Geometria das moléculas

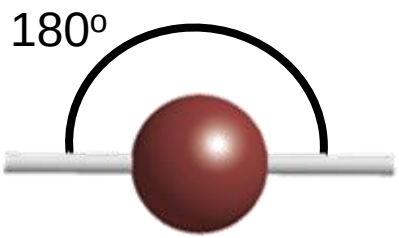
Prof. Dr. Andrei Leitão

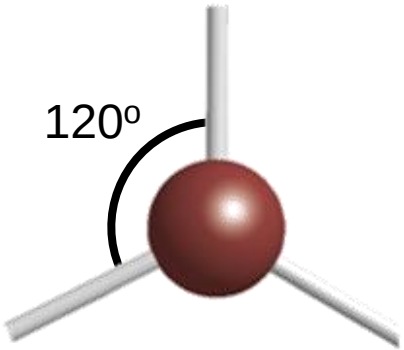
Modelo da Repulsão dos Pares de Elétrons da Camada de Valência

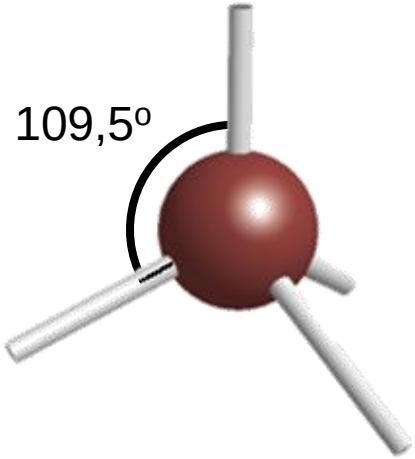
- ✓ Estrutura das moléculas → repulsões entre elétrons na camada de valência;
- ✓ Par de elétrons não-ligante (maior volume)
- ✓ Disposição dos átomos (A - central e X - outros) e par de elétrons (E): AX_nE_m
- ✓ Presença de insaturações
- ✓ Influência da eletronegatividade

Formas

Ângulos







linear

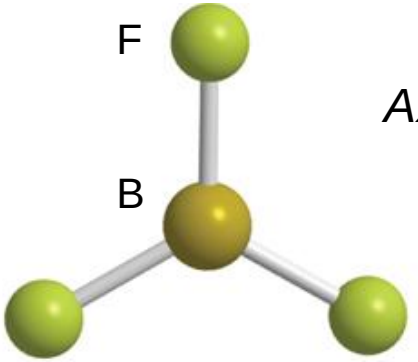
trigonal plana

tetraédrica

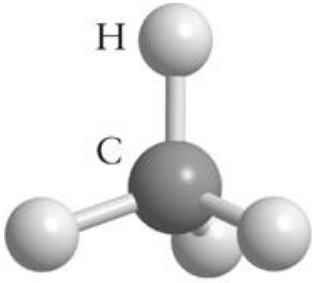
AX

HF

AX$_3$



AX$_4$



AX$_2$

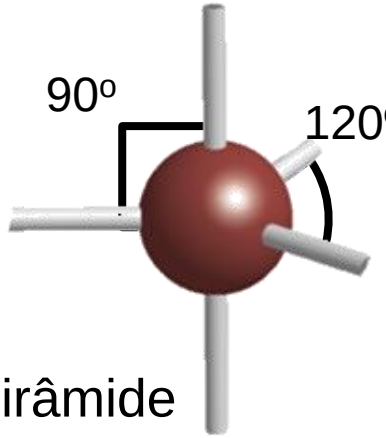
$BeCl_2$

BF_3

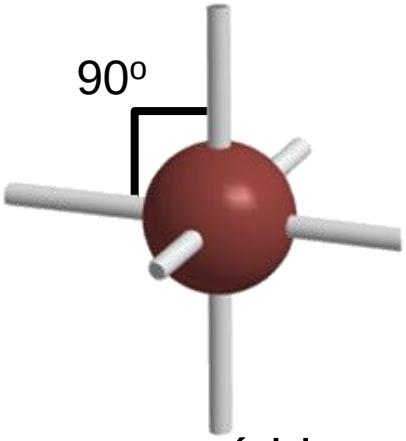
CH_4

Formas

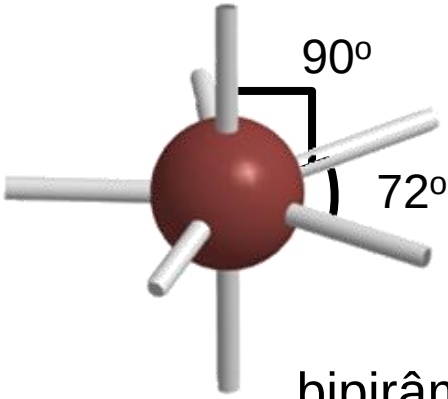
Ângulos



bipirâmide trigonal

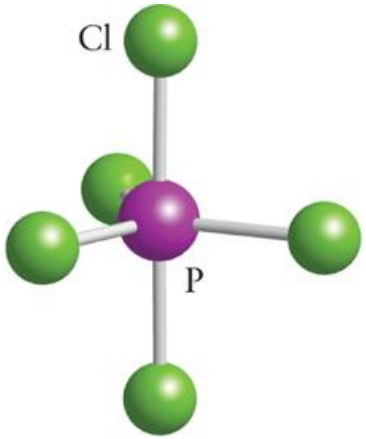


octaédrica



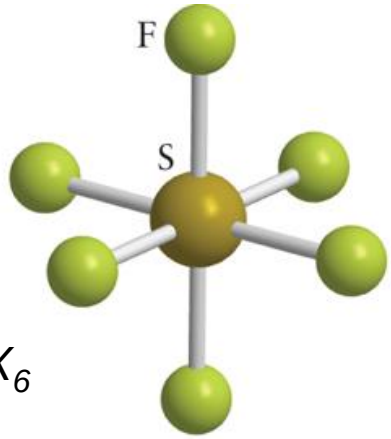
bipirâmide pentagonal

AX_5



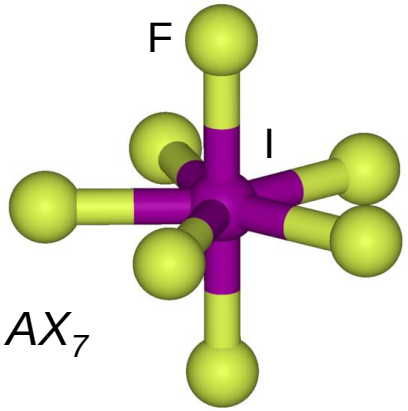
PCl_5

AX_6



SF_6

AX_7

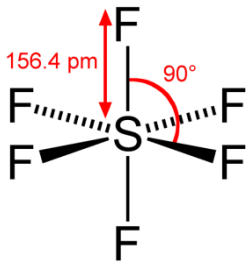


IF_7

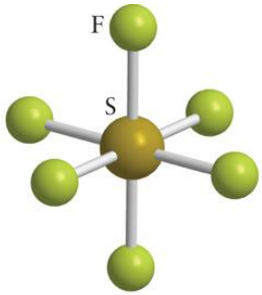
Arranjo dos elétrons e forma

SF_6

- ✓ Estabelecer a estrutura de Lewis



- ✓ Estabelecer o arranjo dos elétrons



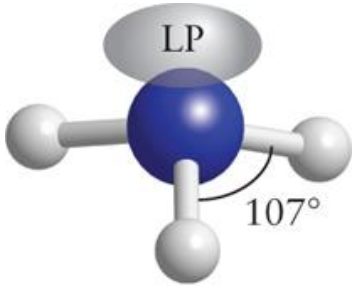
- ✓ Identificar da geometria (forma) **AX_6 octaédrica**

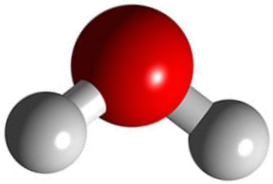
- ✓ Verificar as distorções **Não há**

Arranjo dos elétrons e forma

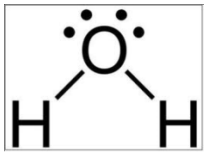
- ✓ A amônia (NH_3) não é trigonal plana e a água (H_2O) não é planar

AX_3E



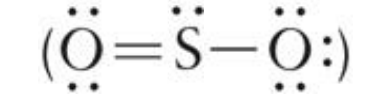


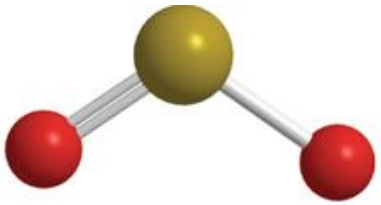
Arranjo dos elétrons	tetraédrico	tetraédrico
Forma (geometria)	pirâmide trigonal	angular



- Repulsão elétron-elétron > elétron-átomo > átomo -átomo

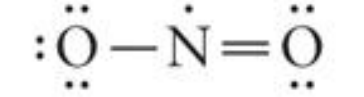
Presença de elétrons não-ligantes no átomo central

