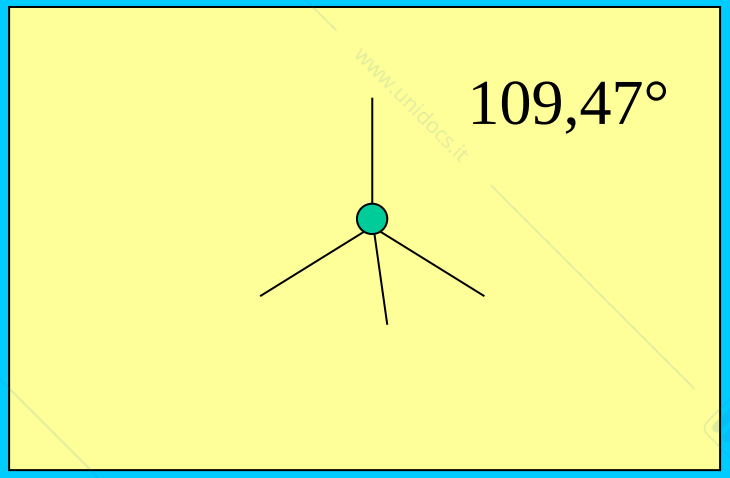
Ibridizzazione di S: sp^3

Geometria : tetraedrica





NS = 4



SO_2

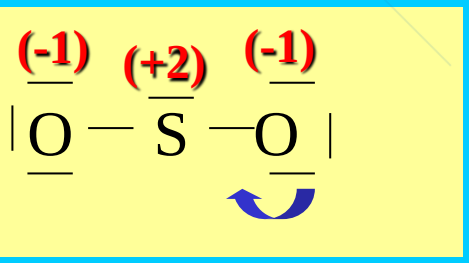
elettroni di valenza

O 6 x 2 = 12 +

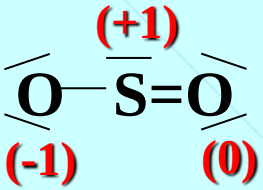
S 6

18

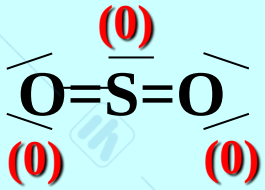
Doppietti = 18 : 2 = 9



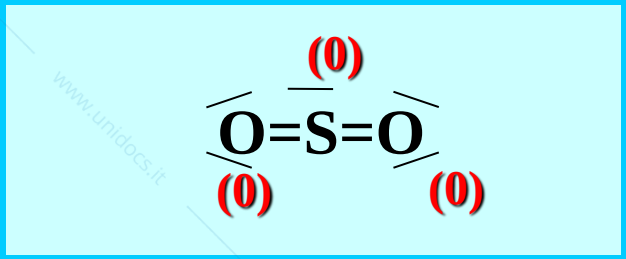
Lo zolfo non ha l'ottetto completo



Possiamo ancora minimizzare le CF poiché
S è del terzo periodo ed ha
orbitali d disponibili(espansione del guscio di valenza)

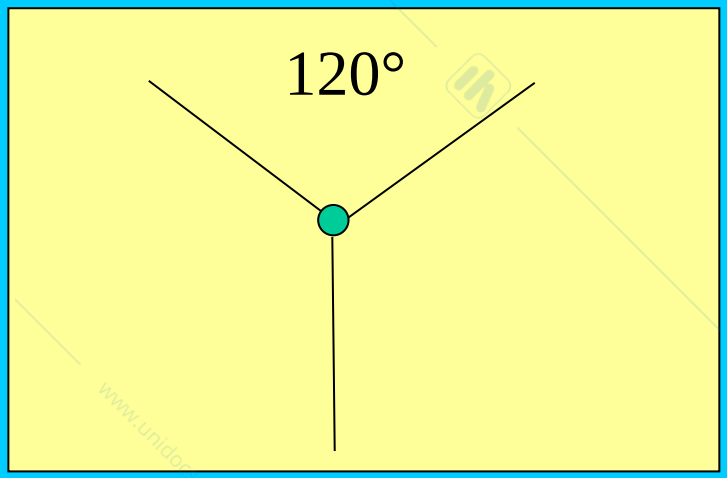


SO_2

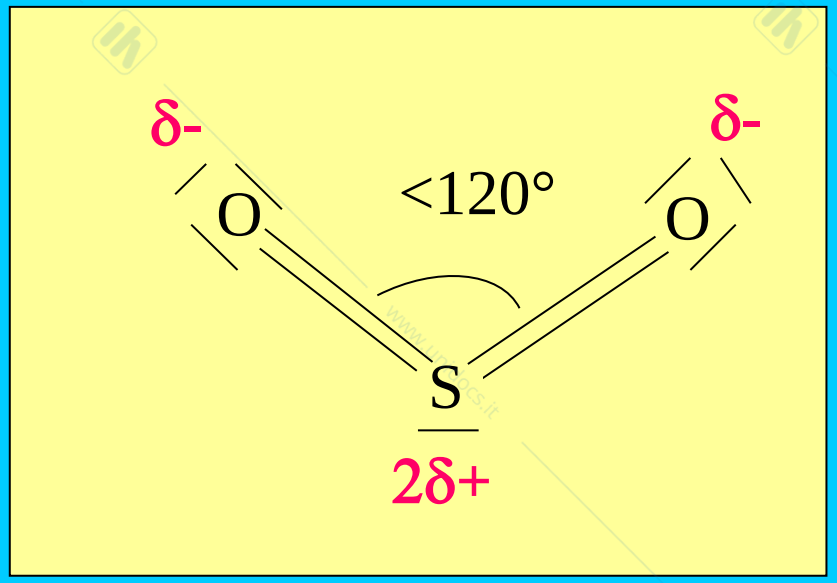


NS = 3

Ibribizzazione dell'atomo centrale = sp^2



Molecola angolata



molecola polare

HNO_2

elettroni di valenza

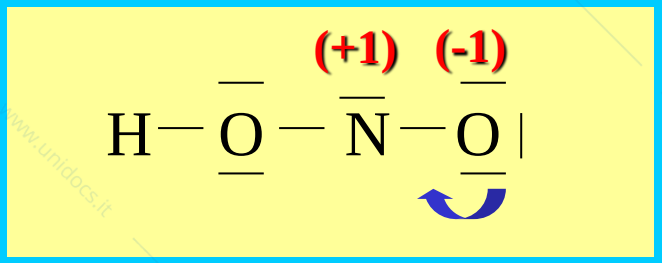
H 1 x1 = 1+

N 5 x 1 = 5 +

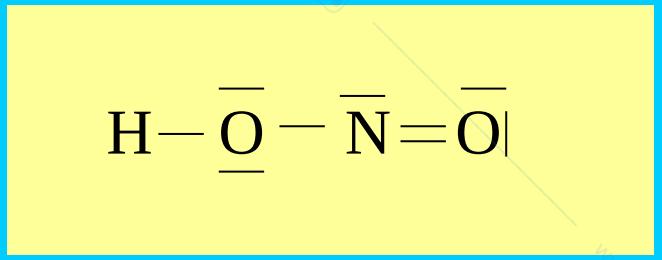
O 6 x 2 = 12

18

Doppietti = 18 : 2 = 9



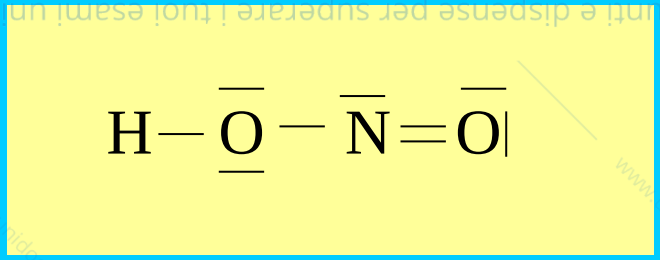
L'azoto non ha l'ottetto completo



CF: assenti

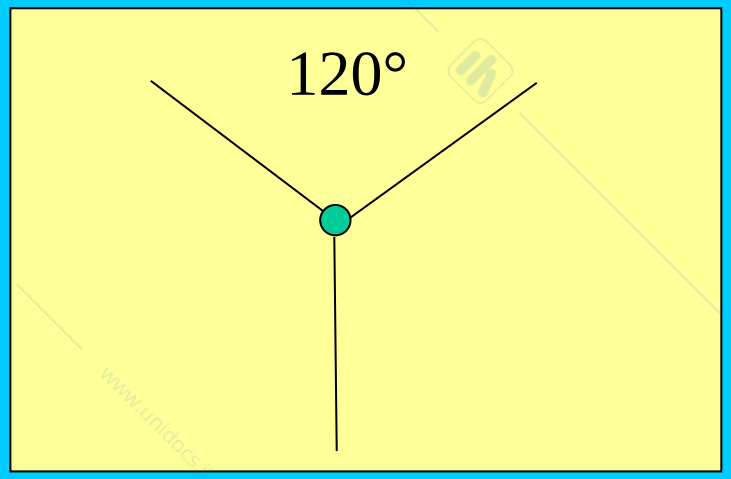
Come in tutti gli ossiacidi di formula HXO(n) l'idrogeno è sempre legato all'ossigeno

