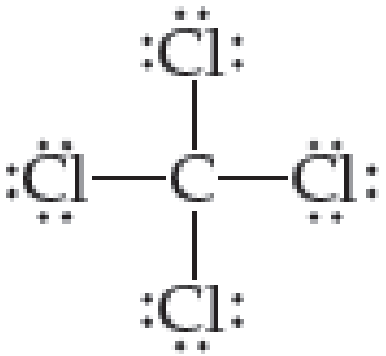
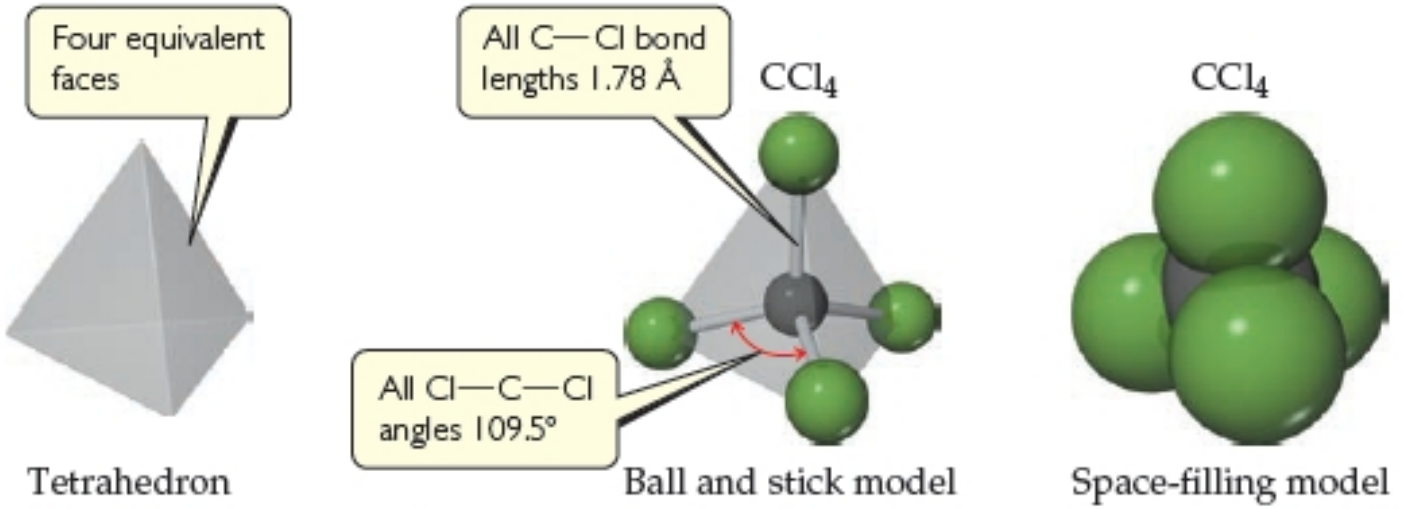
Ligações Químicas – Geometrias Moleculares e Comportamento Químico

US$ 125 bilhões de 1997 a 2011

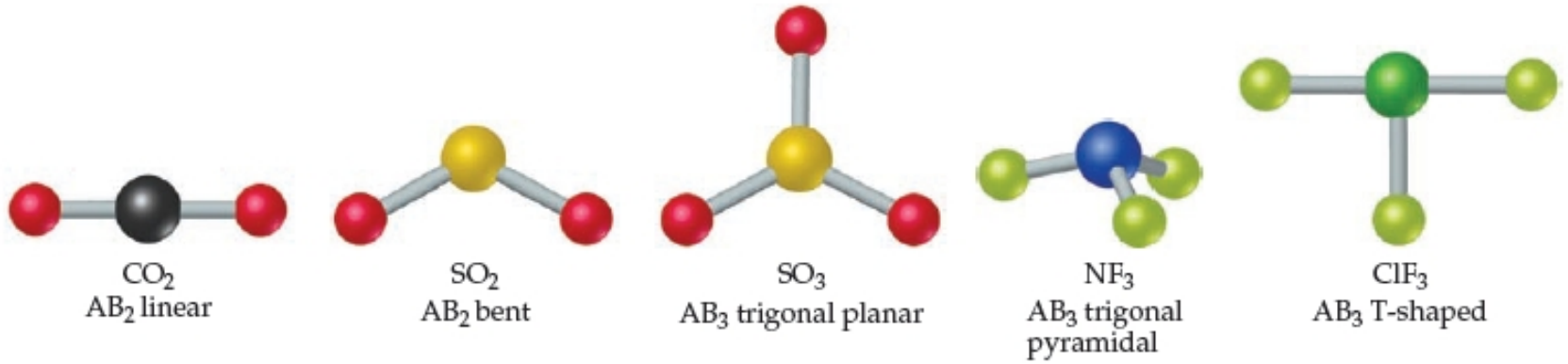


Geometria Planar ?

