Instituto de Química – USP

QFL 0450

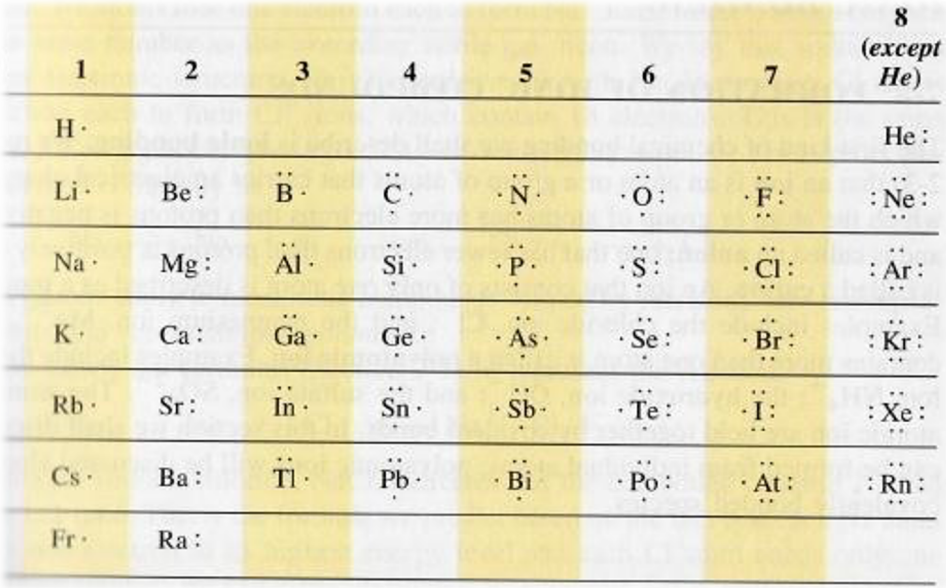
Química Geral e Orgânica para Biomedicina

Ligações Químicas, Teoria dos Orbitais Moleculares e a Teoria da Repulsão dos Pares de Elétrons de Valência

Lewis e os elétrons de valência

Camada de valência: é o nome dado à última camada de um átomo

Representação de Lewis: elemento rodeado de pontos representativos dos elétrons de valência



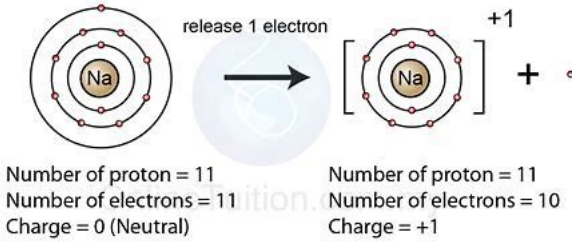
1	2	3	4	5	6	7	8 (except He)
H·							He:
Li·	Be:	·B·	·C·	·N·	·O:	·F:	:Ne:
Na·	Mg:	·Al·	·Si·	·P·	·S:	·Cl:	:Ar:
K·	Ca:	·Ga·	·Ge·	·As·	·Se:	·Br:	:Kr:
Rb·	Sr:	·In·	·Sn·	·Sb·	·Te:	·I:	:Xe:
Cs·	Ba:	·Tl·	·Pb·	·Bi	·Po:	·At:	:Rn:
Fr·	Ra:						

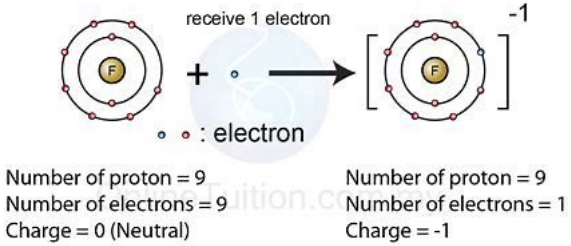
← Elétrons de valência

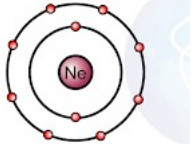
Ligações iônicas vs ligações covalentes

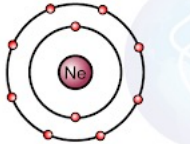
Lewis e a regra do octeto → tendência de formar a camada do gás nobre mais próximo