HNO_2

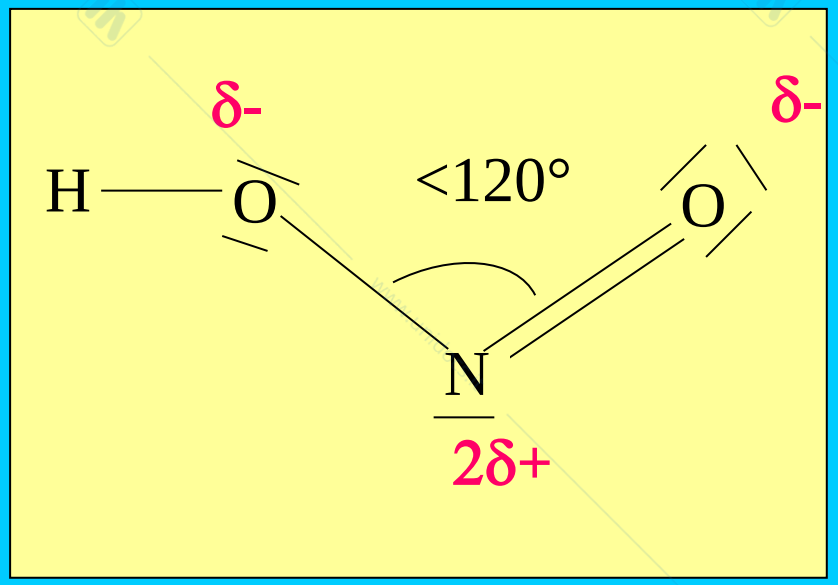


NS = 3

Ibribizzazione dell'atomo centrale = sp^2



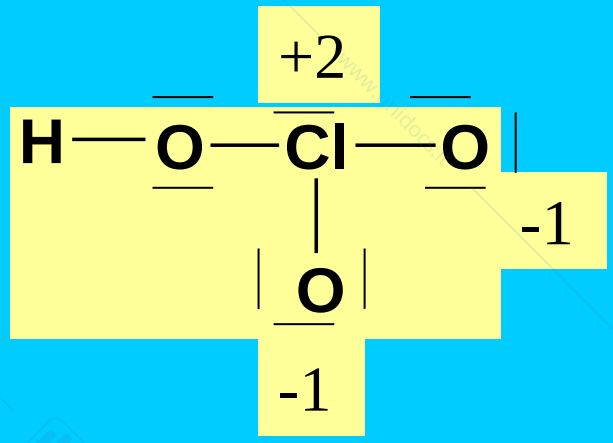
Molecola angolata



molecola polare

$HClO_3$

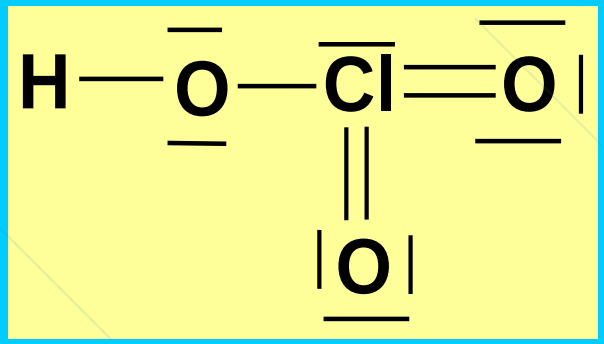
Come in tutti gli ossiacidi di formula HXO(n) l'idrogeno è sempre legato all'ossigeno



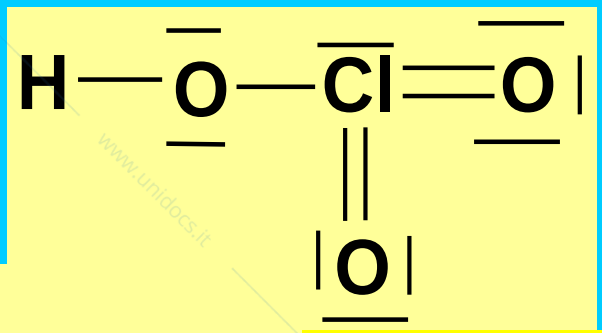
elettroni di valenza

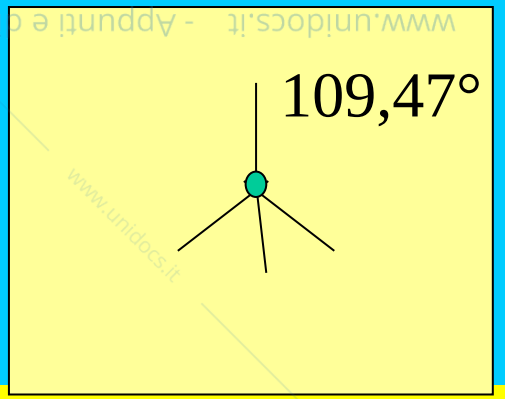
H 1 x1 = 1+
Cl 7 x 1 = 7 +
O 6 x 3 = 18
26

