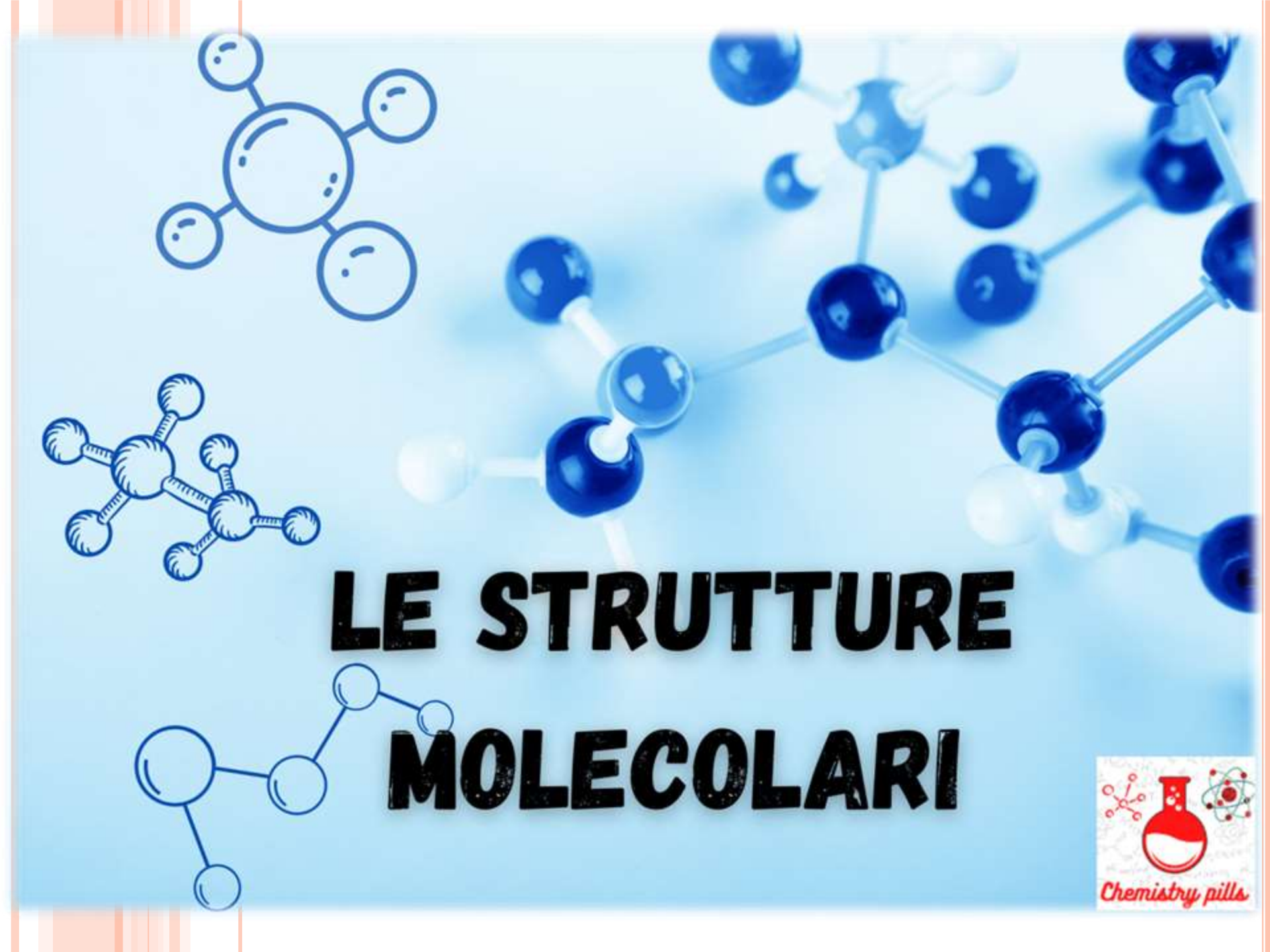

LE STRUTTURE
MOLECOLARI
Chemistry pills

MA CHE FORMA HANNO LE MOLECOLE???

STRUTTURE DI LEWIS

↓

V.S.E.P.R.

↓

ORBITALI IBRIDI

TEORIE SEMPLIFICATE SULLA MECCANICA QUANTISTICA

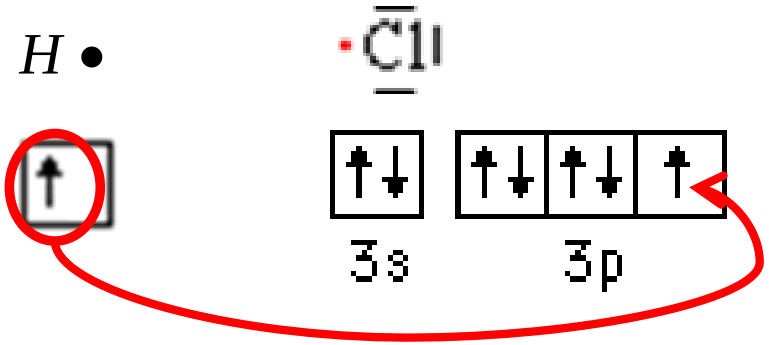
TEORIA DEL LEGAME DI VALENZA (VB)

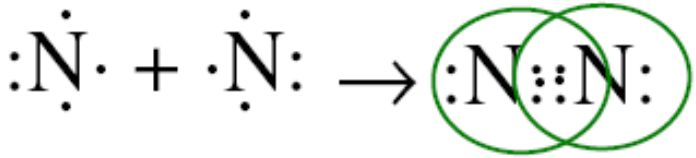
TEORIA DEGLI ORBITALI MOLECOLARI (MO)

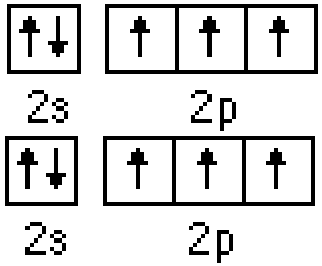
STRUTTURE DI LEWIS

Gli elettroni di un elemento chimico partecipano alla formazione dei legami e che determinano la sua reattività sono gli elettroni esterni, detti di valenza.