Eletrovalência vs Covalência

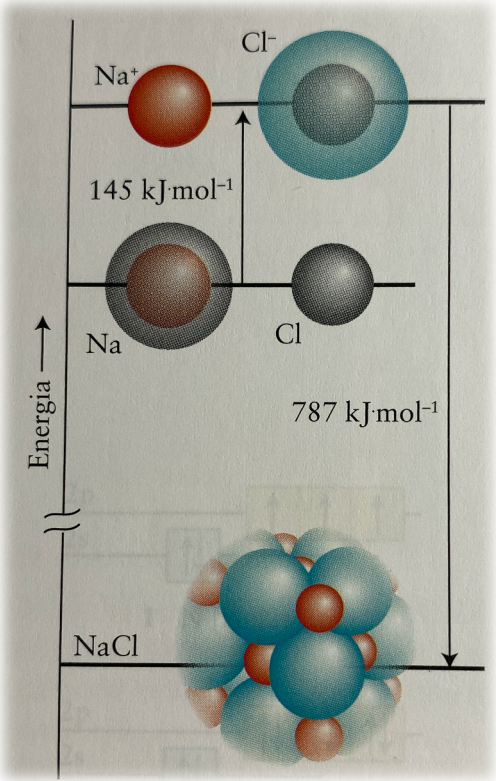






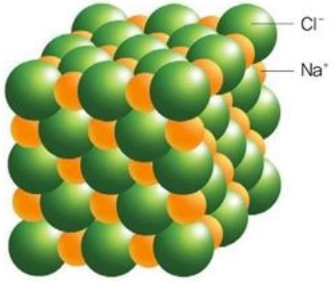


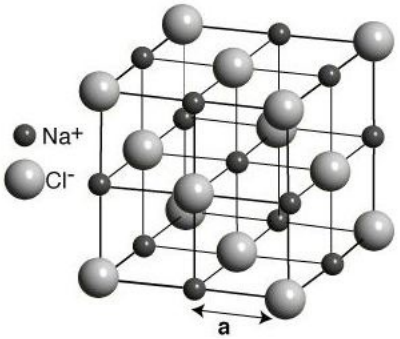
A ligação iônica



EI (Na) = 494 kJ/mol
AE (Cl) = -349 kJ/mol
Net = 145 kJ/mol

Energia de rede cristalina = 787 kJ/mol
Net = -642 kJ/mol

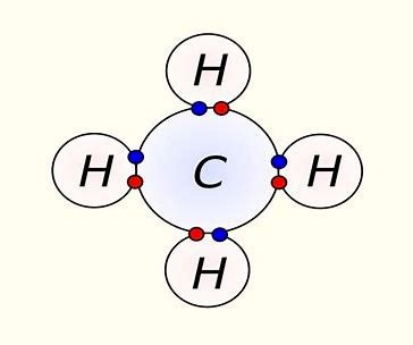


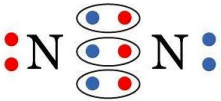


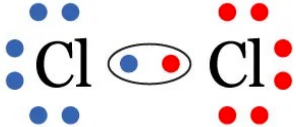
A ligação covalente

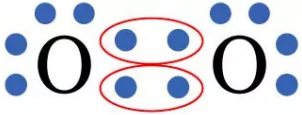
Lewis e a regra do octeto → tendência de formar a camada do gás nobre mais próximo

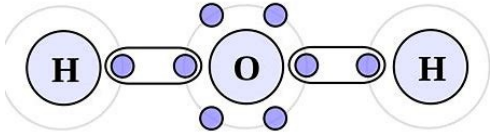
Compartilhamento de elétrons → ligação covalente











Triângulo de Ketelaar

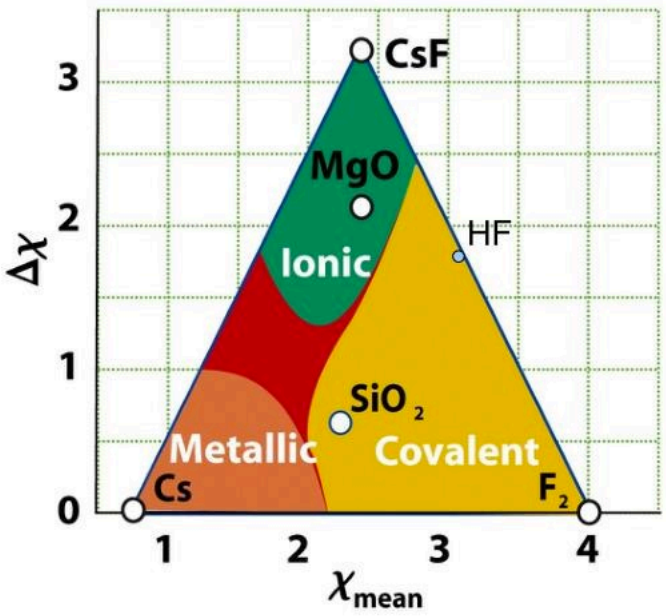
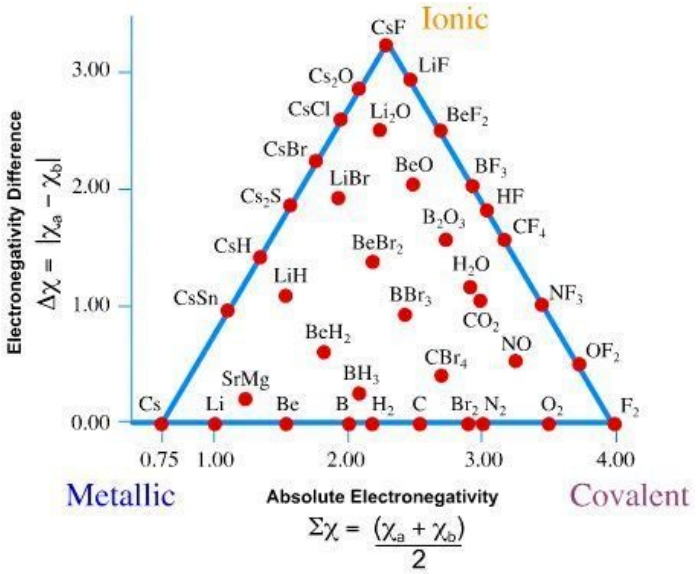
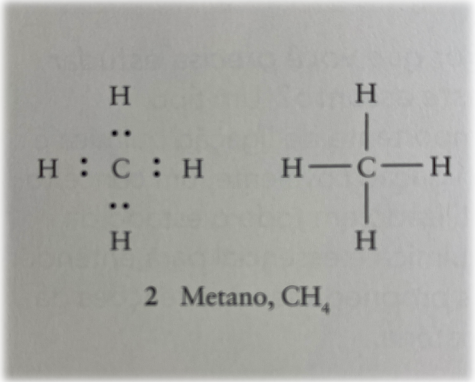
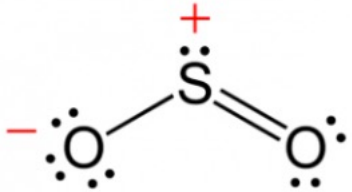