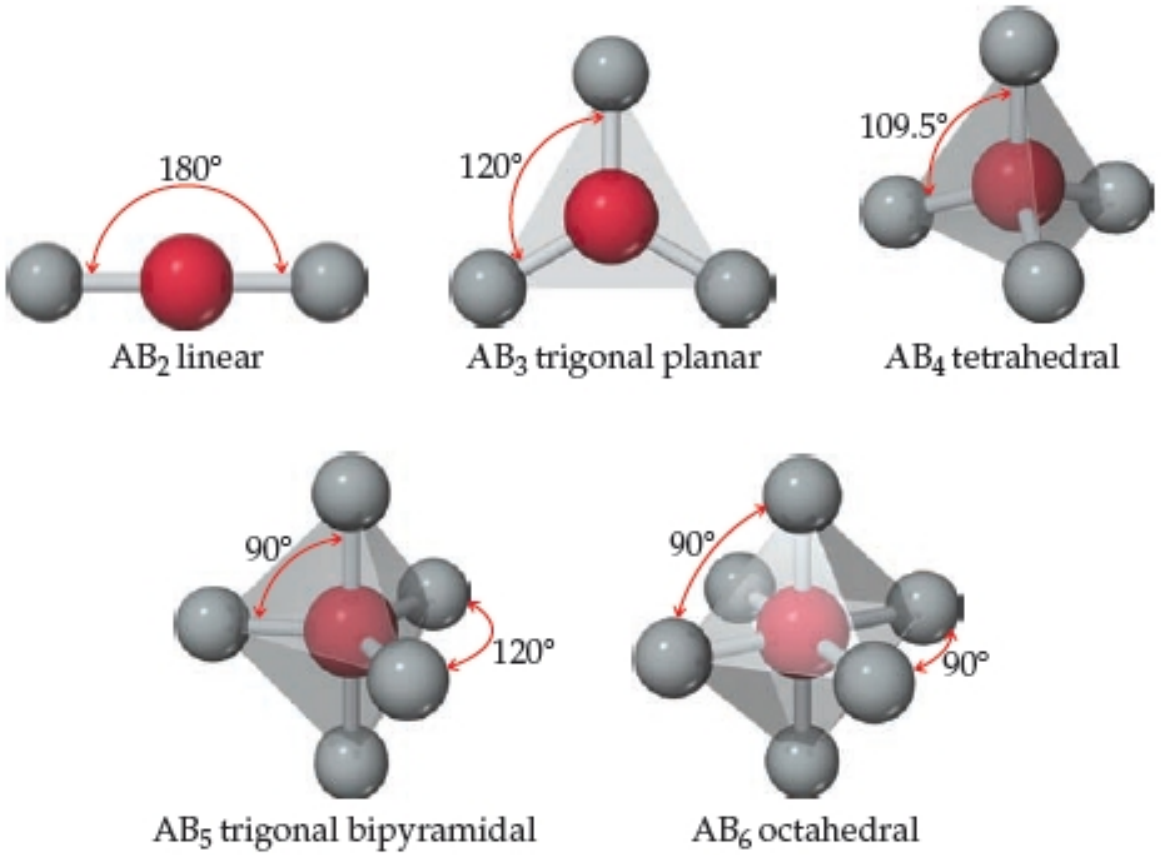


▲ **Figure 9.1** **Tetrahedral shape of CCl_4.**

Geometrias Moleculares de compostos simples



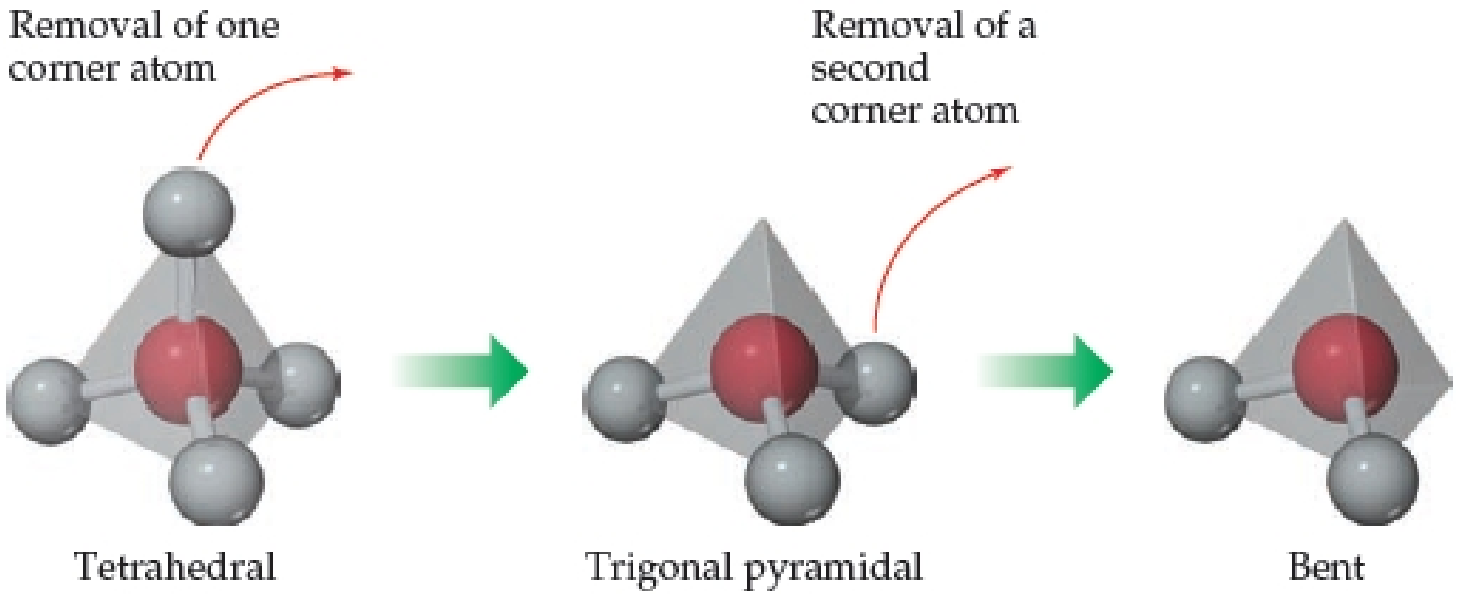
▲ Figure 9.2 Shapes of AB_2 and AB_3 molecules.



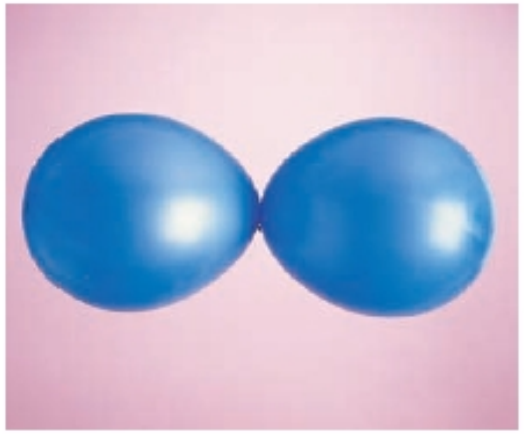
▲ **Figure 9.3** **Shapes allowing maximum distances between B atoms in AB_n molecules.**

Por que as distâncias interatômicas são **maximizadas** ?

E, se um átomo fosse removido de um tetraedro ?



