

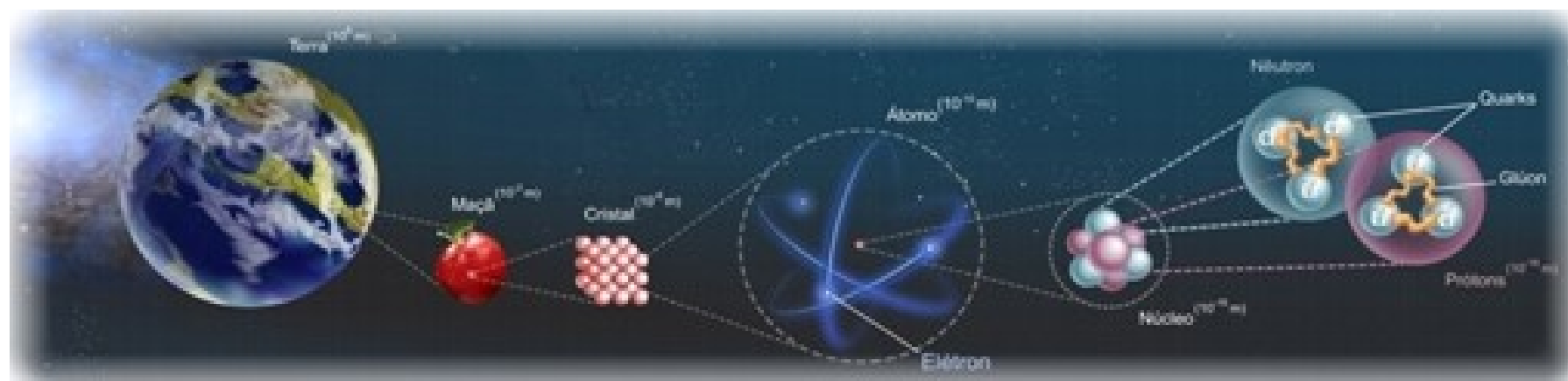


Estrutura da Matéria

2018-2 – Prof. Célio

BIK0102 – S.A.

Aula 12 – Forma e estrutura das moléculas II



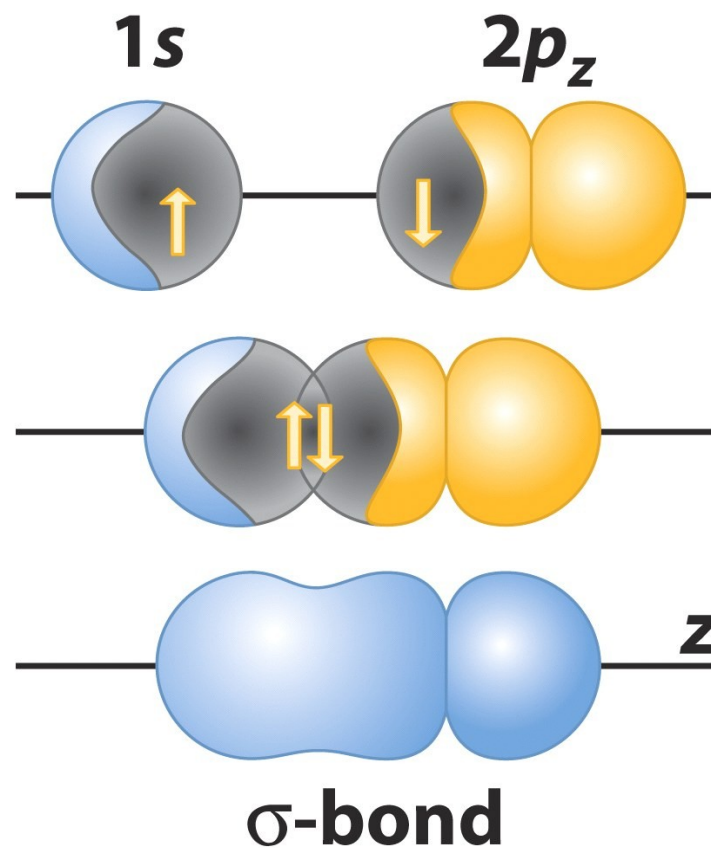
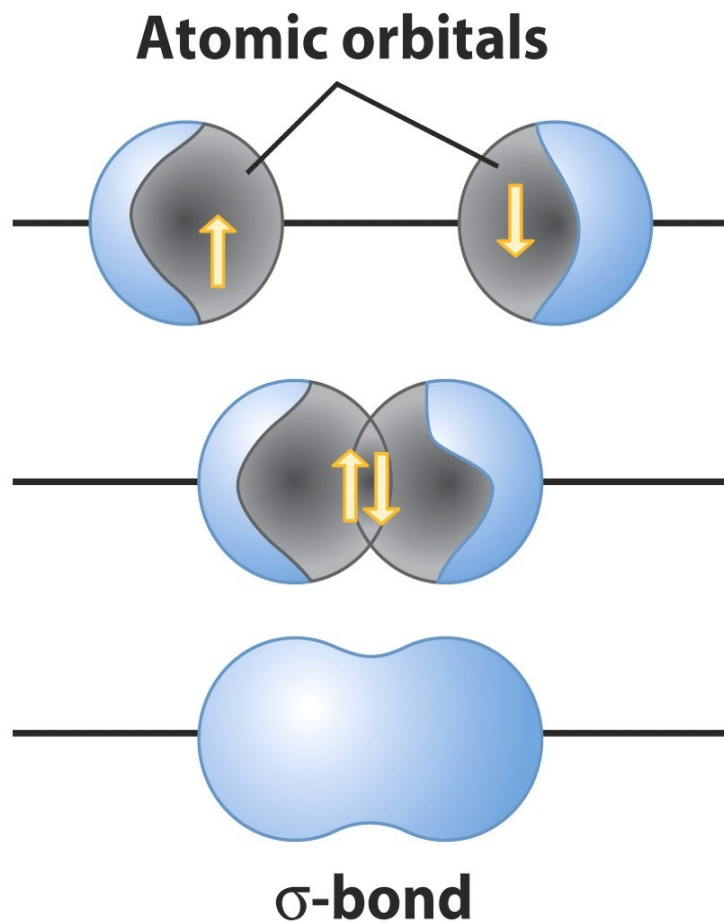
Teoria da Ligação de Valência