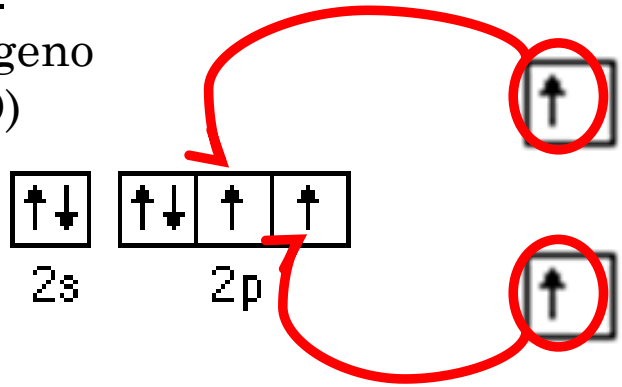
H-Cl

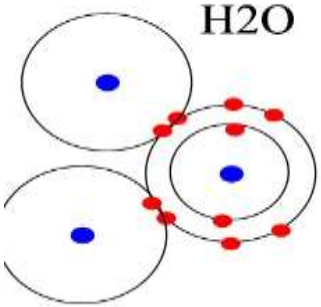






Ossigeno (O)





Formule di Lewis per…
…SPECIE POLIATOMICHE

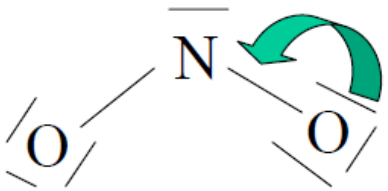
1) Contare gli elettroni di valenza (le cariche!!)
2) Individuare l'atomo centrale (di solito è il meno elettronegativo, no H!)
3) Scrivere lo scheletro σ
4) Distribuire gli elettroni restanti sugli atomi (prima su quelli periferici)
5) Tutti gli atomi (diversi da H) hanno 8 elettroni?
6) Eventualmente usare i lone pair per fare legami doppi
7) Controllare le cariche formali (cf)

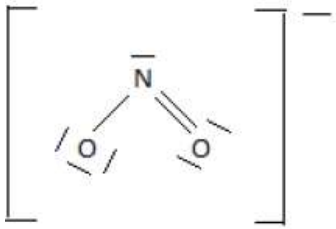
N.B. non sempre 8 elettroni

- Specie elettron povere <8
  - BCl_3
- Specie elettron ricchi >8
  - PF_5 SF_6 SO_4^{2-} n>3

IONE NITRITO

$$NO_2^- \qquad 5+6(2)+1=\frac{18}{2}=9 coppie$$



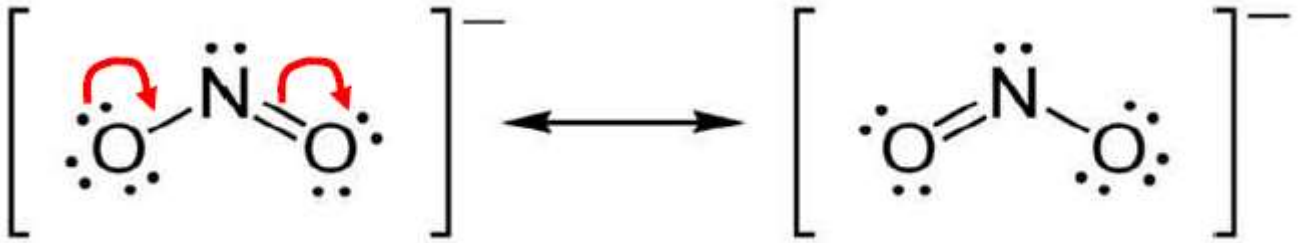


Ione nitrito

- N=O 115 pm
- N-O 136 pm

- nello ione nitrito la distanza N---O è 124

RISONANZA



LA FORMA DELLE MOLECOLE: LA TEORIA VSEPR

Molte proprietà delle sostanze dipendono non solo dalla composizione chimica delle molecole, ma anche dalla loro forma. La forma complessiva di una molecola dipende dalle interazioni tra le forze repulsive e attrattive degli elettroni esterni (sia quelli di legame che i doppietti liberi), che determinano sia la lunghezza sia l'angolo di legame.

La teoria VSEPR (Valence Shell Electron-Pair Repulsion, teoria della repulsione delle coppie di elettroni del "guscio" di valenza) consente di ricavare la geometria, ossia la forma delle molecole, a partire dalle rappresentazioni delle formule di struttura di Lewis, partendo dal presupposto che le coppie di elettroni esterni tendono a respingersi reciprocamente. Secondo questa teoria, gli angoli di legame che si vengono a formare tra 3 atomi di una molecola dipendono dal numero di doppietti elettronici presenti intorno all'atomo centrale (sia condivisi, ossia impegnati nei legami, sia liberi), che, per la loro azione repulsiva, tendono a disporsi reciprocamente il più lontano possibile