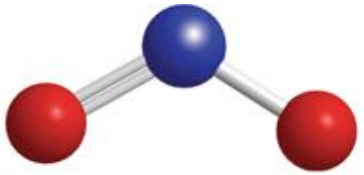




SO_2

AX_2E angular

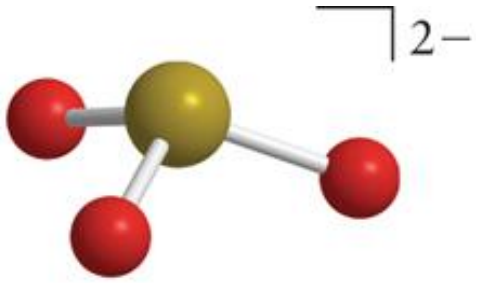




NO_2

angular

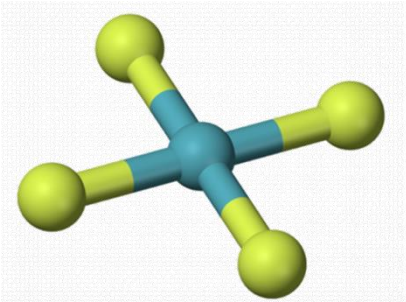
AX_3E



SO_3^{2-}

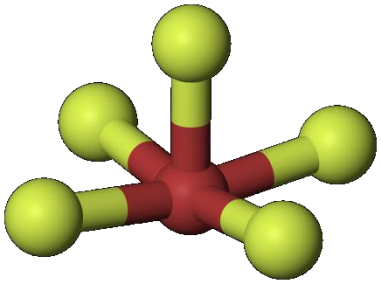
tetraédrica

Formas



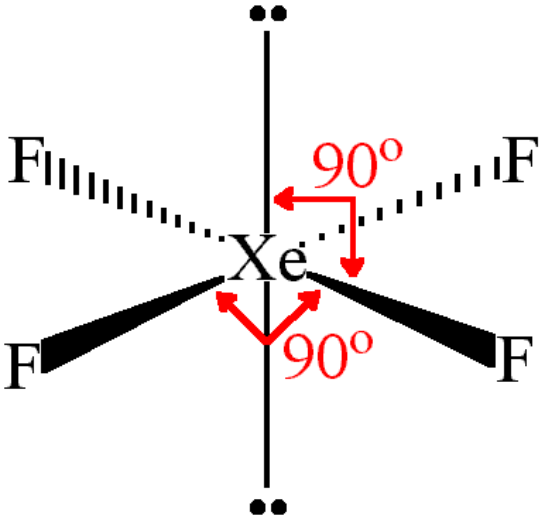
XeF_4

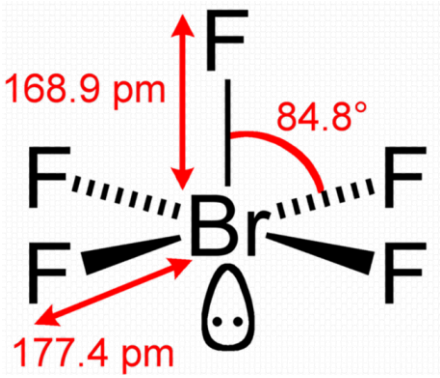
AX_4E_2 quadrática



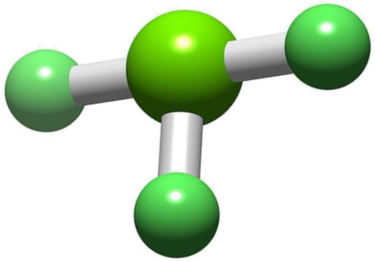
BrF_5

AX_5E Pirâmide quadrada



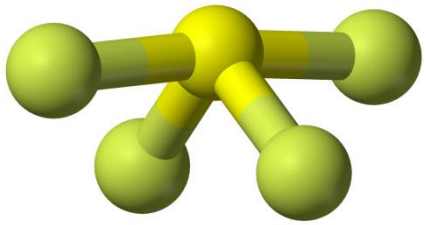


Formas



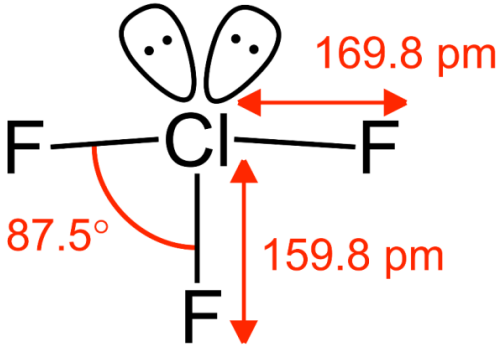
ClF_3

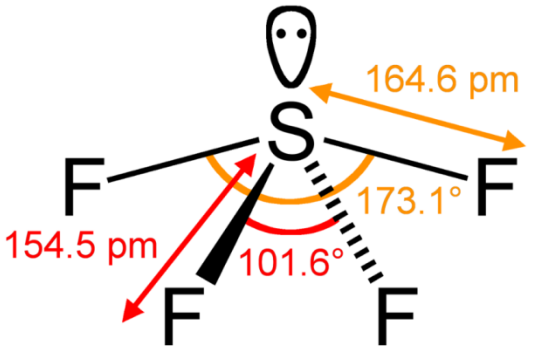
AX_3E_2 forma de T



SF_4

AX_4E gangorra

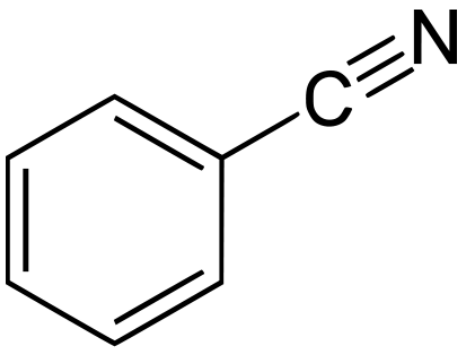




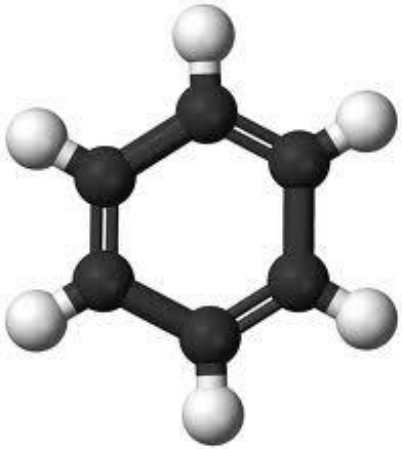
Presença de insaturações

CO_2

AX_2



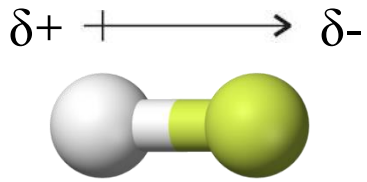
C_7H_5N



C_6H_6

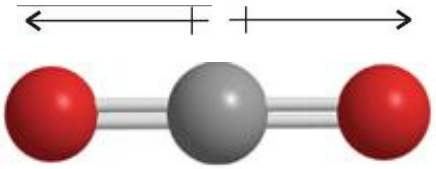
Moléculas polares e apolares

H-F
$\mu = 1{,}91$ D



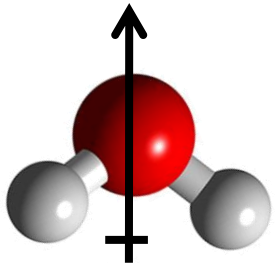
CO
$\mu = 0{,}12$ D

CO_2
$\mu = 0$ D



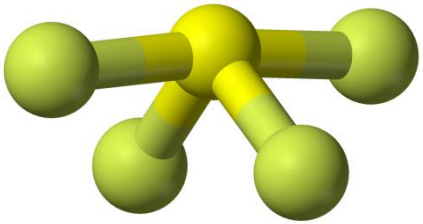
HO
$\mu = 0{,}?5$ D

H_2O
$\mu = 1{,}85$ D



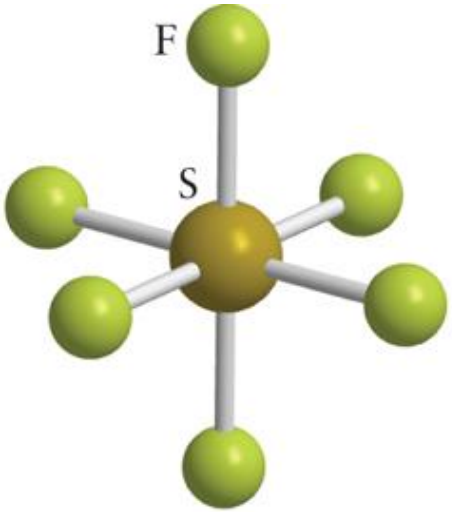
Moléculas polares e apolares

Quais moléculas são polares?