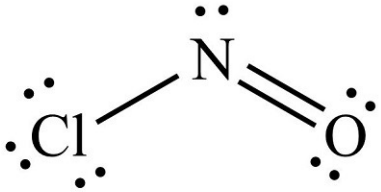
Figure 2-2
Shriver & Atkins Inorganic Chemistry, Fourth Edition
© 2006 by D. F. Shriver, P. W. Atkins, T. L. Overton, J. P. Rourke, M. T. Weller, and F. A. Armstrong

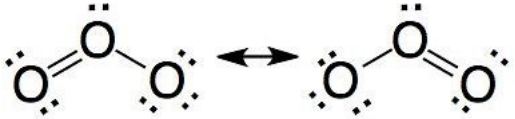


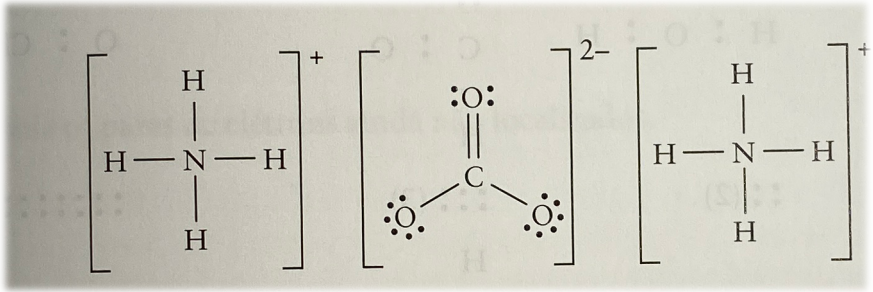
Representação de Lewis e carga formal











$$[carga\ formal] = [e^{-}val] - \left[[e^{-}\text{não } lig] + \frac{[e^{-}lig]}{2}\right]$$

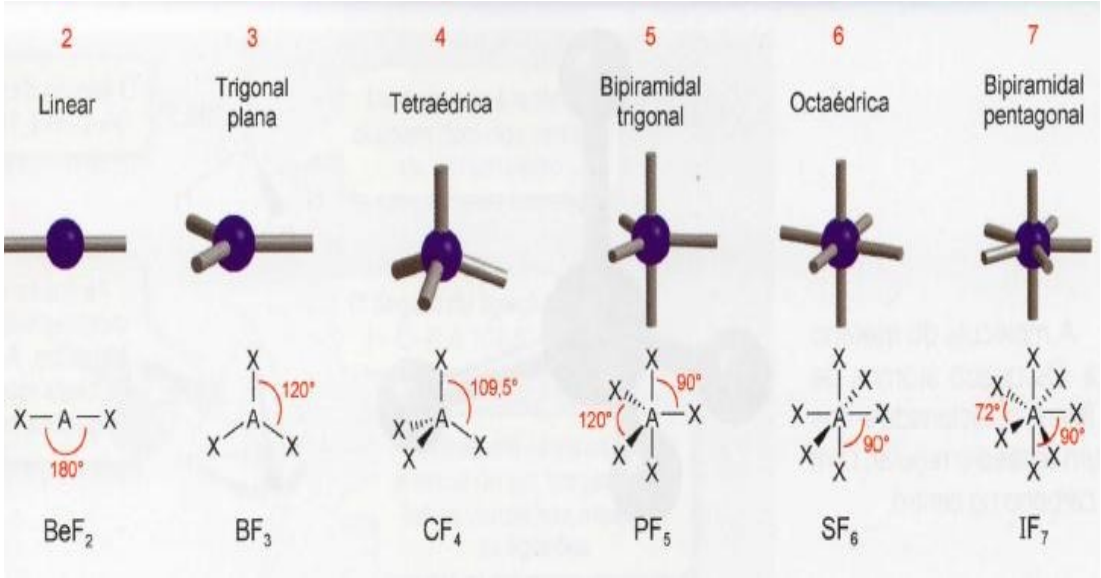
Teoria da repulsão dos pares de elétrons da camada de valência

(Valence shell electron pair repulsion theory)