Doppietti = 26 : 2 = 13



$HClO_3$



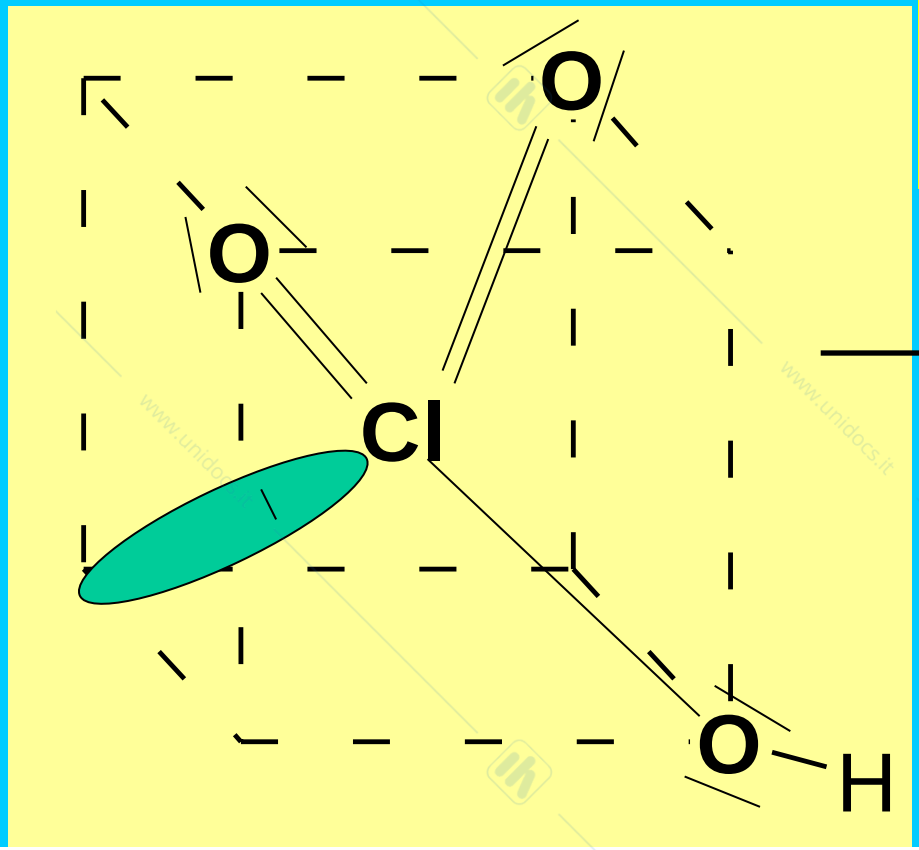


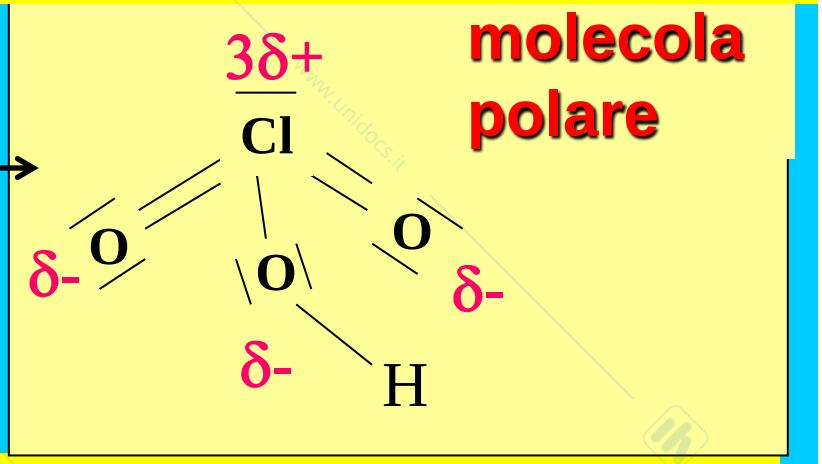
NS = 4

Ibribizzazione dell'atomo centrale = sp^3

Disposizione delle coppie di elettroni: tetraedrica

Espansione del guscio di valenza





molecola polare

Geometria: piramide a base triangolare

$HClO_2$

elettroni di valenza

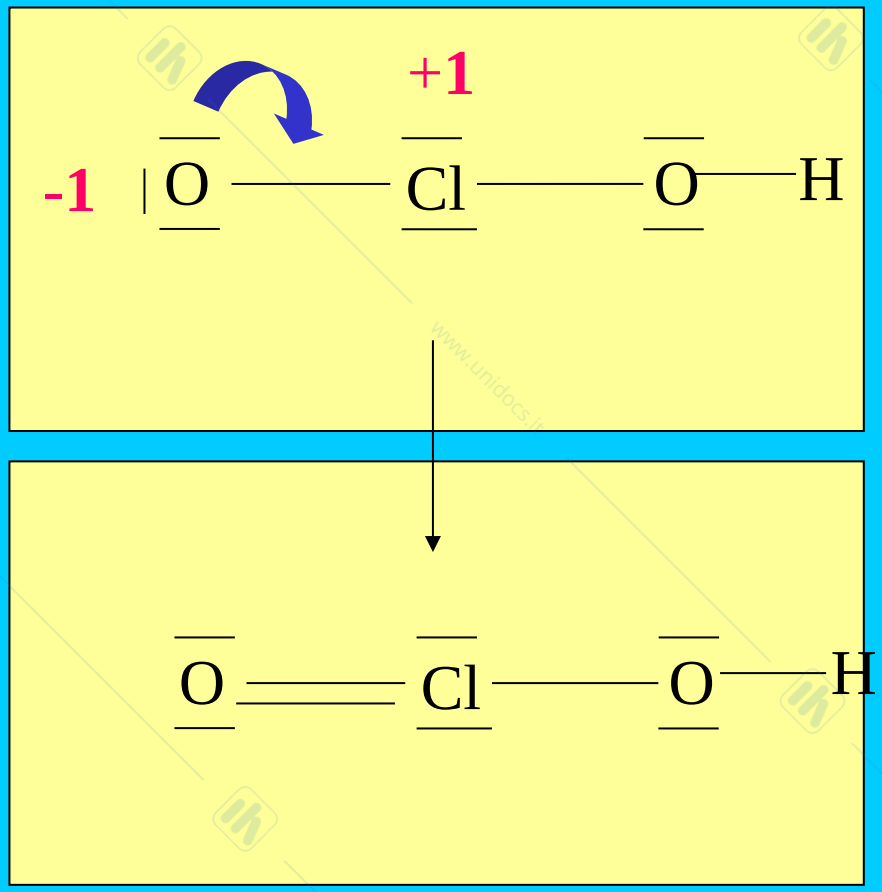
H 1 x1 = 1+

Cl 7 x 1 = 7 +

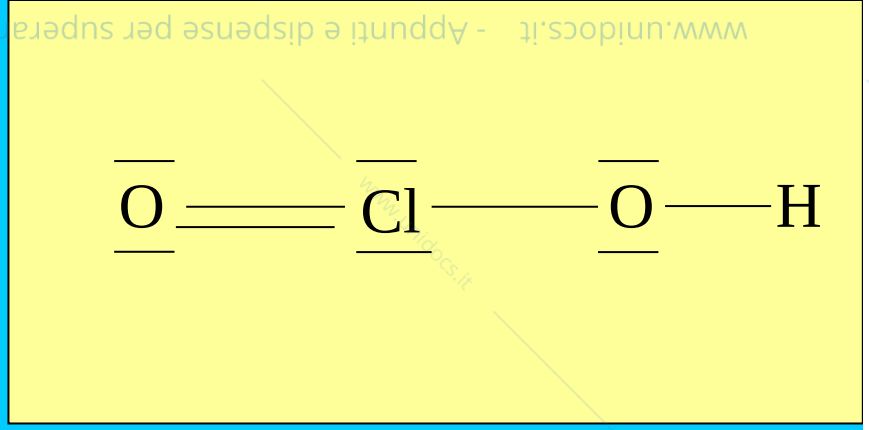
O 6 x 2 = 12

20

Doppietti = 20 : 2 = 10



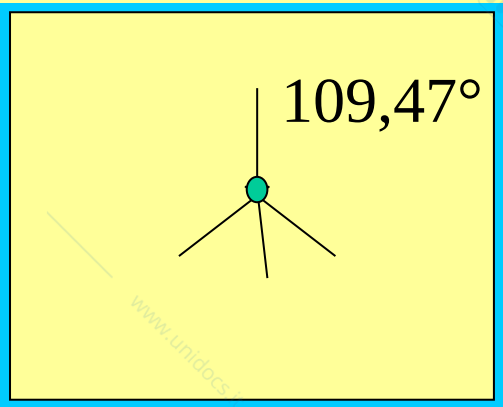
$HClO_2$

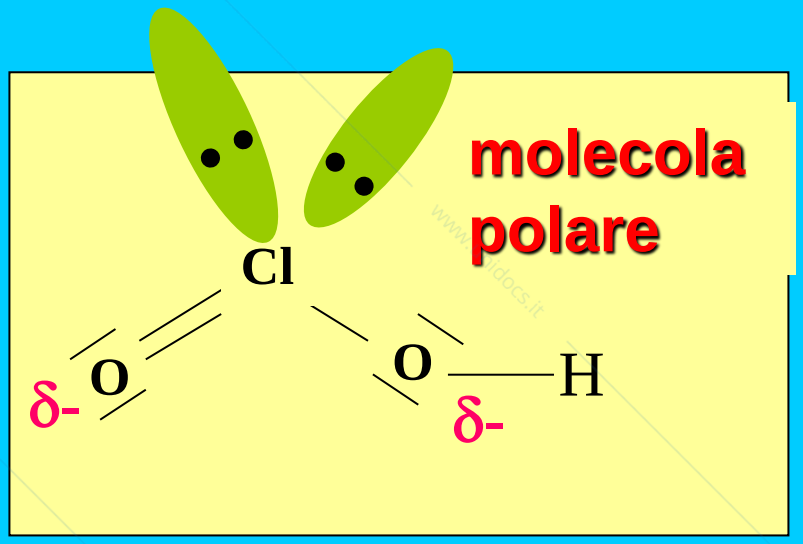


NS = 4

Disposizione delle coppie di elettroni: tetraedrica

Ibribizzazione dell'atomo centrale = sp^3





Geometria: angolata

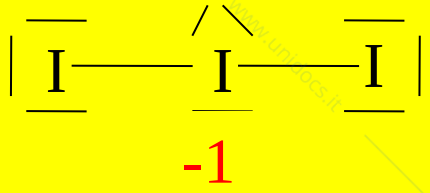
I_3^-

elettroni di valenza

I 7 x 3 = 21 +
- 1 = 1

22

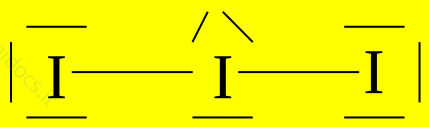
Doppietti = 22 : 2 = 11



I_3^-

Geometria

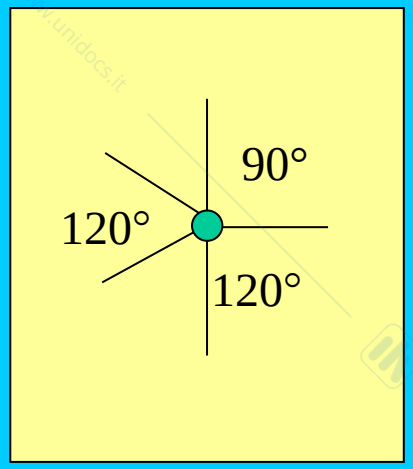
NS = 5



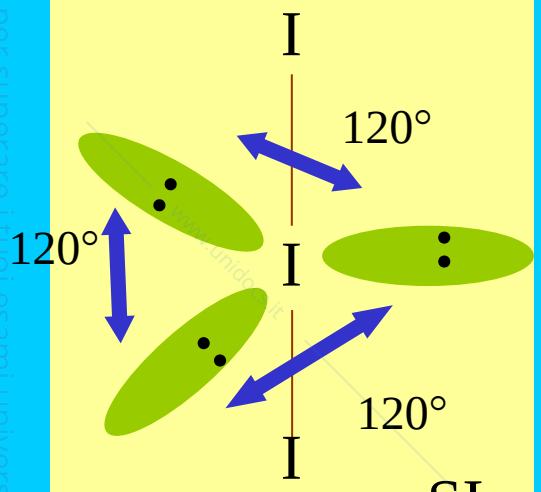
-1

Ibridizzazione di I = sp^3d

Disposizione dei doppietti: Bipiramide trigonale

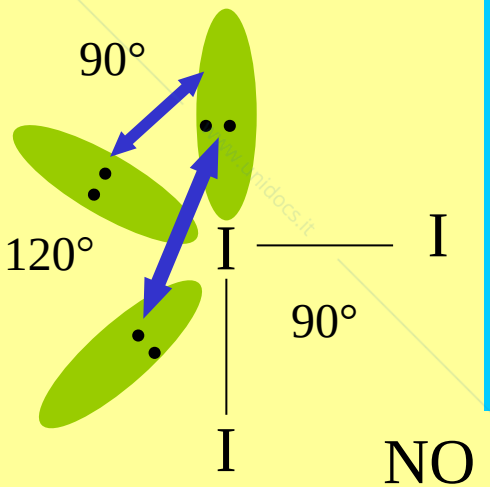


Stabile:



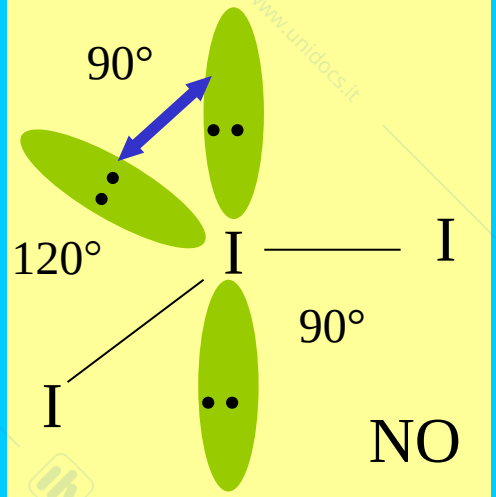
SI

Instabile:



NO

Instabile:



NO

Geometria lineare

$HPO_4^{=}$

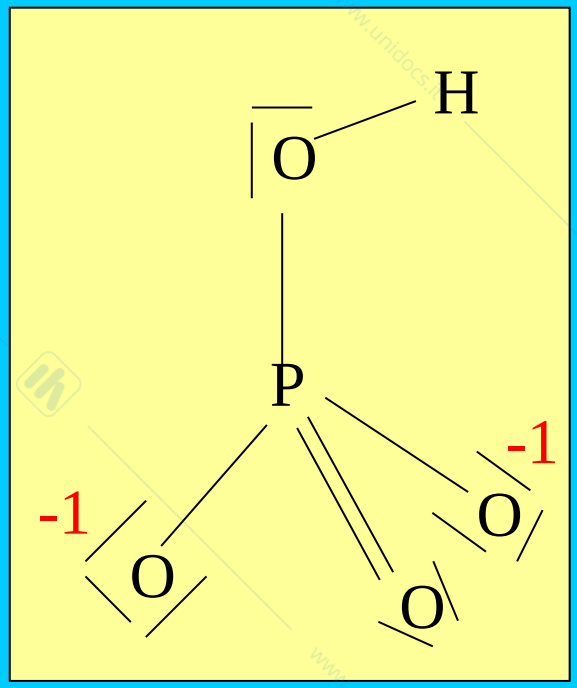
Ione idrogeno fosfato

elettroni di valenza

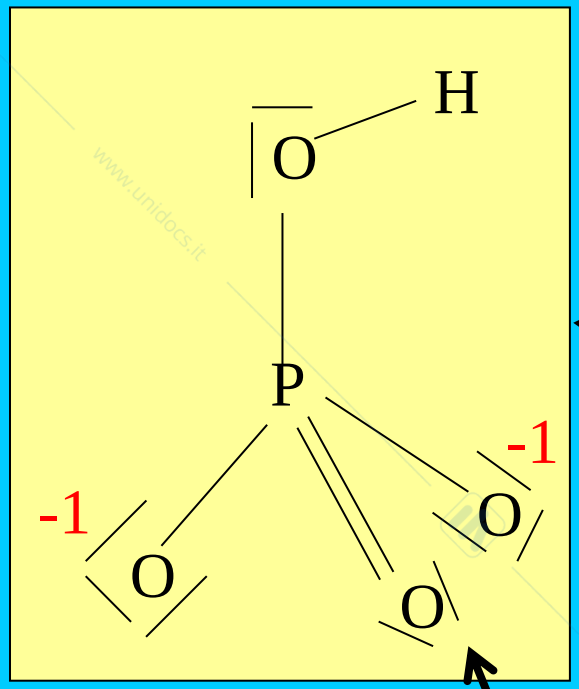
P x 1 = 5 +
4O x 6 = 24 +
H x 1 = 1
e x 2 = 2