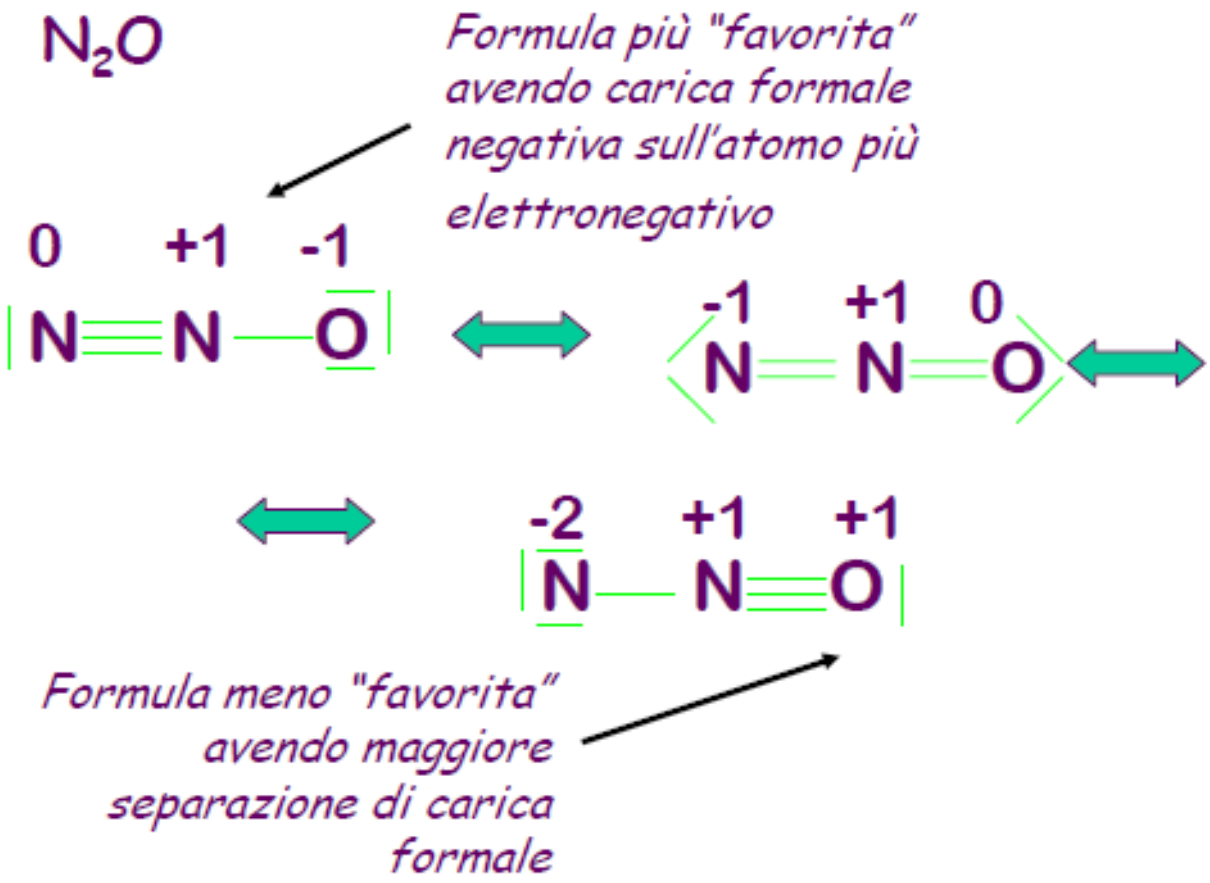
Cariche formali

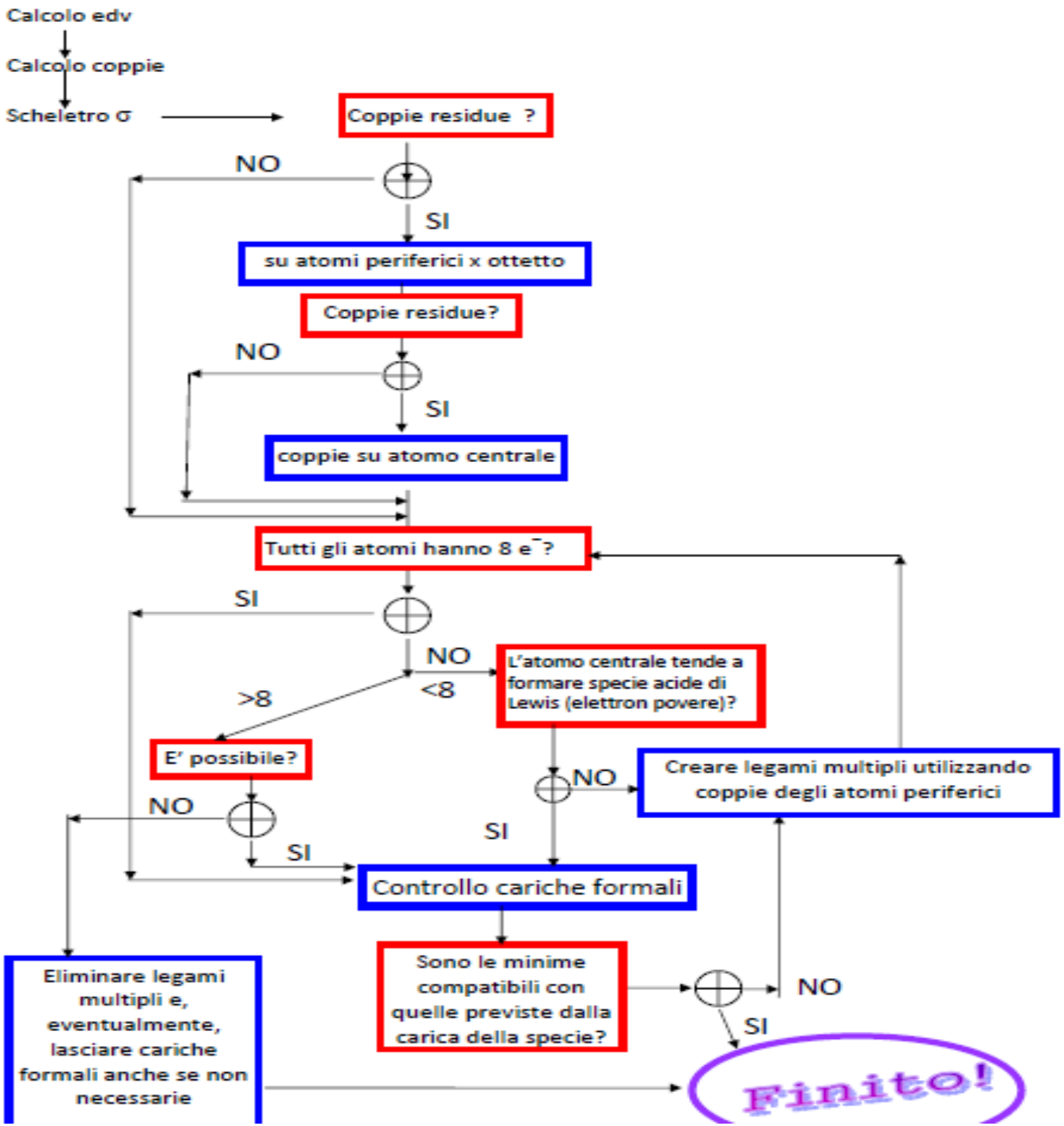
$$cf = V - N - B$$

V = e- di valenza

N = numero di e- di valenza di non legame dell'atomo nella molecola

B = numero totale dei legami (coppie di e-)




Calcolo edv
Calcolo coppie
Scheletro σ
Coppie residue ?
NO
SI
su atomi periferici x ottetto
Coppie residue?
NO
SI
coppie su atomo centrale
Tutti gli atomi hanno 8 e⁻?
SI
NO
<8
L'atomo centrale tende a formare specie acide di Lewis (elettron povere)?
>8
E' possibile?
NO
SI
NO
Creare legami multipli utilizzando coppie degli atomi periferici
SI
Controllo cariche formali
Sono le minime compatibili con quelle previste dalla carica della specie?
NO
SI
Eliminare legami multipli e, eventualmente, lasciare cariche formali anche se non necessarie
Finito!