SF_4

AX_4E gangorra



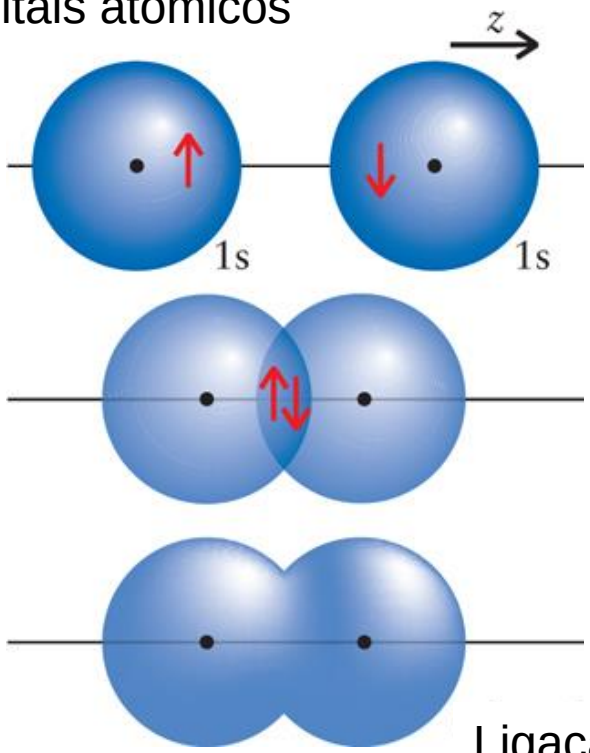
SF_6

AX_6 octaédrica

Teoria de ligação de valência (TLV)

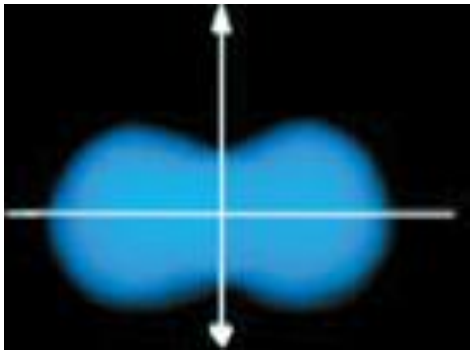
✓ Descreve a formação da ligação química a partir da química quântica

Orbitais atômicos



Ligação σ

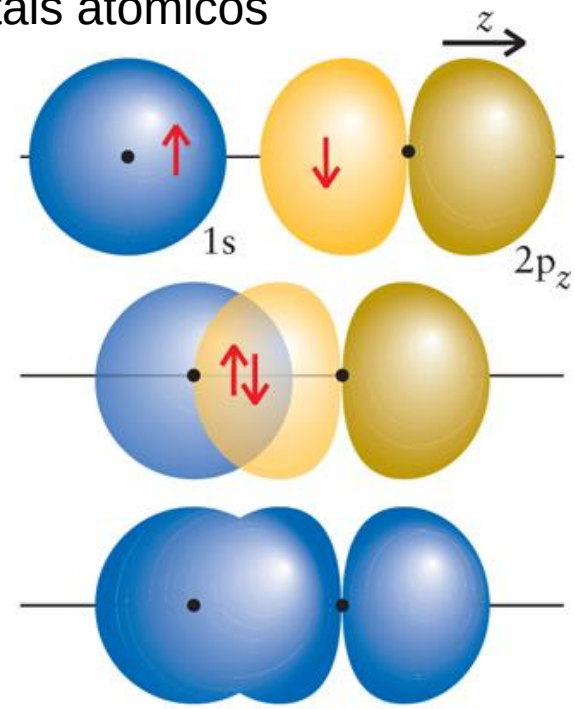
Ligação σ



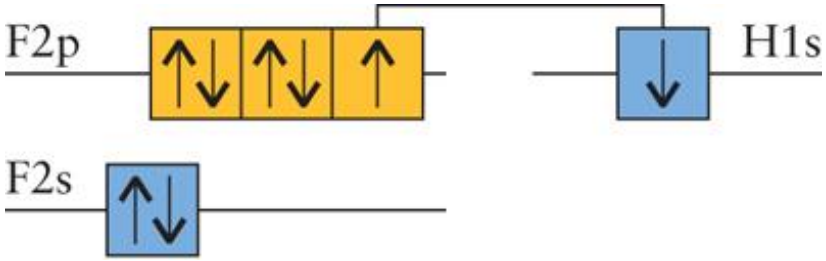
H-H

Ligação σ

Orbitais atômicos



Ligação σ

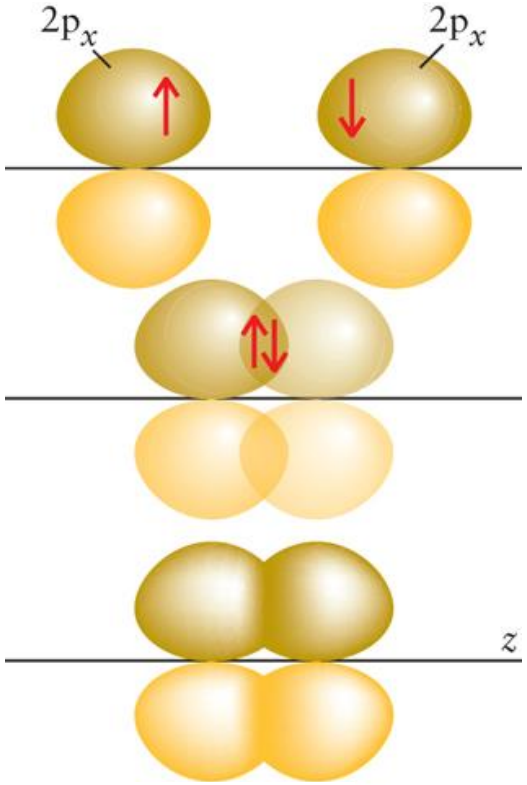


Ligação σ

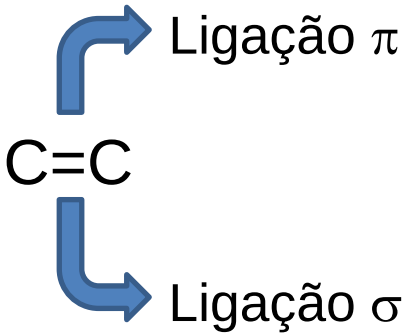
H-F

Ligação π

Orbitais atômicos

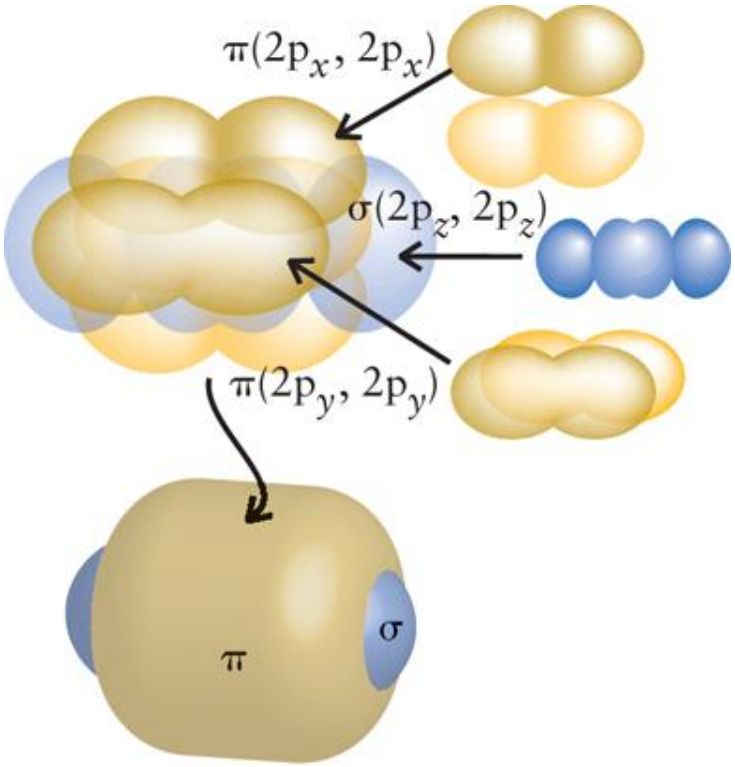


Ligação π

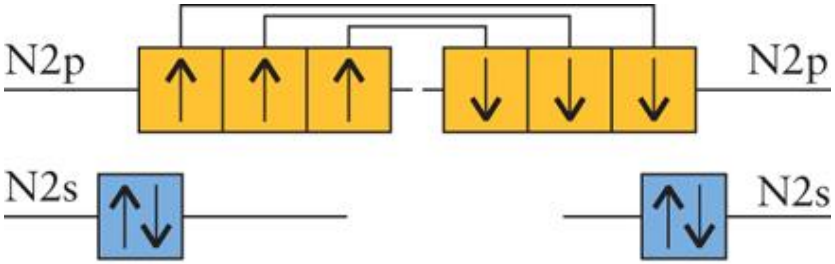


Ligação π

Orbitais atômicos



2 ligações π e 1 σ



N_2

N≡N

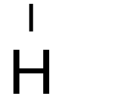
- Ligação π
- Ligação π
- Ligação σ

Moléculas

CO_2

O=C=O

NH_3



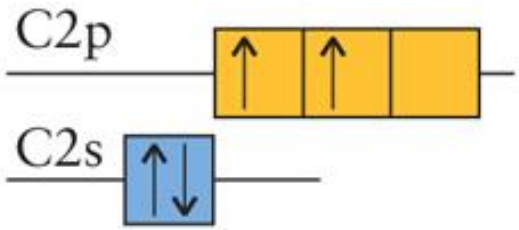
HCN

H-C≡N

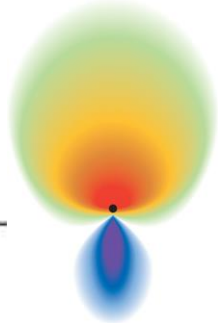
Qual é o número de ligações σ e π formadas?