▲ **Figure 9.4** **Derivatives of the tetrahedral molecular shape.**



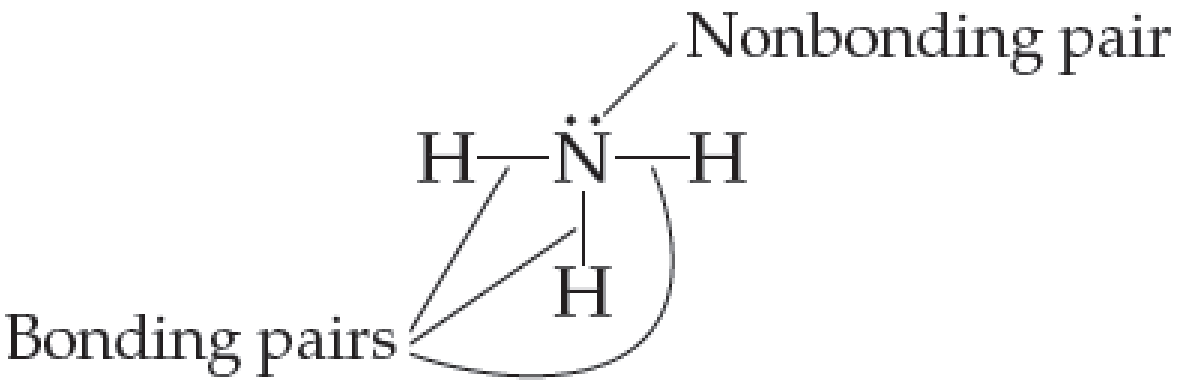
Two balloons
linear orientation

Three balloons
trigonal-planar orientation

Four balloons
tetrahedral orientation

VSEPR : **V**alence **S**hell **E**lectron **P**air **R**epulsion

Domínios de elétrons



1) Os elétrons são domínios negativamente carregados, logo eles se repelem ao máximo

2) O melhor arranjo é aquele onde a repulsão é minimizada

3) Pares não-ligados, ligações simples e ligações múltiplas produzem um único domínio

Geometria Molecular

1) A regra do octeto é seguida ?

2) Qual a geometria molecular ?

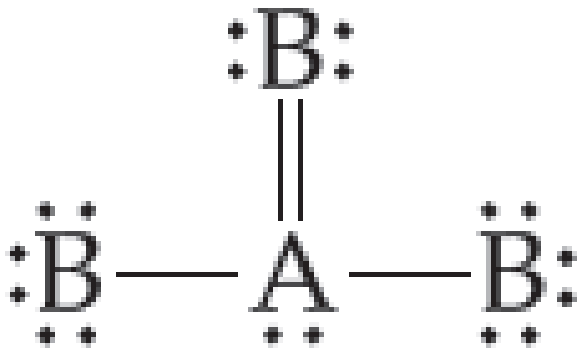
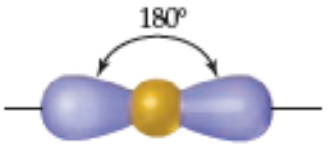
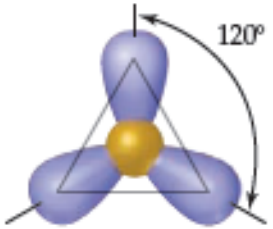
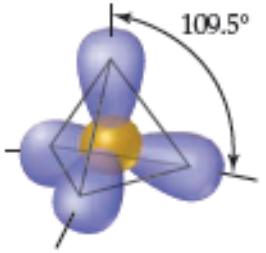
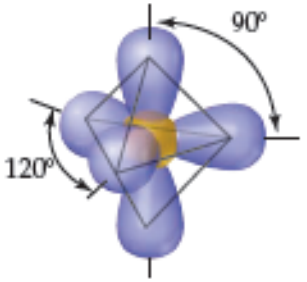
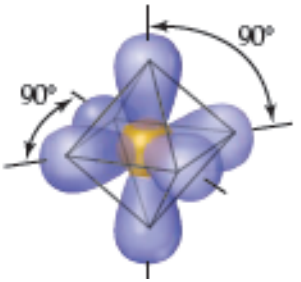
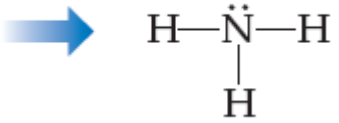
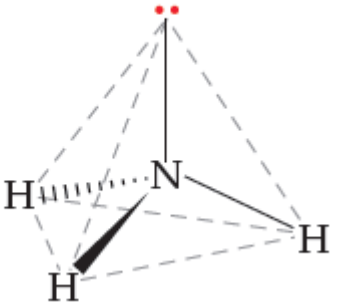


Table 9.1 Electron-Domain Geometries as a Function of Number of Electron Domains

Number of Electron Domains	Arrangement of Electron Domains	Electron-Domain Geometry	Predicted Bond Angles
2		Linear	180°
3		Trigonal planar	120°
4		Tetrahedral	109.5°
5		Trigonal bipyramidal	120° 90°
6		Octahedral	90°

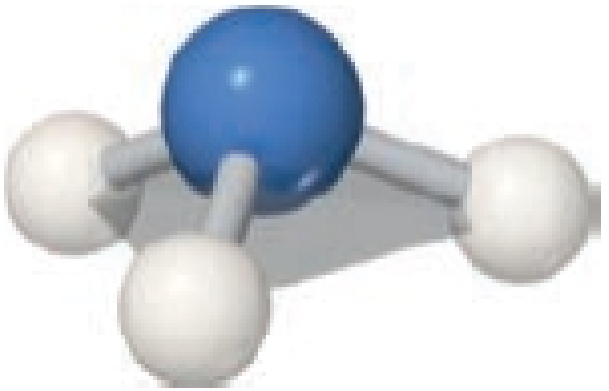
NH_3





1 Draw Lewis structure.

2 Determine electron-domain geometry by counting *all* electron domains, then use Table 9.1 to determine the appropriate electron domain geometry.



3 Determine molecular geometry by counting *only bonding* electron domains to see the arrangement of bonded atoms (trigonal pyramidal).