1 coppia di $e^- \leftrightarrow$ 1 palloncino

Lineare

Trigonale planare

Tetraedrica

Trigonale bipiramidale

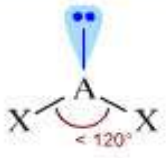
Ottaedrica

Charles D. Winters

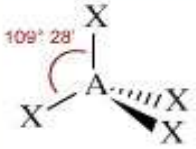
FIGURA 8.4 Modelli a palloncino della geometria delle coppie elettroniche per sistemi da due a sei coppie elettroniche. Quando due, tre, quattro, cinque o sei palloncini di forma e grandezza simili sono legati l'uno all'altro in un unico punto centrale, essi assumono le geometrie che sono rappresentate sotto. Le figure rappresentano le previsioni della teoria VSEPR.

AX_2
Linear

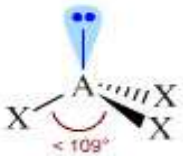
AX_3
Trigonal planar



AX_2E_1
Bent or Angular

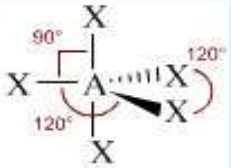


AX_4
Tetrahedral

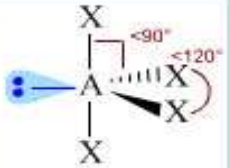


AX_3E_1
Trigonal pyramidal

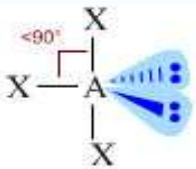
AX_2E_2
Bent or Angular



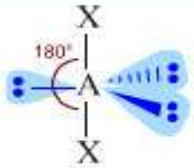
AX_5
Trigonal bipyramidal



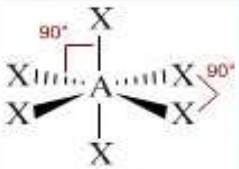
AX_4E_1
Sawhorse or Seesaw



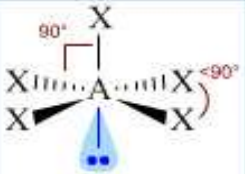
AX_3E_2
T-shape



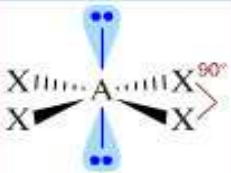
AX_2E_3
Linear



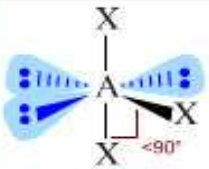
AX_6
Octahedral



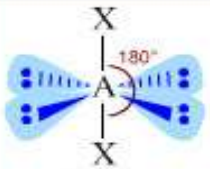
AX_5E_1
Square pyramidal



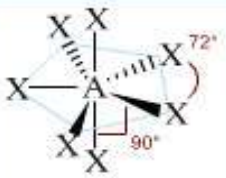
AX_4E_2
Square planar



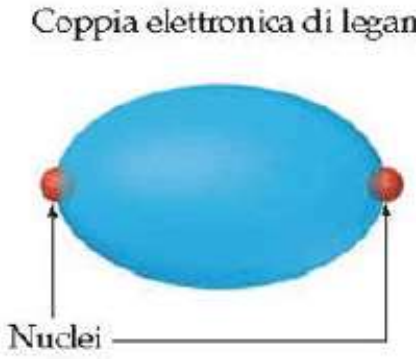
AX_3E_3
T-shape



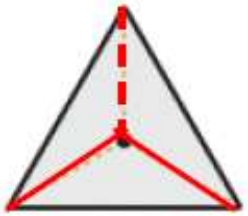
AX_2E_4
Linear



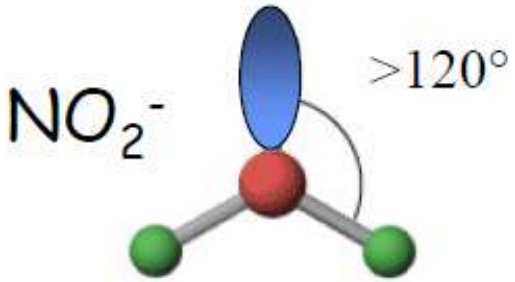
AX_7
Pentagonal bipyramidal



- deformazione della geometria ideale prevista per quel n.ro di coppie



▲ **Figura 9.7 Dimensioni relative dei domini elettronici di legame e non legame.**



nella notazione AB_mE_n (o AX_mE_n)