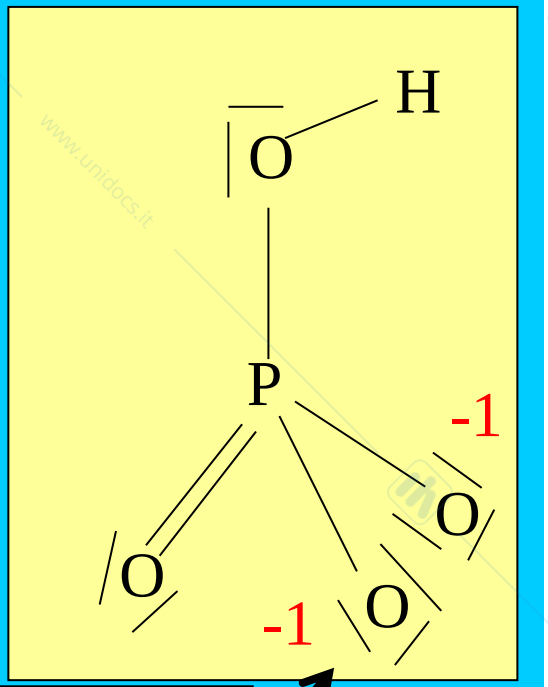
32

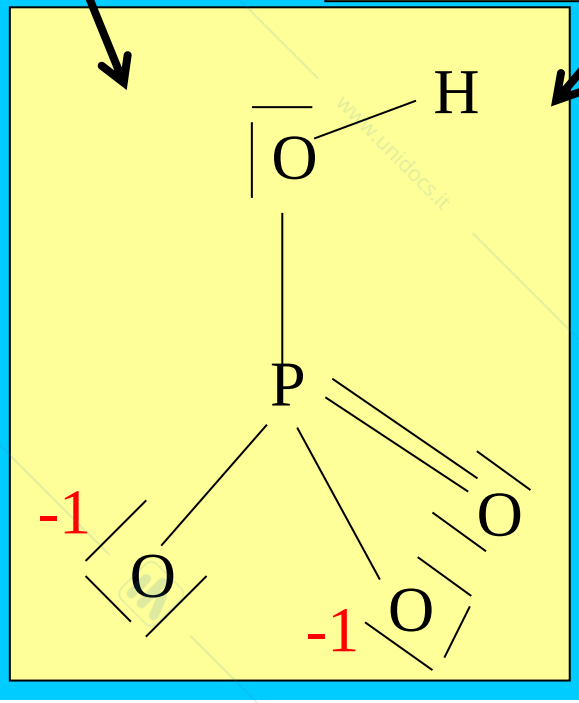
Doppietti = 32 : 2 = 16

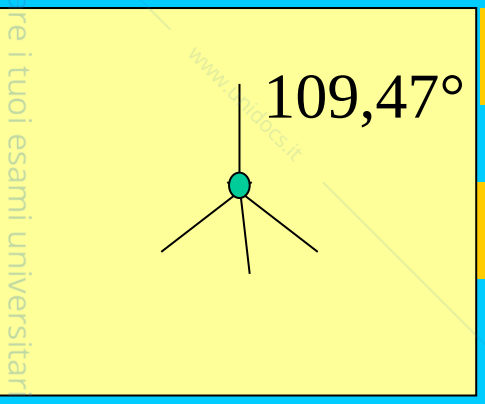


$HPO_4^{=}$









NS: 4

Ibridi sp^3

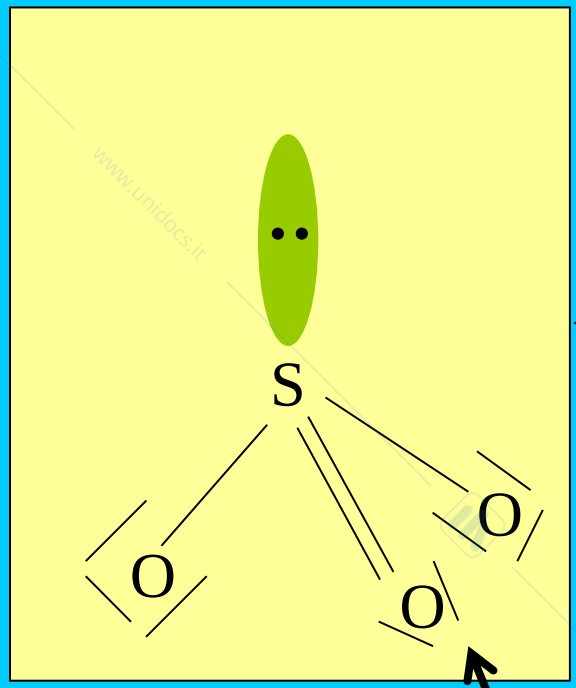
Geometria: tetraedro

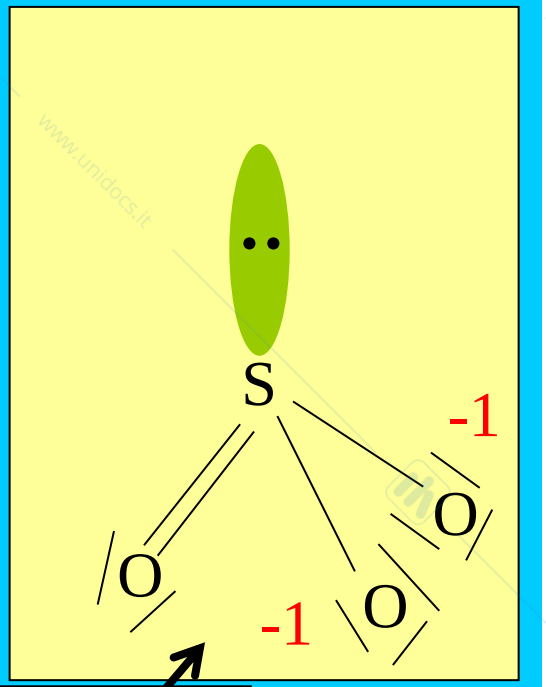
$SO_3^{=}$

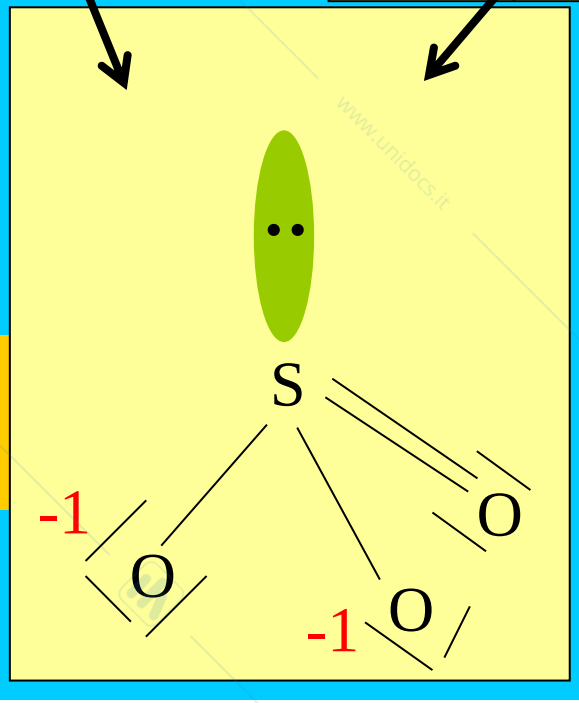
elettroni di valenza

S x 1 = 6 +
3 O x 6 = 18 +
e x 2 = 2

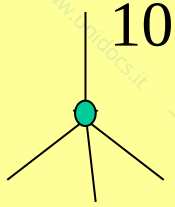
26







Doppietti = 26 : 2 = 13



NS: 4 sp^3

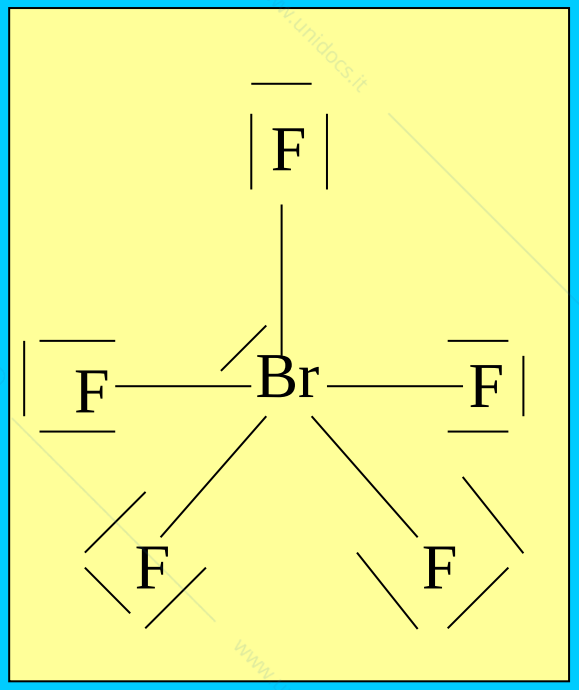
Geometria: Piramide a base triangolare

BrF_5

elettroni di valenza

Br	**7 x 1**	**=**	**7 +**
F	**7x 5**	**=**	**35 +**
			42

Doppietti = 42 : 2 = 21



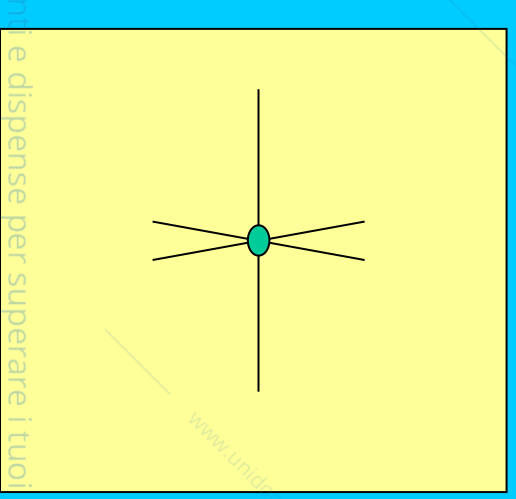
Cariche formali: Nessuna

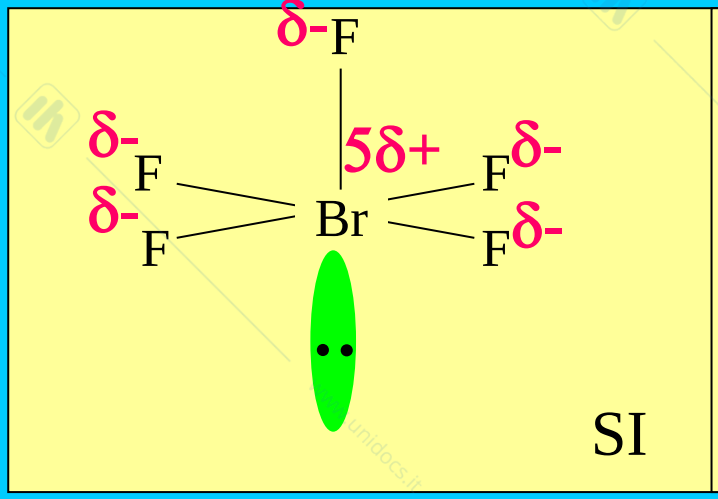
BrF_5

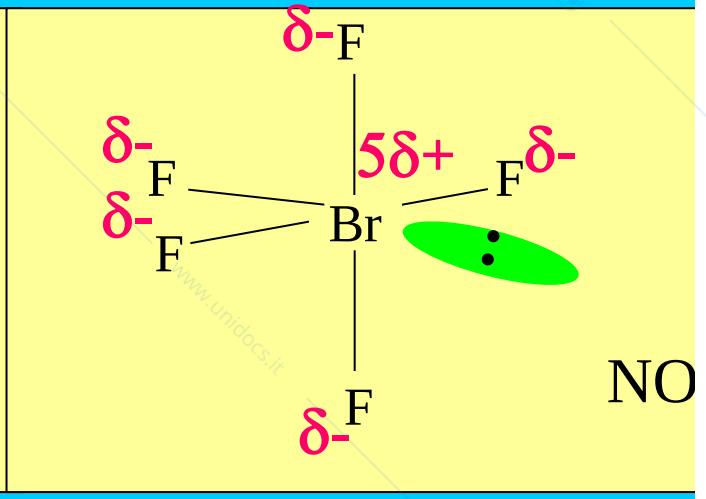
NS = 6 Disposizione dei doppietti: ottaedrica