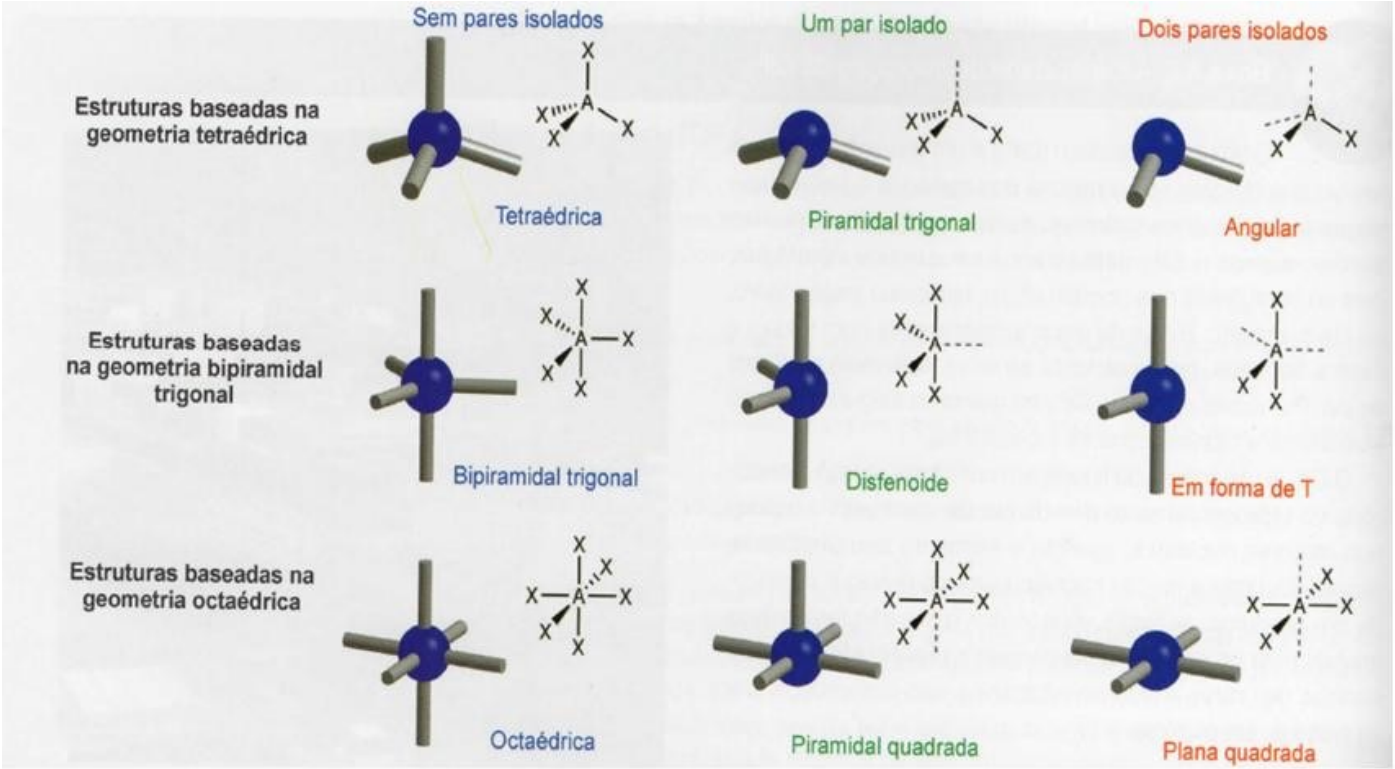
número de densidades eletrônicas

ângulos de ligação

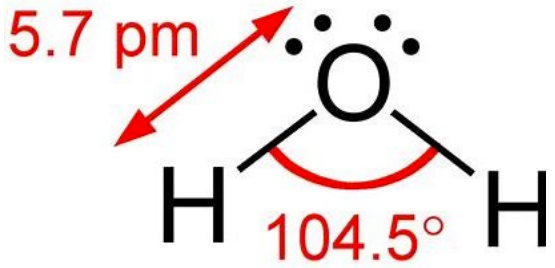
exemplos

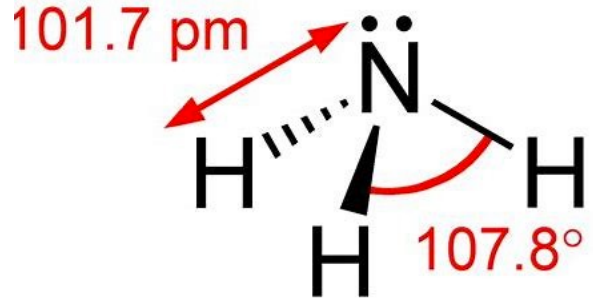


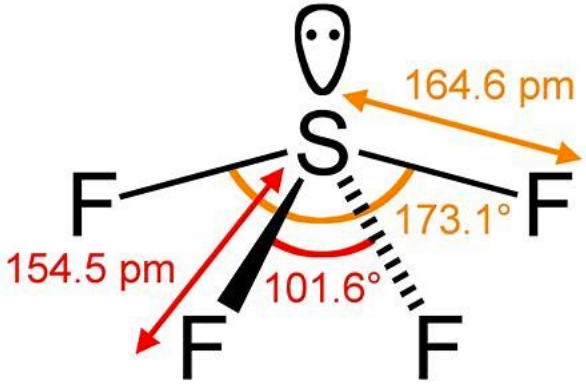
há pares eletrônicos solitários quando ...



