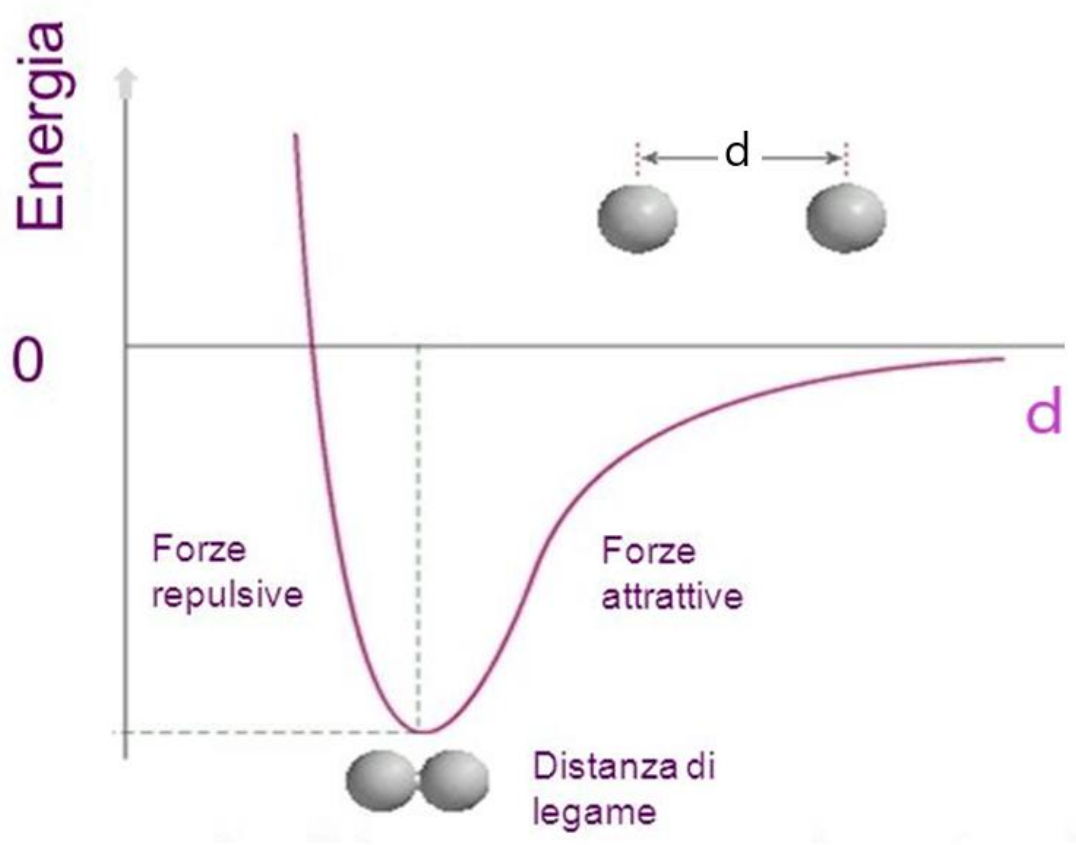
LEGAME CHIMICO

ATOMI → MOLECOLE
- FORMULA BRUTA (es. H_2O, C_2H_4, H_2SO_4)
- FORMULA DI STRUTTURA

- LEGAME CHIMICO
  - IONICO
  - COVALENTE
    - OMEOPOLARE
    - POLARE
  - METALLICO
- FORZE INTERMOLECOLARI
  - VAN DER WAALS
  - LEGAME IDROGENO



ENERGIA DI LEGAME
DISTANZA DI LEGAME

LEGAME IONICO

Ioni positivi e negativi tenuti insieme da interazioni elettrostatiche

Ioni positivi (cationi) → elementi aventi basso I (metalli)

$Na \rightarrow Na^+ + e^-$

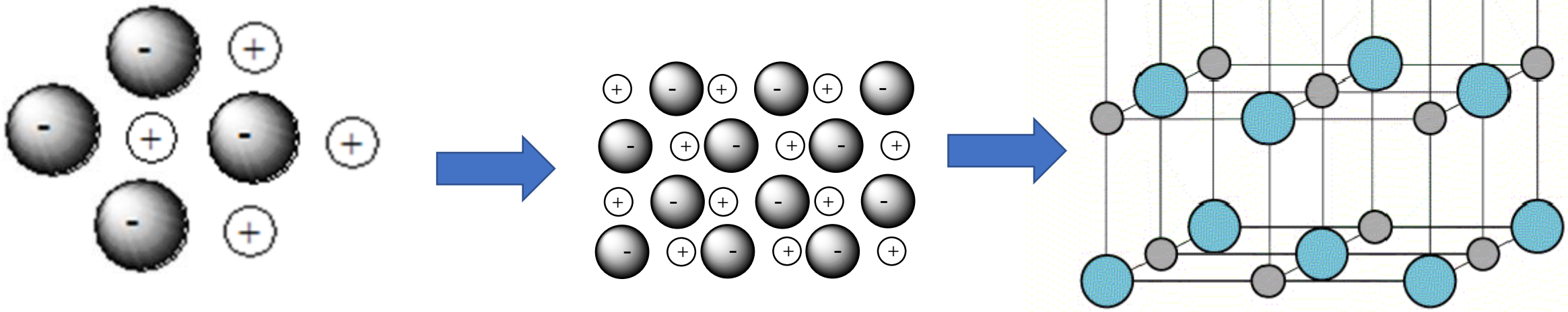
$[Ne]3s^1 \rightarrow [Ne]$

Ioni negativi (anioni) → elementi aventi alta A_e (non metalli)

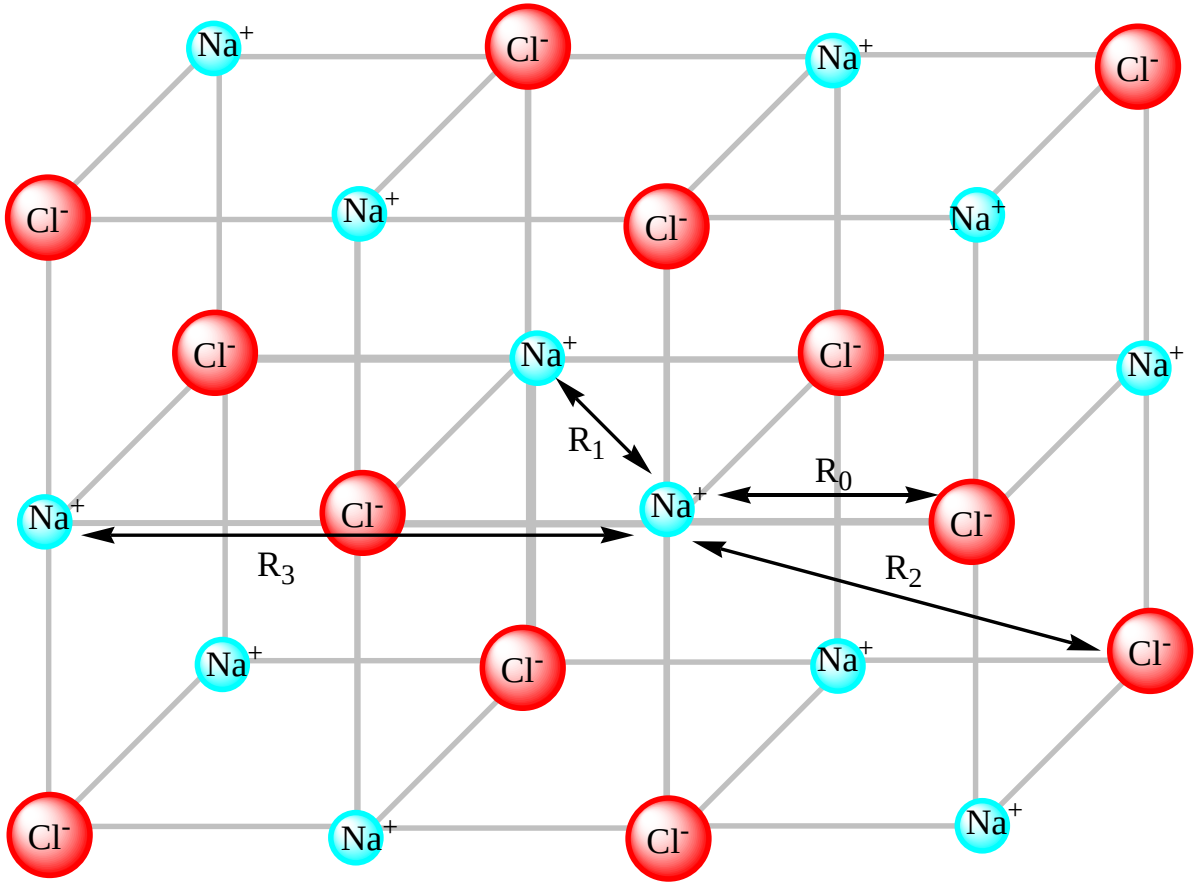
$Cl + e^- \rightarrow Cl^-$

$[Ne]3s^23p^5 \rightarrow [Ne]\ 3s^23p^6 = [Ar]$

$Na^+ + Cl^- \rightarrow Na^+Cl^- = NaCl$



Costanti di Madelung



$$R_1 = \sqrt{2}R_0; R_2 = \sqrt{3}R_0; R_3 = 2R_0 .....$$

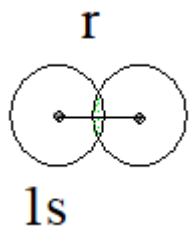
$$E_{MAD} = -6\frac{e^2}{R_0} + 12\frac{e^2}{\sqrt{2}R_0} - 8\frac{e^2}{\sqrt{3}R_0} + 6\frac{e^2}{2R_0} + ... = -E_{Ret}$$