AB_2E

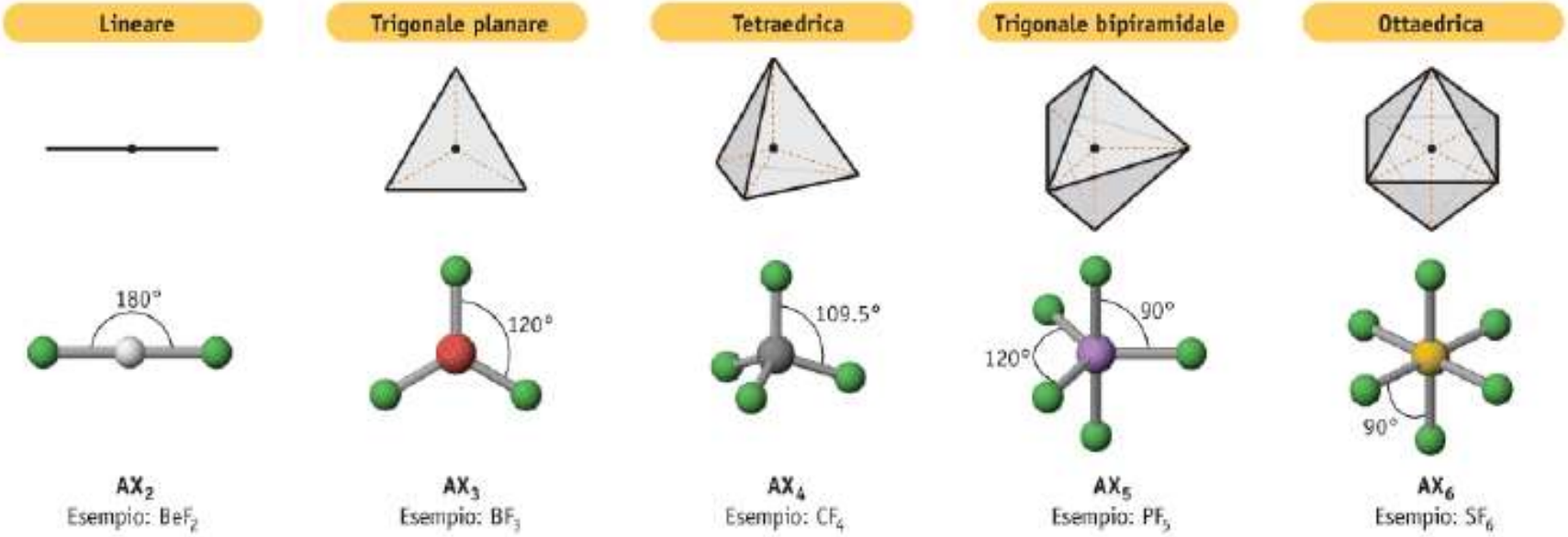


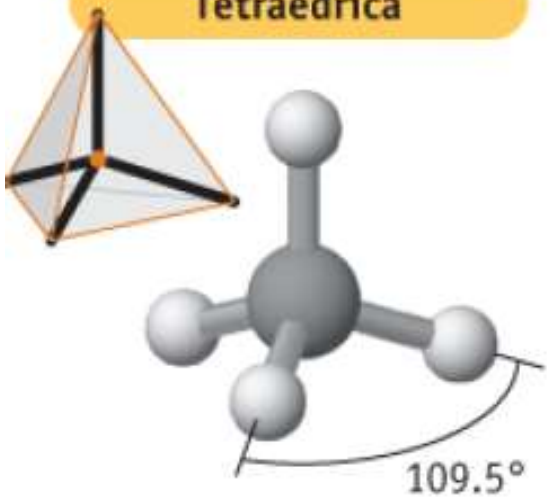
FIGURA 8.5 Varie geometrie previste dal modello VSEPR. Geometrie previste dalla teoria VSEPR che contengono solo legami covalenti singoli attorno all'atomo centrale.

Kotz, Treichel, Townsend
Chimica
EdiSES

QUATTRO COPPIE ELETTRONICHE

Geometria delle coppie = tetraedrica

Tetraedrica



Metano, CH_4

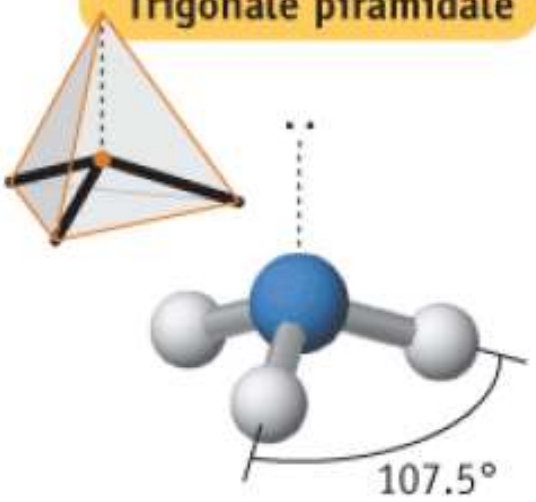
4 coppie di legame

nessuna coppia solitaria

(a)

AB_4

Trigonale piramidale



Ammoniaca, NH_3

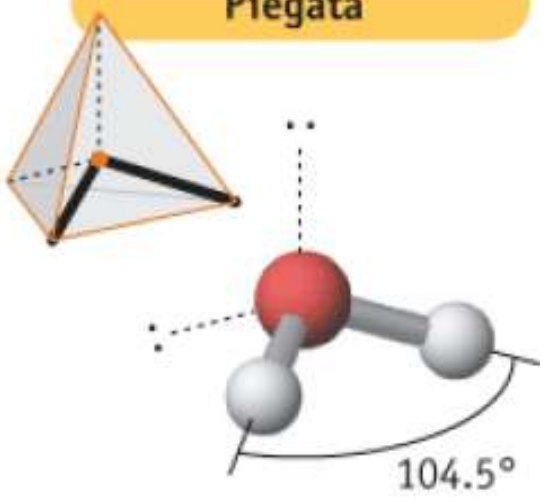
3 coppie di legame

1 coppia solitaria

(b)

AB_3E

Piegata



Acqua, H_2O

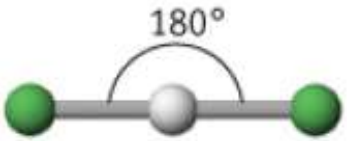
2 coppie di legame

2 coppie solitarie

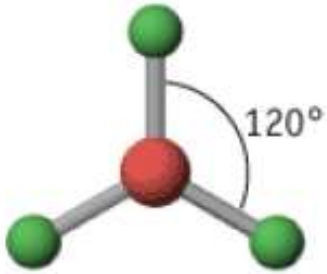
(c)