- Quando dois átomos se aproximam os orbitais atômicos se fundem;
- A fusão dos orbitais é chamada de superposição;
- Quanto maior for a superposição, mais forte é a ligação.

Teoria da ligação de valência

Ligações Sigma e Pi

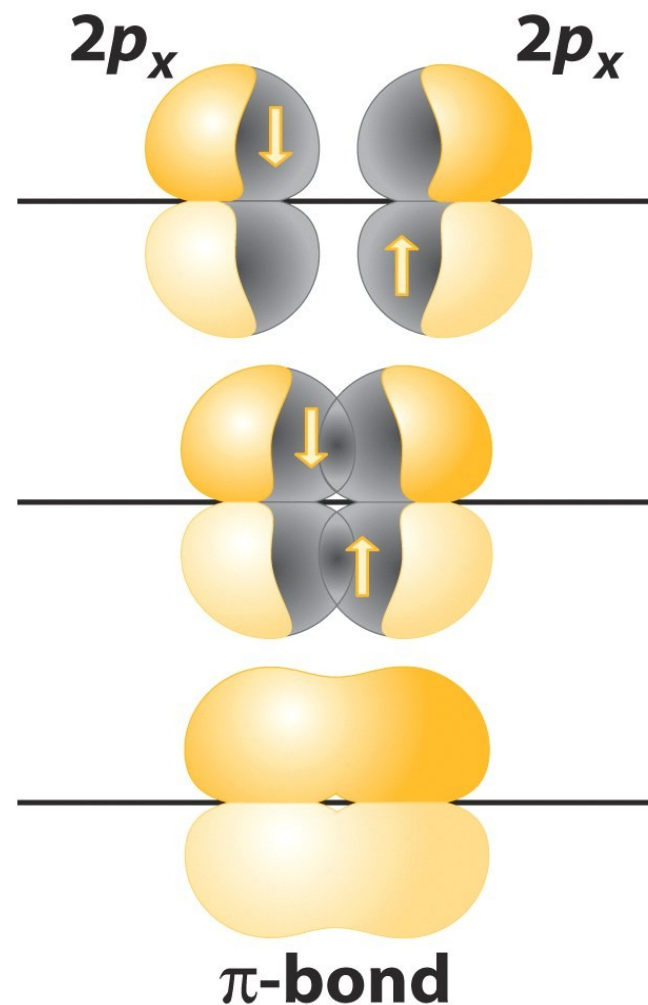
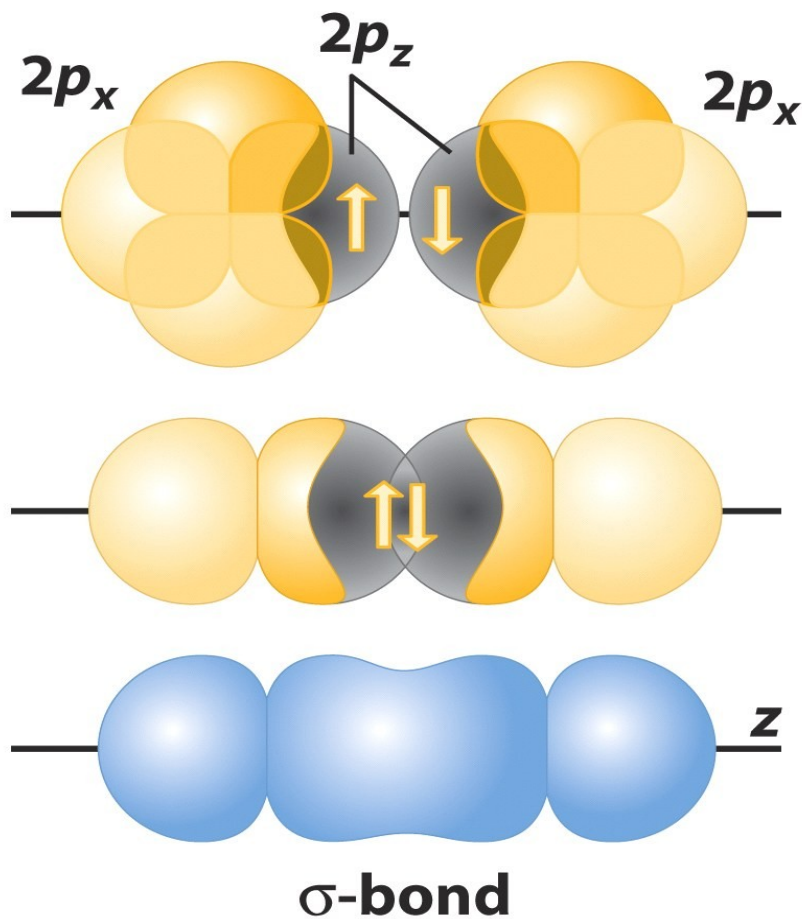
- Ligação Sigma: não tem plano nodal no eixo internuclear.