Hibridização de orbital

Distribuição eletrônica

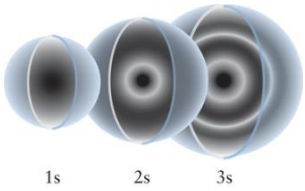


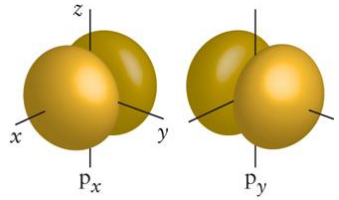
$[He]2s^2 2p_x^{\ 1} 2p_y^{\ 1}$

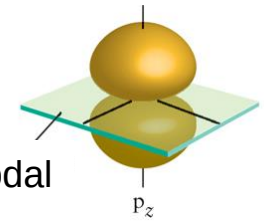


Hibridização

$\mathcal{h}_1 = s + p_x + p_y + p_z$
$\mathcal{h}_2 = s - p_x - p_y + p_z$
$\mathcal{h}_3 = s - p_x + p_y - p_z$
$\mathcal{h}_4 = s + p_x - p_y - p_z$







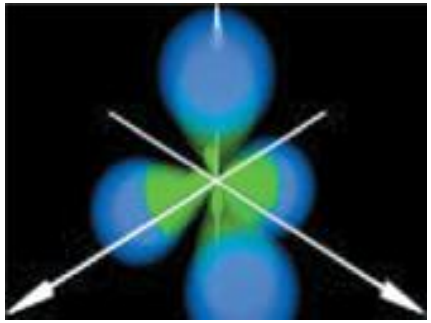
Plano nodal

90º

CH_4

tetraédrico
(109,5º)

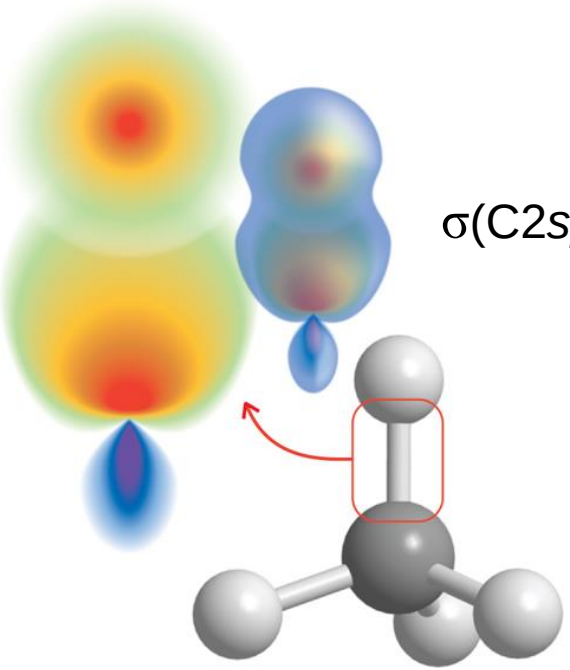
Hibridização - metano



sp^3-s

Hibridização & ligação

H1s



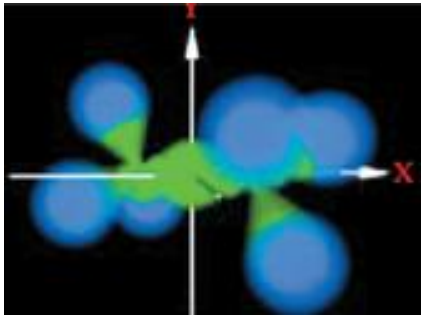
σ(C2sp^3-H1s)

C2sp^3

CH_4

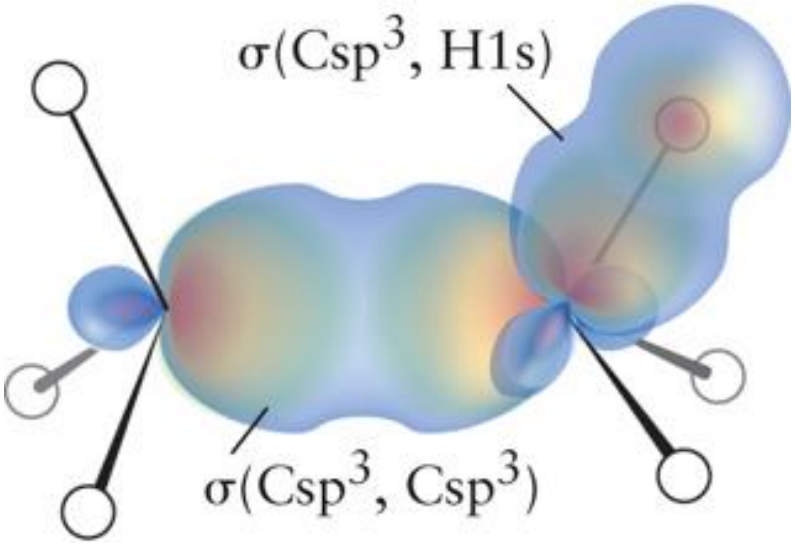
tetraédrico (109,5º)

Hibridização - etano

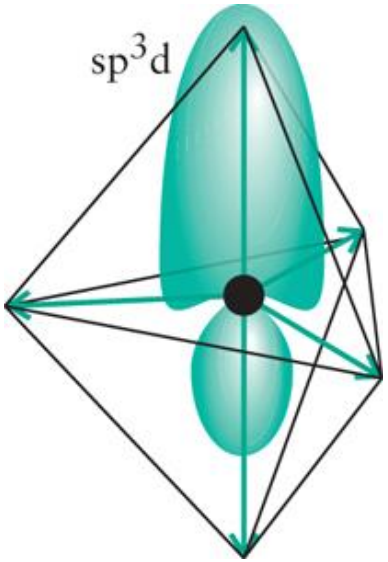


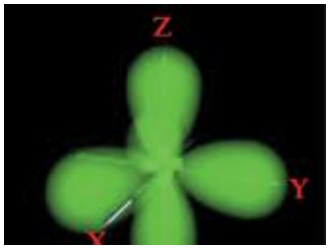
$H_3C\text{-}CH_3$

tetraédrico
(109,5º)

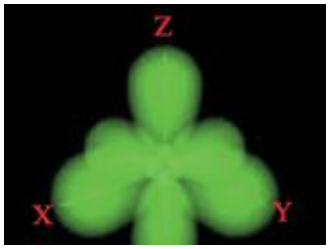


Hibridizações (2)