LEGAME COVALENTE

Teoria a coppia di elettroni (Lewis)
Teoria del legame di valenza (VB)

MOLECOLE BIATOMICHE OMONUCLEARI:

H_2 H 1s H · · H → H-H

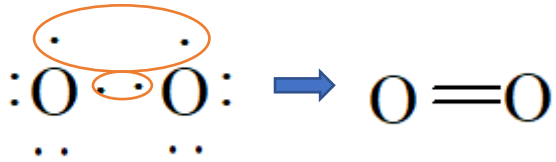


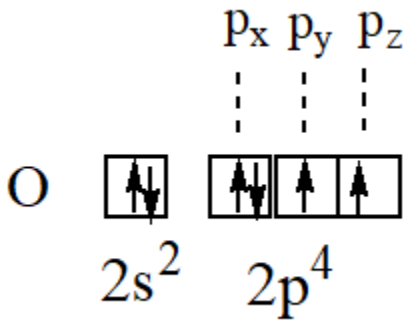
Cl_2 Cl $3s^2$ $3p^5$: Cl · · Cl : → Cl-Cl

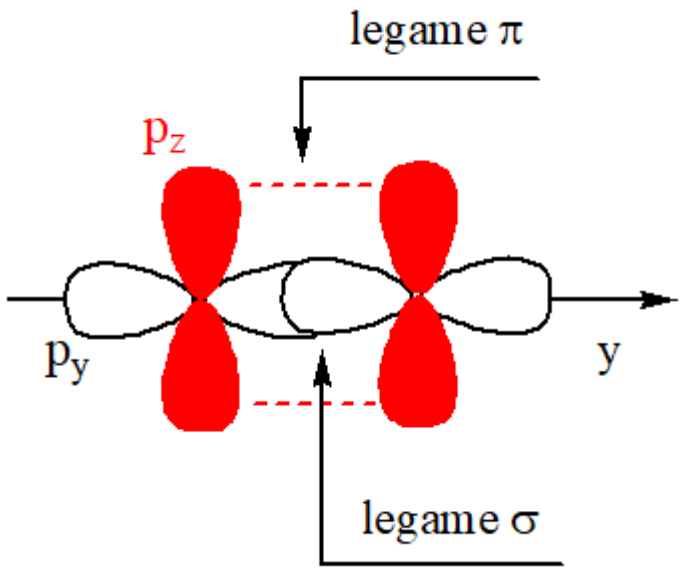
Valenza→ capacità di un atomo di formare legami

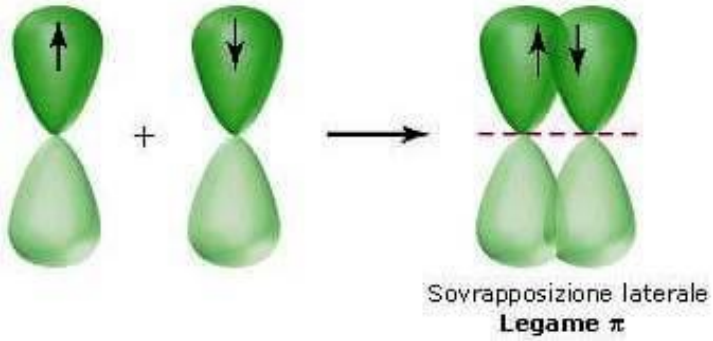
Legami multipli

O_2









O ═ O

$E_\sigma > E_\pi$

σ + π

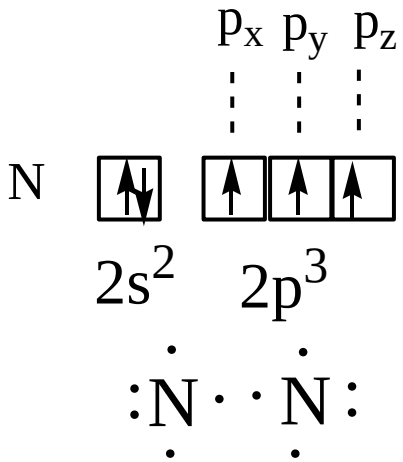
Legame singolo → σ

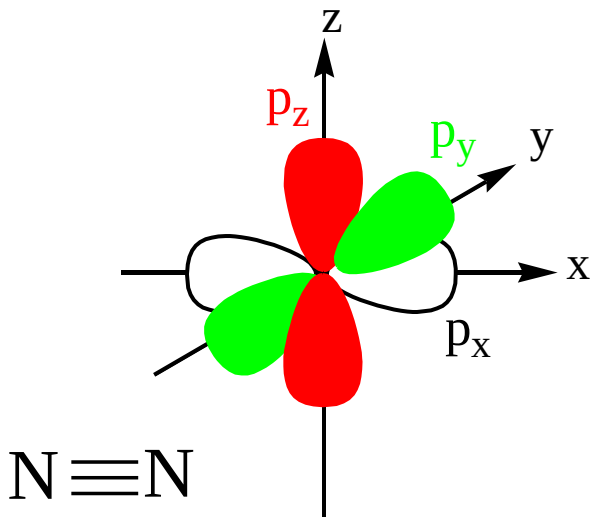
Legame doppio → σ + π

$E_{doppio} > E_{singolo}$

Orbitali s → σ

Orbitali p → σ, π



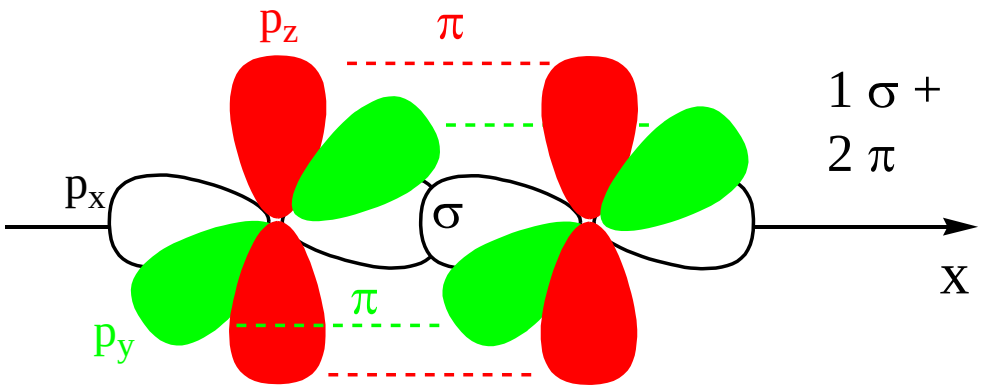


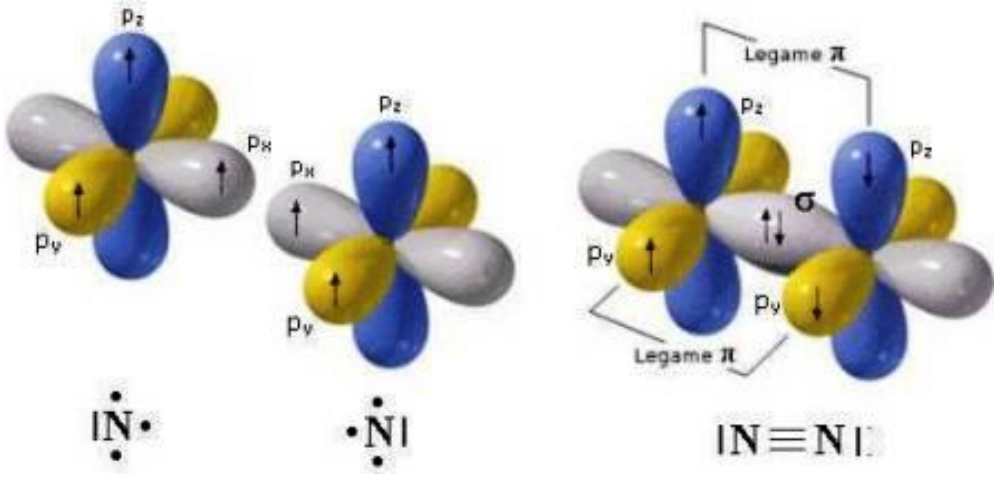
$N \equiv N$

Legame singolo → σ
Legame doppio → σ + π
Legame triplo → σ + 2 π

$E_{triplo} > E_{doppio} > E_{singolo}$

$d_{triplo} < d_{doppio} < d_{singolo}$



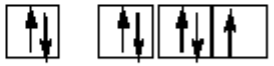


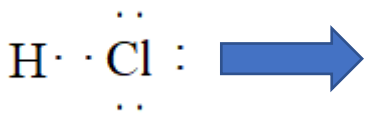
MOLECOLE BIATOMICHE ETERONUCLEARI

LEGAME COVALENTE POLARE

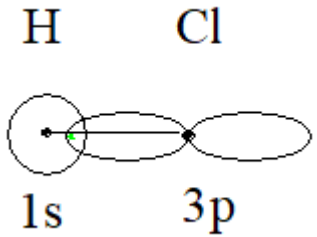
HCl

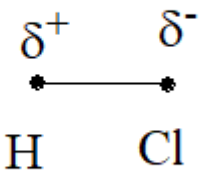
H  1s

Cl  $3s^2$ $3p^5$



H-Cl





Momento di dipolo $\mu = q \times d$

ELETTRONEGATIVITA’ → Tendenza di un atomo ad attrarre su di sè gli elettroni di legame