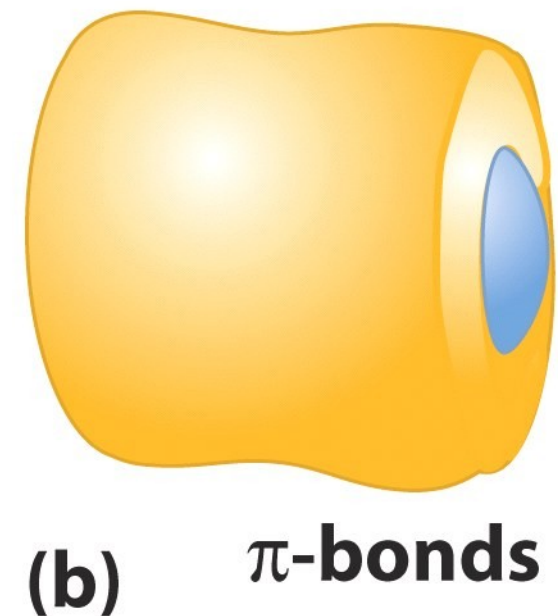
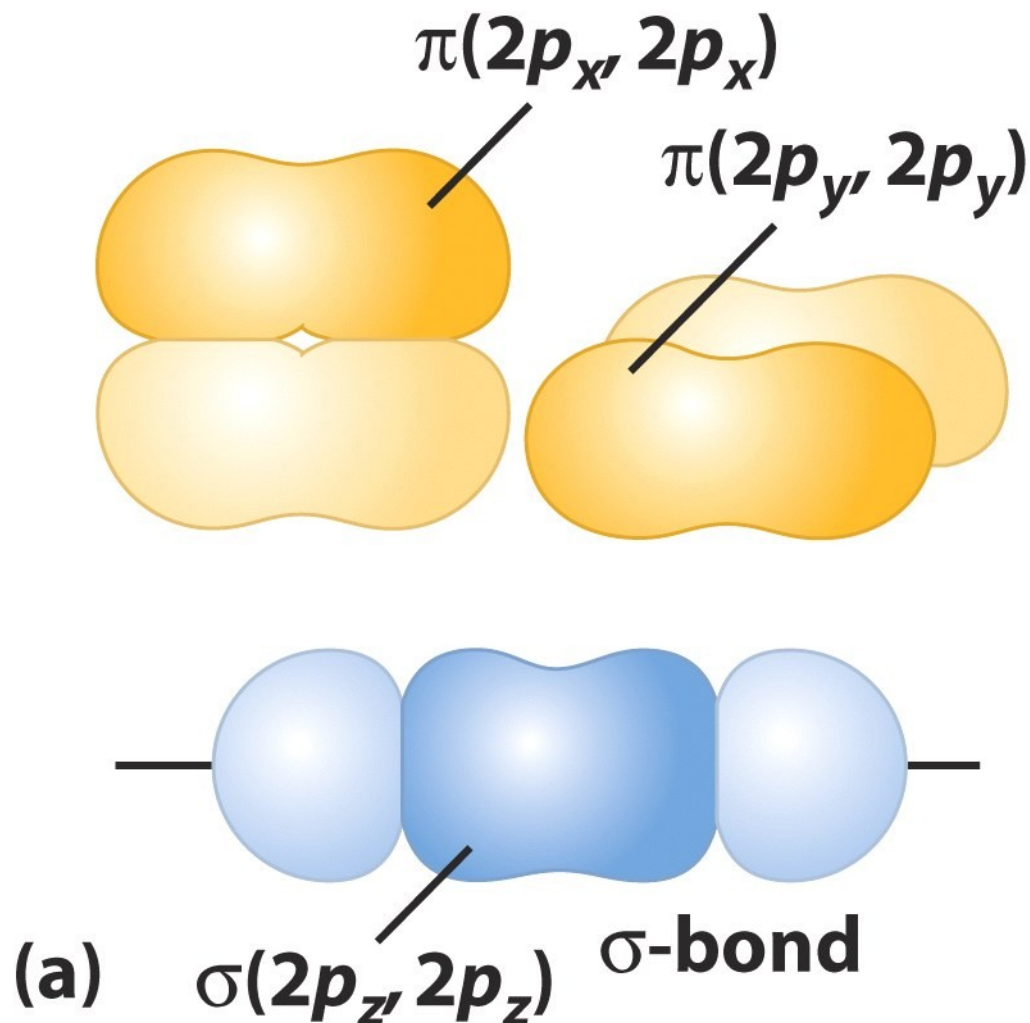
Teoria da ligação de valência

Ligações Sigma e Pi

- Ligação Pi: tem um único plano nodal sobre o eixo internuclear.