Table 9.2 Electron-Domain and Molecular Geometries for Two, Three, and Four Electron Domains around a Central Atom

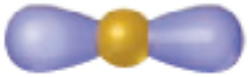
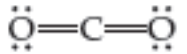
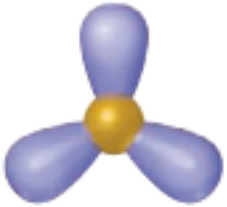
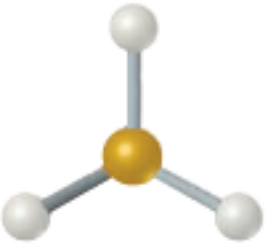
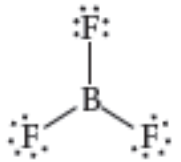
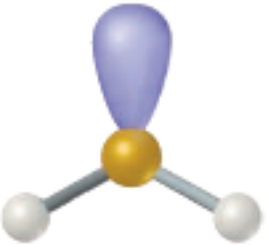
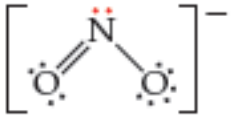
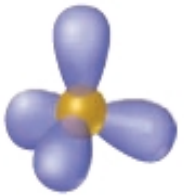
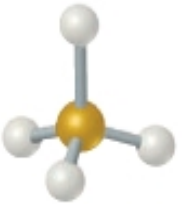
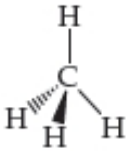
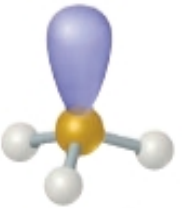
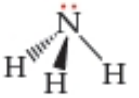
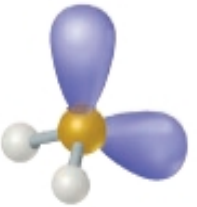
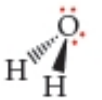
Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
2	 Linear	2	0	 Linear	
3	 Trigonal planar	3	0	 Trigonal planar	
		2	1	 Bent	

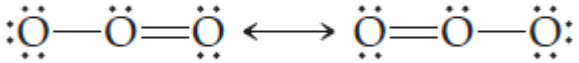
Table 9.2 Electron-Domain and Molecular Geometries for Two, Three, and Four Electron Domains around a Central Atom

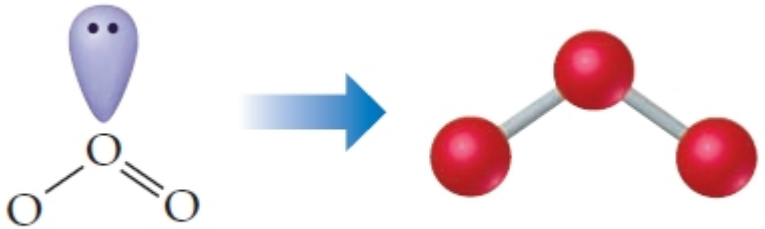
Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
4	 Tetrahedral	4	0	 Tetrahedral	
		3	1	 Trigonal pyramidal	
		2	2	 Bent	

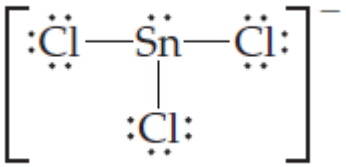
Exercício:

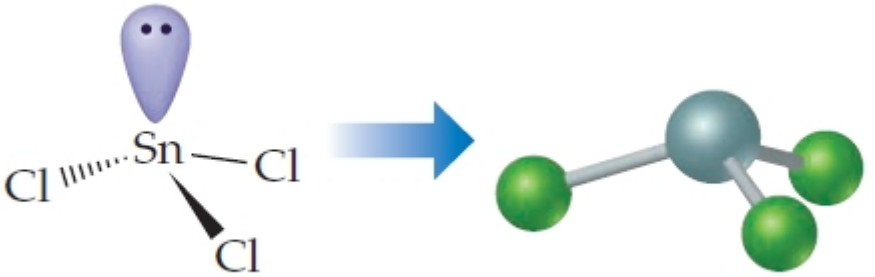
Quais as geometrias moleculares de O_3 e $SnCl_3^-$?

