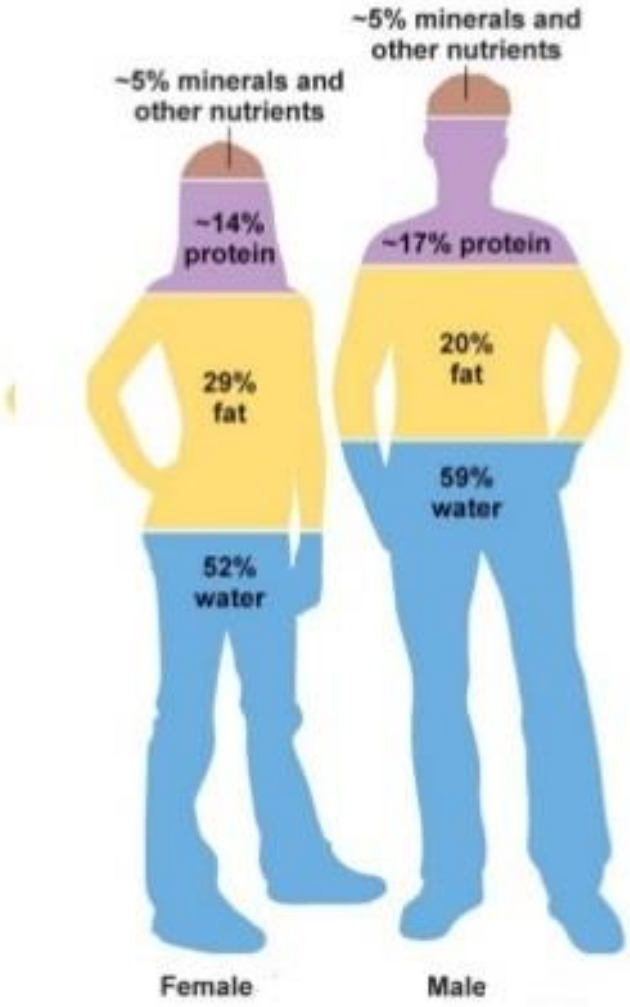
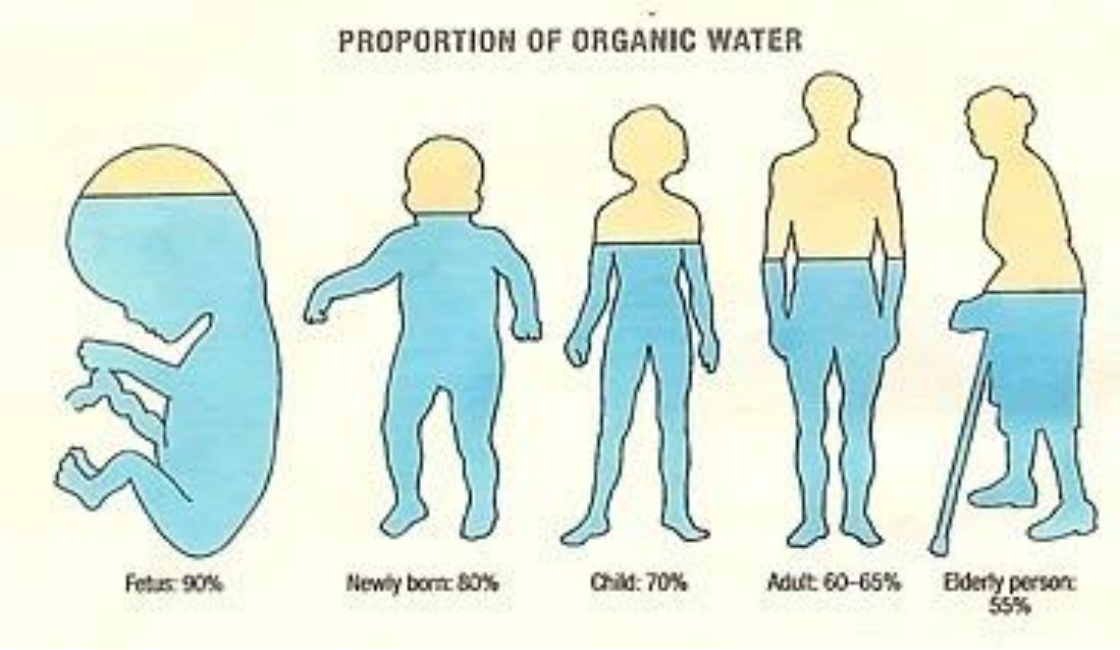
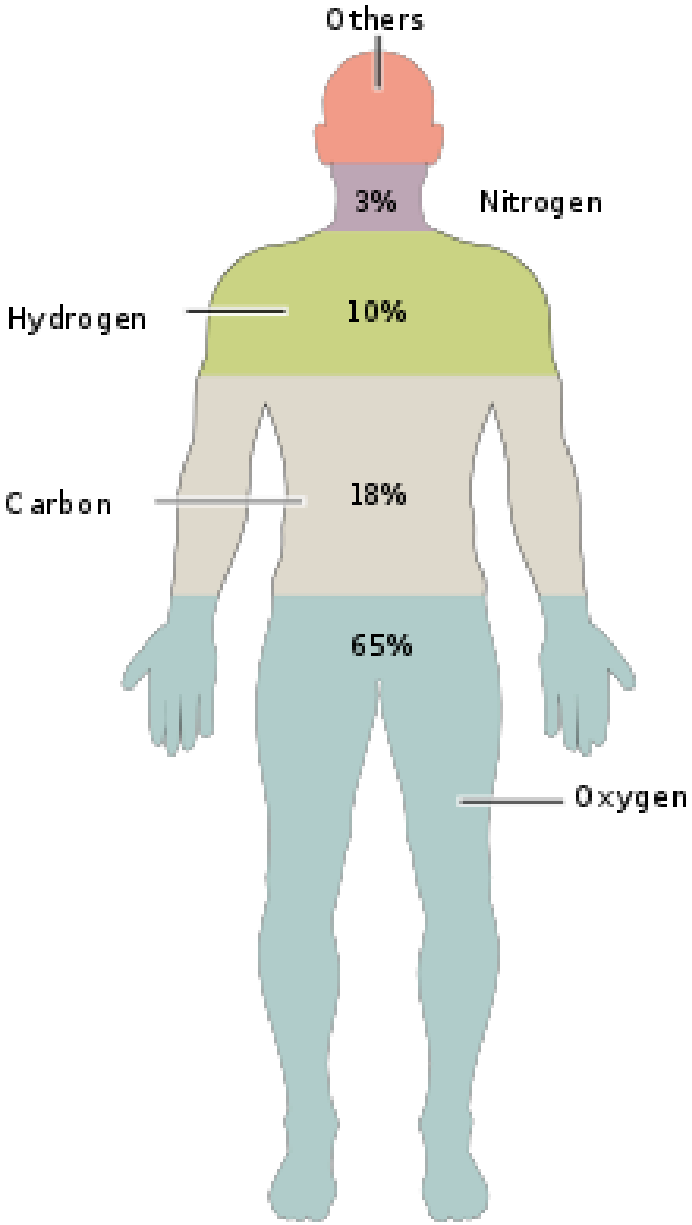
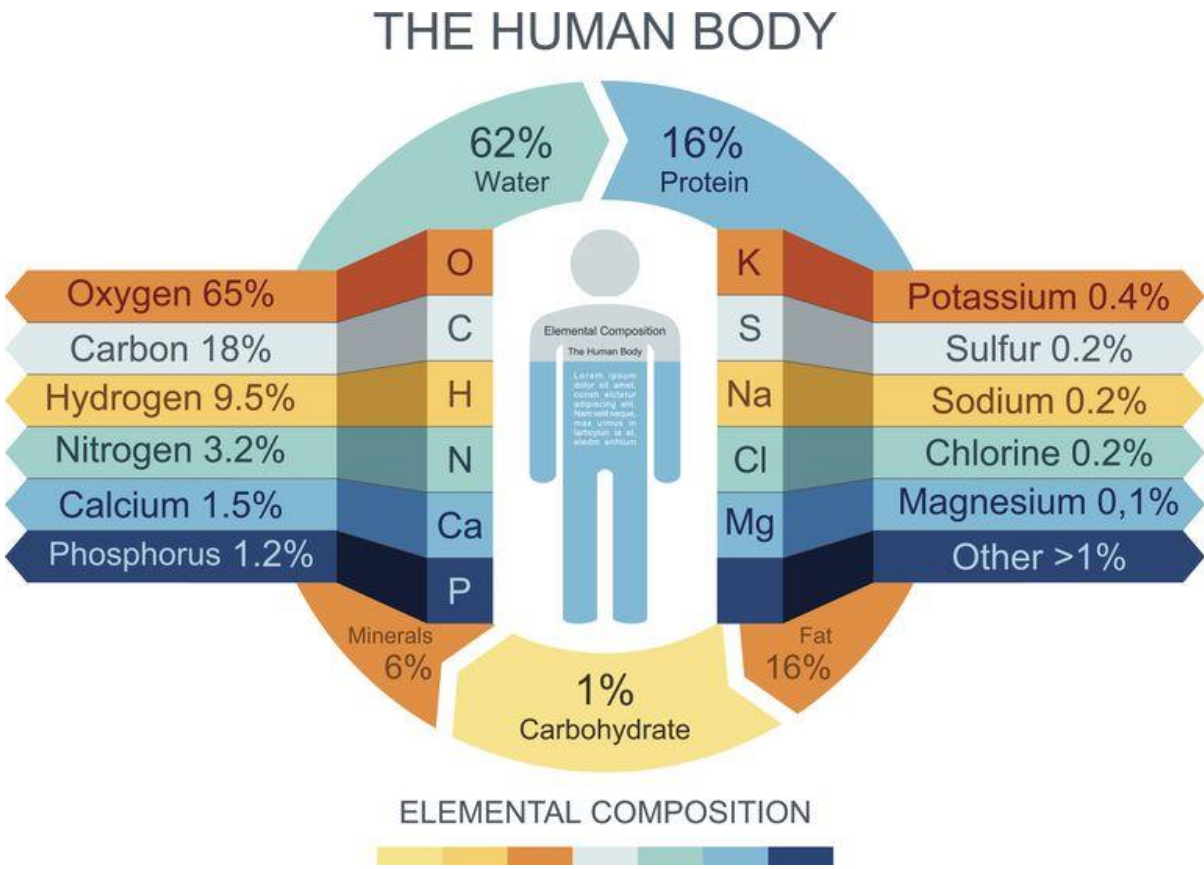
The Composition of the Body