Differenza di elettronegatività

$\Delta E > 2 \rightarrow$ legame ionico

$0 < \Delta E < 2 \rightarrow$ legame covalente polare (eteropolare)

$\Delta E = 0 \rightarrow$ legame covalente puro o omeopolare

ELETTRONEGATIVITA’

Mulliken $x_A = \frac{1}{2}(I + A_e)$

Potenziale di Ionizzazione

Affinità elettronica

Pauling

$\delta^+ \ \delta^-$

A-B E_{A-B}

A-A E_{A-A}

B-B E_{B-B}

$(E_{A-B})_{teor} = \frac{1}{2}(E_{A-A} + E_{B-B})$ $\Delta = (E_{A-B})_{sper} - (E_{A-B})_{teor}$

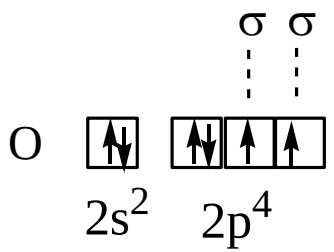
$|x_A - x_B| = 0{,}102\sqrt{\Delta}$

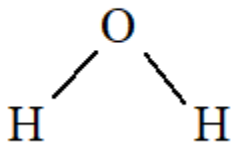
$\%_{ion} = 1 - \exp\{-[\frac{1}{4}(x_A - x_B)^2]\}$

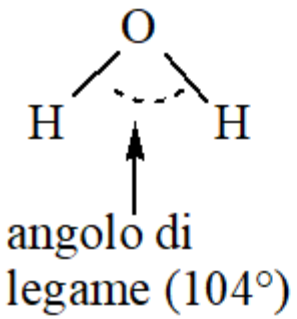
MOLECOLE POLIATOMICHE

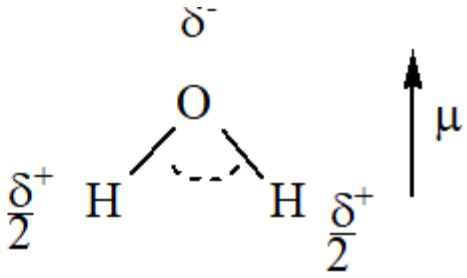
Formula di struttura

H_2O

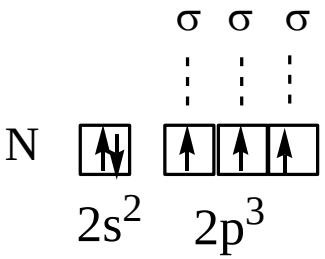


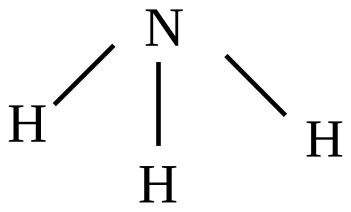






NH_3





Angolo di legame 106°

ORBITALI IBRIDI

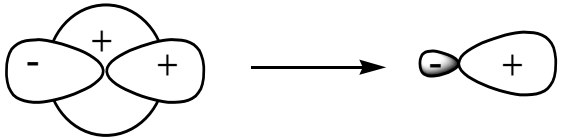
C 

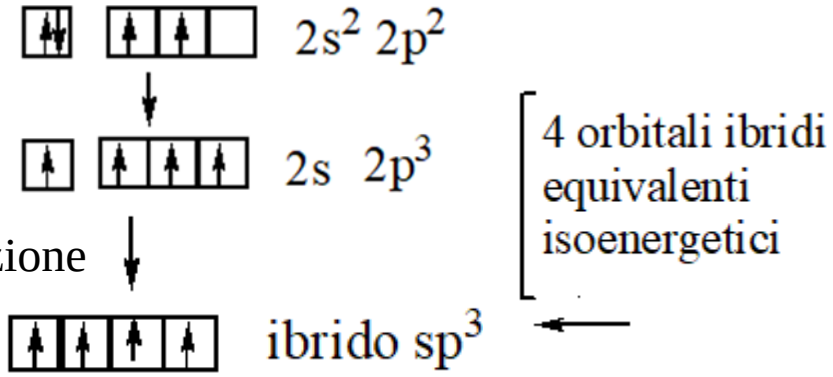
$2s^2$ $2p^2$

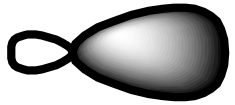
Divalente → no! TETRAVALENTE

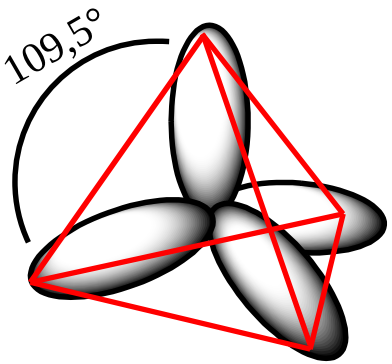
CH_4 4 legami equivalenti

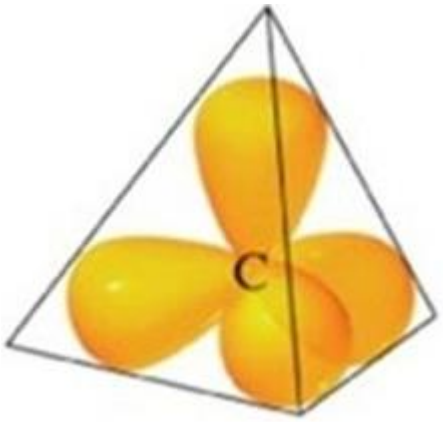
$\Psi_{sp^2} = N (\Psi_{2s} + 3\Psi_{2p})$