Dados: $_{8}O$ $_{17}Cl$ $_{50}Sn$

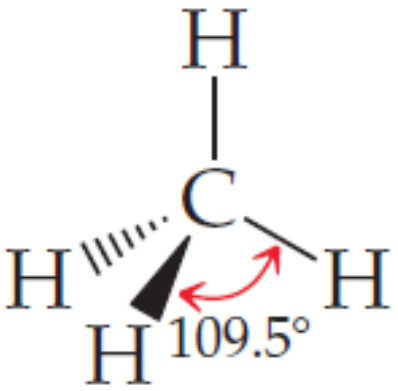


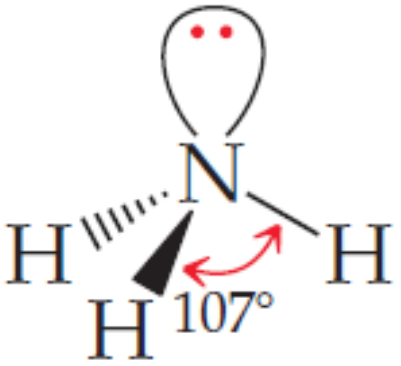


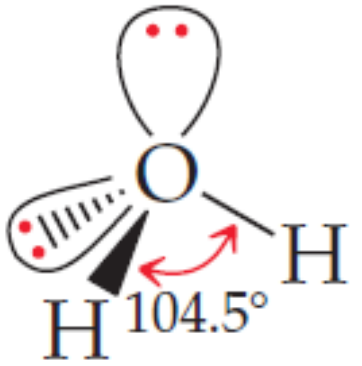


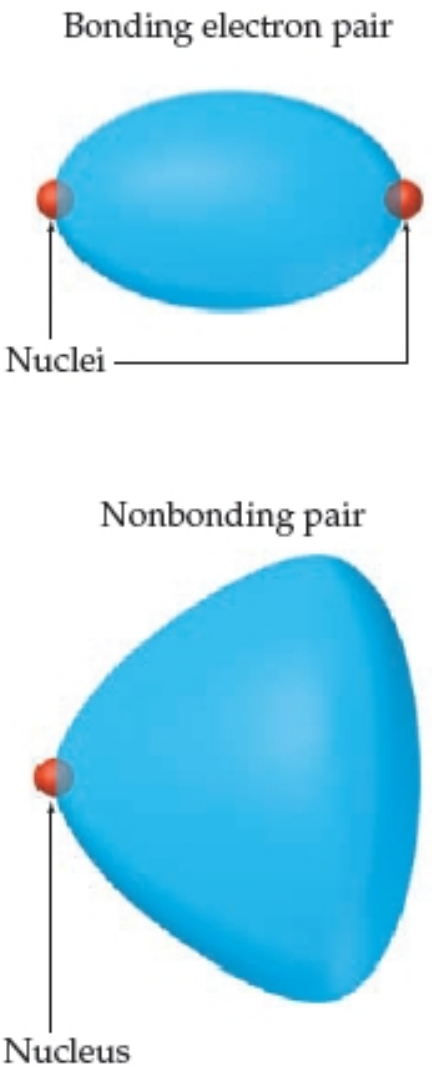


Efeito de Pares eletrônicos não-ligados



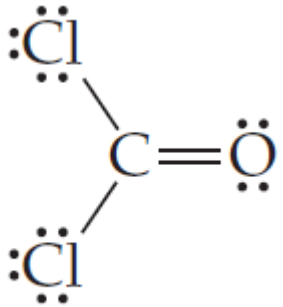




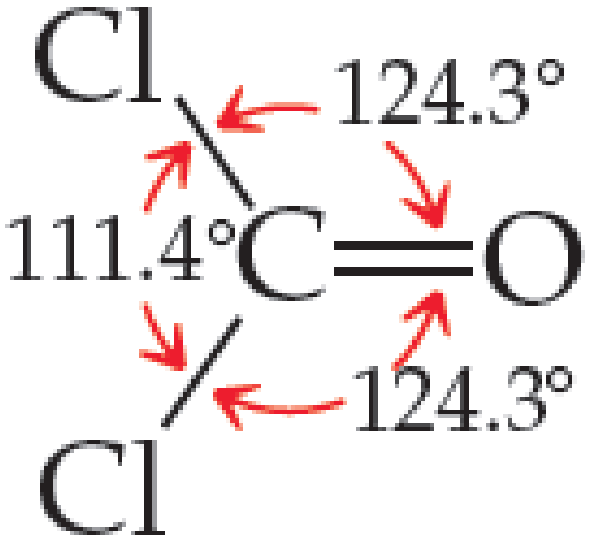


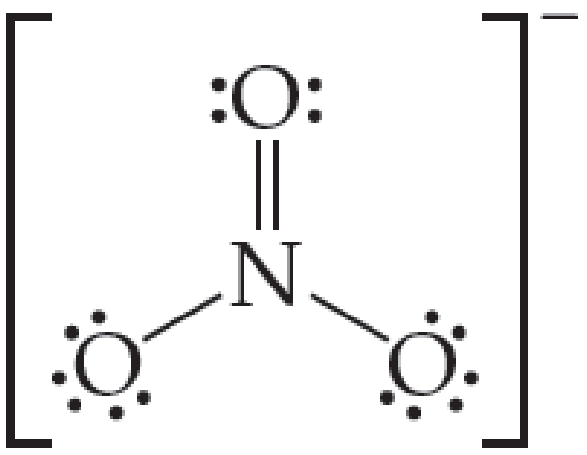
▲ **Figure 9.7** **Relative volumes occupied by bonding and nonbonding electron domains.**

Efeito de Ligações Múltiplas



Fosgênio





Por que os ângulos são todos iguais a 120.0^{o} ?

Átomos centrais com valência estendida

Table 9.3 Electron-Domain and Molecular Geometries for Five and Six Electron Domains around a Central Atom

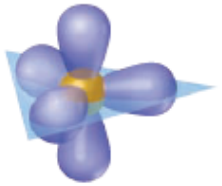
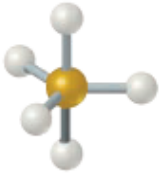
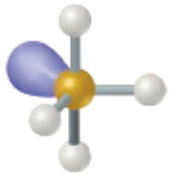
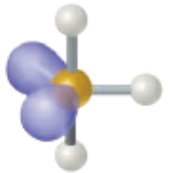
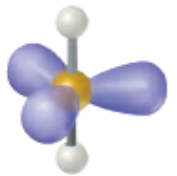
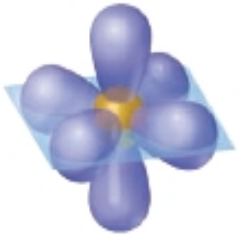
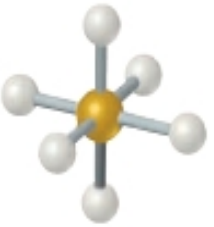
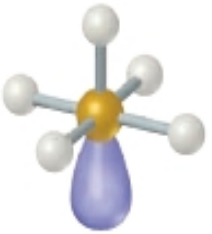
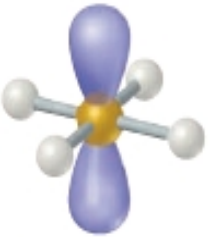
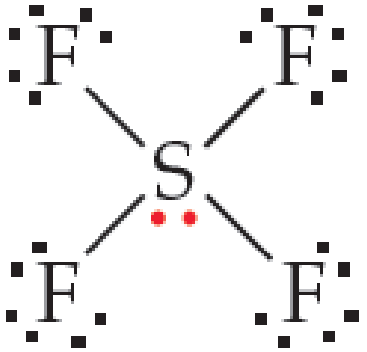
Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
5	 Trigonal bipyramidal	5	0	 Trigonal bipyramidal	PCl_5
		4	1	 Seesaw	SF_4
		3	2	 T-shaped	ClF_3
		2	3	 Linear	XeF_2