Others
3%
Nitrogen
Hydrogen
10%
Carbon
18%
65%
Oxygen


THE HUMAN BODY
62%
Water
16%
Protein
Oxygen 65%
Carbon 18%
Hydrogen 9.5%
Nitrogen 3.2%
Calcium 1.5%
Phosphorus 1.2%
O
C
H
N
Ca
P
K
S
Na
Cl
Mg
Potassium 0.4%
Sulfur 0.2%
Sodium 0.2%
Chlorine 0.2%
Magnesium 0,1%
Other >1%
Elemental Composition
The Human Body
Minerals
6%
Fat
16%
1%
Carbohydrate
ELEMENTAL COMPOSITION

mg kg^{-1}

Inorganic elements in a healthy human adult of 70 kg weight

Elements in red indicate established essentiality for animals, plants, or both. The year in which essentiality was established is also reported.

Element	Quantity (ppm)	Year	Element	Quantity (ppm)	Year
Ca	1.4×10^4		Sn	0.1-1.5	1970
S	6.4×10^3		Al	0.2-0.6	
P	6.3×10^3		Se	0.4	1957
Na	2.6×10^3		Cd	0.3-0.4	
K	2.2×10^3		Ba	0.3	
Cl	1.8×10^3		I	0.2-0.3	
Mg	4.0×10^2		Mn	0.2-0.3	1930
Fe	60-70	1925	Mo	0.2	1953
Si	40	1972	B	0.2	
F	37		As	0.05	
Zn	20-33	1930	Cr	0.04	1959
Rb	5.1		Ni	0.04	1974
Sr	4.6		Li	0.03	
Br	1.7-7.5		V	0.03	1971
Pb	1.7		Co	0.02	1930
Cu	1.1				

Elements of biological relevance

IA	IIA	IIIA	IVA	VA	VIA	VIIA	VIII	VIII	VIII	IB	IIB	IIIB	IVB	VB	VIB	VIIB	0
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	Ln	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Th	Pa	U												

Bulk biological elements

Trace elements believed to be essential for plants or animals

Possibly essential trace elements

Ruolo di alcuni ioni metallici nei processi biologici

Funzione strutturale **Cationi Ca, Mg**
Anioni: P, O, C, Si, S, F

- ***Trasportatori di carica per un veloce trasferimento dell'informazione***
  cationi Na, K e Ca

- ***Trasferimento di elettroni***
  Ioni Fe, Cu, Mn, Mo, Co, Ni

- ***Formazione, Metabolismo e Degradazione di composti organici***
  Catalisi (acidi e basi di Lewis)

Biomolecole contenenti metalli di transizione

Proteine

Proteine di trasporto e di accumulo

- **Vettori di elettroni (*es. citocromi*)**
- **Strutturali e di accumulo di metalli (*es. Transferrina e Ferritina*)**
- **Leganti di ossigeno (*es. Emoglobina e Mioglobina*)**

Enzimi

- **Idrolasi (*es. Carbossipeptidasi*)**
- **Ossidoriduttori (*es. Superossidodismutasi*)**
- **Mutasi (*es. Cobalammine*)**

Catalizza lo spostamento di un gruppo funzionale da una posizione ad un'altra all'interno della stessa molecola