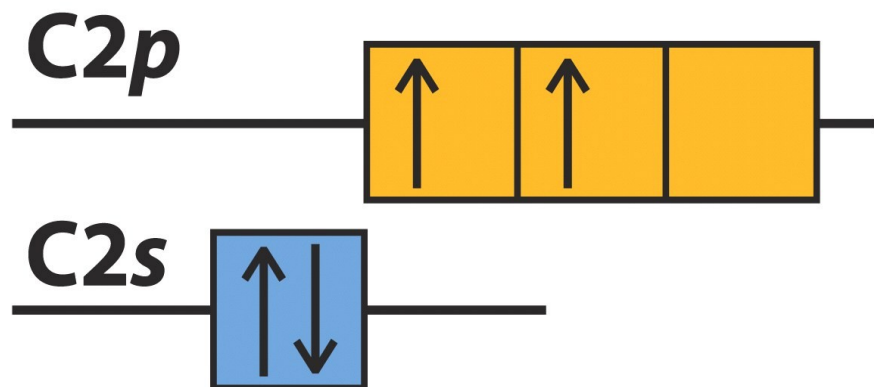
Padrão de ligação da molécula de nitrogênio



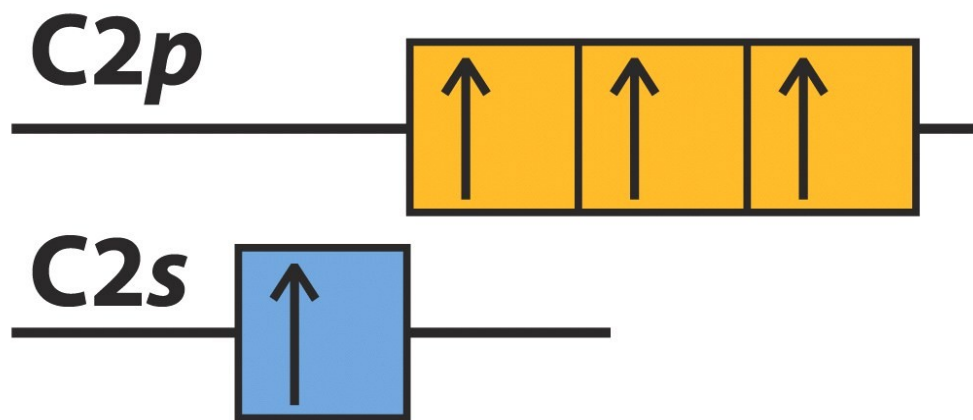
Ligações Sigma e Pi

- Simples \rightarrow Sigma;
- Dupla \rightarrow Sigma + Pi;
- Tripla \rightarrow Sigma + 2 ligações Pi.
- Os orbitais atômicos que os elétrons ocupam se superpõem:
 - Cabeça-cabeça para formar ligações Sigma;
 - Lateralmente para formar ligações Pi.

Hibridação dos Orbitais



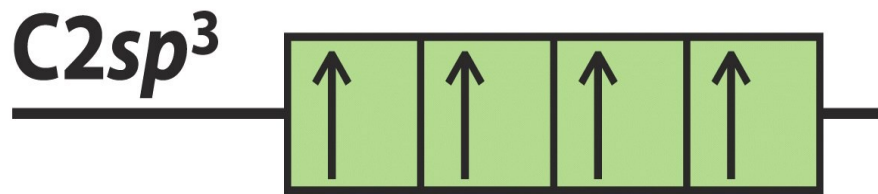
35 Carbon, $[\text{He}]2s^2 2p_x^1 2p_y^1$



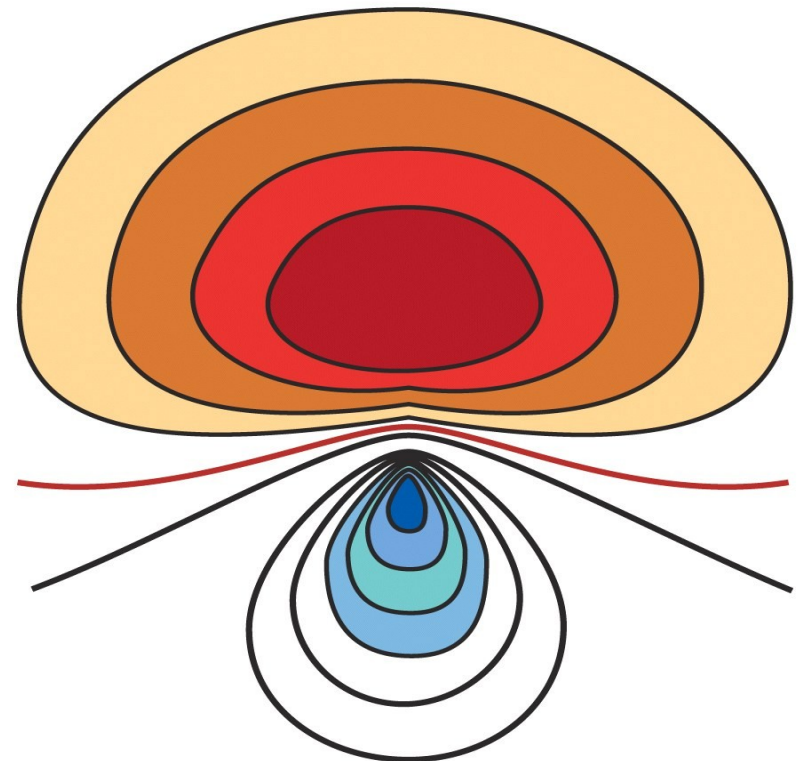
36 Carbon, $[\text{He}]2s^1 2p_x^1 2p_y^1 2p_z^1$