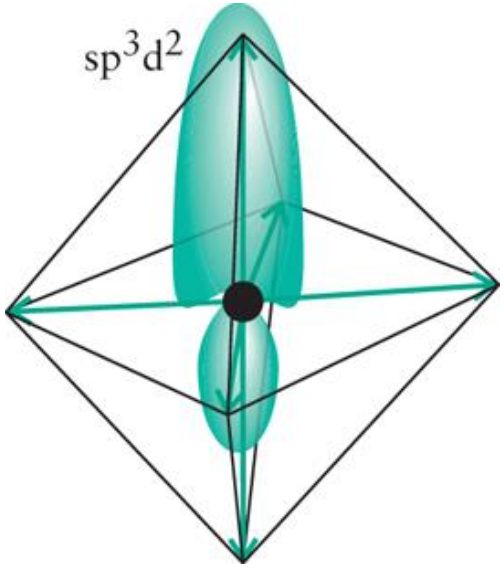




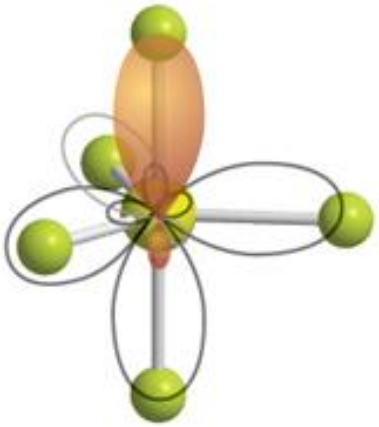
bipirâmide trigonal

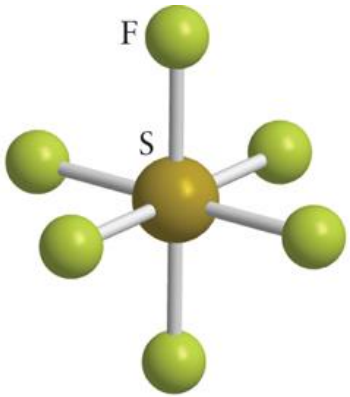


octaédrica



PCl_5

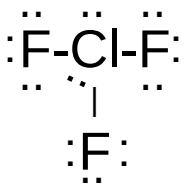




SF_6

Exemplo – ClF_3

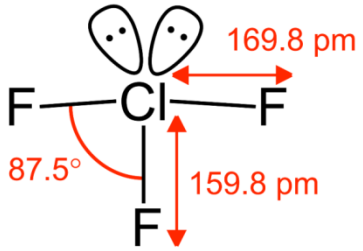
1. ***Estrutura de Lewis:***



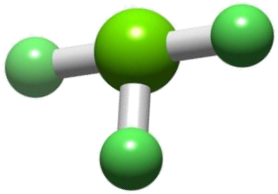
AX_3E_2

Cl = [Ne]$3s^2 3p^5$

2. ***Arranjo dos elétrons:*** bipirâmide trigonal



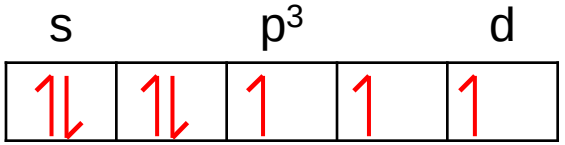
3. ***Geometria da molécula:***



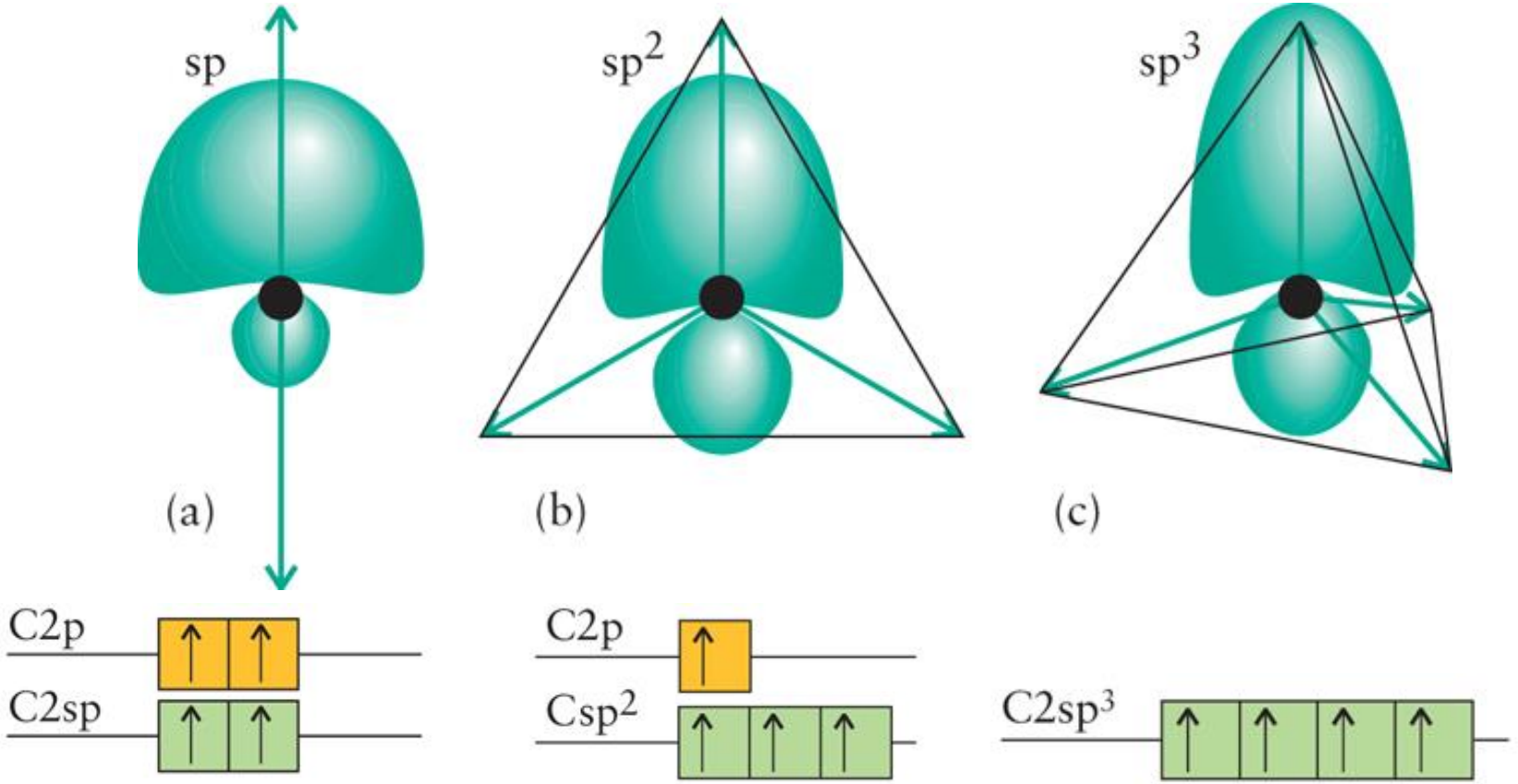
forma de T

4. ***Número de orbitais atômicos:*** 5

5. ***Construção dos orbitais híbridos:*** sp^3d



Hibridizações e insaturações