Exemplos


5.7 pm
O
H
104.5°
H

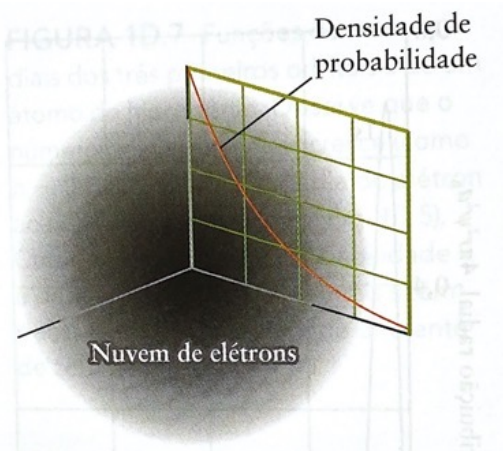

101.7 pm
N
H
H
H
107.8°


164.6 pm
S
F
F
173.1°
154.5 pm
101.6°
F
F

O modelo atômico atual

Modelo Quântico

- Núcleo envolto por nuvem eletrônica
- Probabilidade de encontrar o elétron
- O átomo de hidrogênio e a seu espectro de emissão



A teoria dos orbitais atômicos

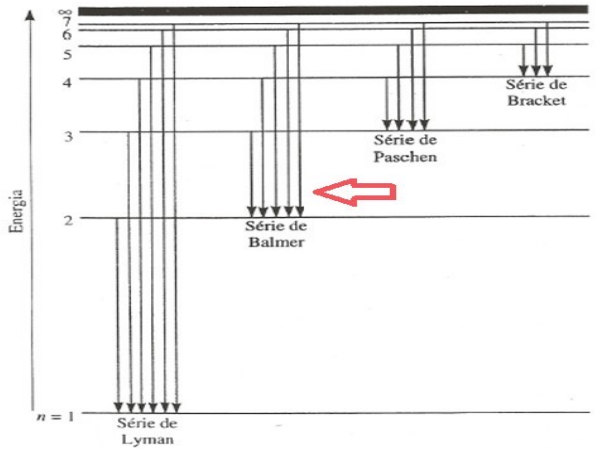
Equação de Schödinger

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\boldsymbol{x})\psi = E\psi$$

$$E_n = -\frac{Z^2 h\mathcal{R}}{n^2}$$

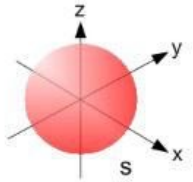
$$n = 1,2,3, \ldots$$

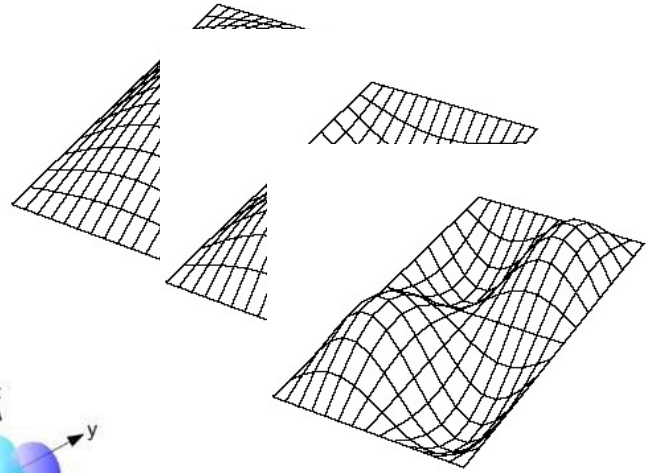
Séries	n_f	n_i	Região espectral
Lyman	1	2, 3, 4, ...	Ultravioleta
Balmer	2	3, 4, 5, ...	Visível e ultravioleta
Paschen	3	4, 5, 6, ...	Infravermelho
Brackett	4	5, 6, 7, ...	Infravermelho