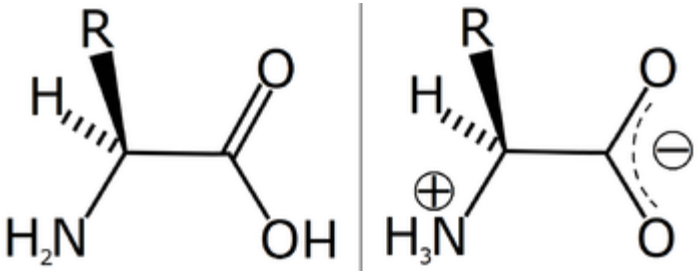
Non Proteine

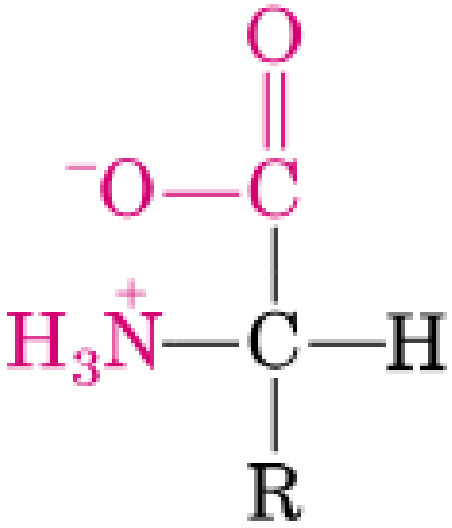
Siderofori

Bioleganti

- ***peptidi (proteine)***
- ***leganti tetrapirrolici***
- ***nucleobasi, nucleotidi ed acidi nucleici (DNA, RNA)***

Amino Acids

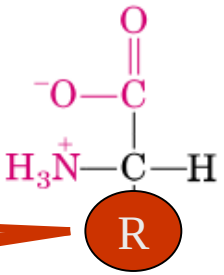




Zwitterionic form

Classification of amino acids

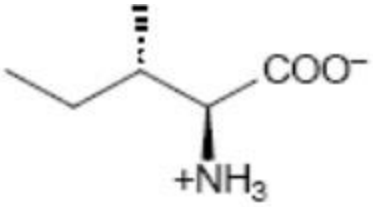
- Side chains of amino acids are responsible for many of the unique properties of proteins
- 3 major classes of sides chains
  - hydrophobic
  - charged
  - polar
  - can also count 4 classes if Gly considered in own class
- The 20 different amino acids are commonly abbreviated with 1 or 3-letter codes



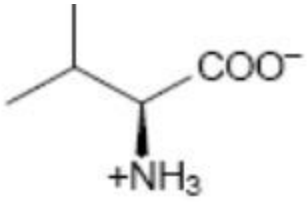
Zwitterionic form

R = H *Gly*

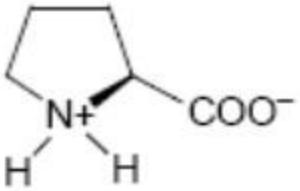
Gruppi R non polari (idrofobici)