Orbitais Híbridos

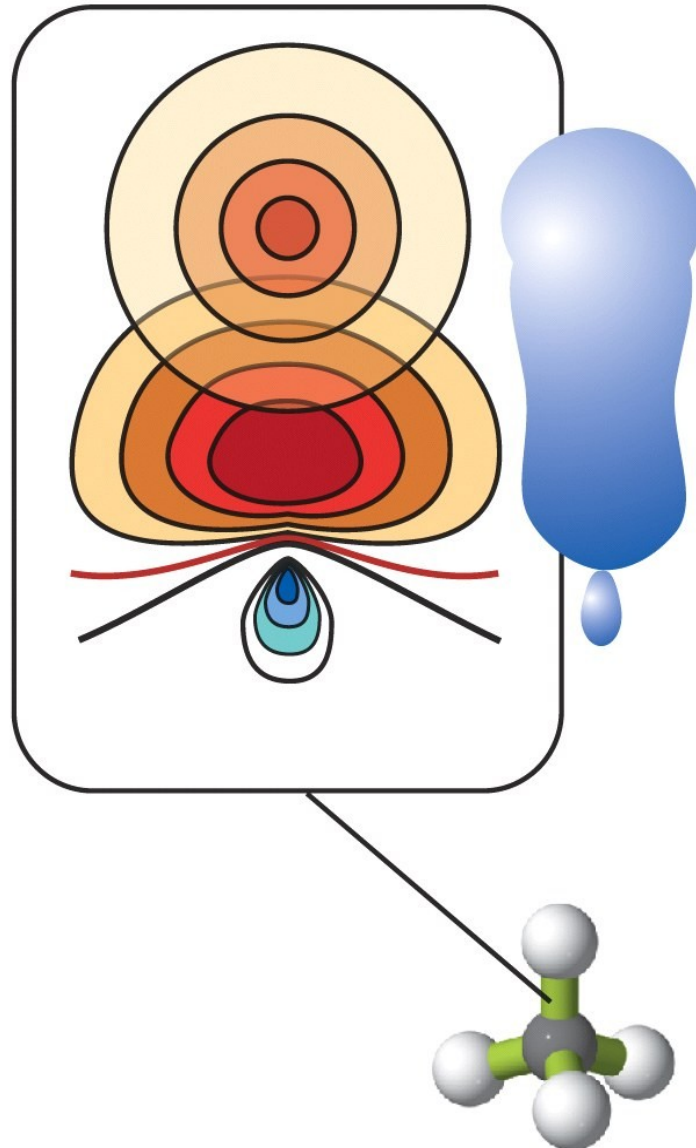
- Vão diferir somente na orientação, cada um apontando para o vértice de um tetraedro.