***Geometria*: piramide a base quadrata**

Ibridizzazione: sp^3d^2







molecola polare

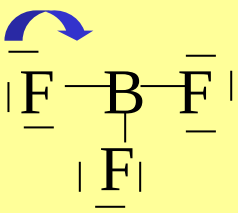
BF_3

elettroni di valenza

F 7 x 3 +

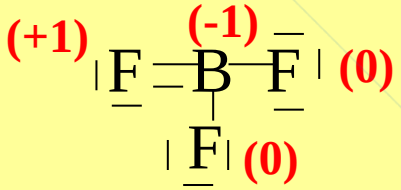
B 3

24



Il boro non ha l'ottetto completo

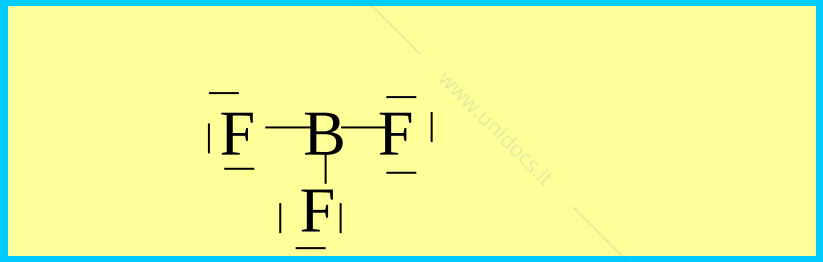
Doppietti = 24 : 2 = 12

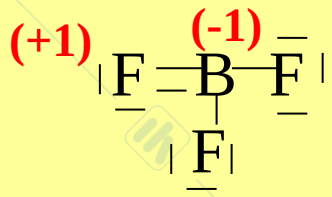


C.F. fluoro = 7 –4 –2 = +1

C.F. fluoro = 7 – 6 –1 = 0

C.F. boro = 3 – 0 –4 = -1

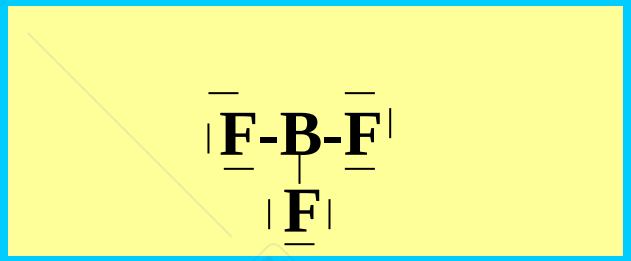




La seconda struttura rispetto alla prima introduce delle cariche formali (*regola 5*). E' pertanto sfavorita.

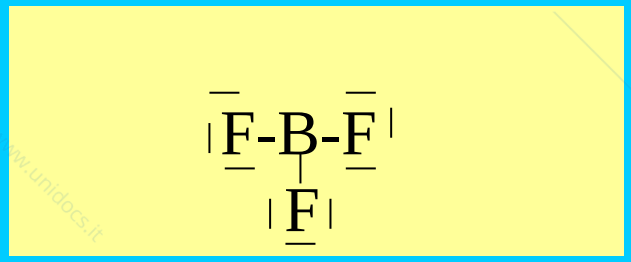
E' vistosissima l'incompatibilità di una carica formale positiva sull'atomo di fluoro che è l'elemento più elettronegativo.

BF_3

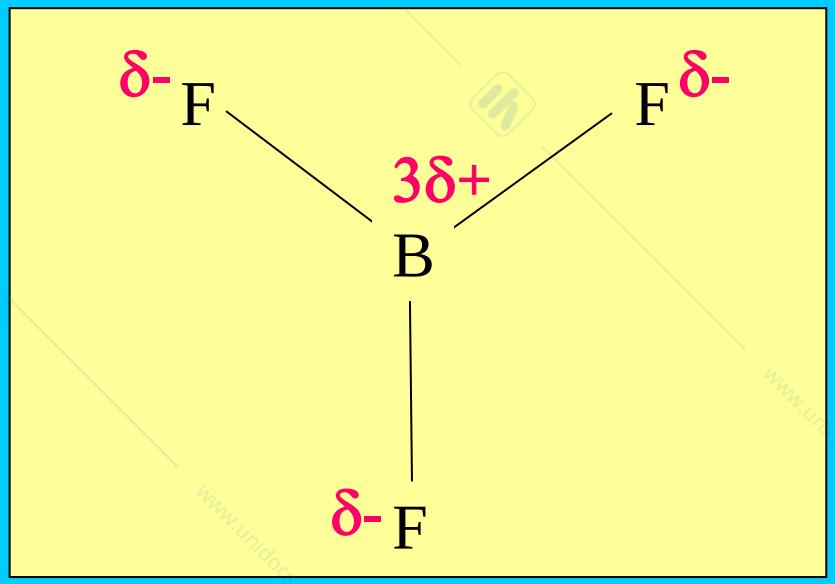


Boro (B) e Alluminio (Al) costituiscono delle eccezioni e possono avere meno di 8 elettroni.