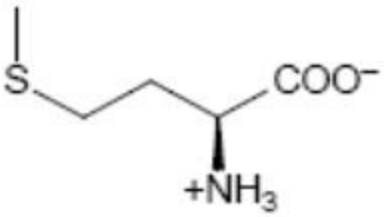
(2S,3S)-(+)-Isoleucine *(Ile, I)*



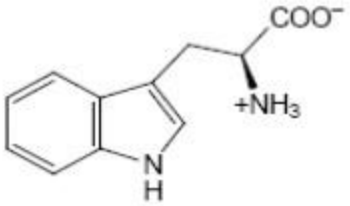
(S)-(+)-Valine *(Val, V)*



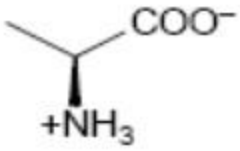
(S)-(–)-Proline *(Pro, P)*



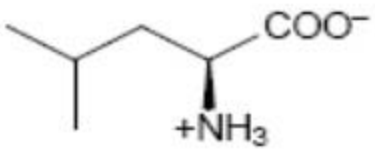
(S)-(–)-Methionine *(Met, M)*



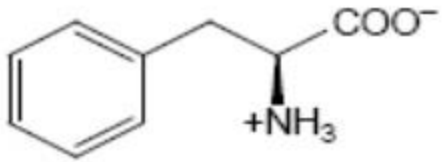
(S)-(–)-Tryptophan *(Trp, W)*



(S)-(+)-Alanine *(Ala, A)*

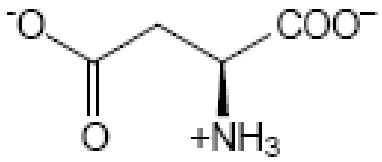


(S)-(–)-Leucine *(Leu, L)*

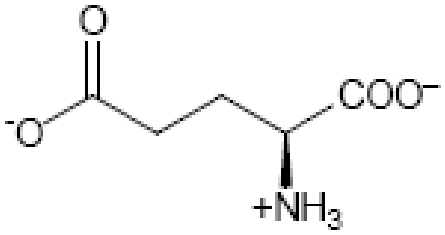


(S)-(–)-Phenylalanine *(Phe, F)*

Gruppi R carichi **negativamente**

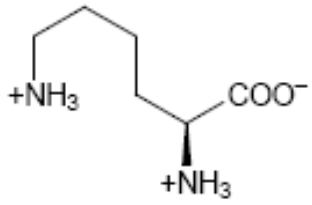


(S)-(+)-Aspartic Acid *(Asp, D)*

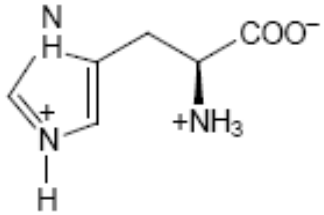


(S)-(+)-Glutamic Acid *(Glu, E)*

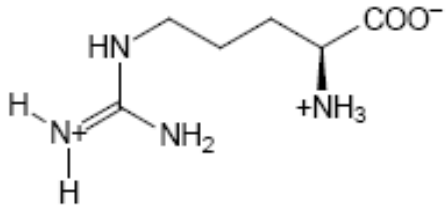
Gruppi R carichi **positivamente**



(S)-(+)-Lysine *(Lys, K)*

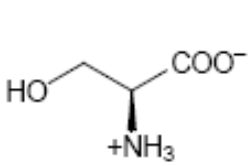


(S)-(–)-Histidine *(His, H)*

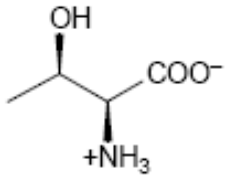


(S)-(+)-Arginine *(Arg, R)*

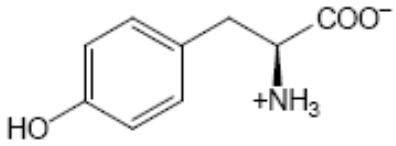
Gruppi R polari ma non carichi



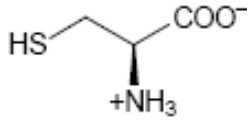
(S)-(–)-**Serine** *(Ser, S)*



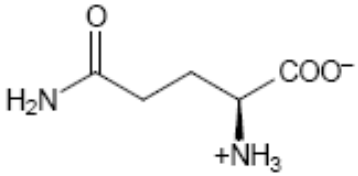
(2S,3R)-(–)-**Threonine** *(Thr, T)*



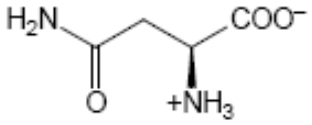
(S)-(–)-**Tyrosine** *(Tyr, Y)*



(R)-(–)-Cysteine *(Cys, C*



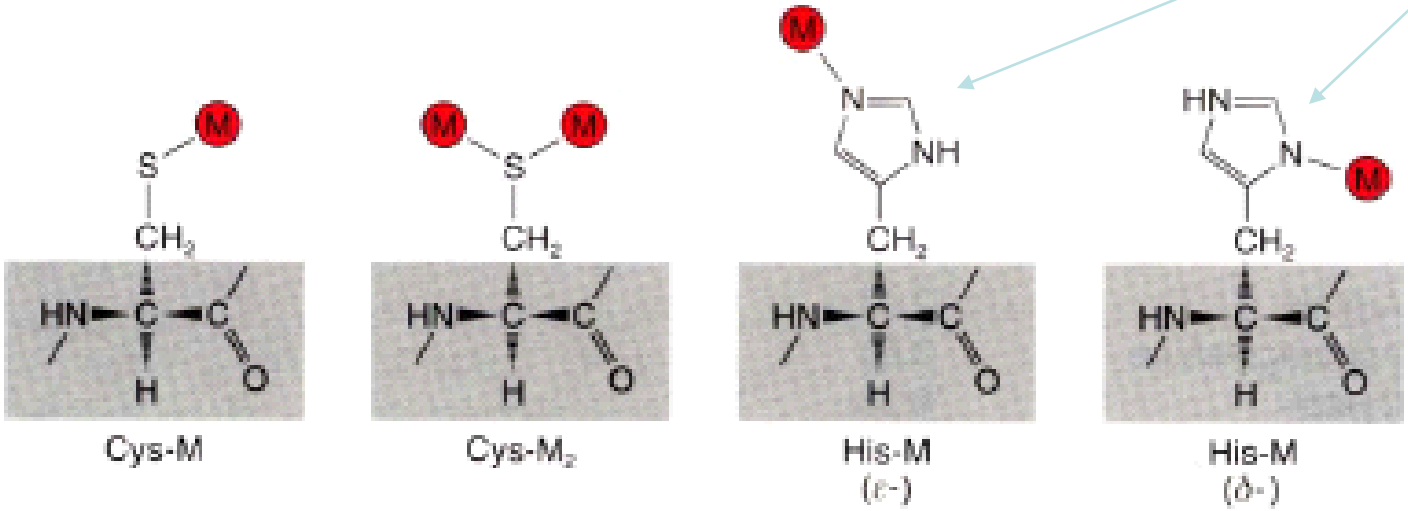
(S)-(+)-Glutamine *(Gln, Q)*



(S)-(–)-**Asparagine** *(Asn, N)*

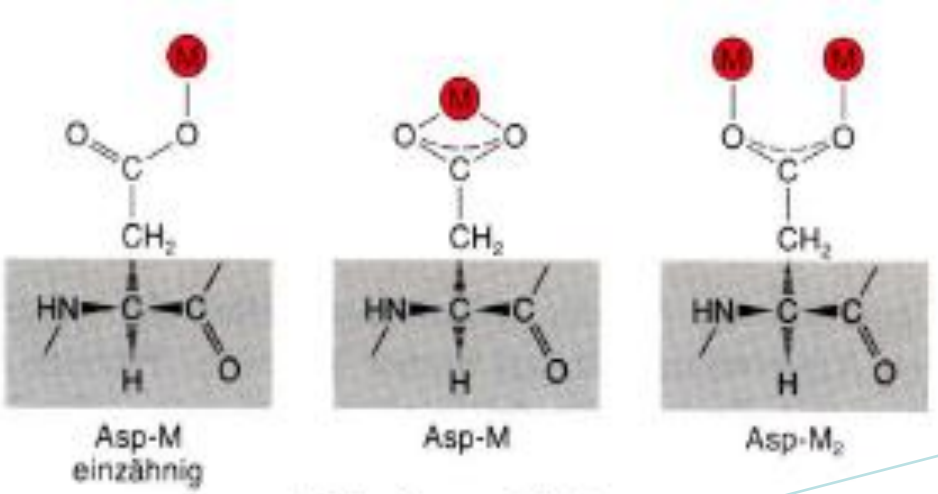
Bioligands – Amino Acids

Imidazole

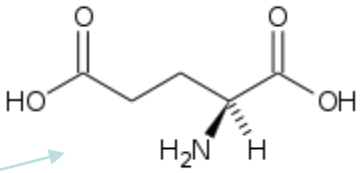


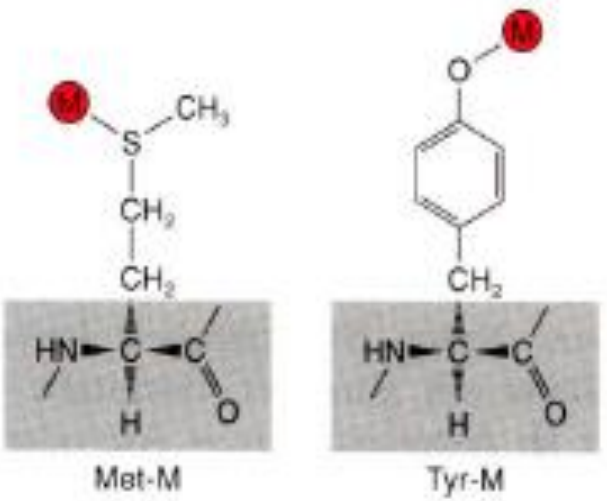
Cysteine and histidine binding modes

Aspartic acid binding modes



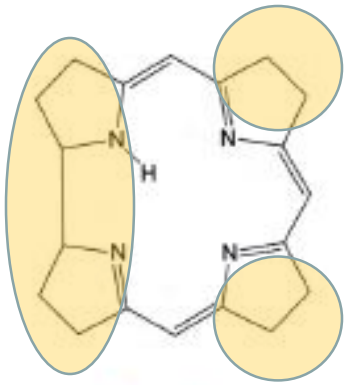
(Similar: Glu)