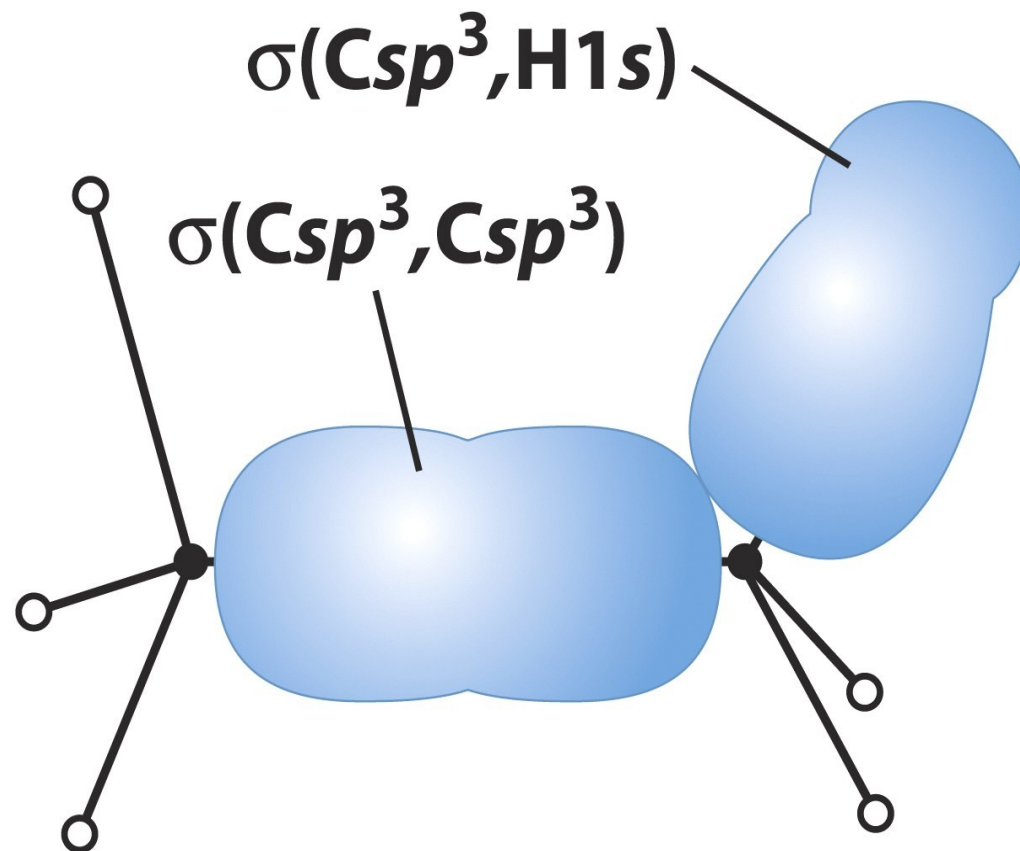
38 sp^3 hybridized carbon



Hibridação no Metano



Hibridação em moléculas mais complexas: Etano

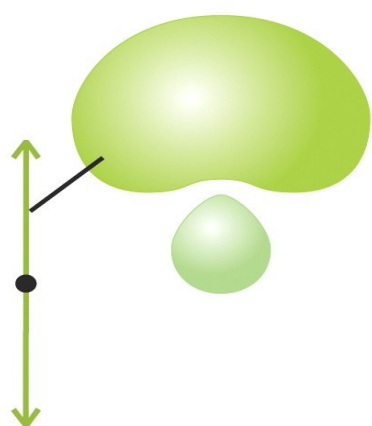


Hibridação e forma molecular

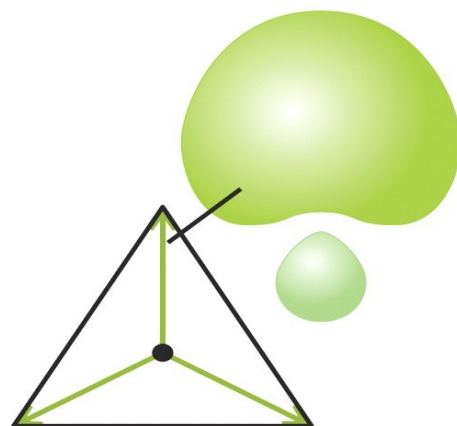
TABLE 3.2 Hybridization and Molecular Shape*

Electron arrangement	Number of atomic orbitals	Hybridization of the central atom	Number of hybrid orbitals
linear	2	sp	2
trigonal planar	3	sp^2	3
tetrahedral	4	sp^3	4
trigonal bipyramidal	5	sp^3d	5
octahedral	6	sp^3d^2	6

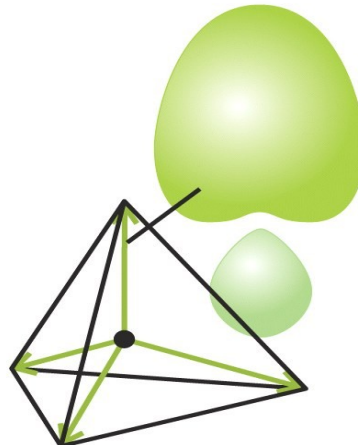
*Other combinations of s -, p -, and d -orbitals can give rise to the same or different shapes, but these combinations are the most common.