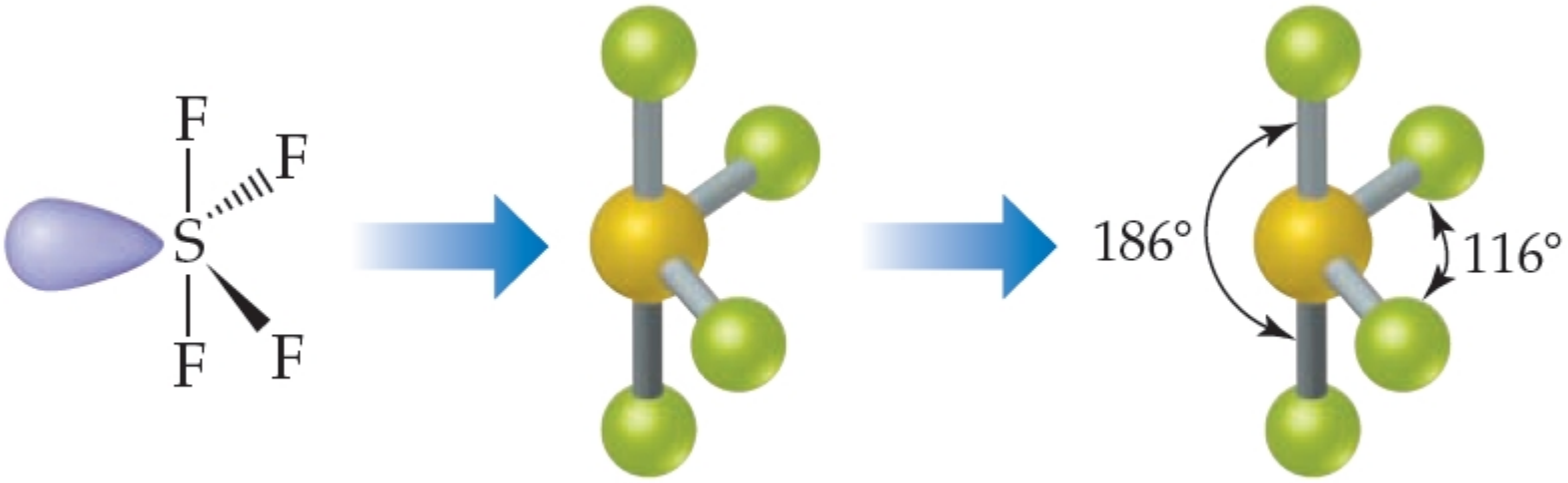
Table 9.3 Electron-Domain and Molecular Geometries for Five and Six Electron Domains around a Central Atom

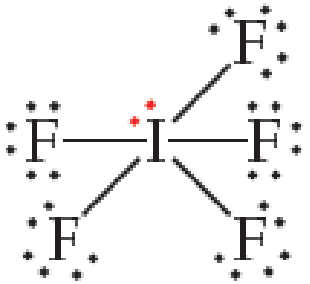
Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
6	 Octahedral	6	0	 Octahedral	SF_6
		5	1	 Square pyramidal	BrF_5
		4	2	 Square planar	XeF_4

Exemplos

SF_4



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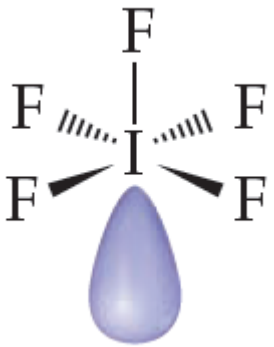
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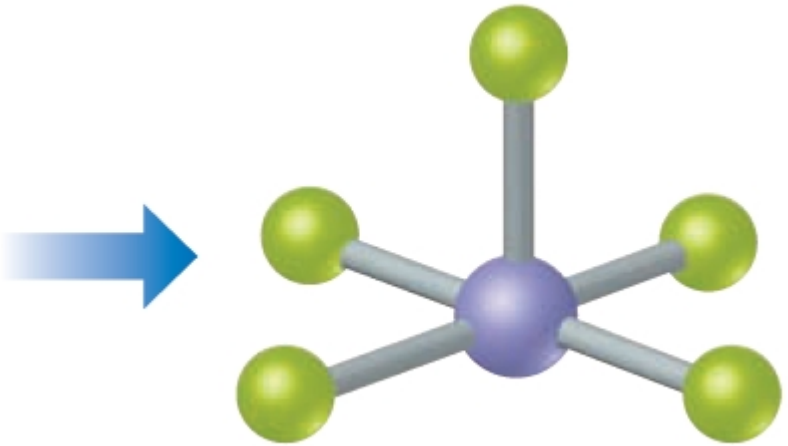
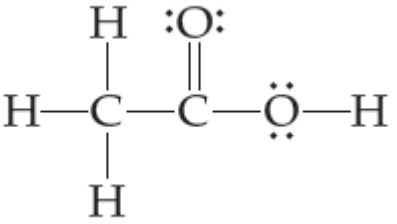
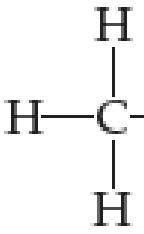
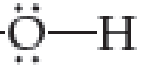
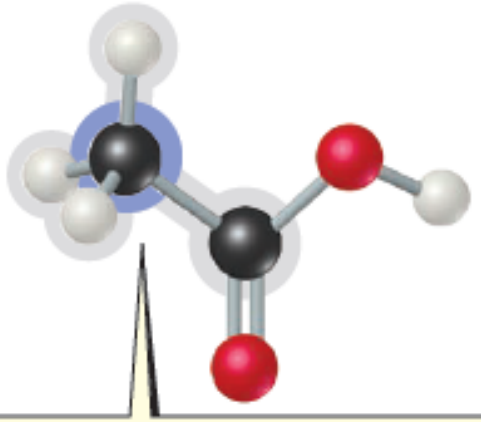


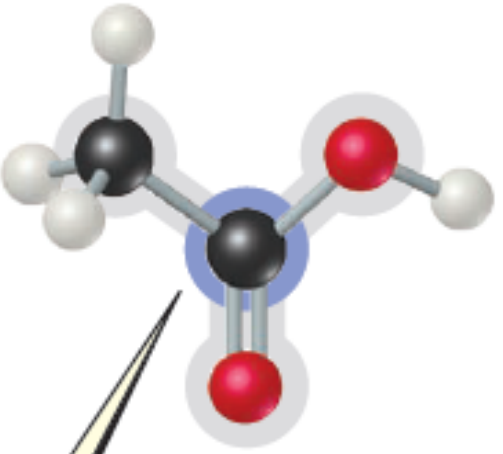
Moléculas Maiores



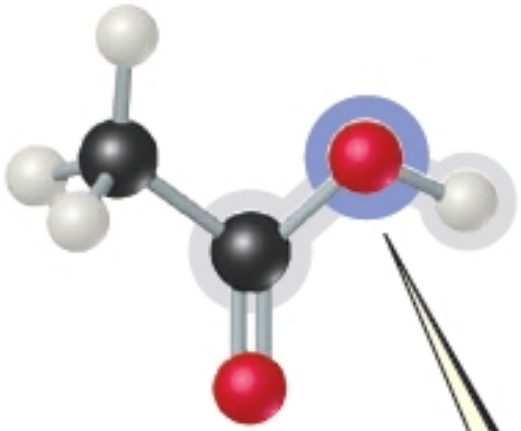
			
Number of electron domains	4	3	4
Electron-domain geometry	Tetrahedral	Trigonal planar	Tetrahedral
Predicted bond angles	109.5°	120°	109.5°