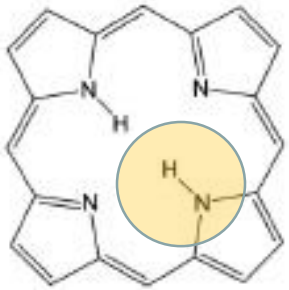


Methionine and tyrosine binding modes

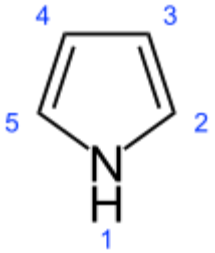
Bioligands – Porphyrins and Related



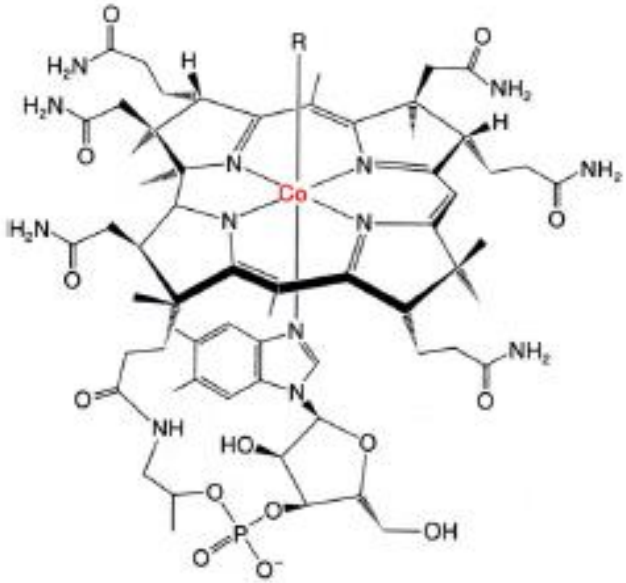
Corrin

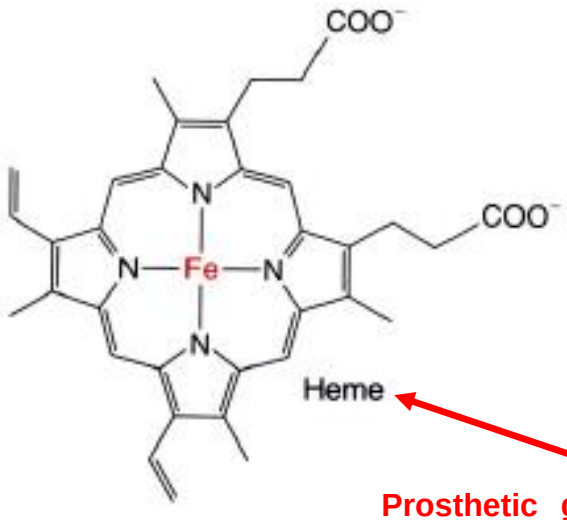


Porphyrin



pyrrole

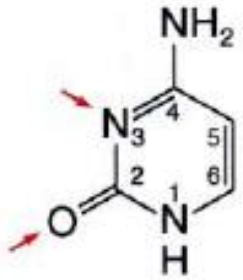




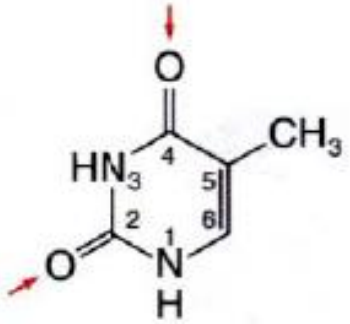
Prosthetic group in – among others – hemoglobin, myoglobin, cytochromes