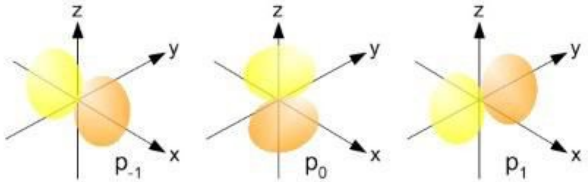


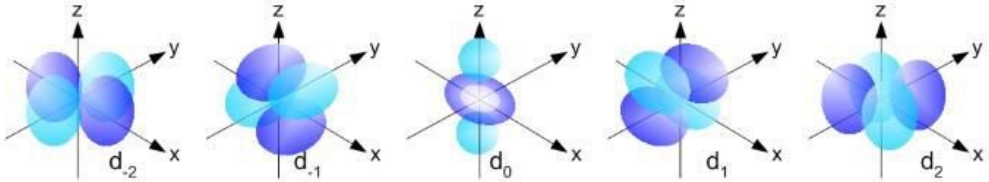
A teoria dos orbitais atômicos

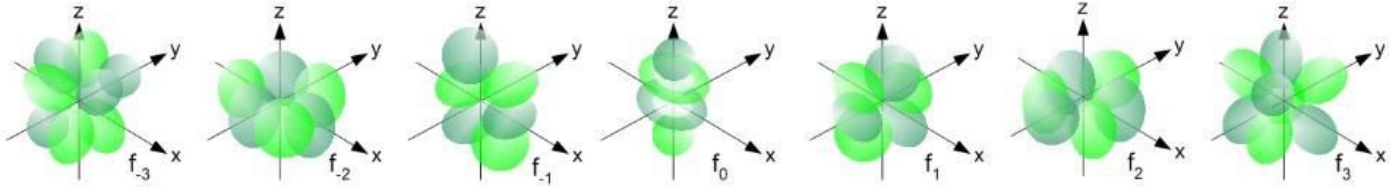
$$L^2\Psi = \hbar^2\, \ell(\ell+1)\, \Psi$$