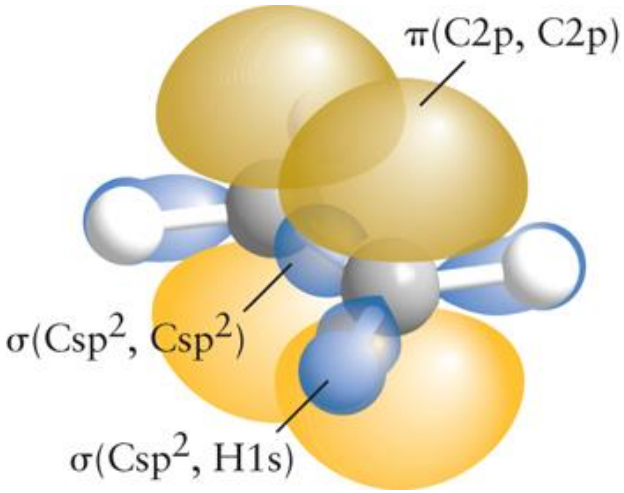


HC≡N
O=C=O

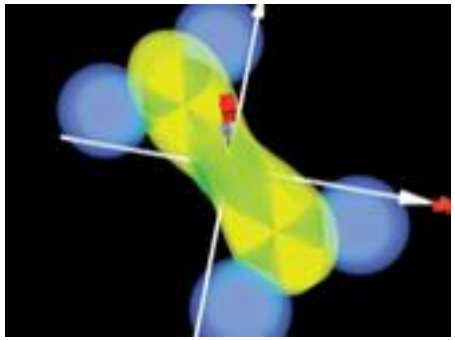
$H_2C=CH_2$
$O=CH_2$

H_3C-NH_2
$HO-CH_2$

sp^2

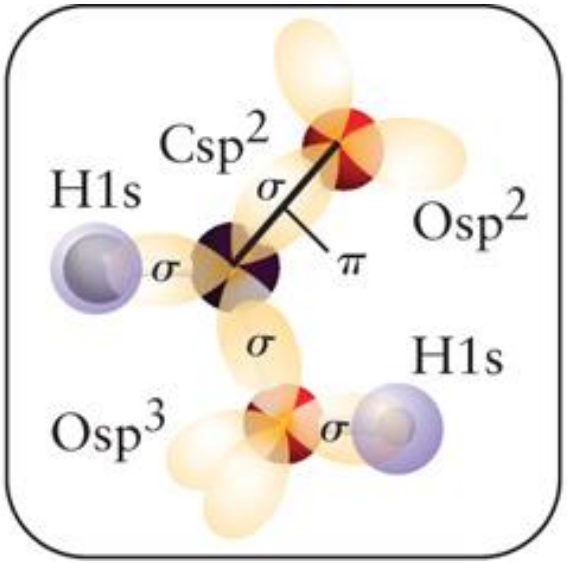


$H_2C=CH_2$

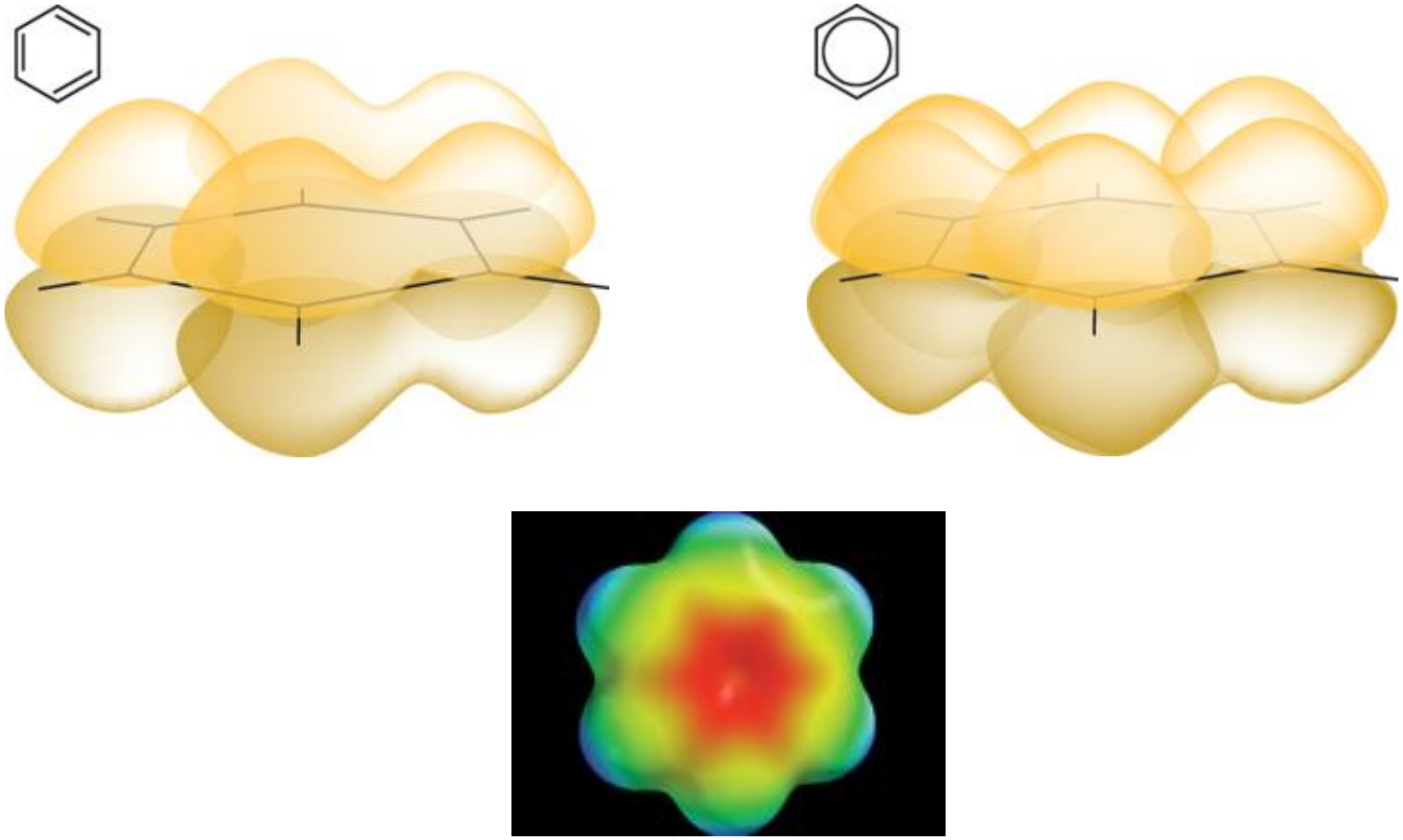


HCOOH

ácido fórmico

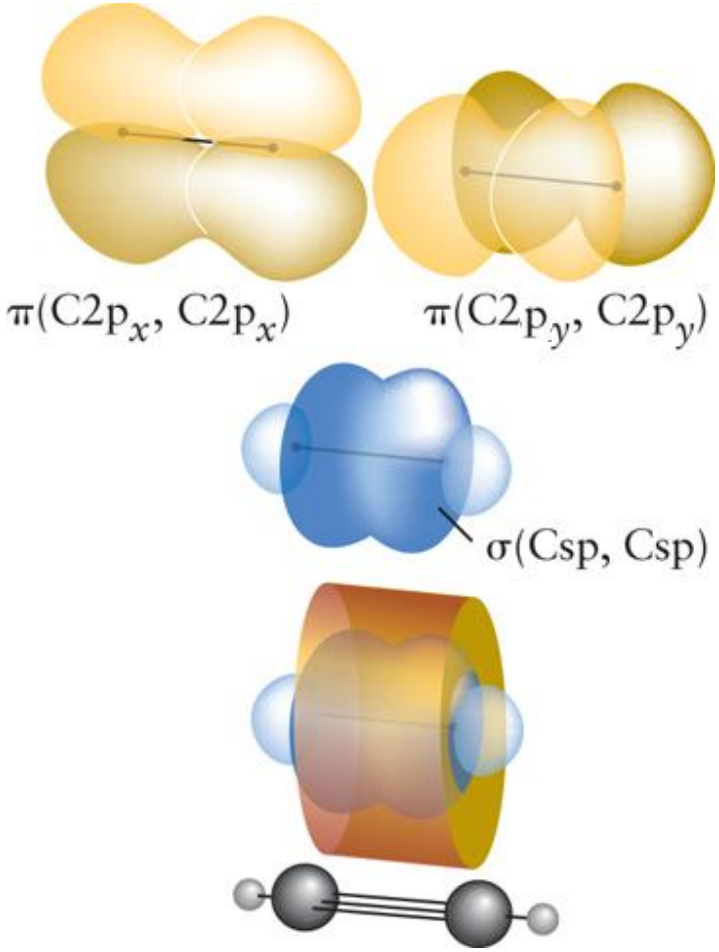


sp^2 - benzeno



sp

H-C≡C-H



Teoria do orbital molecular (TOM)

- ✓ **TOM**: elétrons distribuídos nos orbitais moleculares (deslocalização)

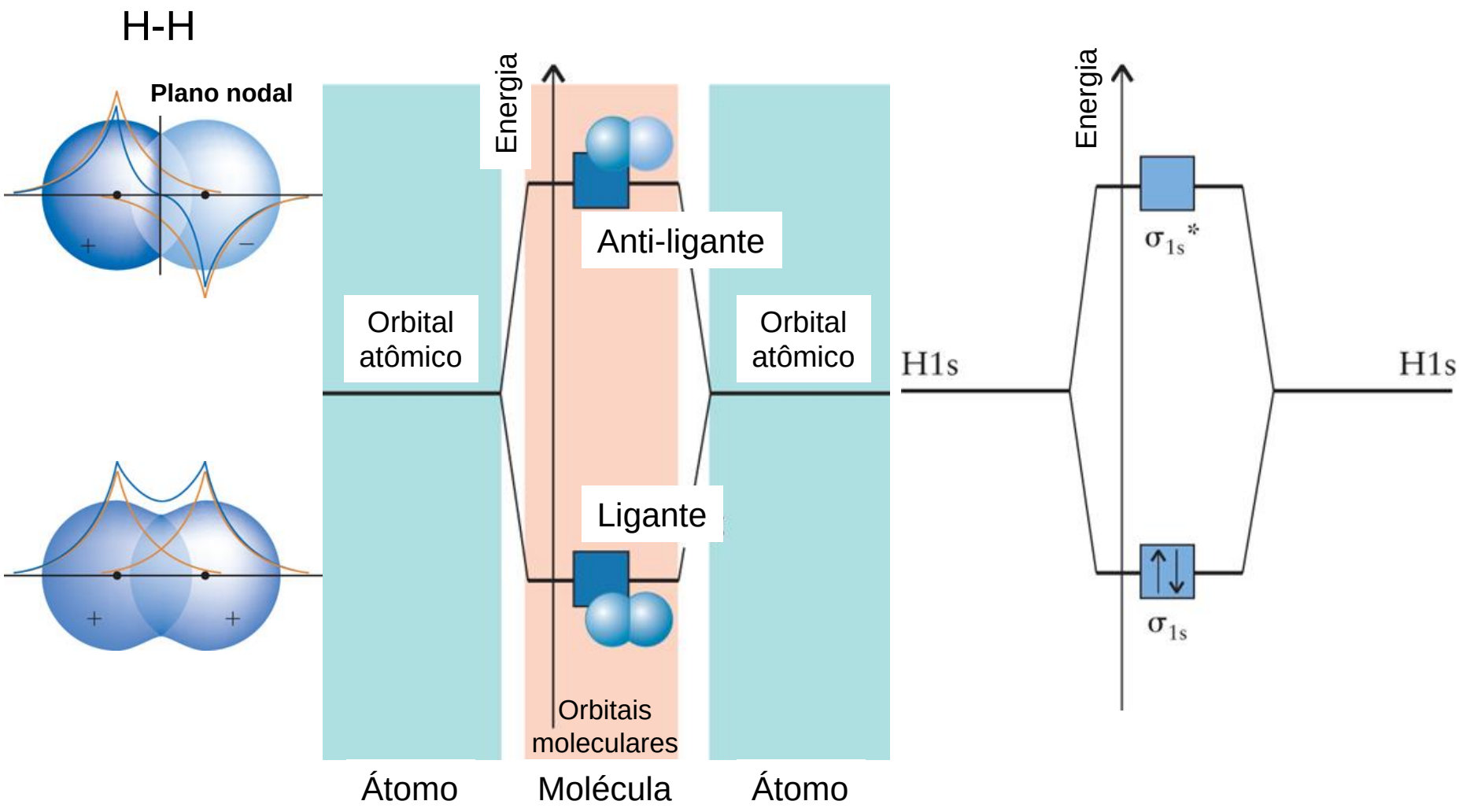
- ✓ Paramagnetismo de O_2 não é explicado por Lewis ou TLV

  Composto diagmagnético: e^- emparelhados (repulsão por um campo magnético)

  Composto paramagnético: e^- desemparelhados (atração por um campo magnético)