Bioligands – Nucleobases

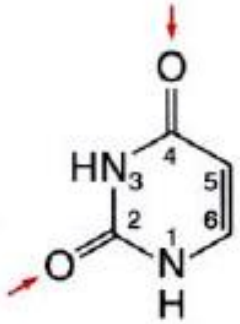
binding sites



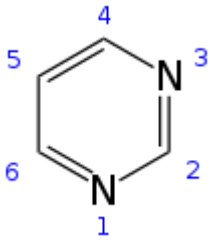
Cytosine



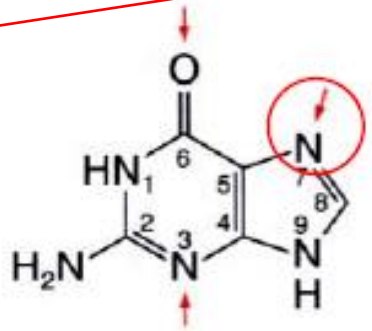
Thymine



Uracil

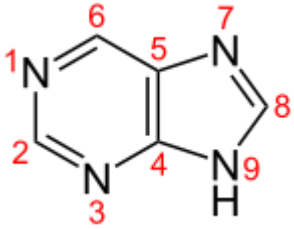


Pyrimidine



Guanine

Adenine

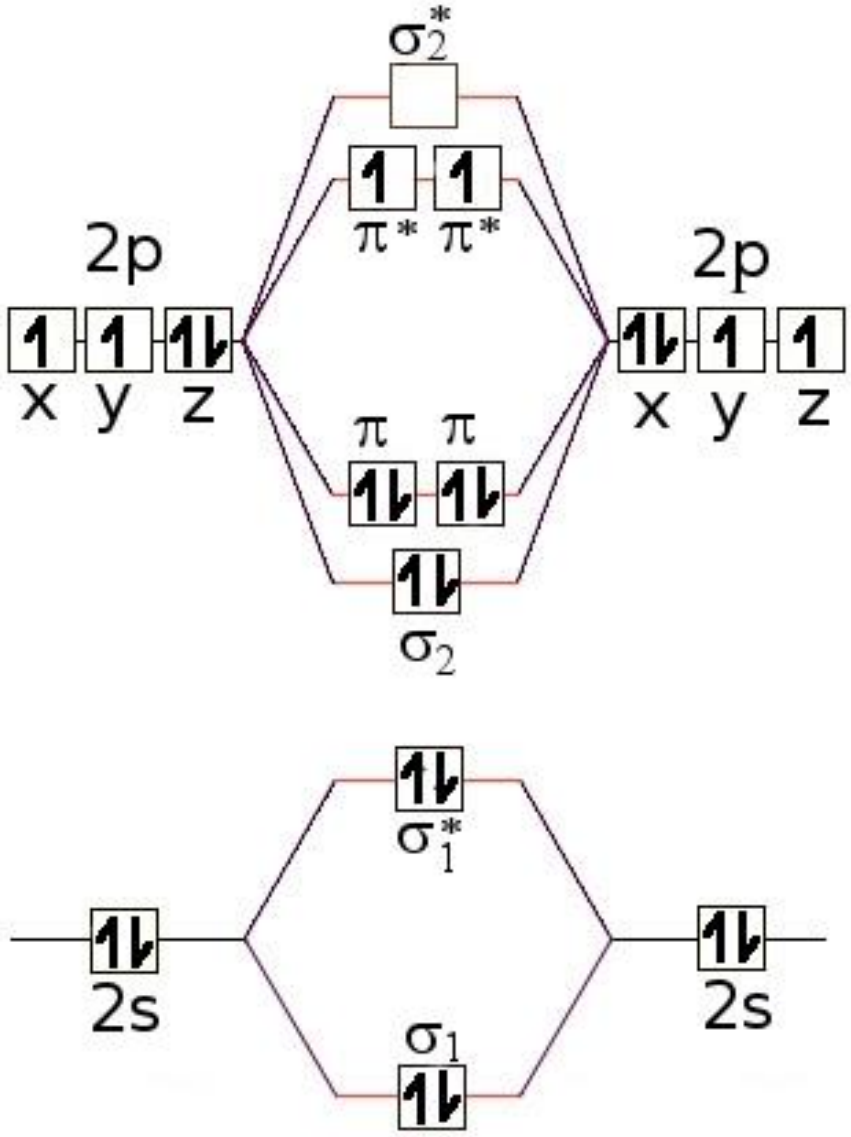


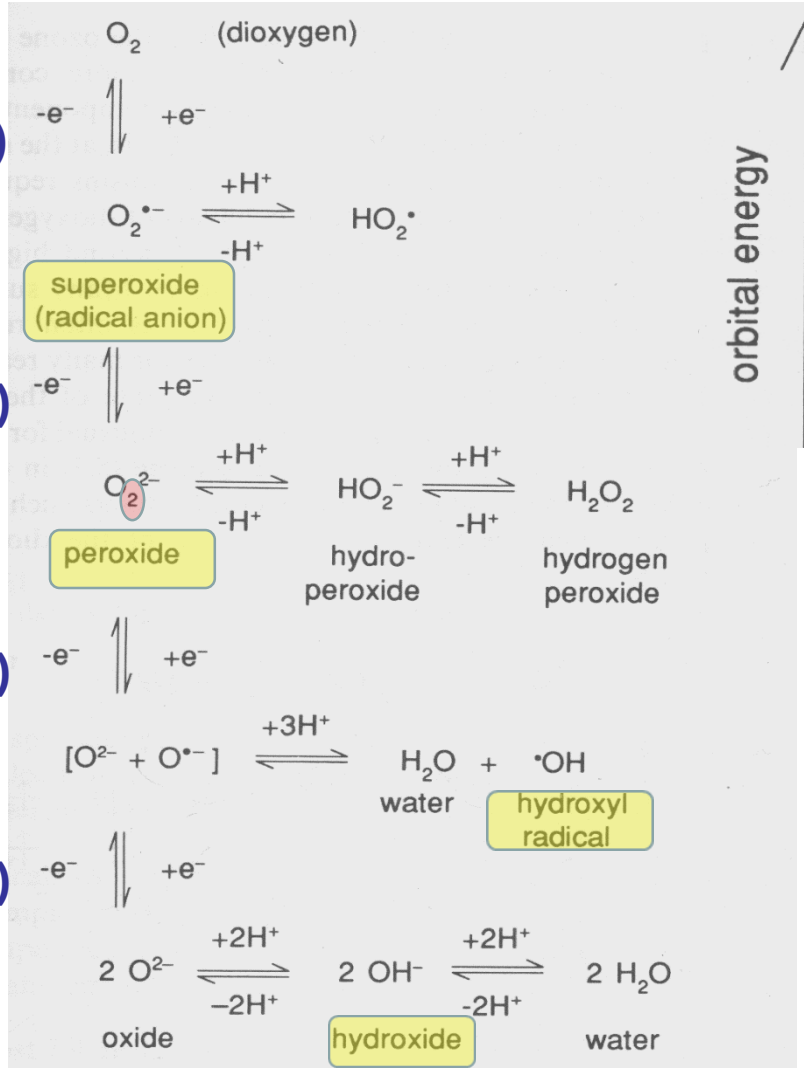
Purine

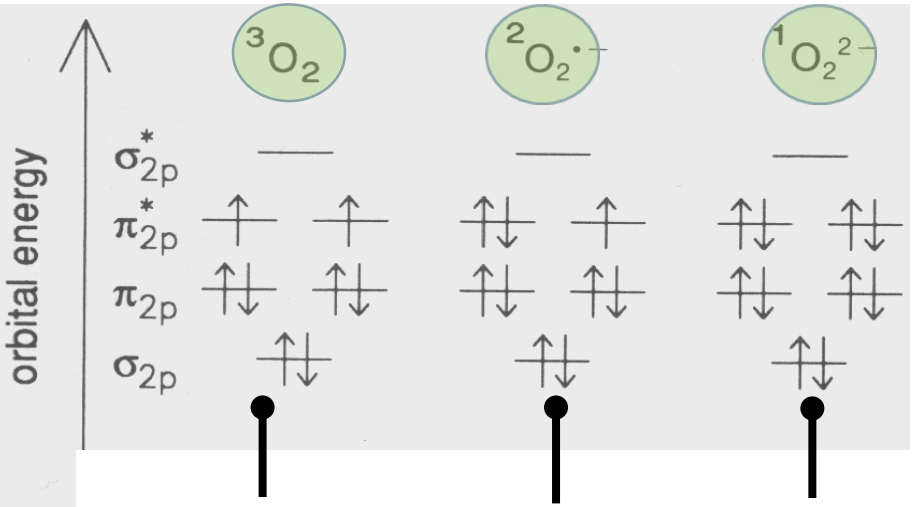
L’ossigeno come accettore di :

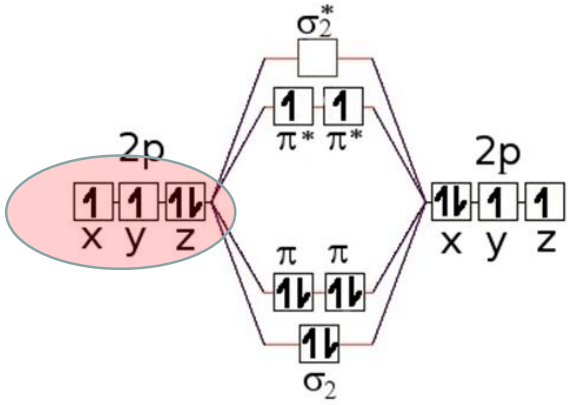
- elettroni
- energia

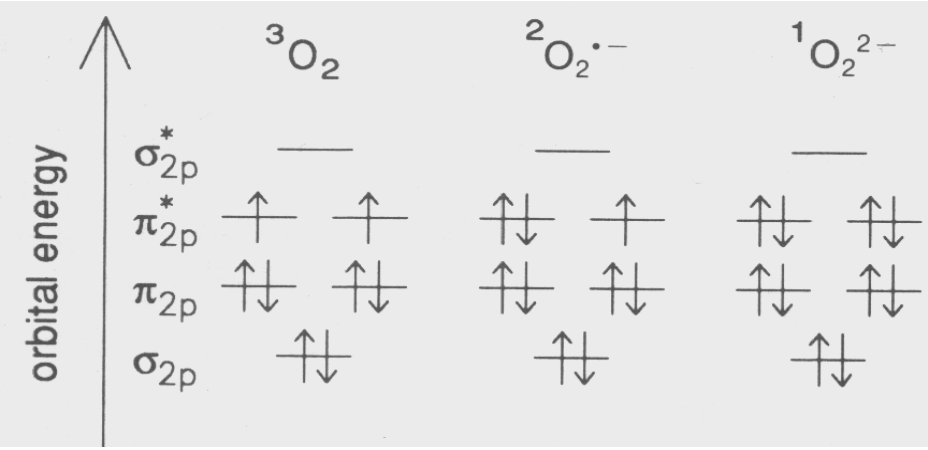
L’ossigeno come accettore di elettroni




O2 (dioxygen)
1)
-e⁻ +e⁻
O2•⁻ +H⁺ -H⁺ HO2•
superoxide (radical anion)
2)
-e⁻ +e⁻
O2 2⁻ +H⁺ -H⁺ HO2⁻ +H⁺ -H⁺ H2O2
peroxide
hydro-peroxide
hydrogen peroxide
3)
-e⁻ +e⁻
[O²⁻ + O•⁻] +3H⁺ H2O + •OH
water
hydroxyl radical
4)
-e⁻ +e⁻
2 O²⁻ +2H⁺ −2H⁺ 2 OH⁻ +2H⁺ -2H⁺ 2 H2O
oxide
hydroxide
water