AB_2E_2

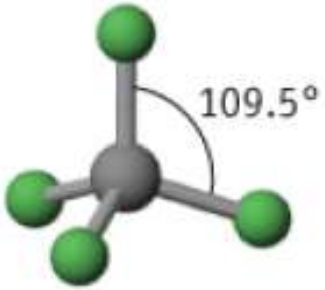
GEOMETRIA DELLE COPPIE



LINEARE AX_2 BeF_2

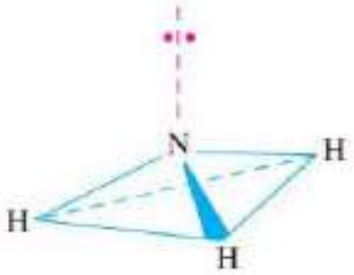


TRIGONALE PLANARE AX_3 BeF_3



TETRAEDRICA AX_4 CH_4

GEOMETRIA DELLA MOLECOLA

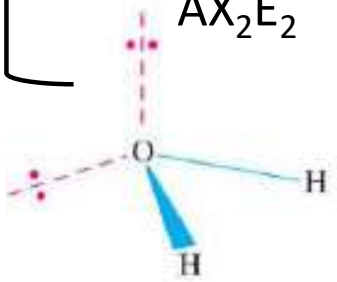


TRIGONALE PIRAMIDALE

AX_3E NH_3

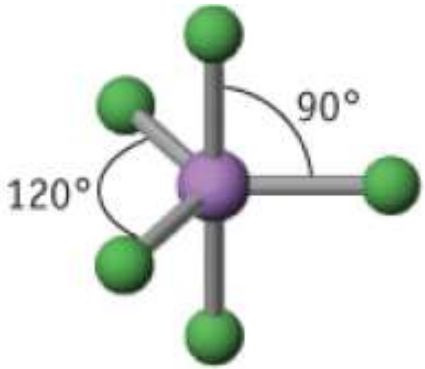
PIEGATA

AX_2E_2 H_2O



GEOMETRIA DELLE COPPIE

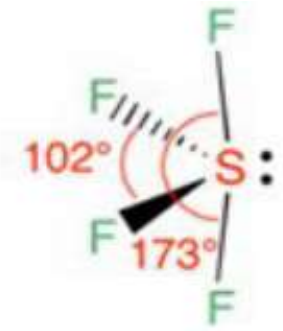
GEOMETRIA DELLA MOLECOLA



TRIGONALE BIPIRAMIDALE

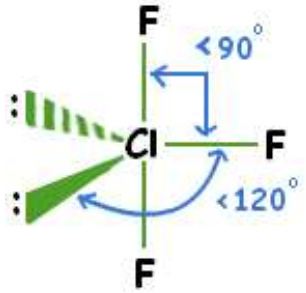
AX_5

PF_5



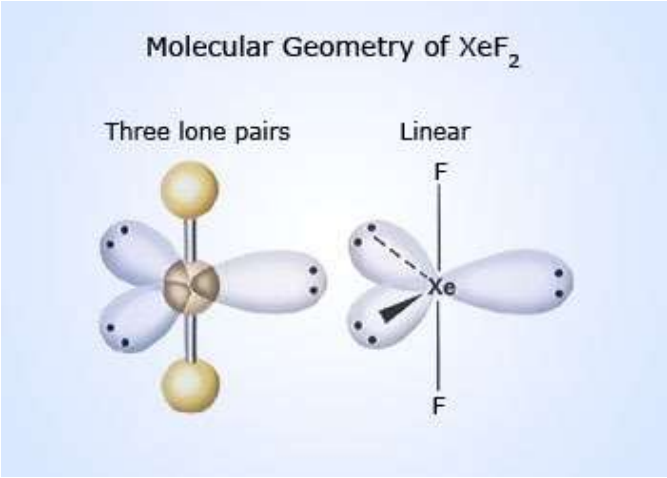
ALTALENA

AX_4E SF_4



A «T»

AX_3E_2 ClF_3

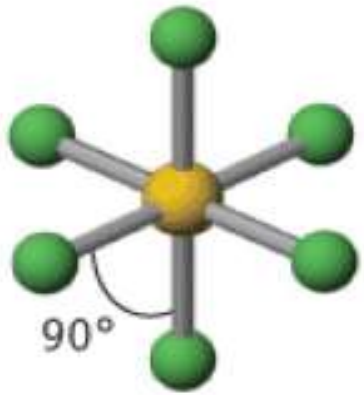


LINEARE

AX_2E_3 XeF_2

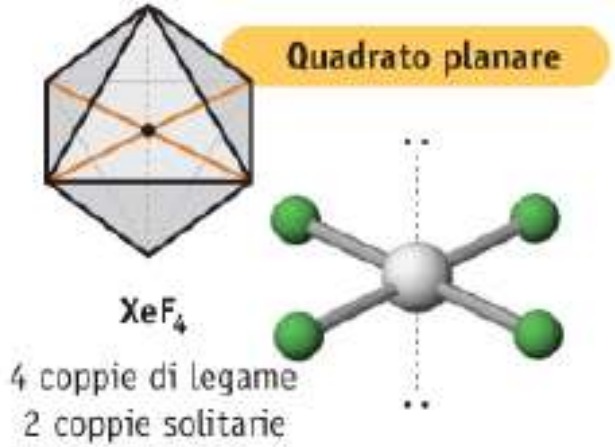
GEOMETRIA DELLE COPPIE

GEOMETRIA DELLA MOLECOLA



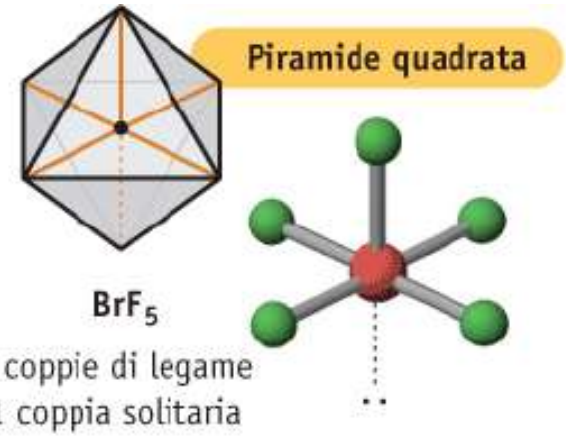
AX_6

Esempio: SF_6



QUADRATO PLANARE

AX_4E_2 XeF_4



PIRAMIDE QUADRATA

AX_5E BrF_5

ESERCIZIO 1.

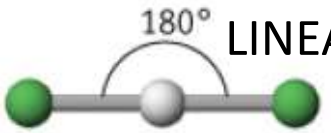
$$cf = V - N - B$$

V = e- di valenza
N = numero di e- di valenza di non legame dell'atomo nella molecola
B = numero totale dei legami (coppie di e-)

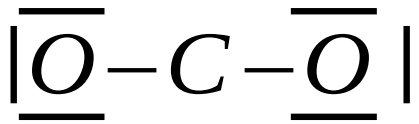
DIOSSIDO DI CARBONIO
ANIDRIDE CARBONICA

CO_2

$$4 + 6(2) = \frac{16}{2} = 8 coppie$$

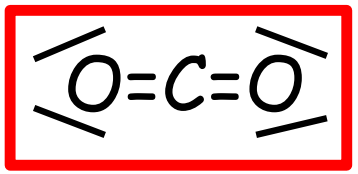


LINEARE

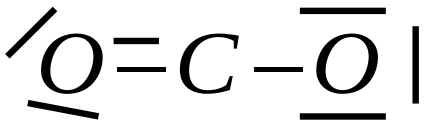


Tutti 8 elettroni?
NO!!!