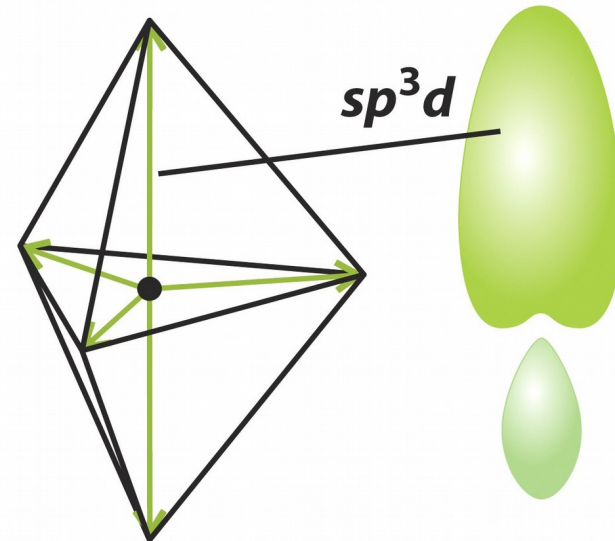
(a) sp



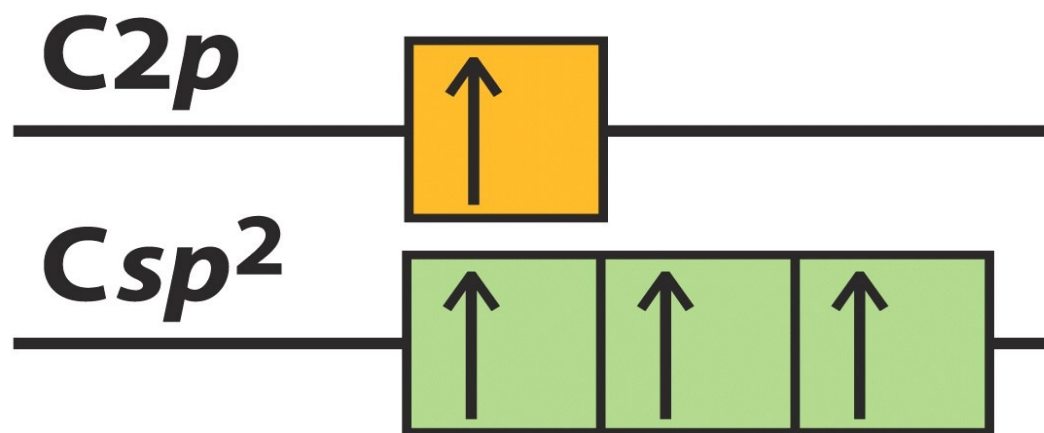
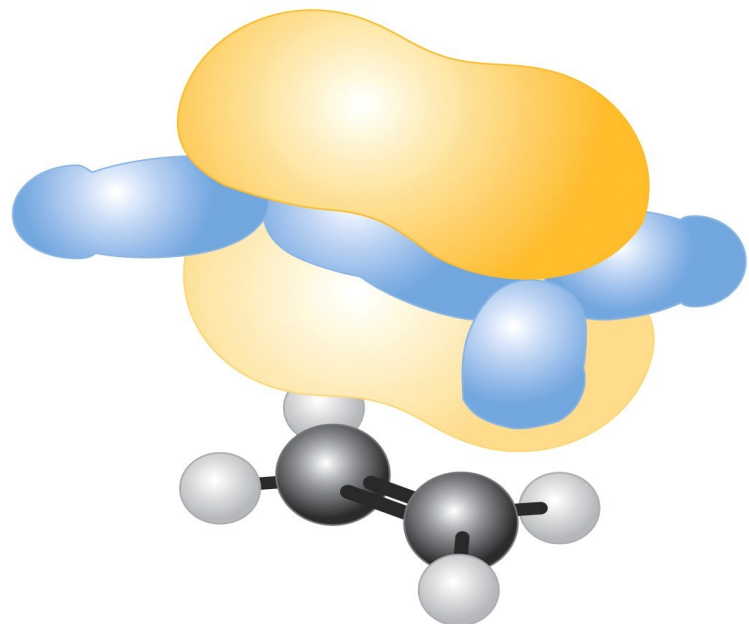
(b) sp^2