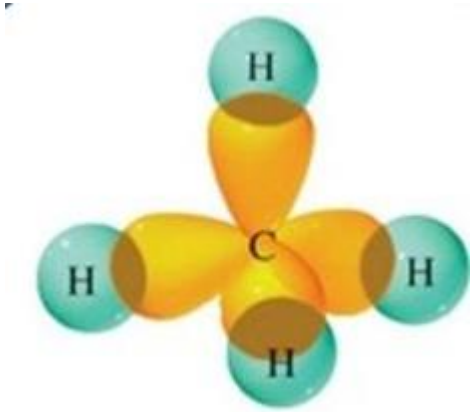


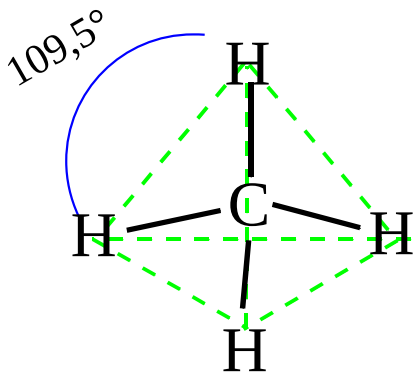


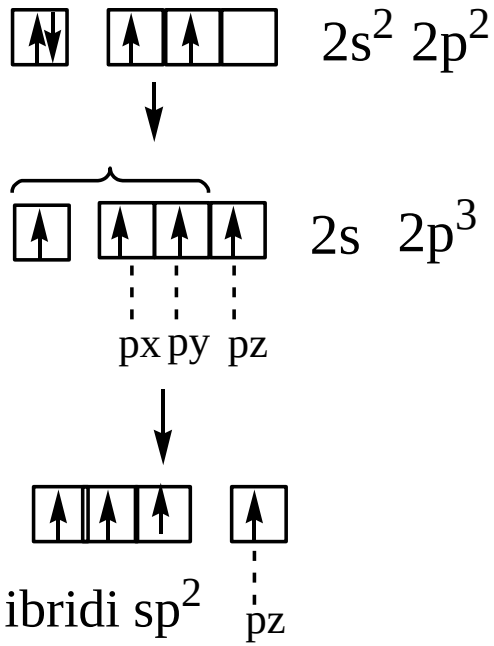




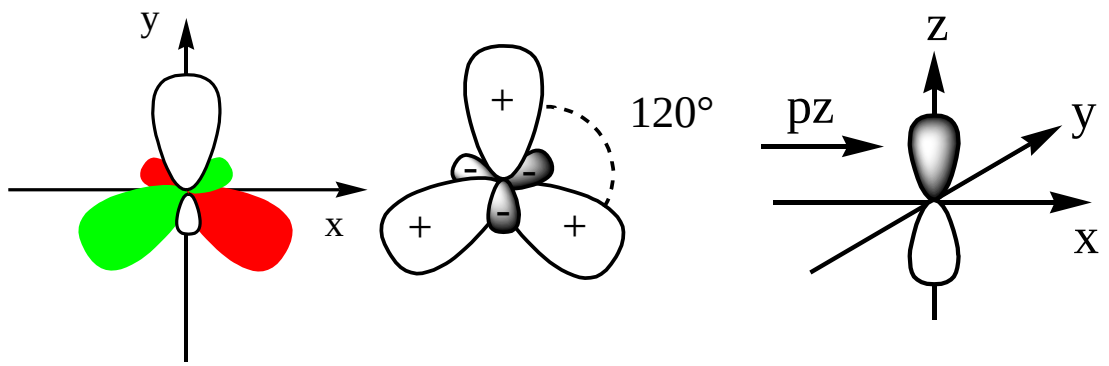








$$\Psi_{sp^2} = N\,(\Psi_{2s} + \Psi_{2px} + \Psi_{2py})$$

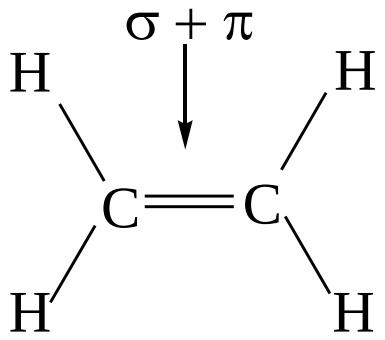


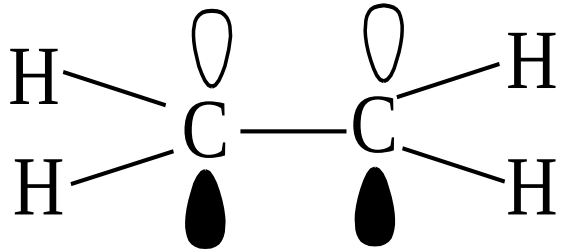
L'orbitale pz non ibridizzato rimane lungo l'asse z
⊥ al piano degli orbitali ibridi

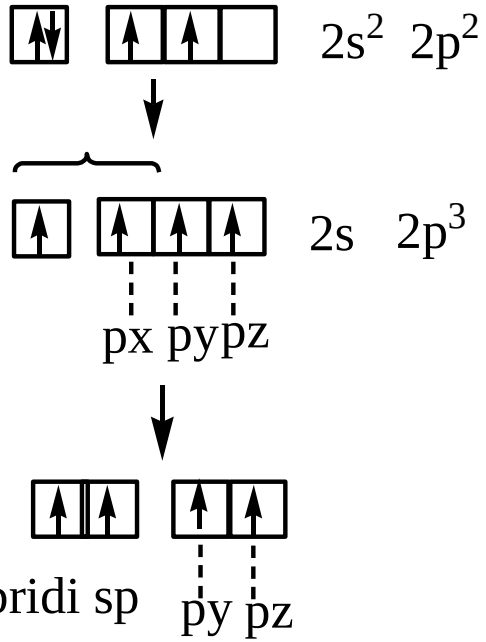
Orbitali ibridi: legami σ
Orbitale non ibrido: legame π

3 legami σ + 1 legame π

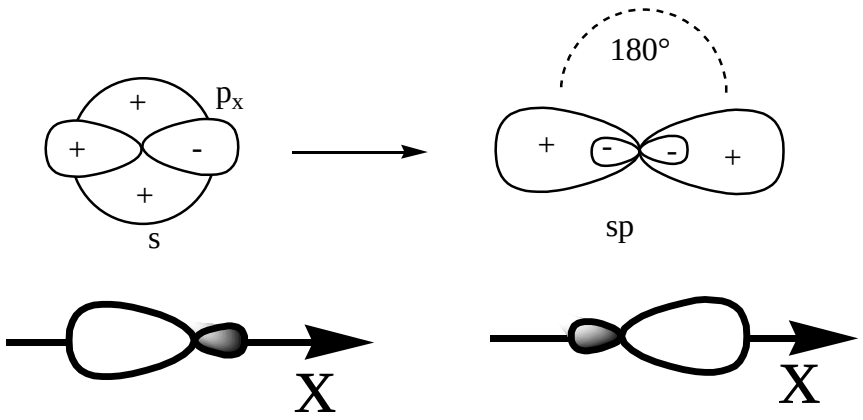
Un legame doppio (σ+π)
Due legami semplici (σ)







$\Psi_{sp} = N (\Psi_{2s} + \Psi_{2px})$



Orbitali ibridi: 2 legami σ
Orbitali non ibridi: 2 legame π

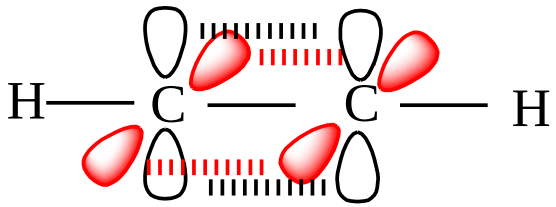
orbitali py e pz non ibridizzati
⊥ tra loro e alla direzione degli orbitali ibridi

C_2H_2 H-C≡C-H

↑

σ+2π

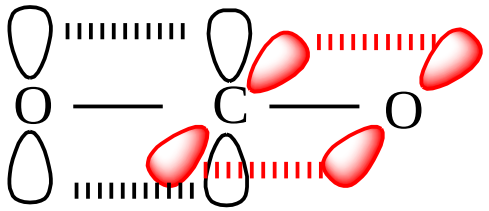
1 legame singolo
+ 1 legame triplo



CO_2 O = C = O

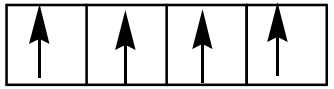
↑ ↑

σ+π σ+π



2 doppi legami

SOMMARIO



sp^3

Ibridazione $sp^3 \rightarrow$ tetraedrica
angoli di 109°
4 orbitali ibridi $\rightarrow$ 4 legami σ $\rightarrow$ 4 legami singoli

sp^2 p

Ibridazione $sp^2 \rightarrow$ trigonale planare
angoli di 120°
3 orbitali ibridi $\rightarrow$ 3 legami σ
1 orbitale p non ibridato $\perp$ al piano $\rightarrow$ 1 legame π
2 legami singoli + un legame doppio

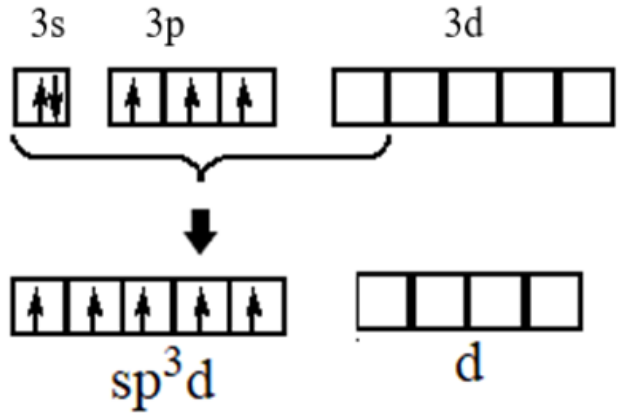
sp p

Ibridazione sp $\rightarrow$ lineare
angoli di 180°
2 orbitali ibridi $\rightarrow$ 2 legami σ
2 orbitali p non ibridati $\rightarrow$ 2 legame π