orbital energy
σ*2p
π*2p
π2p
σ2p
molecular oxygen
superoxide
peroxide


σ*2
π* π*
2p
x y z
π π
σ2
2p
x y z



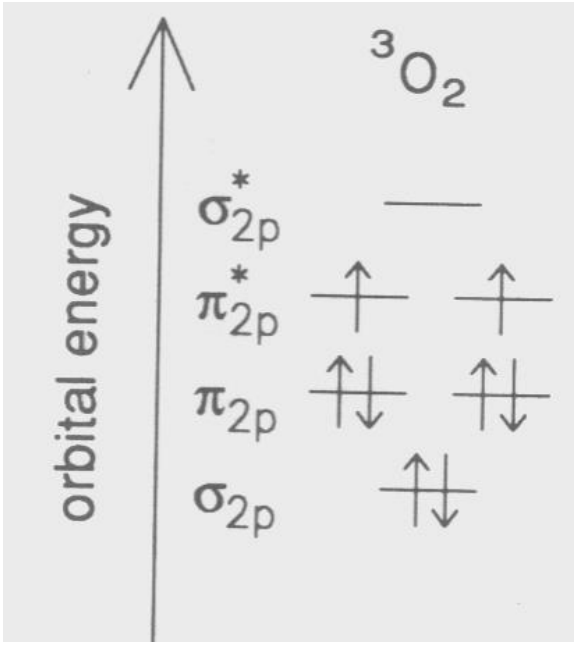
la molteplicità di spin* vale $2S + 1$

Stato	S	**Molteplicità di spin**	**Valori possibili di $m_S=S_Z/\hbar$**
Singoletto	0	1	0
Doppietto	1/2	2	±½
Tripletto	1	3	0, ±1
Quadrupletto	3/2	4	±1/2, ±3/2
...	...	...	...
(2S + 1)-pletto	S	$2S + 1$	S, S-1, ..., -S+1, -S

***numero di stati degeneri in energia per un sistema avente molteplici valori della componente di *s* lungo una direzione**