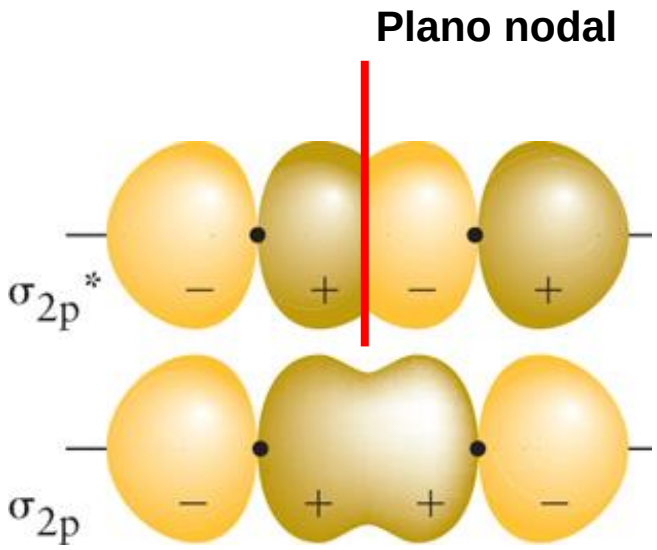
- ✓ Ordem de ligação química menor do que 1

TOM: ligação química



Ligações químicas: σ e π

Ligação σ



Ligação π

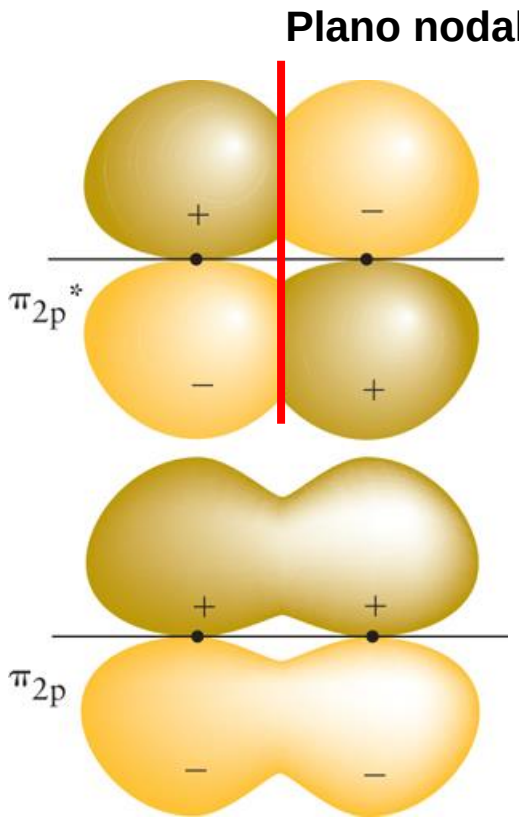
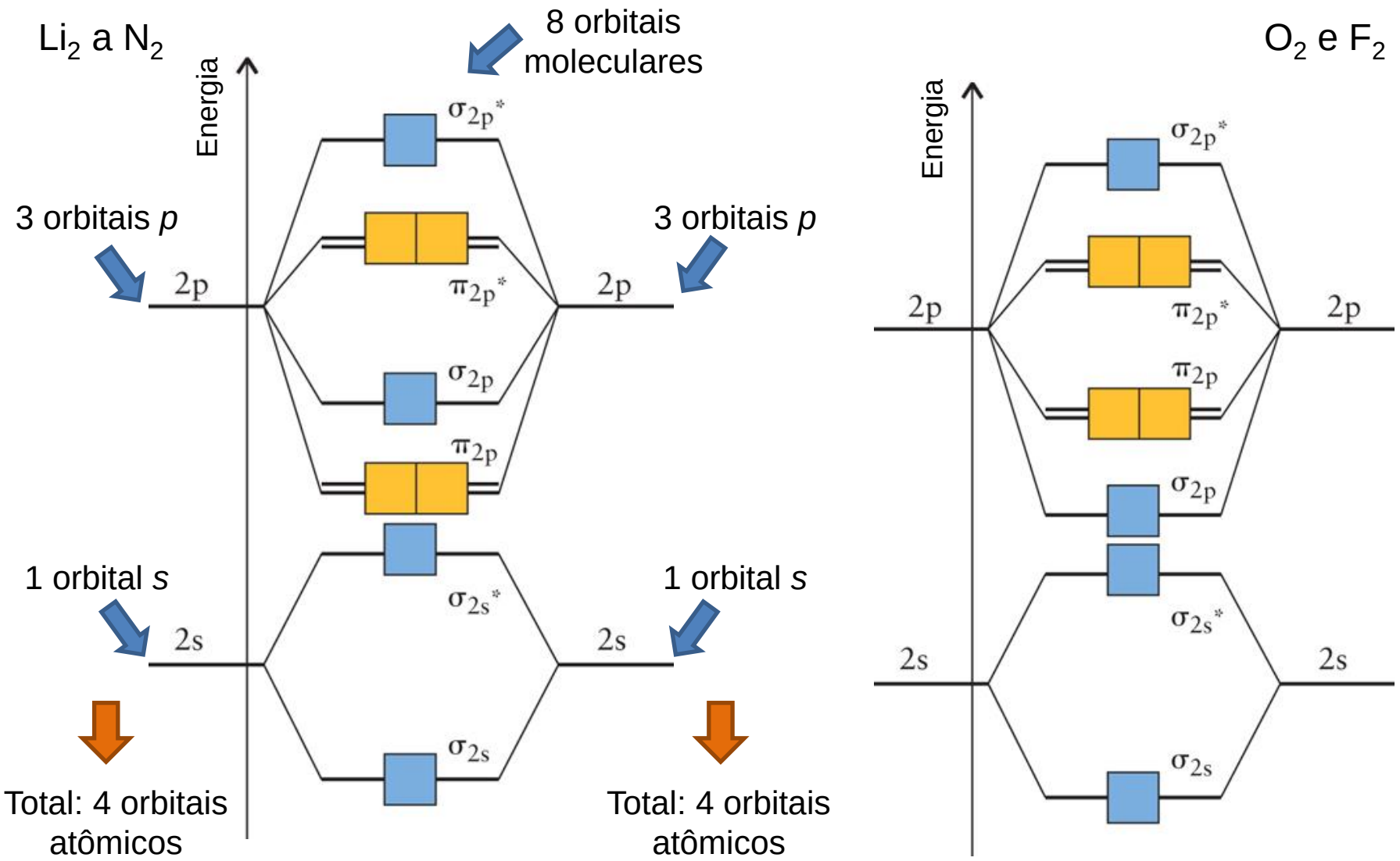
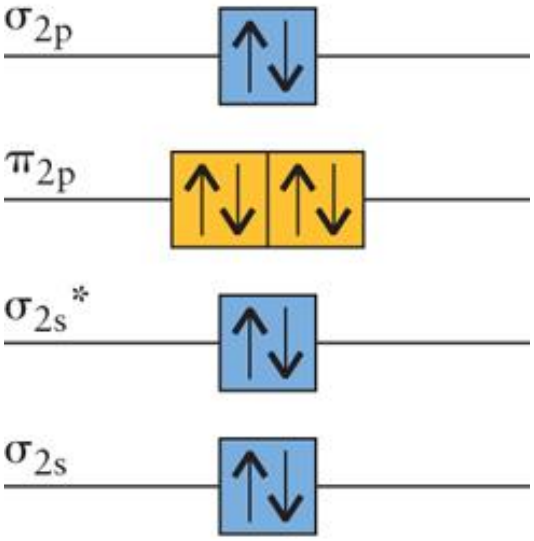


Gráfico de energia



Exemplo – N_2

✓ Esquema de preenchimento para o N_2 (10 elétrons)



Ordem de ligação (*b*):

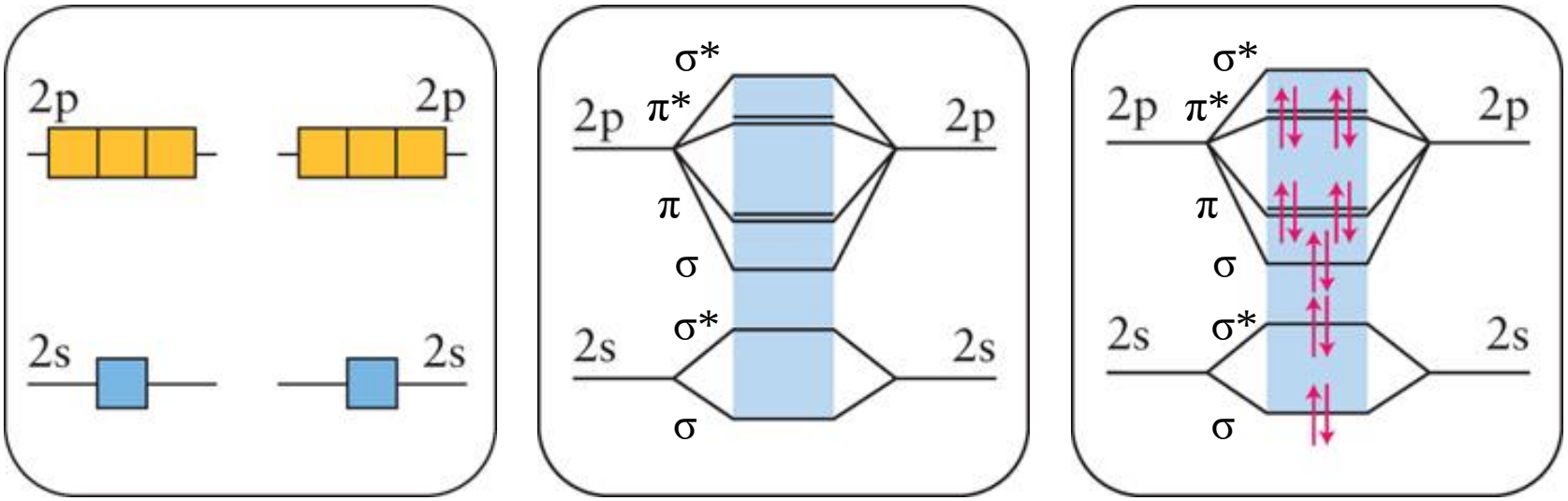
$b = 0{,}5(e^-_{\text{OM ligantes}} - e^-_{\text{OM anti-ligantes}})$