6-4-2=0 4-0-4=0



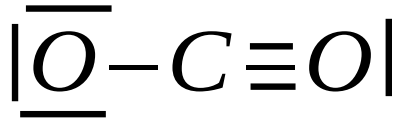
6-4-2=0



6-4-2=0 4-1-3=0

6-6-1=-1

4-0-4=0

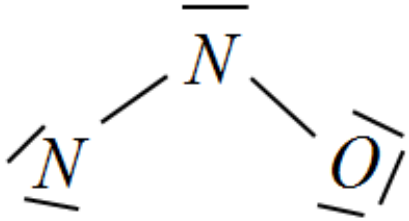


6-6-1=-1 6-2-3=+1

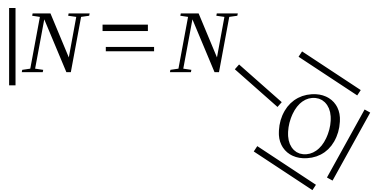
ESERCIZIO 2.

MONOSSIDO DI DIAZOTO

$$N_2O \qquad 5(2)+6=\frac{16}{2}=8 coppie$$



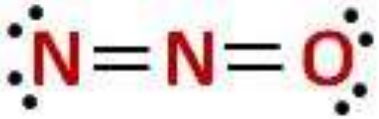
Tutti 8 elettroni?
NO!!!



Tutti 8 elettroni?
NO!!!

5-0-4=+1 6-4-2=0

5-4-2=-1



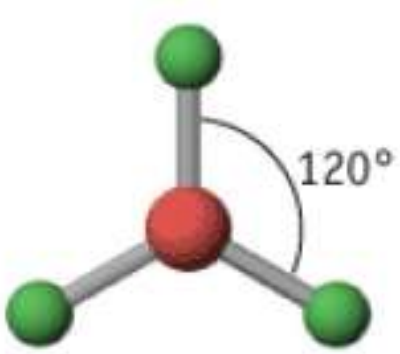
5-2-3=0 5-0-4=+1

6-6-1=-1

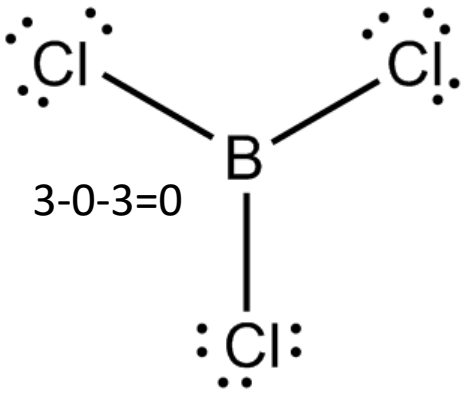
ESERCIZIO 3.

TRICLORURO DI BORO

$$BCl_3 \qquad 3+7(3)=\frac{24}{2}=12 coppie$$



7-6-1=0

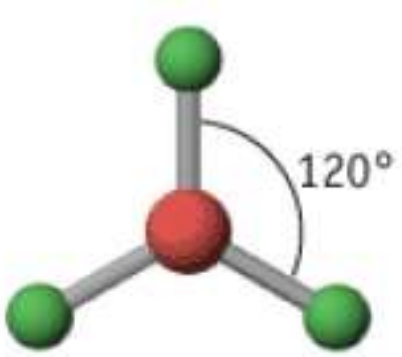


3-0-3=0

B specie e- povere

ACIDI DI LEWIS

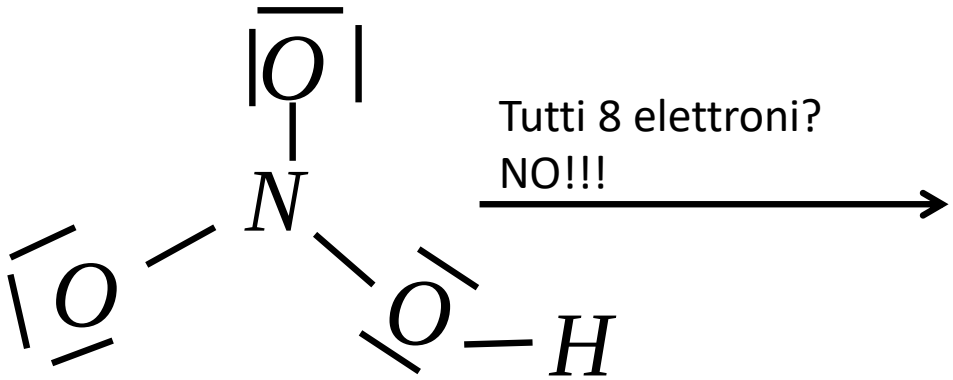
ESERCIZIO 4.



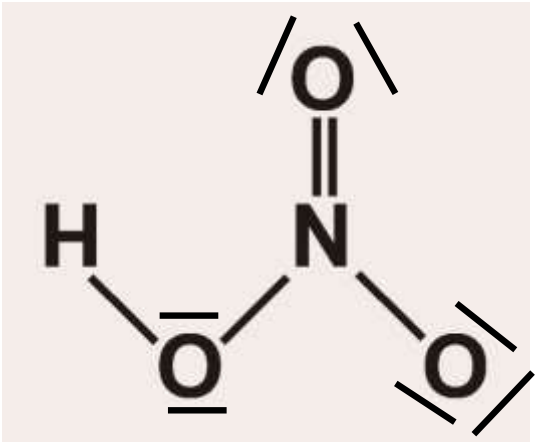
ACIDO NITRICO

HNO_3

$$1+5+6(3)=\frac{24}{2}=12 coppie$$



6-4-2=0



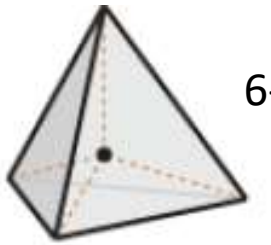
6-4-2=0

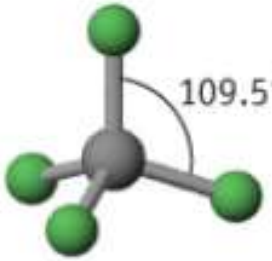
6-6-1=-1

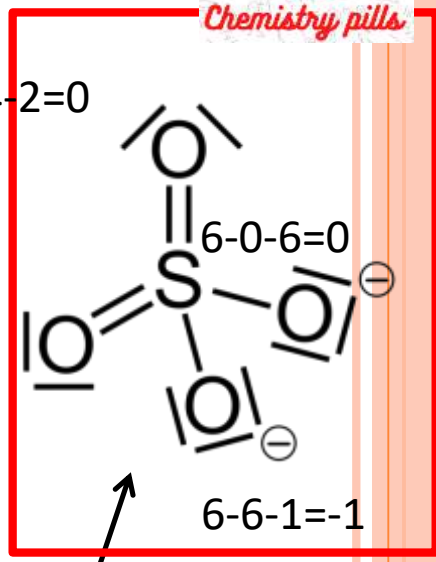
ESERCIZIO 5.