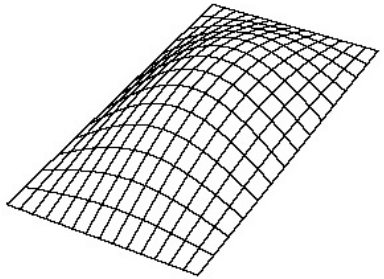


A teoria dos orbitais atômicos

Modos vibracionais de uma membrana retangular

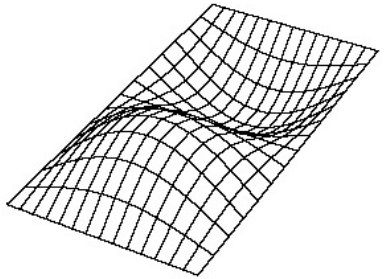
$\ell = 0(s)$

(1,1) mode



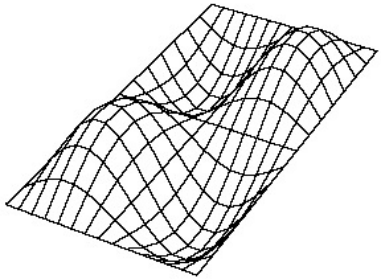
$\ell = 1(p)$

(1,2) mode



$\ell = 2(d)$

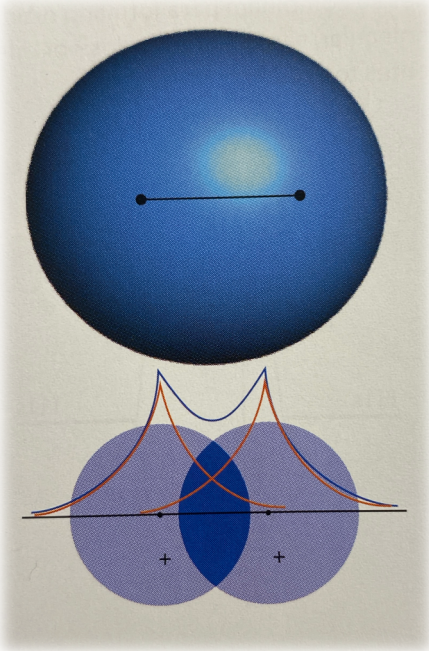
(2,2) mode

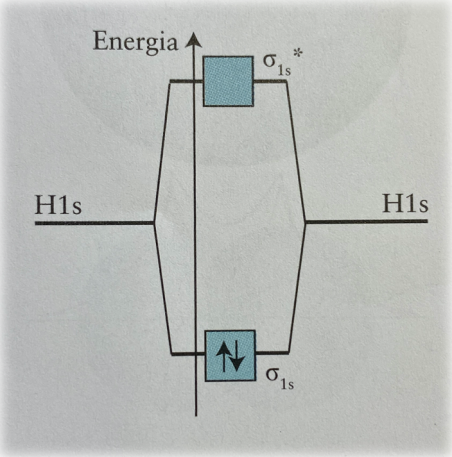


l	SÍMBOLO	SIGNIFICADO
0	S	Sharp
1	p	Principal
2	d	Difuse
3	f	Fundamental

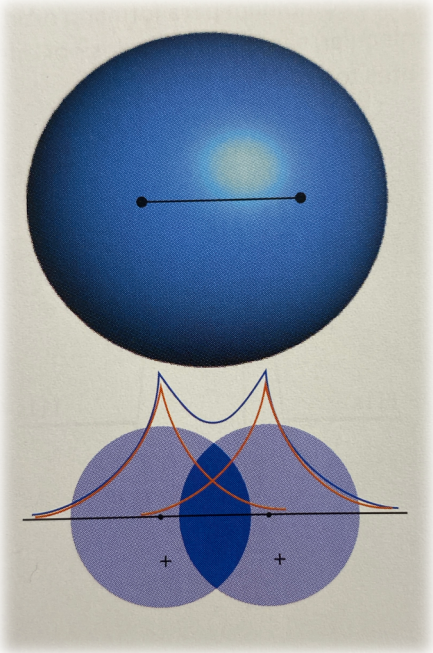
Teoria dos orbitais moleculares

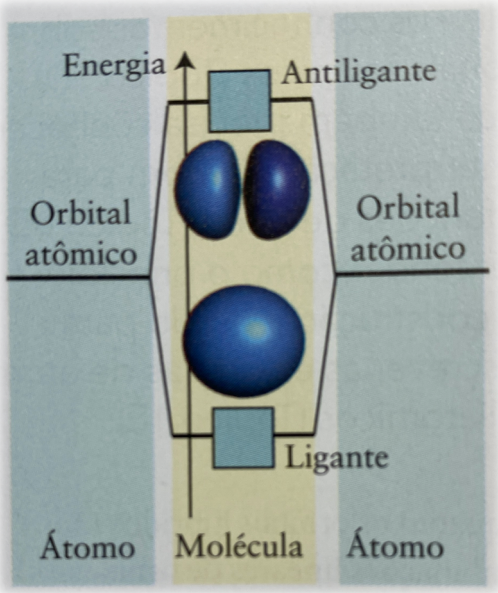
ligação entre dois átomos → orbitais moleculares
formados a partir da combinação linear de orbitais atômicos
(LCAO – linear combination of atomic orbitals)





Teoria dos orbitais moleculares





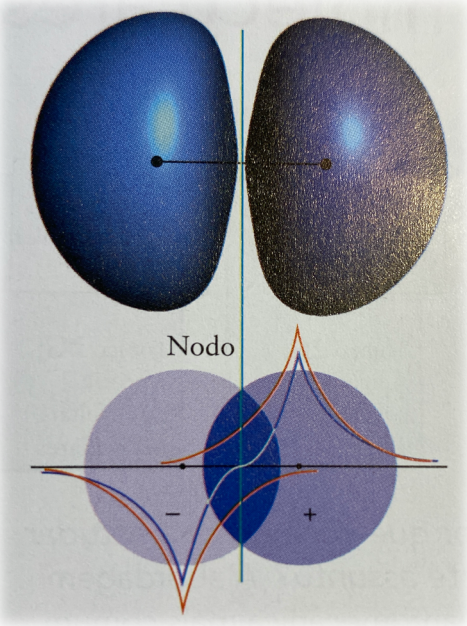
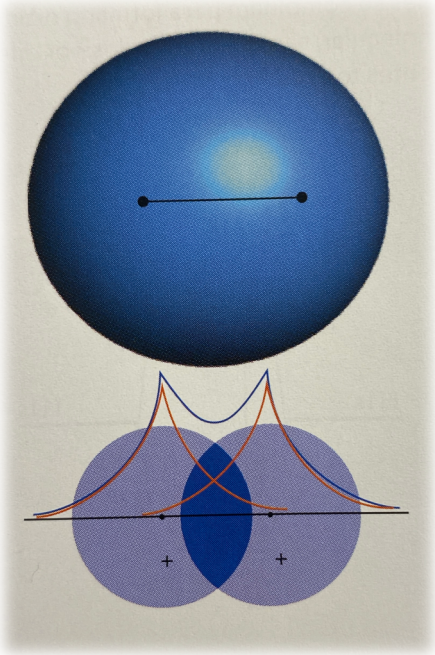
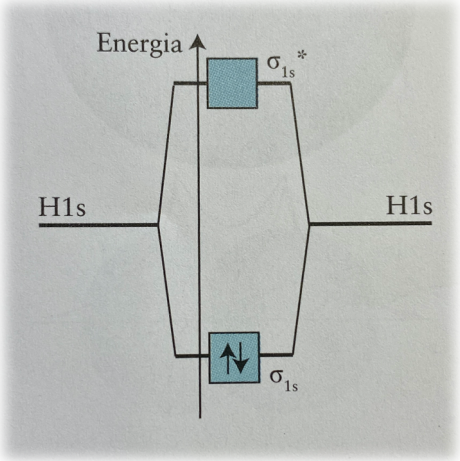


Diagrama de níveis de energia

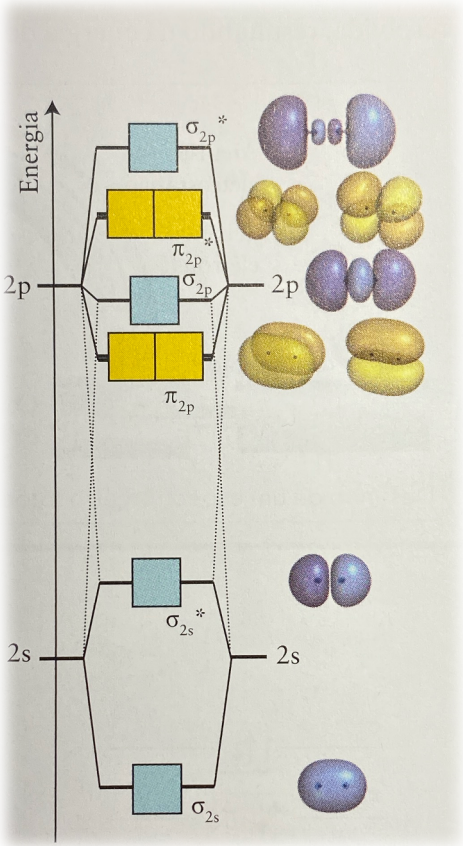
A ocupação dos OM segue a mesma ordem dos AO (Pauli e Hund)