BF_3



NS = 3



Molecola triangolare

molecola apolare

H_2O

H-$\underline{\overline{O}}$-H

elettroni di valenza

H 1 x 2 +

O 6

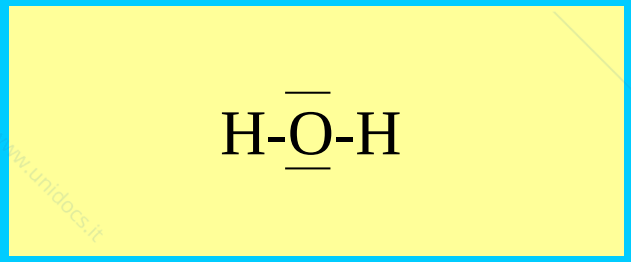
8

Doppietti = 8 : 2 = 4

C.F. ossigeno = 6 – 4 –2 = 0

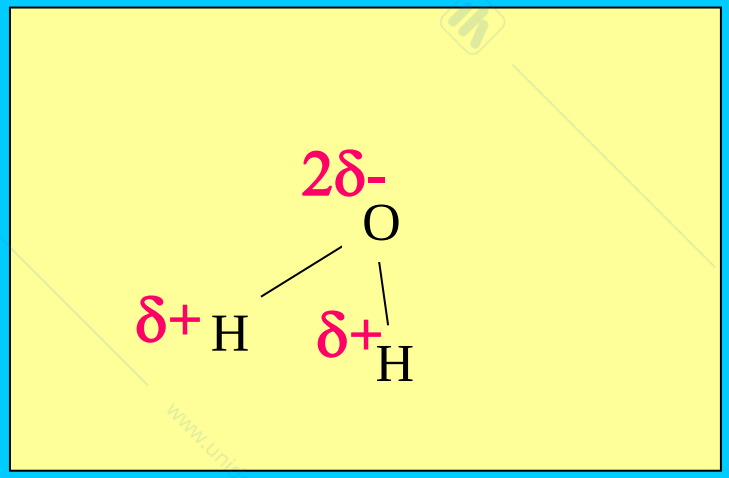
C.F. idrogeno = 1 – 0 –1 = 0

H_2O



NS = 4

Ibridizzazione degli orbitali: sp^3



molecola angolare

molecola polare

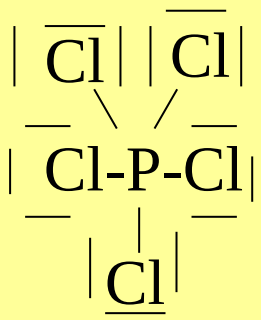
PCl_5

elettroni di valenza

Cl 7 x 5 +

P 5

40

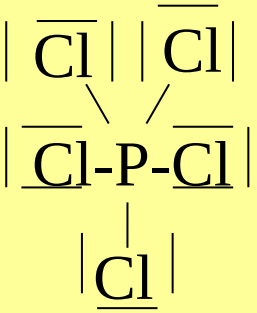


Doppietti = 40 : 2 = 20

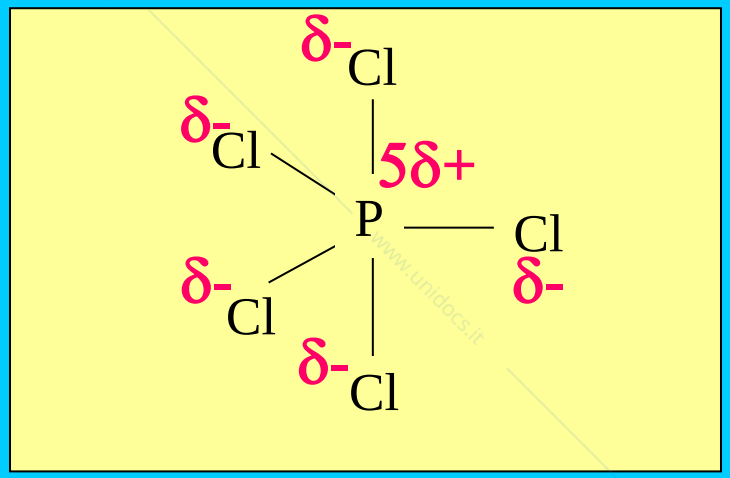
C.F. cloro = 7 – 6 –1 = 0

C.F. fosforo = 5 –0 –5 = 0

PCl_5



NS = 5
Ibridizzazione di P: sp^3d



molecola bipiramidale a base triangolare

molecola apolare

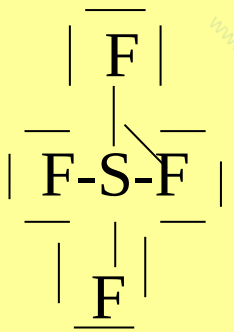
SF_4

elettroni di valenza

F 7 x 4 +

S 6

34

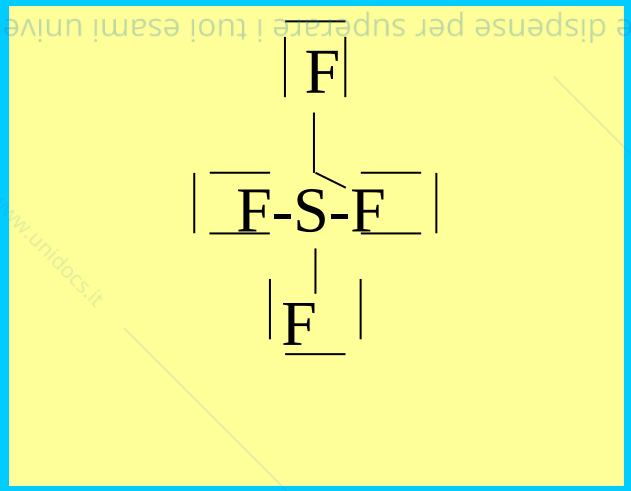


Doppietti = 34 : 2 = 17

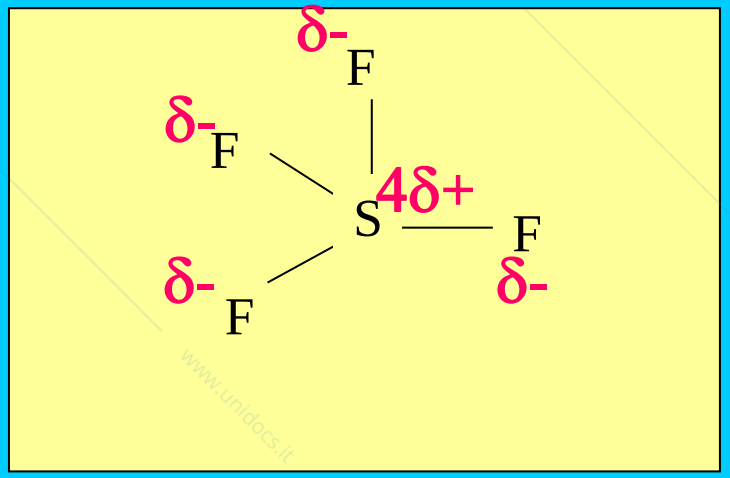
C.F. fluoro = 7 – 6 –1 = 0

C.F. zolfo = 6 – 2 –4 = 0

SF_4



NS = 5

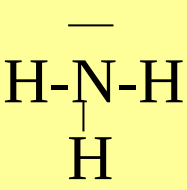


Ibridizzazione di S = sp3d

molecola piramidale a base triangolare

molecola polare

NH_3



elettroni di valenza

H 1 x 3 +

N 5

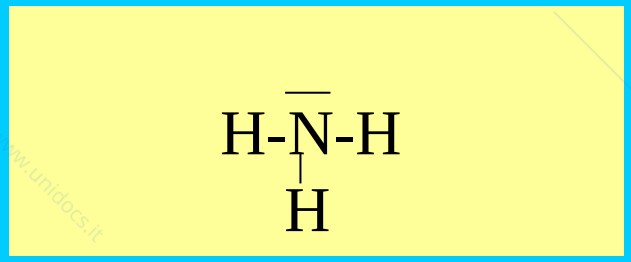
8

Doppietti = 8 : 2 = 4

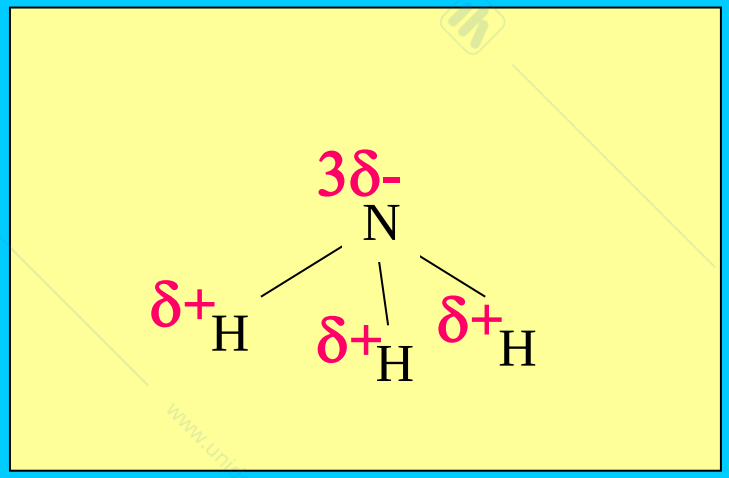
C.F. azoto = 5 – 2 –3 = 0

C.F. idrogeno = 1 – 1 = 0

NH_3



NS = 4
Ibridizzazione di N: sp^3



molecola piramidale a base triangolare

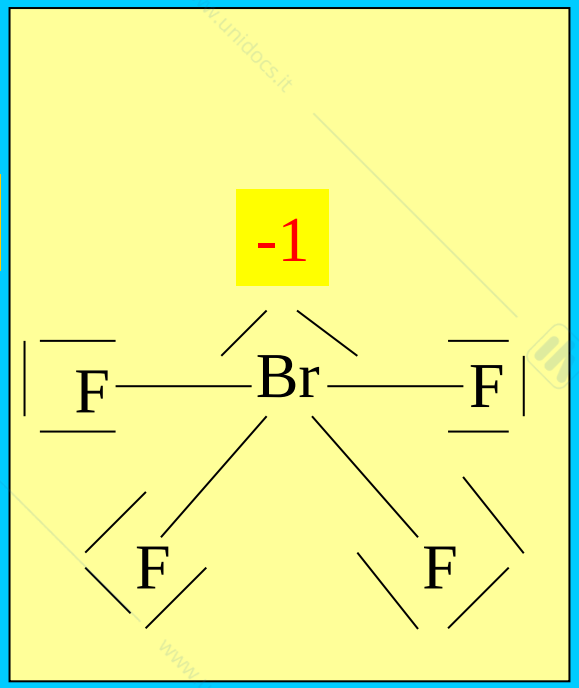
molecola polare

BrF_4^-

elettroni di valenza

Br	**7 x 1**	**=**	**7 +**
F	**7x 4**	**=**	**28 +**
e			**1=**
			36

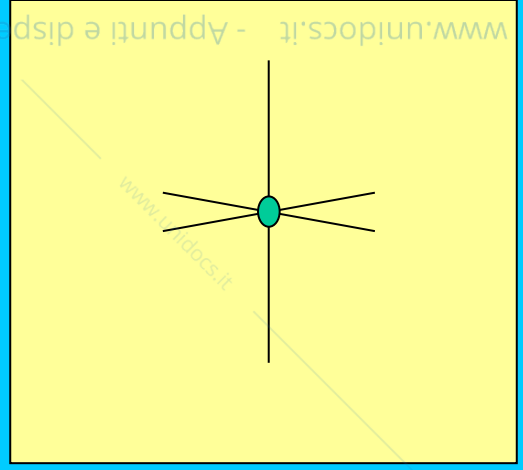
Cariche formali:



Doppietti = 36 : 2 = 18

BrF_4^-

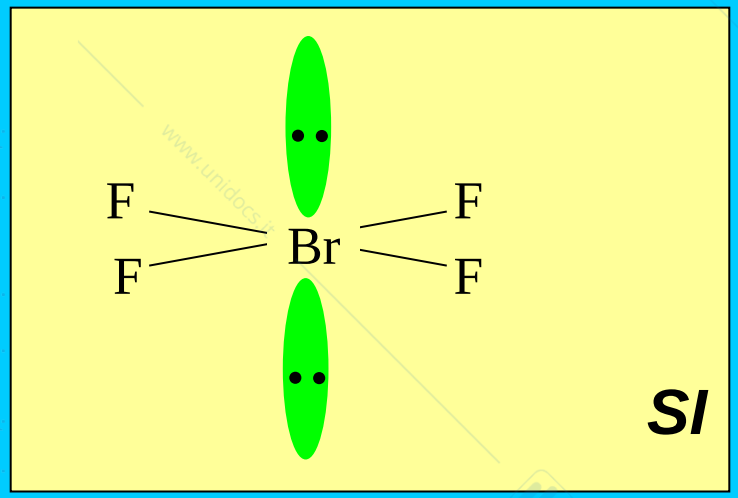
NS = 6 Disposizione dei doppietti: ottaedrica

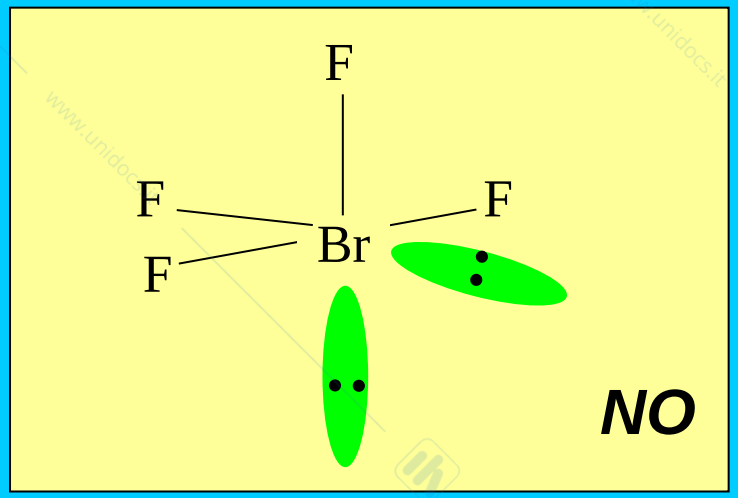


Ibridizzazione di Br: sp^3d^2

***Geometria*: planare quadrato**

molecola ionica





$HClO_2$

Come in tutti gli ossiacidi di formula HXO(n) l'idrogeno è sempre legato all'ossigeno