$b = 0{,}5(N - N^*) = 0{,}5(8 - 2) = 3$

N_2: $\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^2$

Exemplo – F_2

✓ Esquema de preenchimento para o F_2 (14 elétrons)



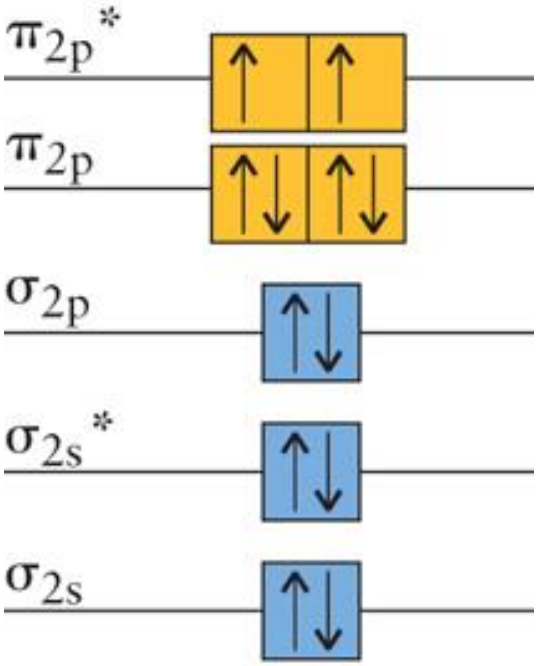
F_2: $\sigma_{2s}^{2}\sigma_{2s}^{*2}\sigma_{2p}^{2}\pi_{2p}^{4}\pi_{2p}^{*4}$

Ordem de ligação (*b*):

$b = 0{,}5(N - N^*) = 0{,}5(8 - 6) = 1$

Exemplo – O_2

✓ Esquema de preenchimento para o O_2 (12 elétrons)

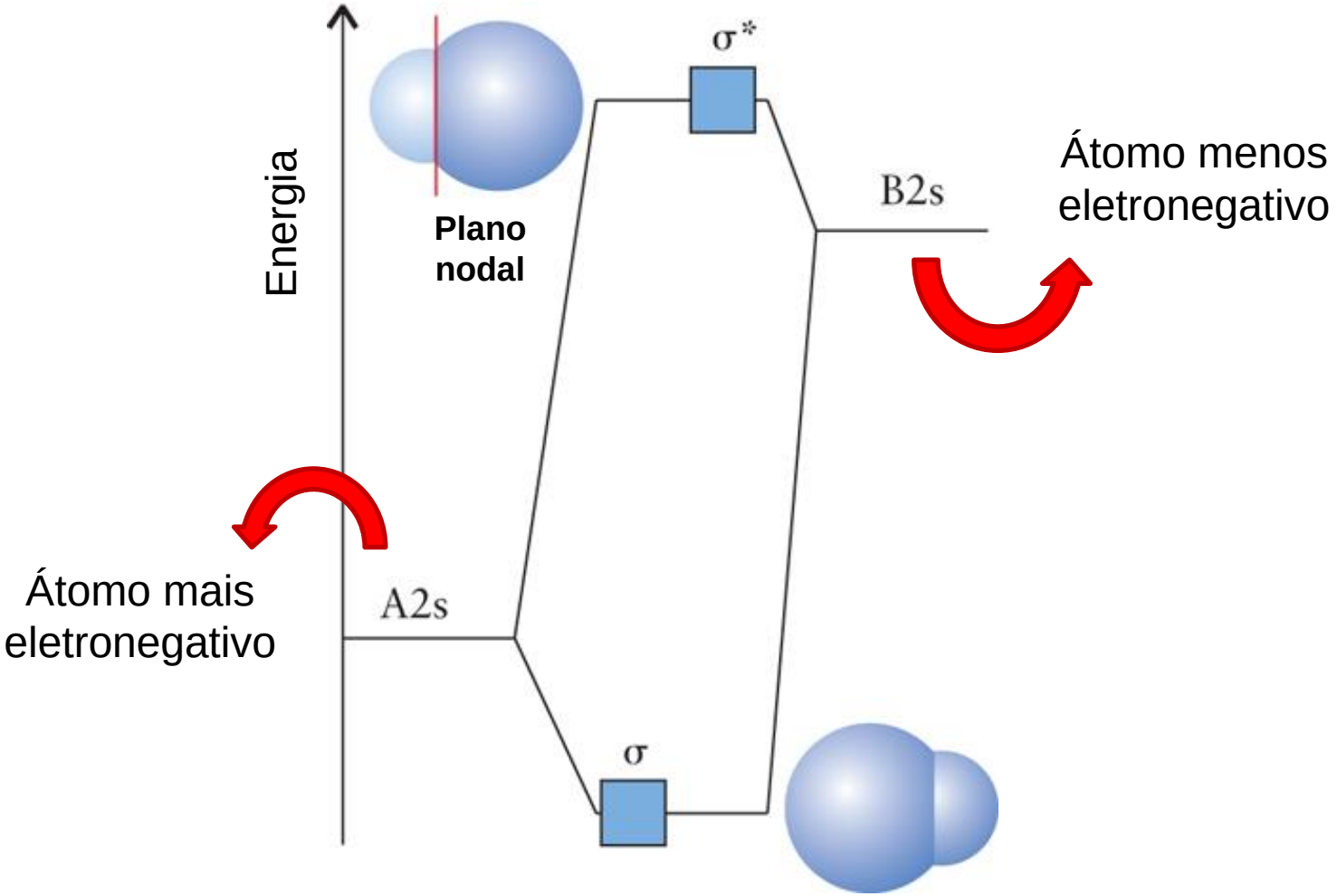


Ordem de ligação (*b*):

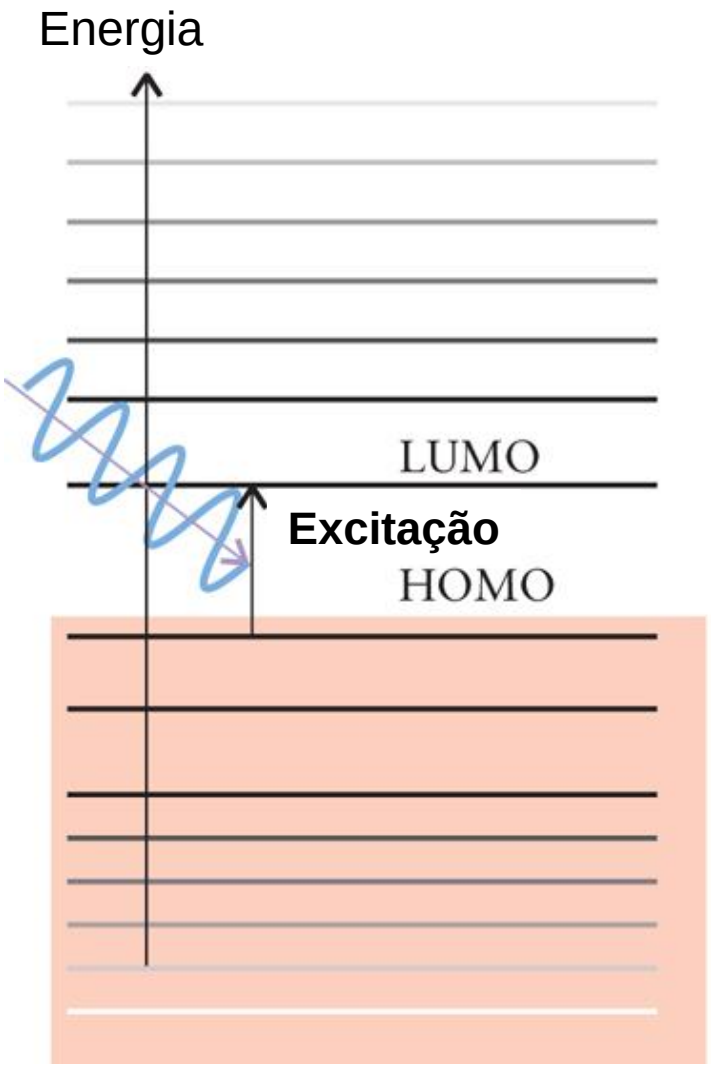
$b = 0{,}5(N - N^*) = 0{,}5(8 - 4) = 2$

O_2: $\sigma_{2s}^2\sigma_{2s}^{*2}\sigma_{2p}^2\pi_{2p}^4\pi_{2p}^{*2}$

Ligação covalente polar



Excitação eletrônica



Orbitais não preenchidos

Orbitais preenchidos com elétrons

Próxima aula

Forças intermoleculares

✓ Veremos como as moléculas interagem entre si no meio líquido e sólido