1 legame triplo +
1 legame singolo

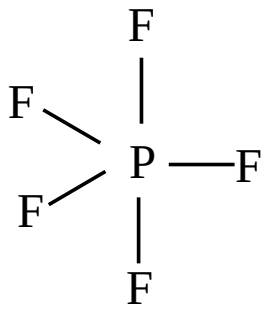
2 doppi legami

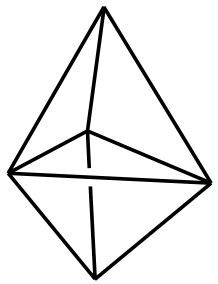
PF_5



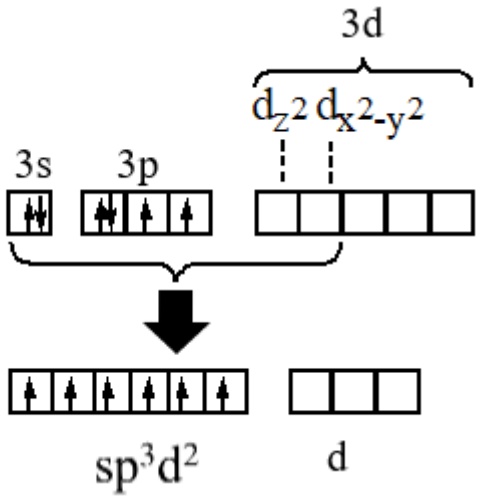
5 legami σ

n c = 5



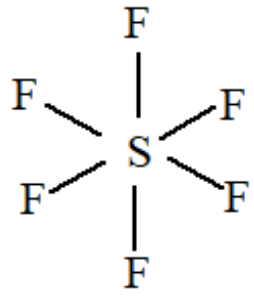


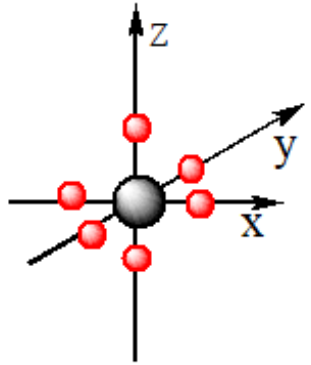
SF_6

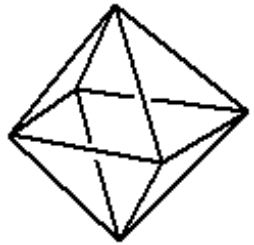


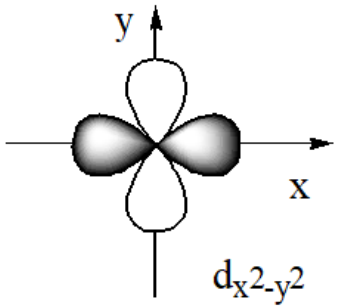
6 legami σ

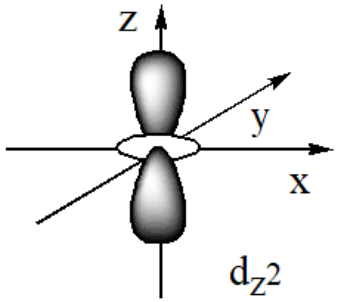
nc = 6





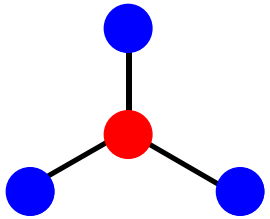




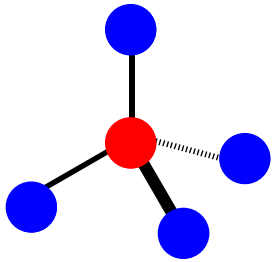


VALENCE SHELL ELECTRON PAIRS REPULSION (VSEPR)

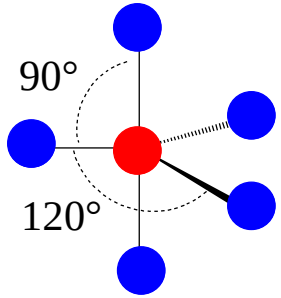
nc=2 180°
lineare
sp



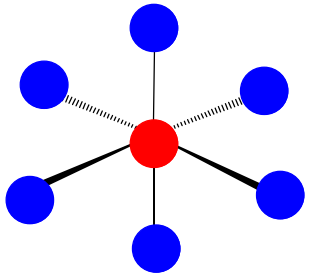
nc=3 120°
trigonale
planare
sp^2



nc=4 109,5°
tetraederica
sp^3

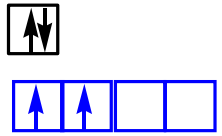


nc=5
bipiramide
trigonale
sp^3d



nc=6 90°
ottraederica
sp^3d^2

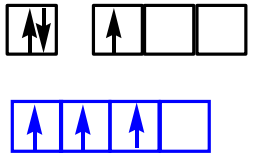
nc = 2

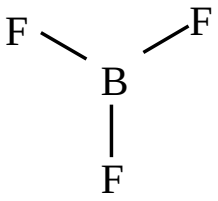
Be 

H-Be-H

2σ 180°

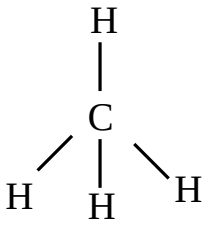
nc = 3

B 



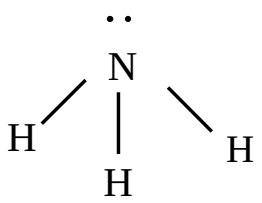
3σ 120°

nc =4 C 



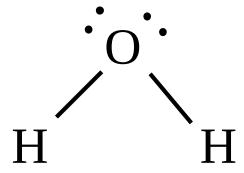
4σ
109,5°

N 



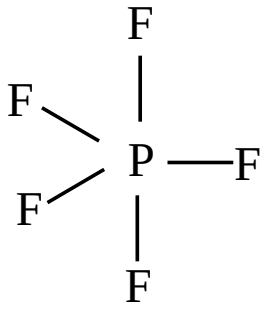
3σ +1 lp
106°

O 

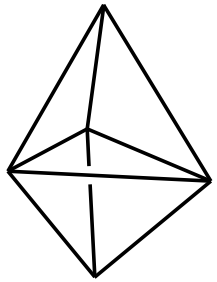


2σ + 2lp
104°

5 legami σ

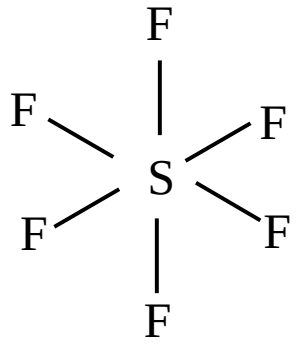


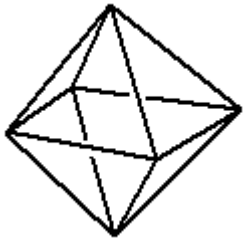
n c = 5



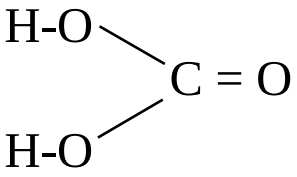
nc = 6

SF_6 6 legami σ

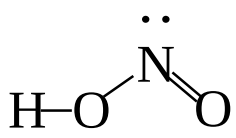




E se ci sono legami π?
Solo legami σ + lone pair determinano la geometria molecolare



3 σ→120°



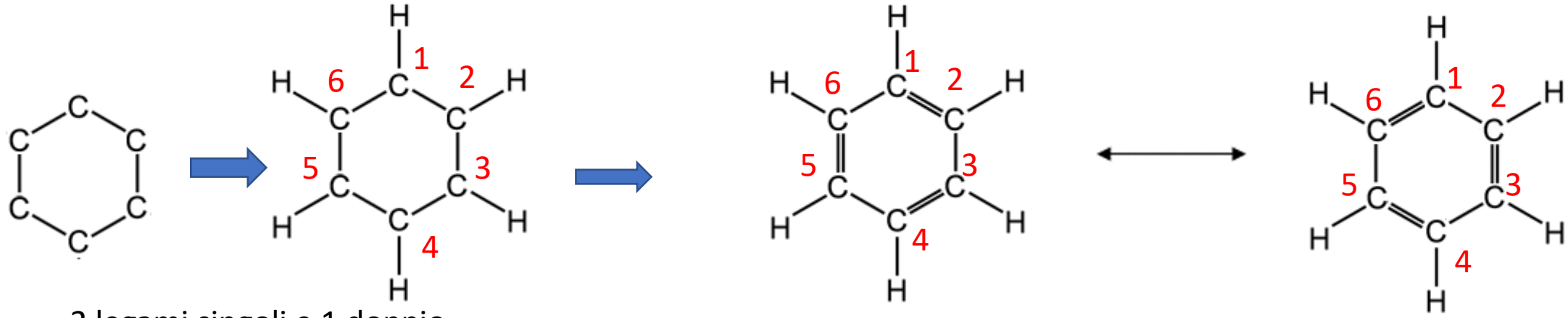
2 σ + 1 lp→120°

H-C≡N
2σ → 180°

O=C=O
2σ → 180°

benzene C_6H_6

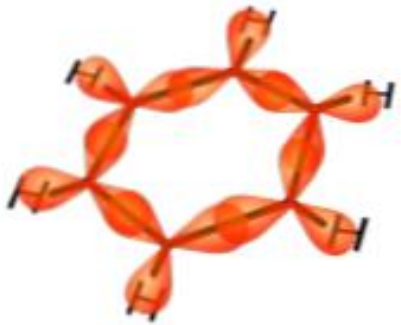
RISONANZA

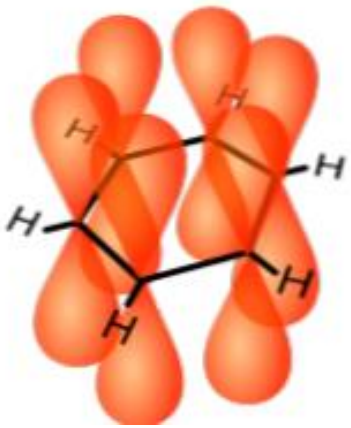


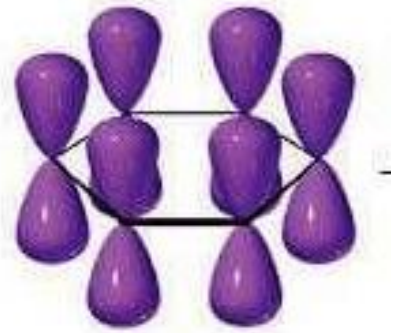
2 legami singoli e 1 doppio
3 σ + 1 π = ibridazione sp^2
Trigonale planare