elettroni di valenza

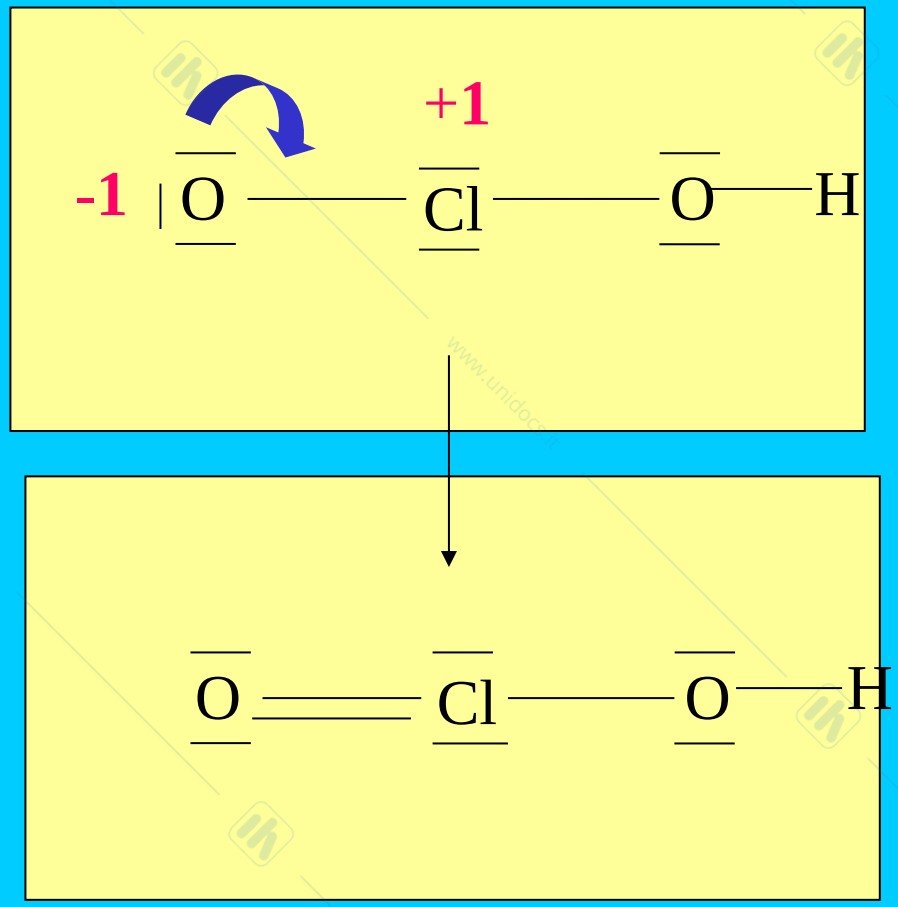
H 1 x1 = 1+

Cl 7 x 1 = 7 +

O 6 x 2 = 12

20

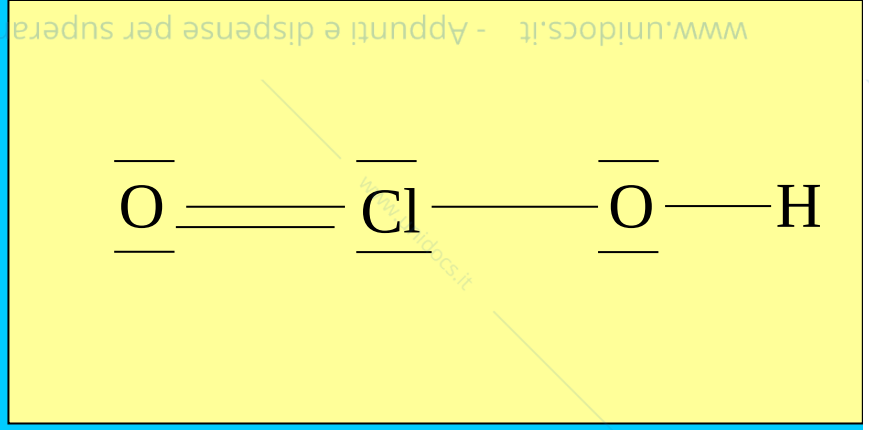
Doppietti = 20 : 2 = 10



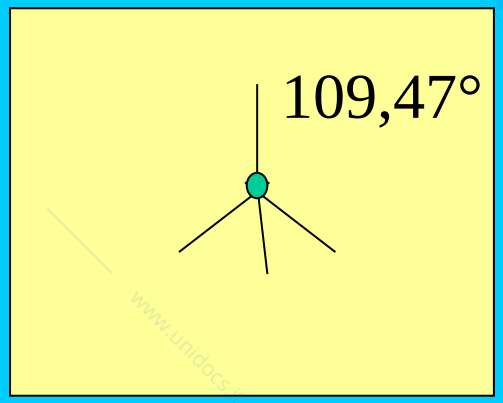
$HClO_2$

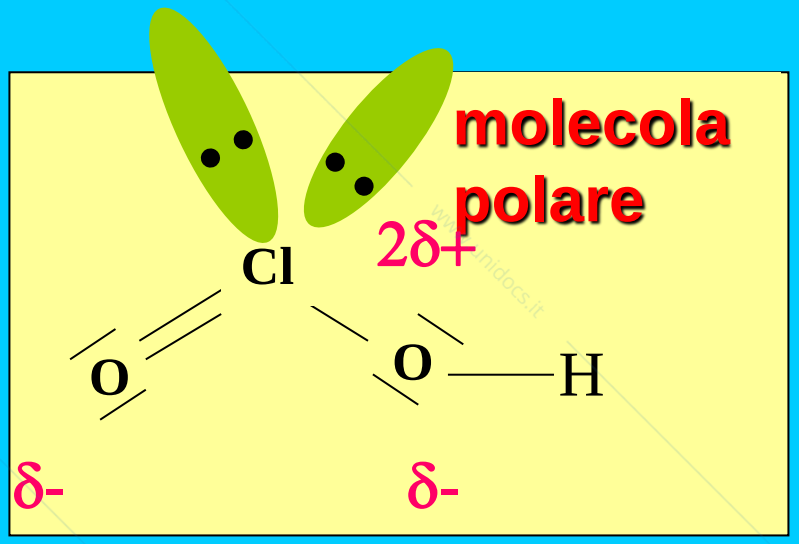
NS = 4

Ibribizzazione
Di Cl = sp^3



Disposizione delle coppie di elettroni del Cl: tetraedrica

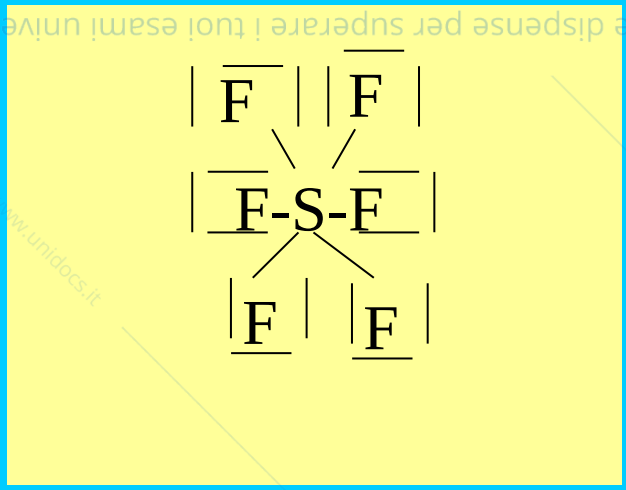


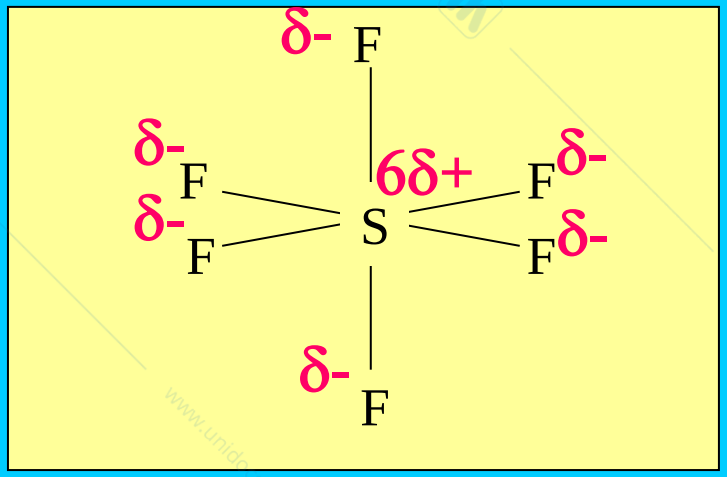


Geometria: angolata

SF_6

NS = 6





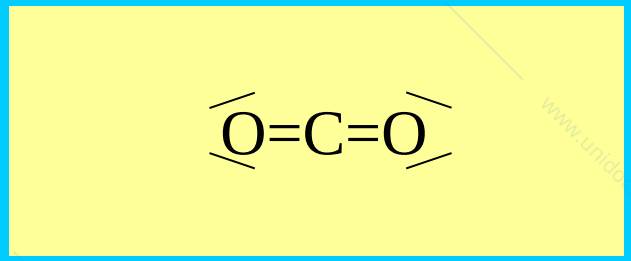
molecola ottaedrica

molecola apolare

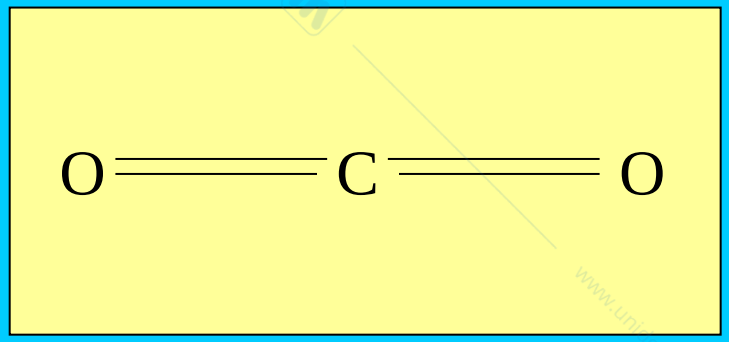
CO_2

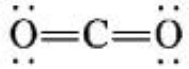
NS = 2

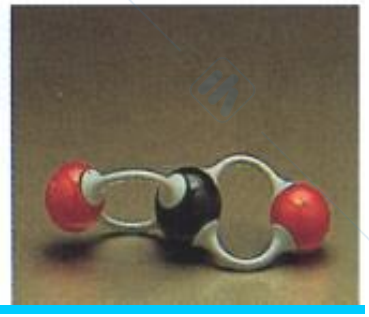
Ibridizzazione di C: sp



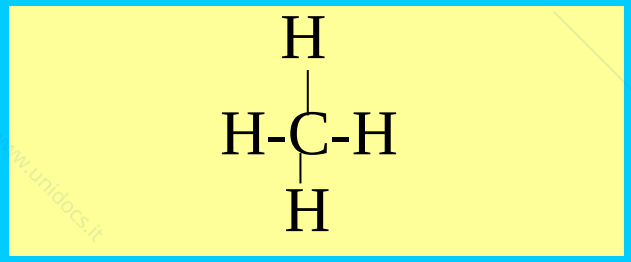
molecola lineare



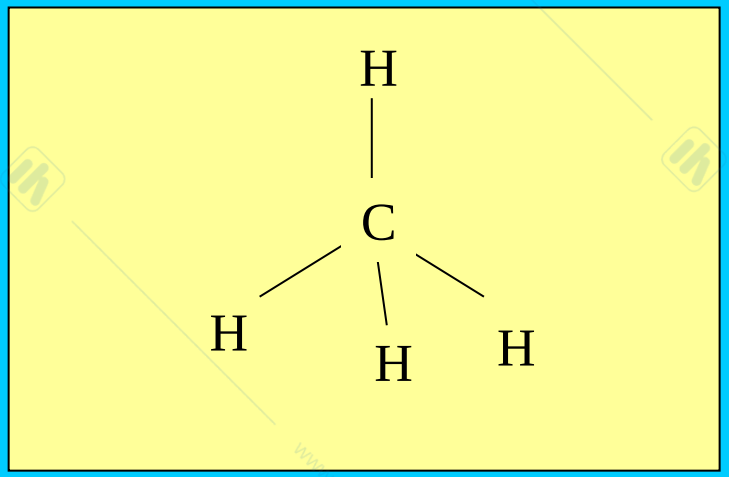
Molecola	*NS*	Geometria	Schizzo in prospettiva	Modello a sfere e bastoncini
CO_2	2	Lineare		



CH_4

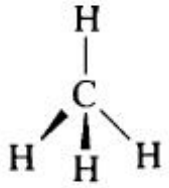


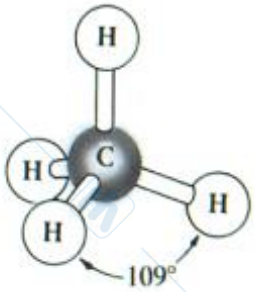
NS = 4
Ibridizzazione di C: sp^3



molecola tetraedrica

CH_4	4	Tetraedrica



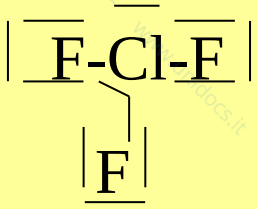


ClF_3

elettroni di valenza

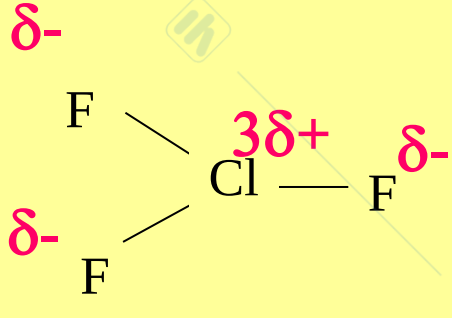
Cl	**1 x 7**	**=**	**7 +**
F	**3 x 7**	**=**	**21 +**
			28

Doppietti 28 : 2 = 14



NS = 5

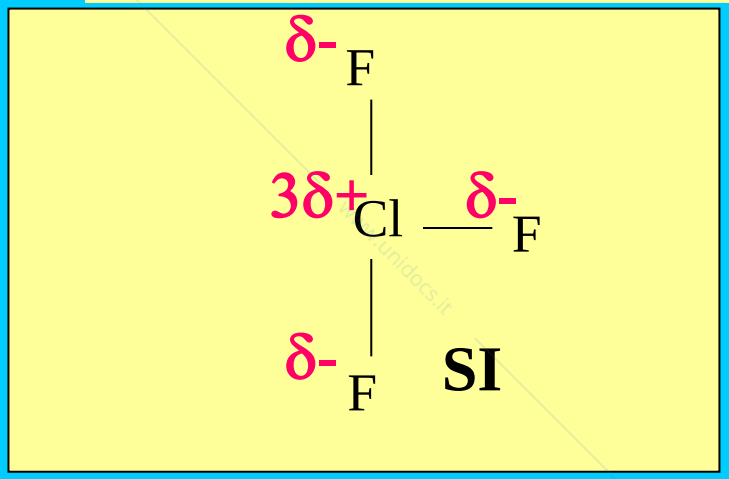
Ibridizzazione di Cl: sp^3d



NO

molecola triangolare

molecola apolare



SI

molecola a T

molecola polare