(c) sp^3

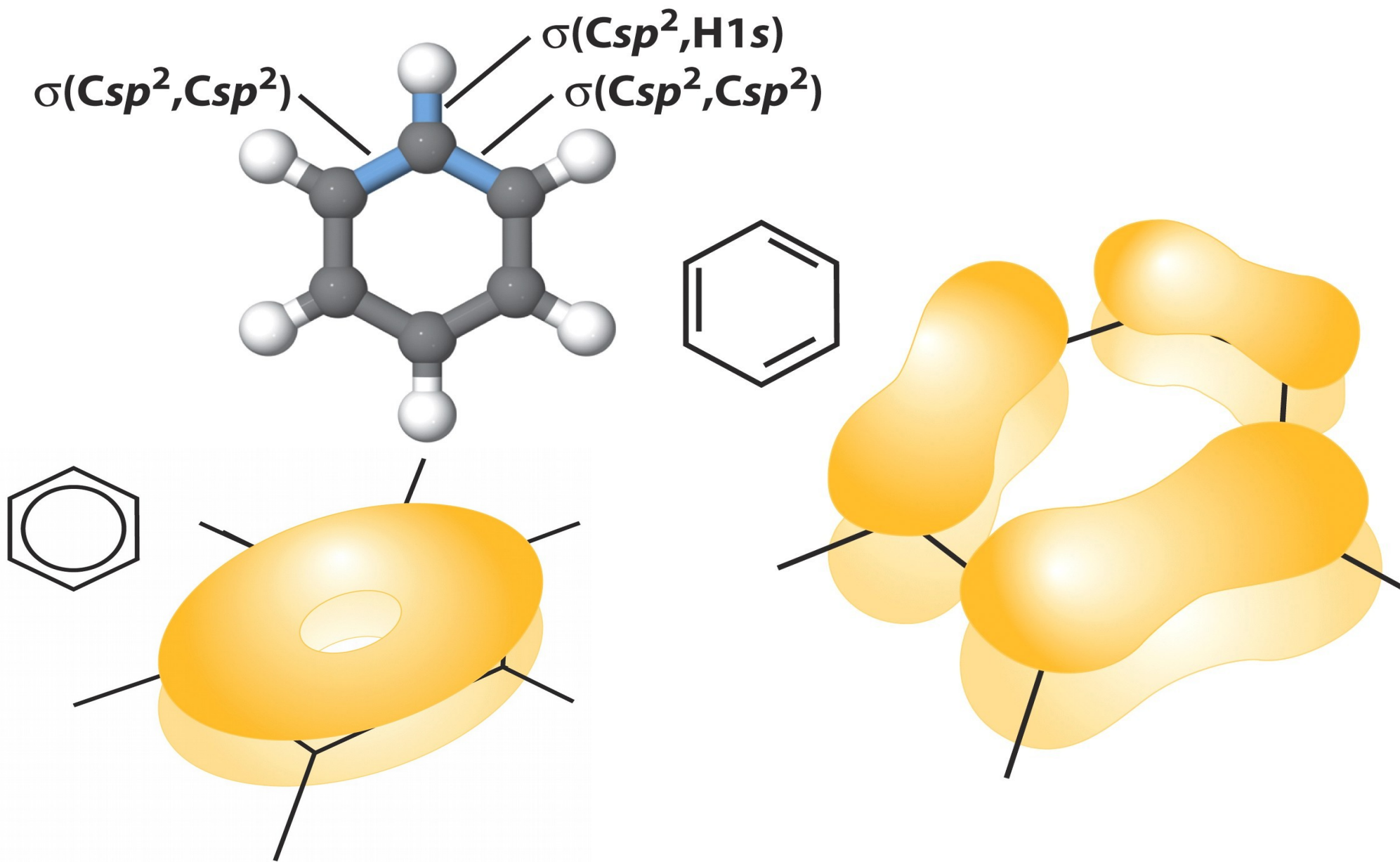


Ligações dos Hidrocarbonetos

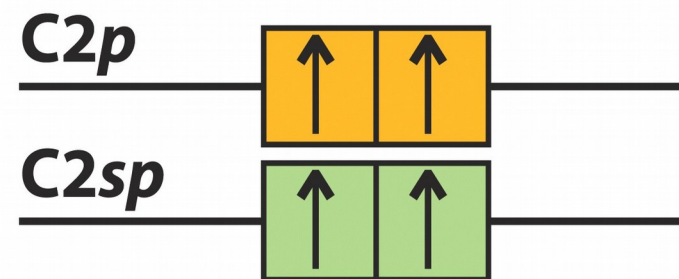


41 sp^2 hybridized carbon

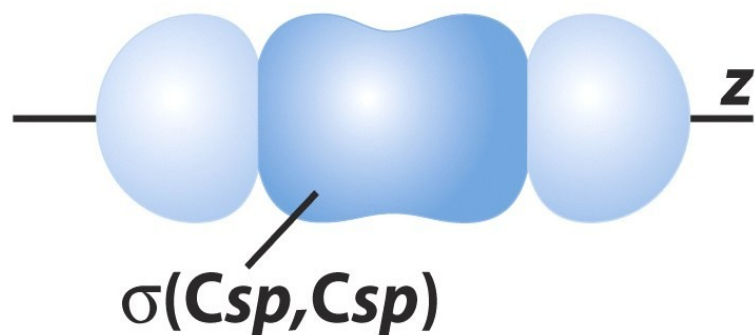
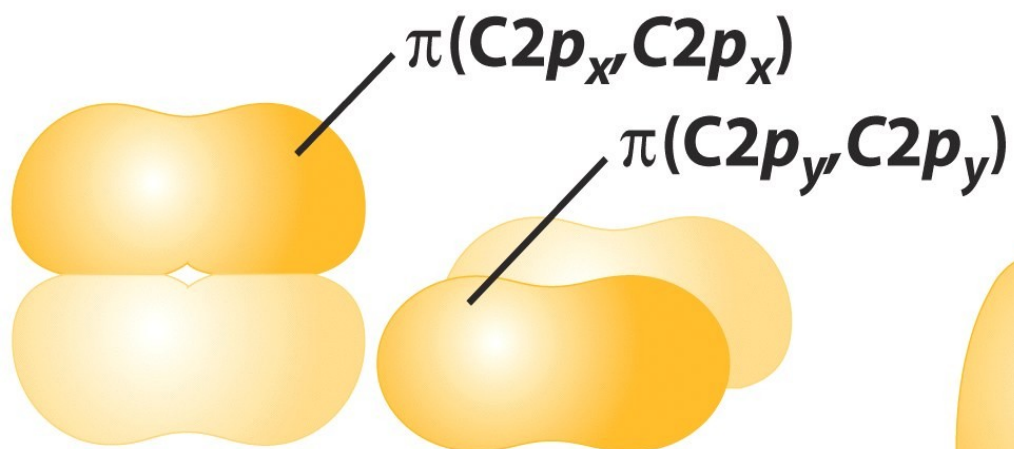
Benzeno



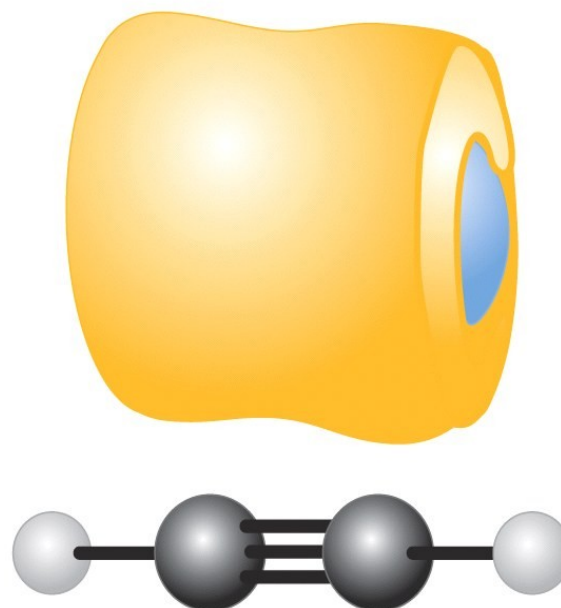
Acetileno



42 sp hybridized carbon



(a)



(b)

Bibliografia

- Atkins e Jones, Princípios de Química, cap. 3, ed. Bookman (2006).