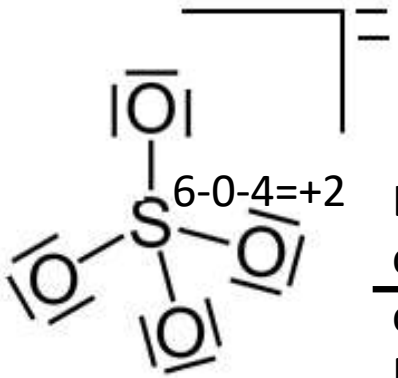
IONE SOLFATO

$$SO_4^{2-} \qquad 6+6(4)+2=\frac{32}{2}=16 coppie$$

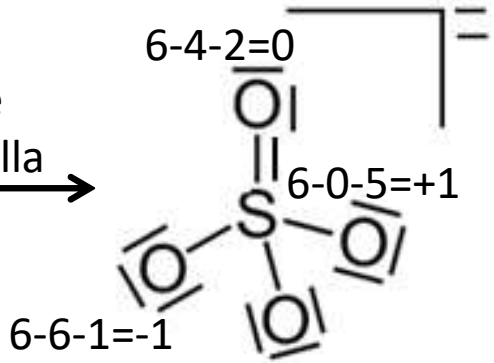








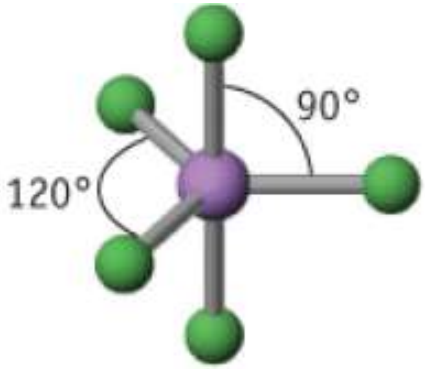
Le cariche formali Sono le minime compatibili con quelle previste dalla carica della specie? ?
NO!!!



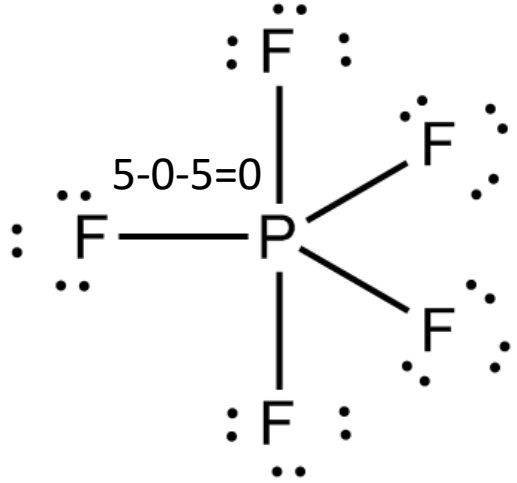
ESERCIZIO 6.

PENTAFLORURO DI FOSFORO

$$PF_5 \qquad 5+7(5)=\frac{40}{2}=20 coppie$$



TRIGONALE BIPIRAMIDALE
AX_5



5-0-5=0

7-6-1=0

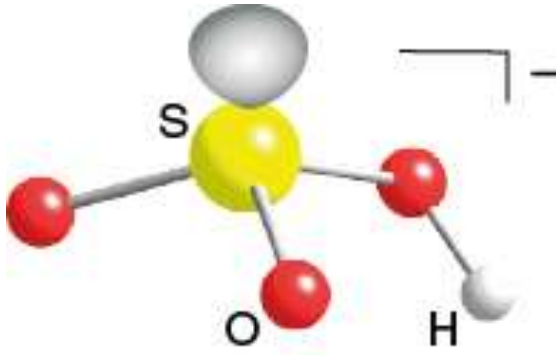
P > 8 elettroni

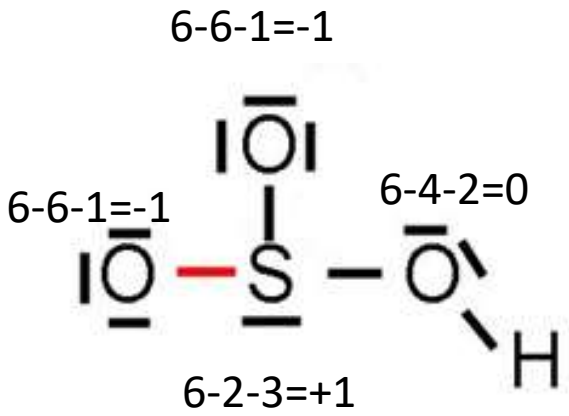
n = 3

ESERCIZIO 7.

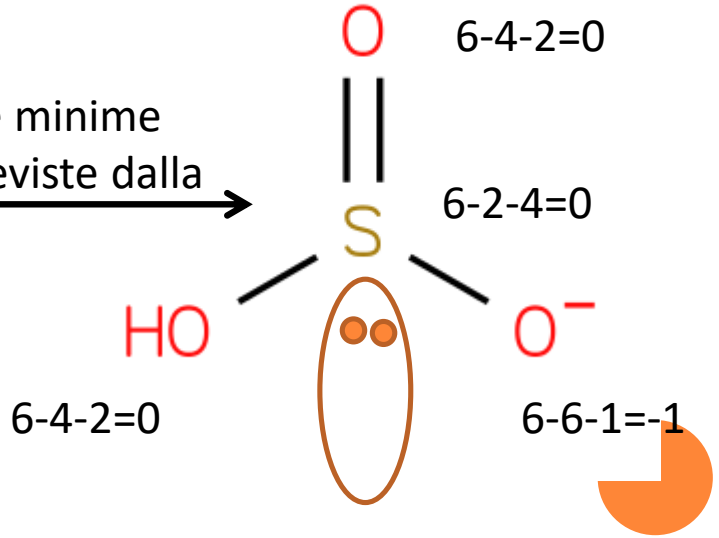
IONE IDROGENO SOLFITO
BISOLFITO

$$HSO_3^- \quad 1+6+6(3)+1=\frac{26}{2}=13 coppie$$





Le cariche formali Sono le minime compatibili con quelle previste dalla carica della specie? ?
NO!!!



S > 8 elettroni
n = 3