OM de moléculas diatômicas

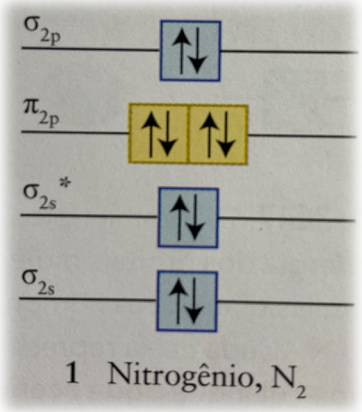




OM de moléculas diatômicas

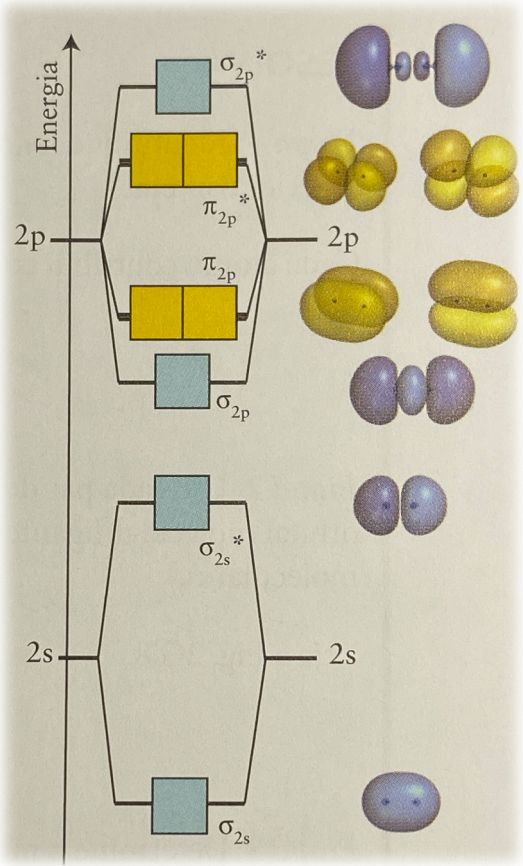


	1s	2s	2p
$_3$Li	↑↓	↑	
$_4$Be	↑↓	↑↓	
$_5$B	↑↓	↑↓	↑ _ _
$_6$C	↑↓	↑↓	↑ ↑ _
$_7$N	↑↓	↑↓	↑ ↑ ↑
$_8$O	↑↓	↑↓	↑↓ ↑ ↑
$_9$F	↑↓	↑↓	↑↓ ↑↓ ↑
$_{10}$Ne	↑↓	↑↓	↑↓ ↑↓ ↑↓

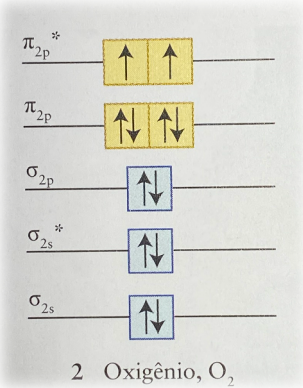


1 Nitrogênio, N_2

OM de moléculas diatômicas

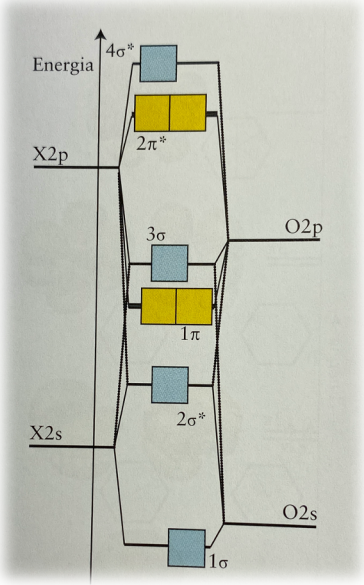


	1s	2s	2p
$_3$Li	↑↓	↑	
$_4$Be	↑↓	↑↓	
$_5$B	↑↓	↑↓	↑ _ _
$_6$C	↑↓	↑↓	↑ ↑ _
$_7$N	↑↓	↑↓	↑ ↑ ↑
$_8$O	↑↓	↑↓	↑↓ ↑ ↑
$_9$F	↑↓	↑↓	↑↓ ↑↓ ↑
$_{10}$Ne	↑↓	↑↓	↑↓ ↑↓ ↑↓



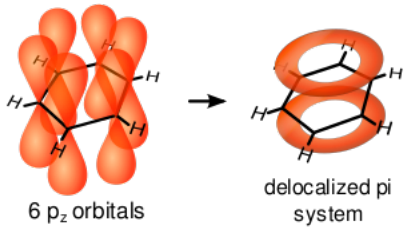
2 Oxigênio, O_2

OM de moléculas hetero- e multiatômicas



:C≡O:

112.8 pm



6 p_z orbitals

delocalized pi system

Benzene ring
Simplified depictior