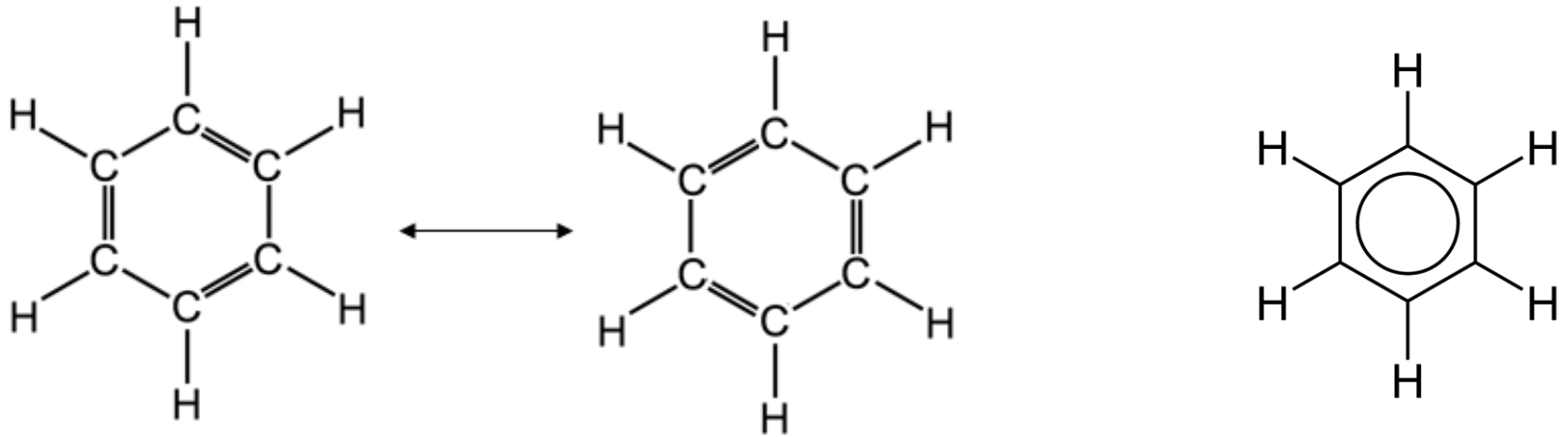
3 C=C e 3 C-C
$E_{C=C} > E_{C-C}$ $d_{C=C} < d_{C-C}$

I 6 legami tra gli atomi di carbonio sono uguali tra loro
Stessa energia di legame
Stessa distanza di legame