Electron-domain geometry tetrahedral, molecular geometry tetrahedral

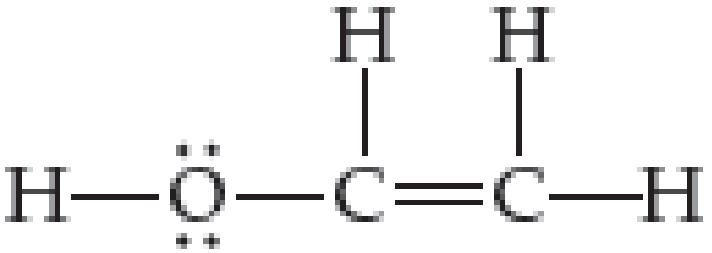


Electron-domain geometry trigonal planar, molecular geometry trigonal planar

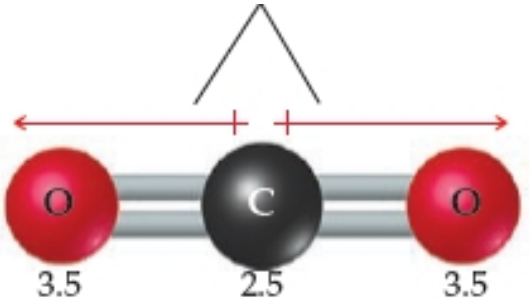


Electron-domain geometry tetrahedral, molecular geometry bent

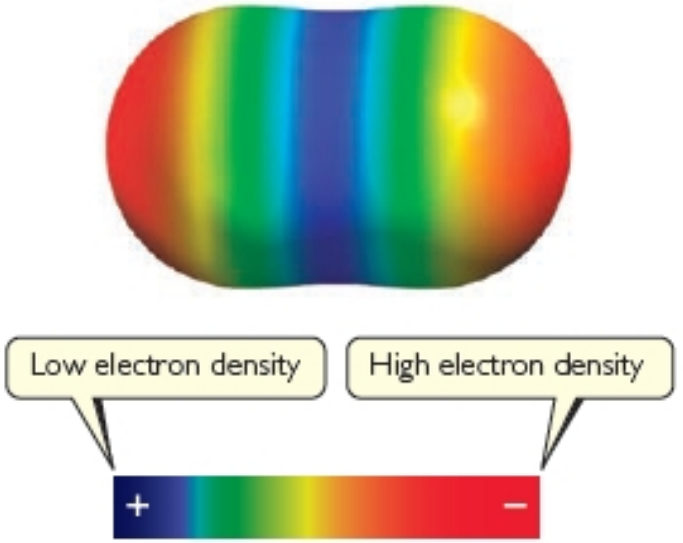
Desenhe a geometria de:

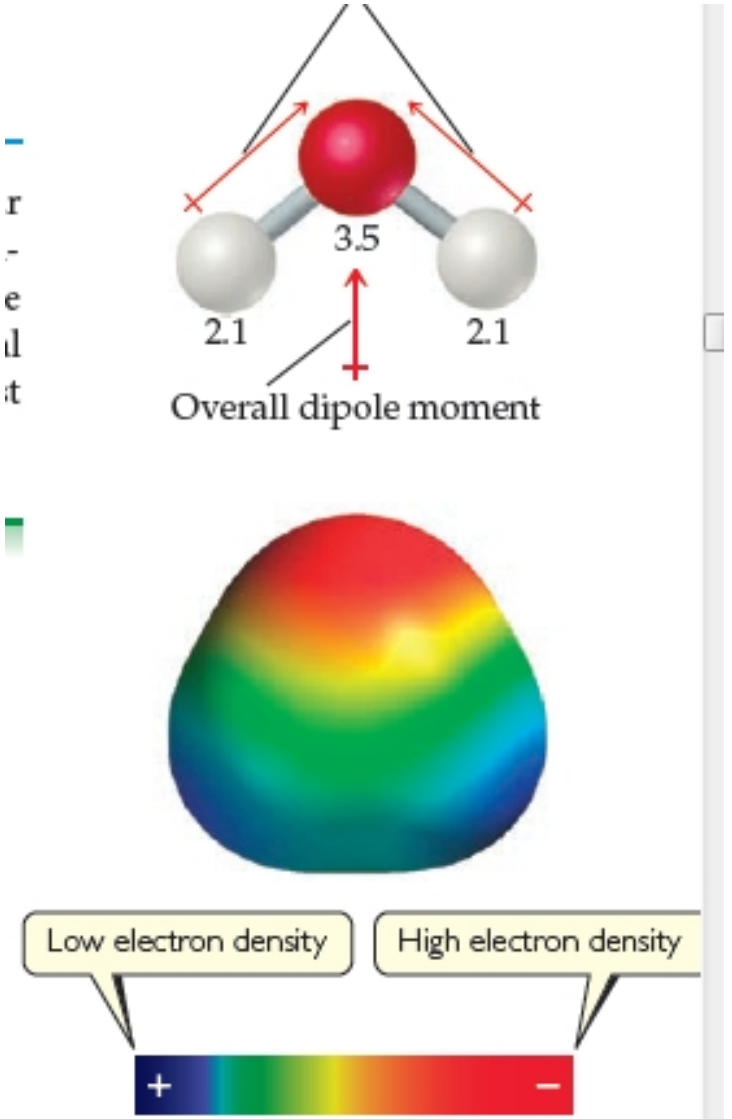


Polaridade e Geometria Molecular

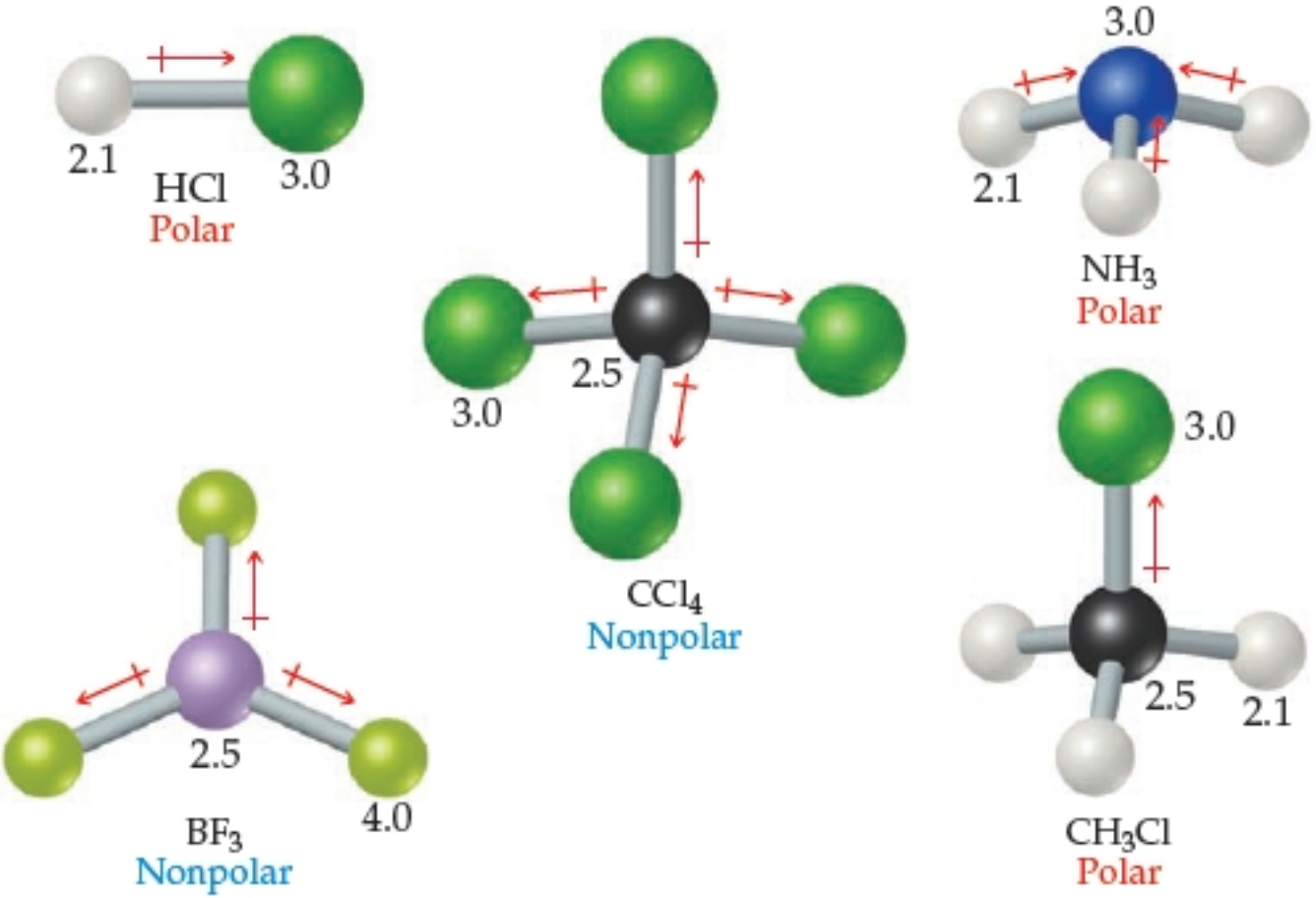


Overall dipole moment = 0



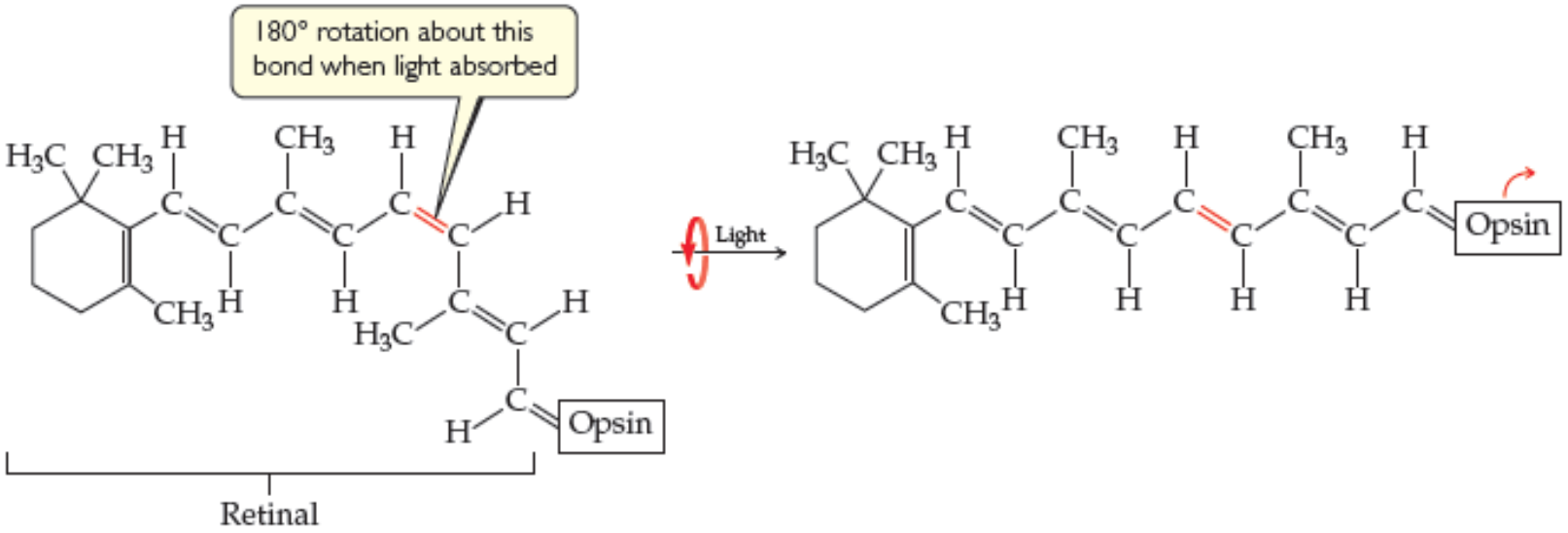


▲ **Figure 9.11** **H_2O, a polar molecule.** The numbers are electronegativity values.



▲ **Figure 9.12** **Polar and nonpolar molecules containing polar bonds.** The numbers are electronegativity values.

A Química da Visão



▲ **Figure 9.31** **The rhodopsin molecule, the chemical basis of vision.** When rhodopsin absorbs visible light, the π component of the double bond shown in red breaks, allowing rotation that produces a change in molecular geometry before the π bond re-forms.