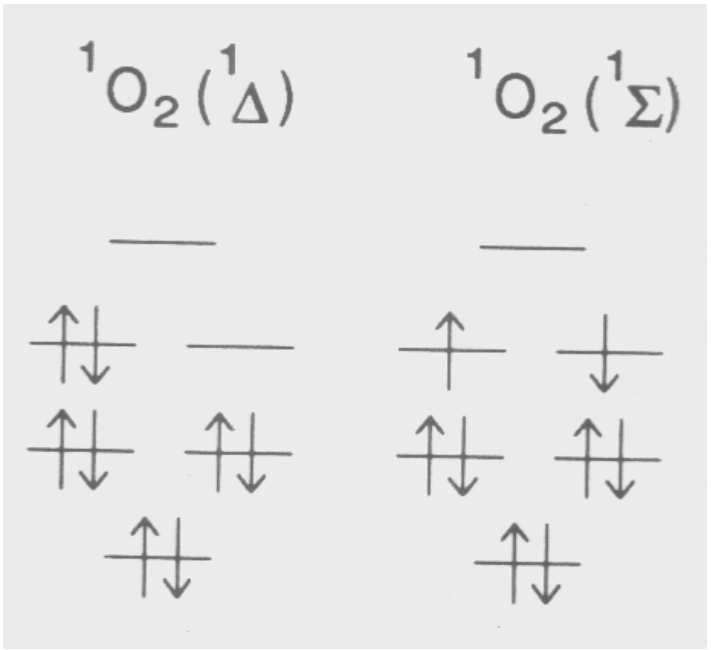
L’ossigeno come accettore di energia

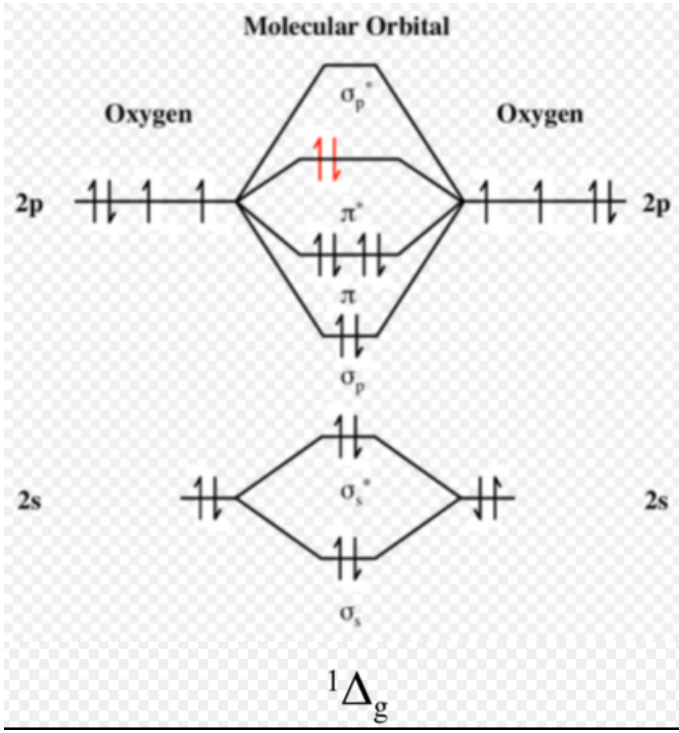
Ossigeno Tripletto



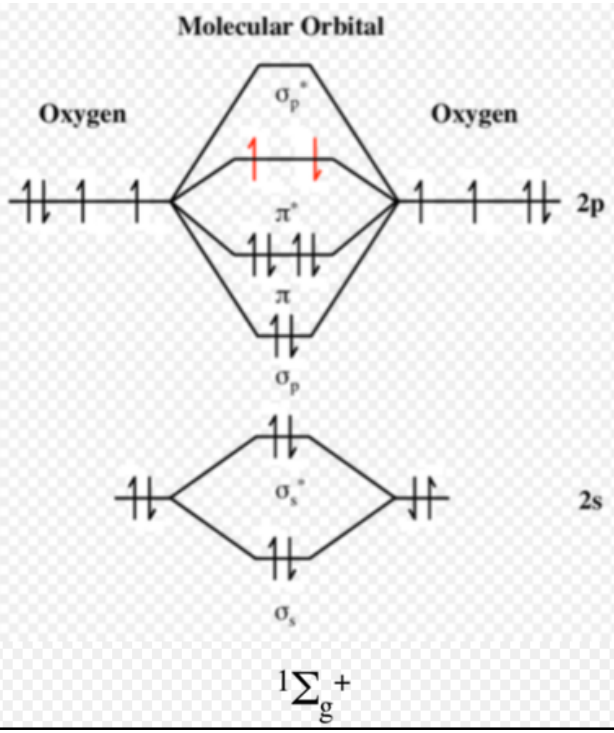
Energia

Ossigeno Singoletto

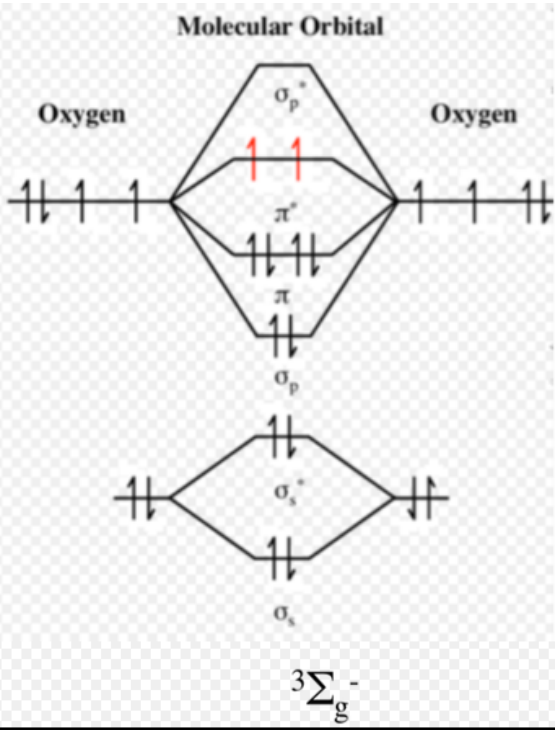




$^1\Delta_g$



$^1\Sigma_g^+$



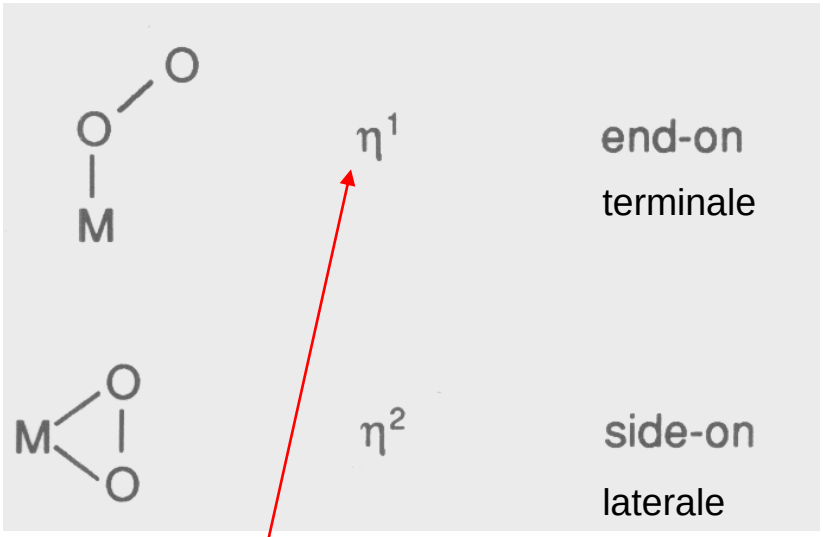
$^3\Sigma_g^-$

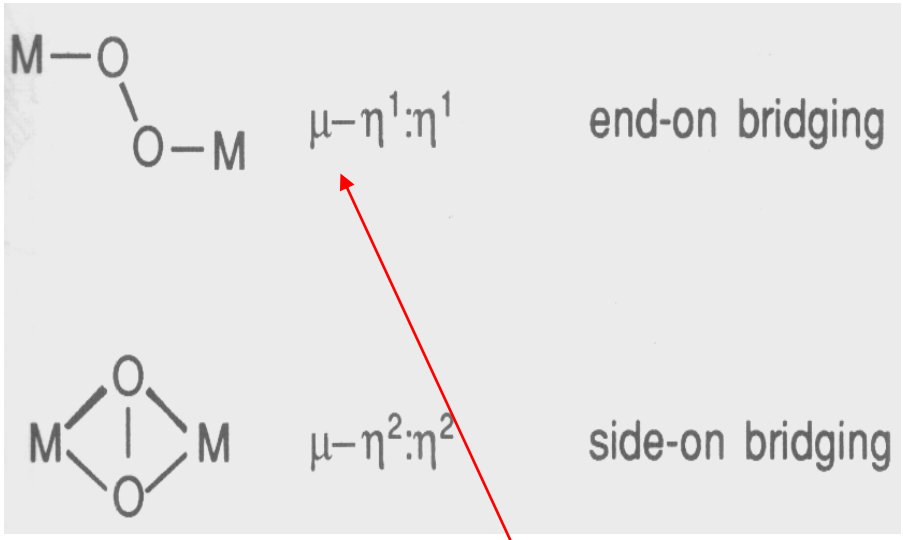
+ 94 kJ/mol

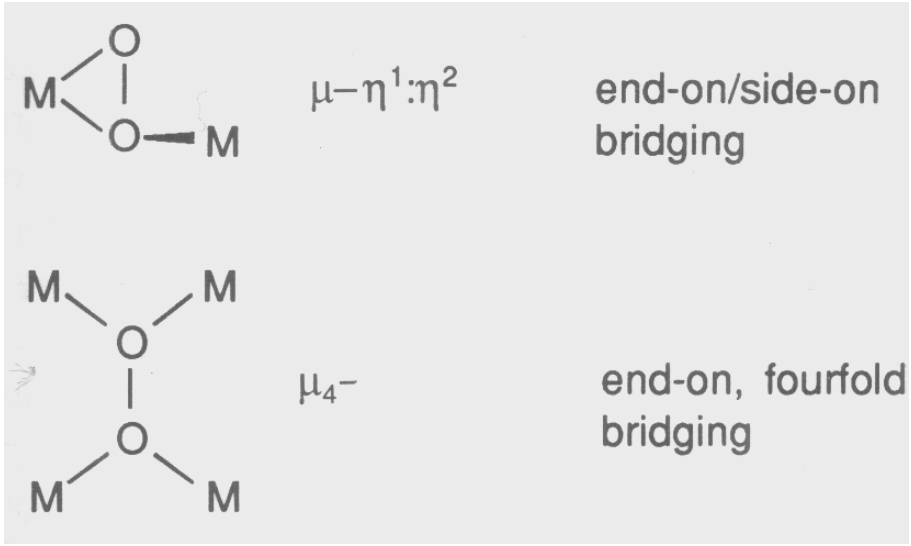
+ 157 kJ/mol

tripletto

L'ossigeno come legante: tipi di coordinazione







il legante a ponte è preceduto dalla lettera greca μ con un numero a pedice per denotare il numero di metalli collegati

apticità: η^n con *n* si indica il numero di atomi contigui del legante che sono legati al metallo