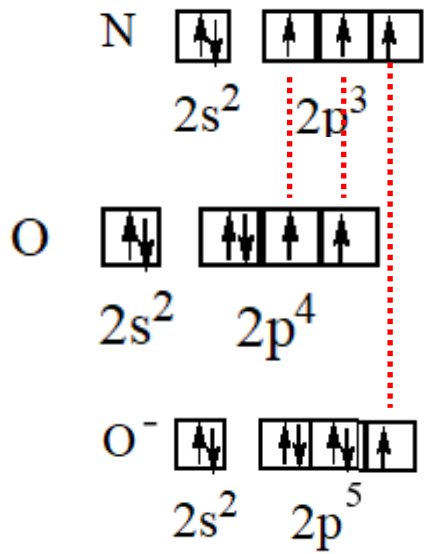


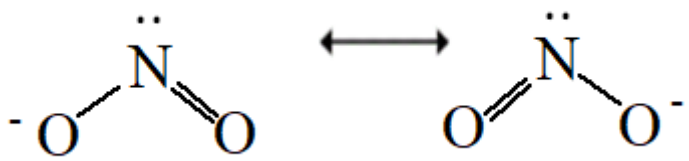






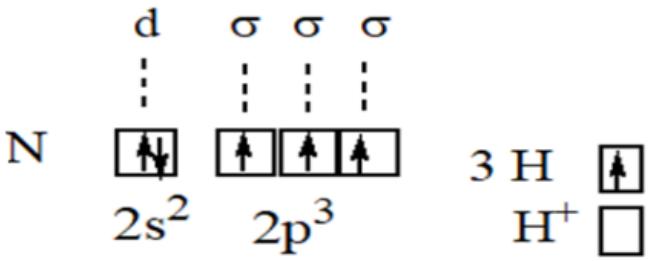
Ione NO_2^-

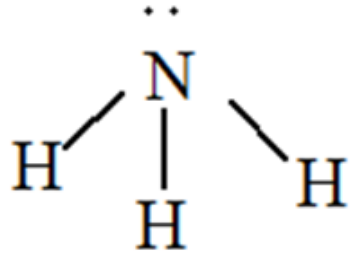


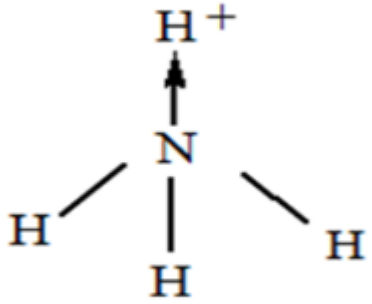


LEGAME DATIVO

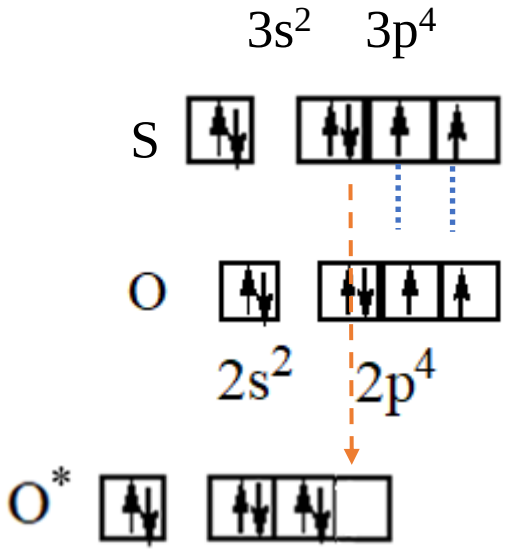
$NH_3 + H^+ \leftrightarrows NH_4^+$

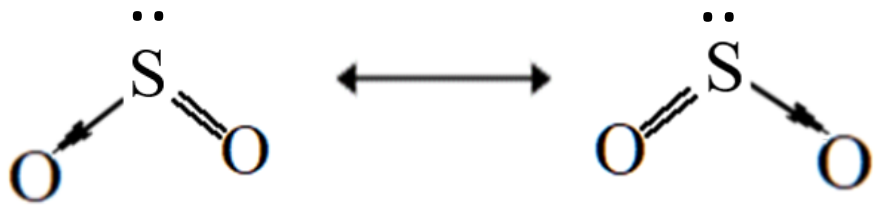






SO_2

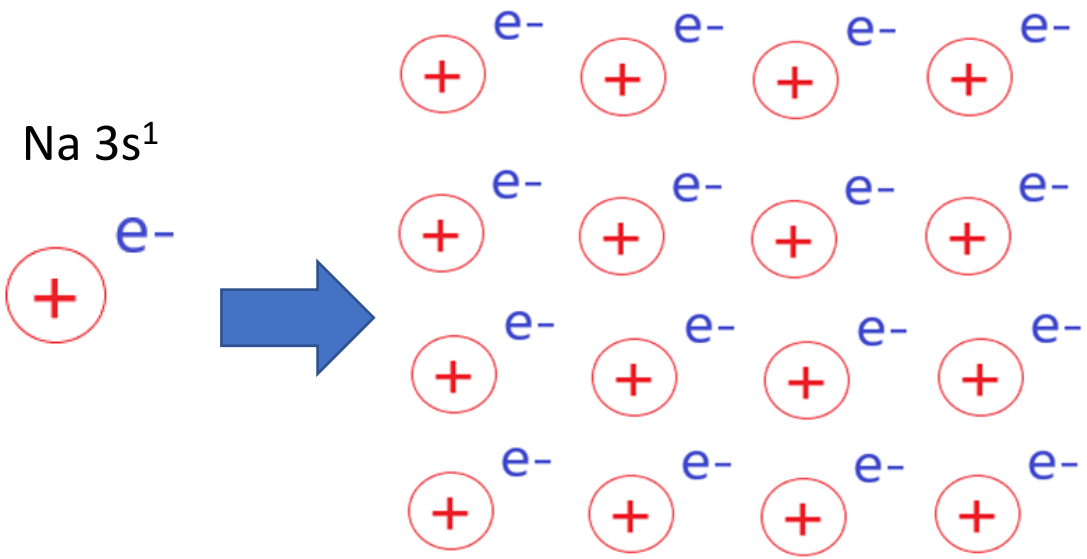


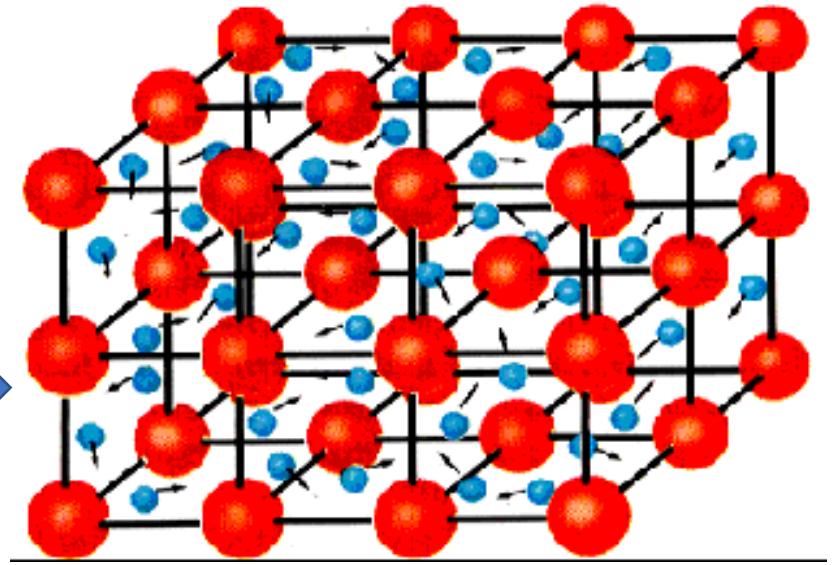


LEGAME METALLICO

Metalli→ Basso I

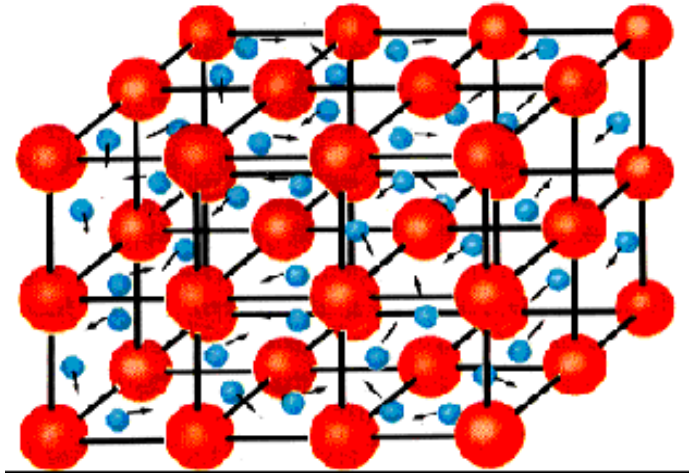
Na $3s^1$





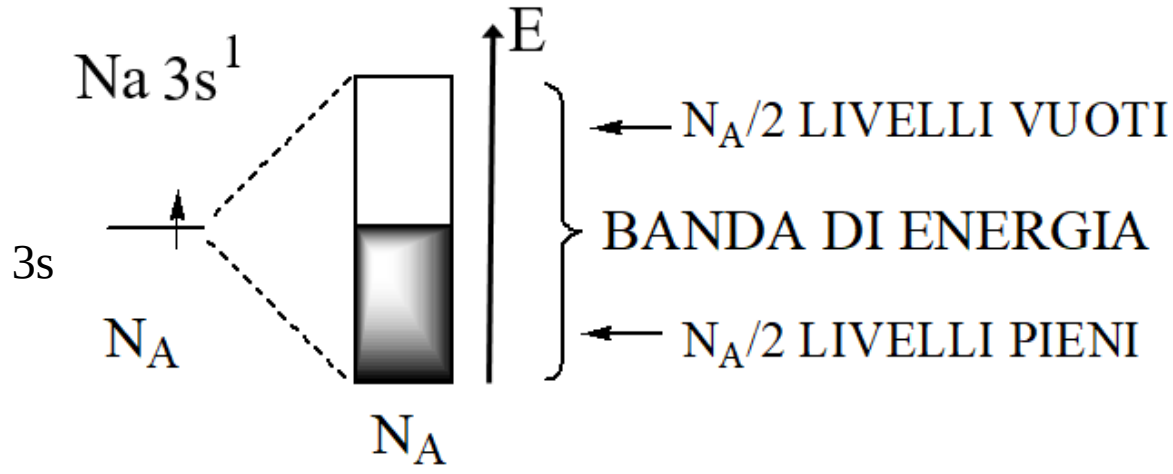
RETICOLO CRISTALLINO
→ IONI METALLICI

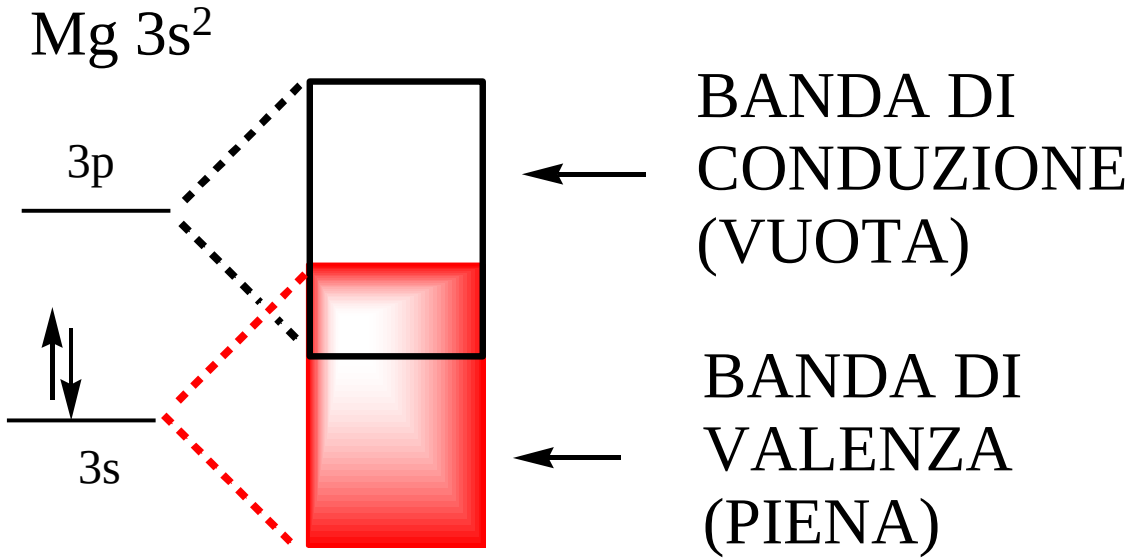
ELETTRONI DI VALENZA
→MARE DI FERMI



CONDUCIBILITA
-ELETTRICA
-TERMICA

MALLEABILITA',
DUTTILITA'





FORZE INTERMOLECOLARI

	Energia
Legami covalenti	100-1000 KJ/mole
Forze intermolecolari	0,1-10 KJ/mole

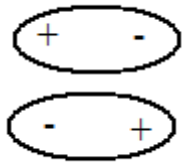
- Van der Waals
  - dipolo-dipolo
  - dipolo-dipolo indotto
  - dipolo istantaneo-dipolo indotto
- Legame idrogeno

Solidi > liquidi >> gas ≈ 0
Gas reali> gas ideali = 0

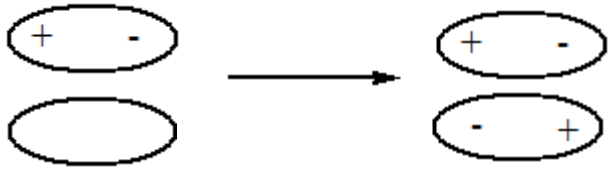
Punto di fusione
Punto di ebollizione

FORZE DI VAN DER WAALS

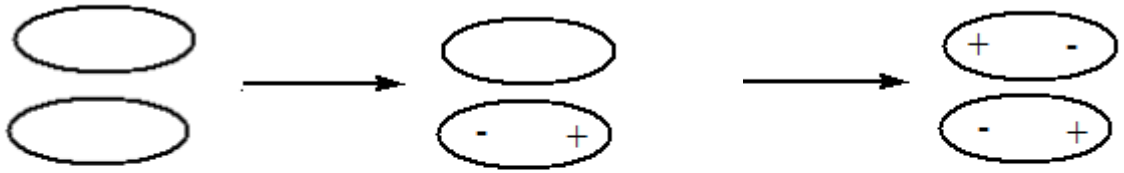
dipolo-dipolo



dipolo-dipolo indotto



dipolo istantaneo-dipolo indotto



molecole apolari

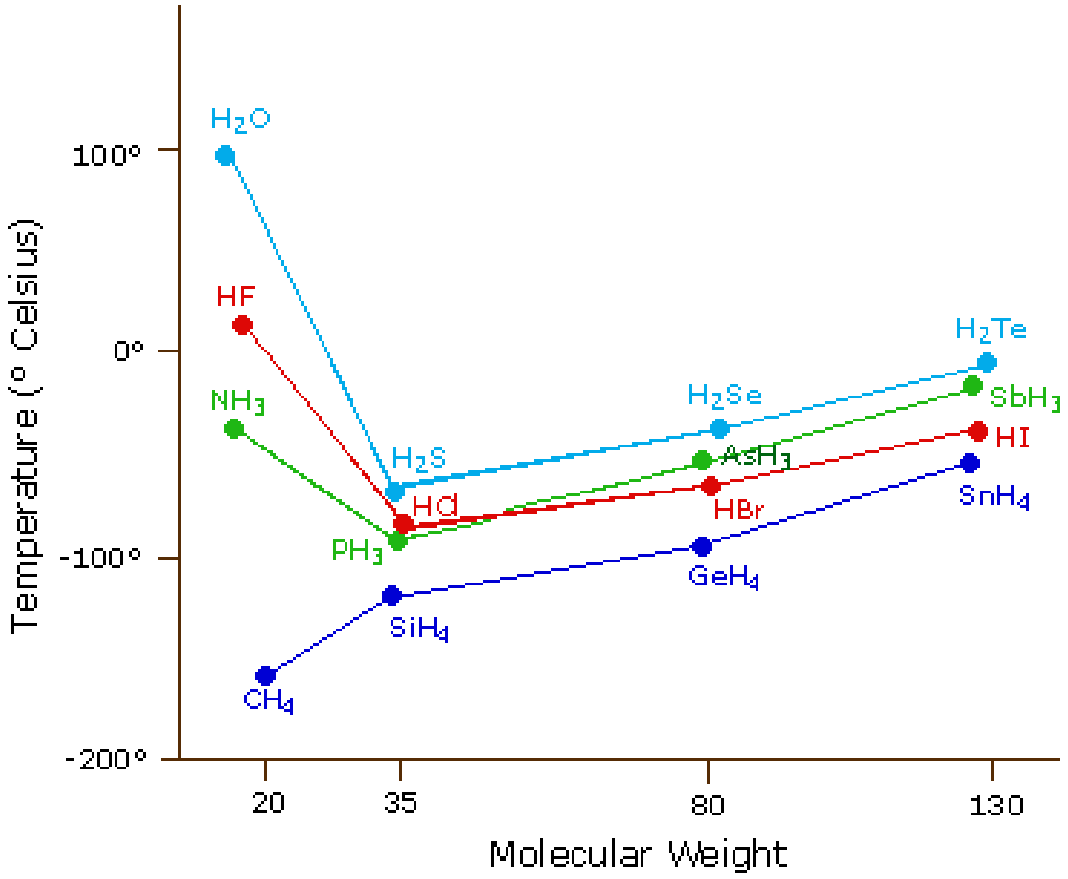
dipolo instantaneo

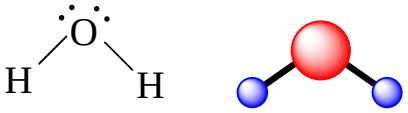
dipolo indotto

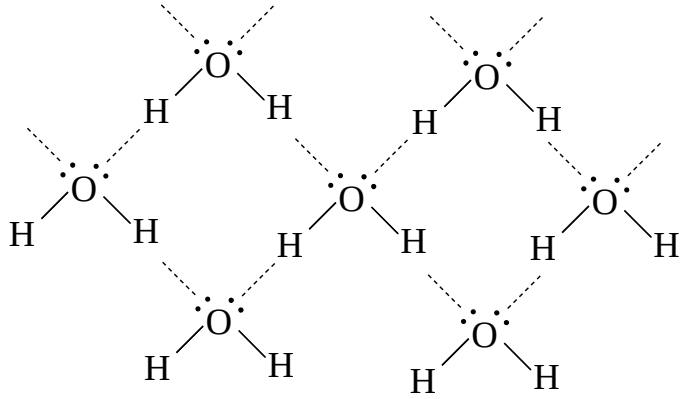
Es F_2, Cl_2, Br_2, I_2

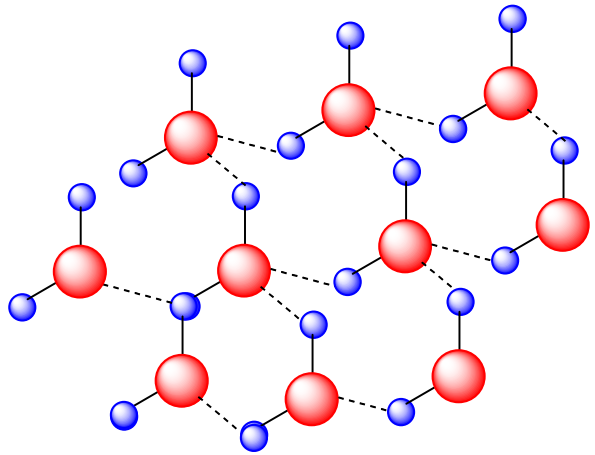
LEGAME IDROGENO

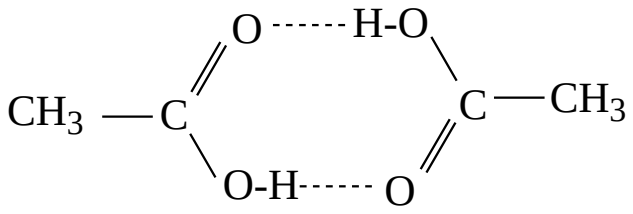
$$X—H\cdots\cdots Y$$
$$\delta^- \ \delta^+ \qquad \delta^-$$

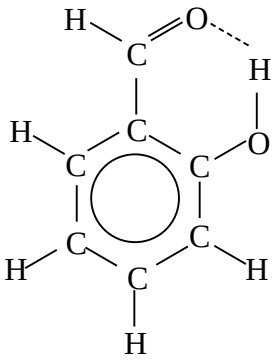


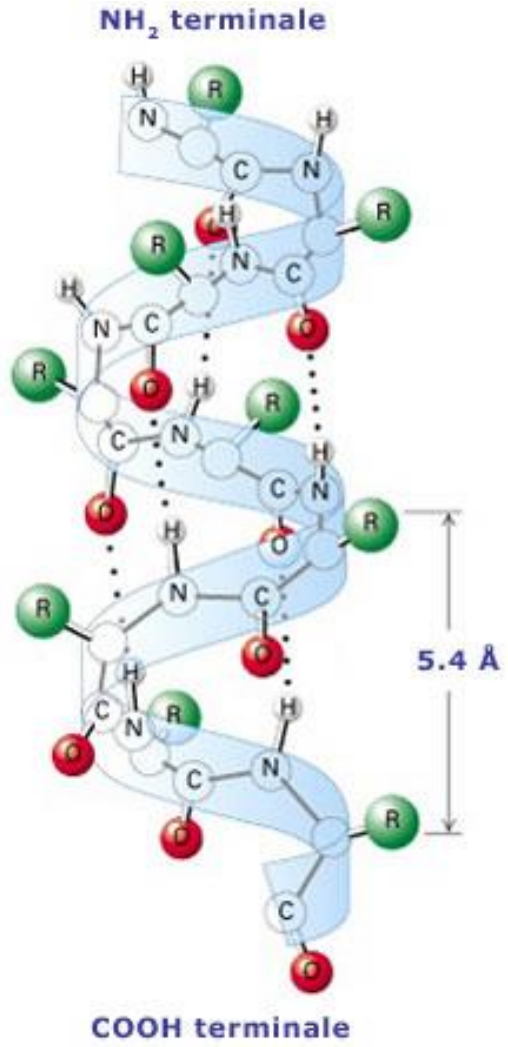


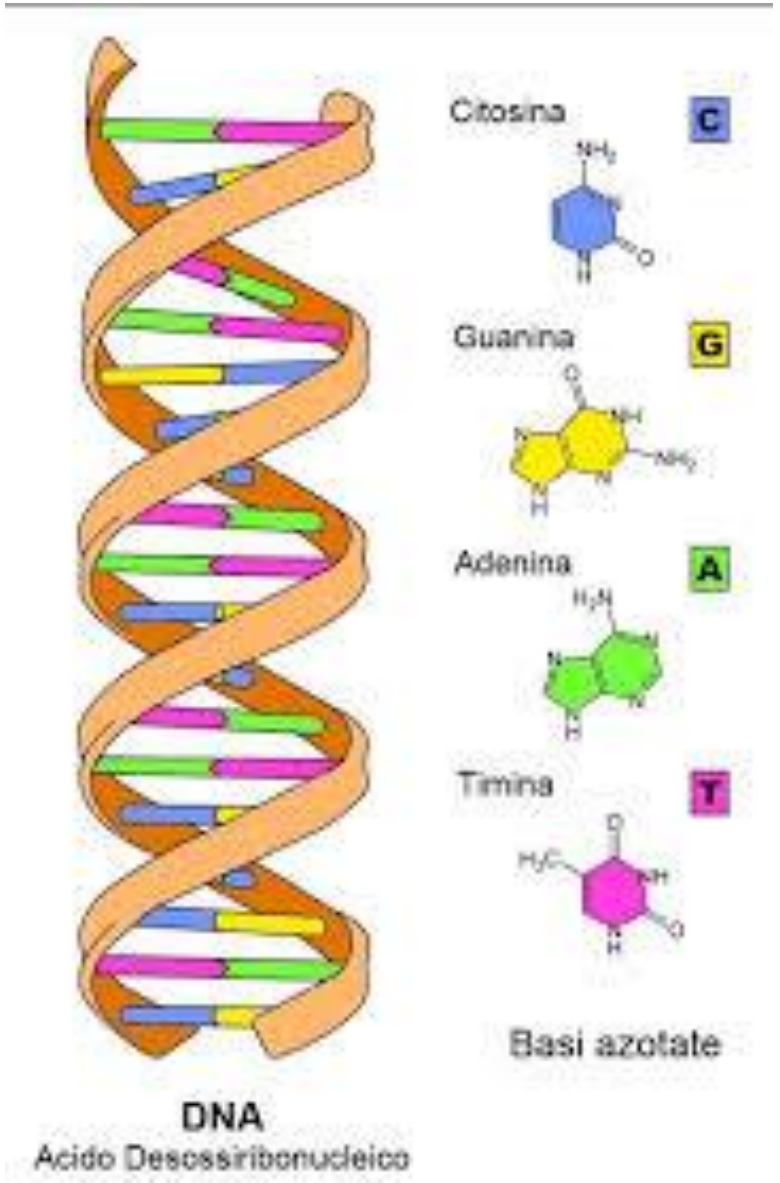









NH2 terminale
5.4 Å
COOH terminale


Citosina
C
Guanina
G
Adenina
A
Timina
T
Basi azotate
DNA
Acido Desossiribonucleico