

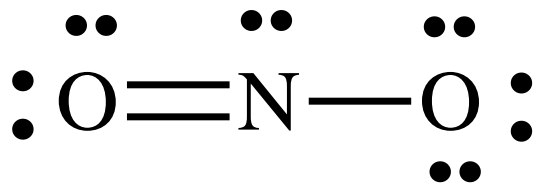
Molecular Shapes

VSEPR Model

- Valence-Shell Electron-Pair Repulsion
- Bonds (single or multiple) and lone pairs are thought of as charge clouds
 - They repel each other and stay as far away from each other as possible
 - Because of this, molecules assume specific 3D geometries based on the lone pairs and bonds made.

Electron Groups

- The Lewis structure predicts the arrangement of valence electrons around the central atom(s).
- Each lone pair of electrons constitutes one electron group on a central atom.
- Each bond constitutes one electron group on a central atom.
 - Regardless of whether it is single, double, or triple.



There are 3 electron groups on N.
1 lone pair.
1 single bond.
1 double bond.

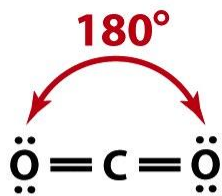
Steps to Predicting a VSEPR Geometry

1. Draw the Electron-Dot Structure
2. Identify the number of bonds and lone pairs.
3. Predict the arrangement assuming that the clouds orient so that they are as far apart as possible.
 - Note that actual shape is based on where atoms are, not the lone pairs.

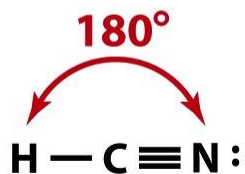
Molecular Shapes: the VSEPR Model

Two Charge Clouds

A CO₂ molecule is linear, with a bond angle of 180°.



An HCN molecule is linear, with a bond angle of 180°.

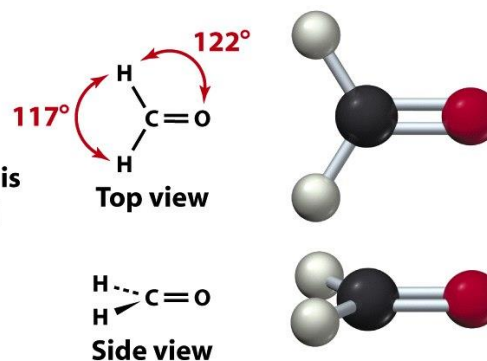


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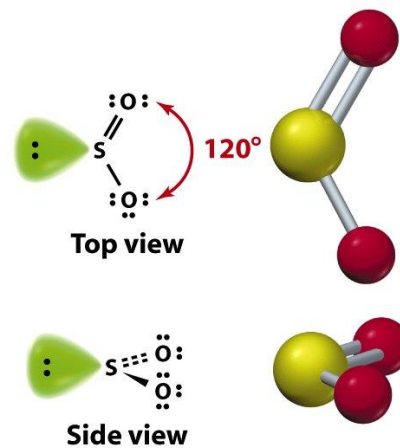
Molecular Shapes: the VSEPR Model

Three Charge Clouds

A formaldehyde molecule is trigonal planar, with bond angles of roughly 120° .



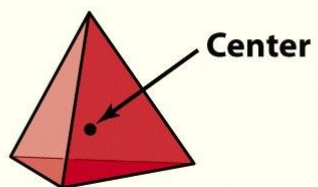
An SO_2 molecule is bent with a bond angle of approximately 120° .



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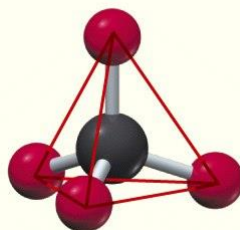
Molecular Shapes: the VSEPR Model

Four Charge Clouds

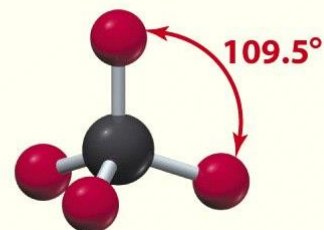


A regular tetrahedron

The atom is located in the center of a regular tetrahedron.



The four charge clouds point to the four corners of the tetrahedron.



A tetrahedral molecule

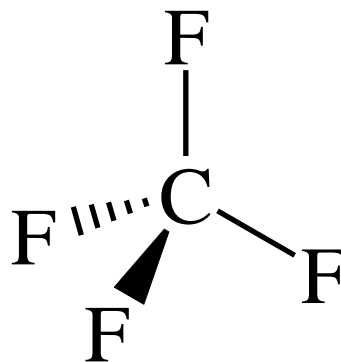
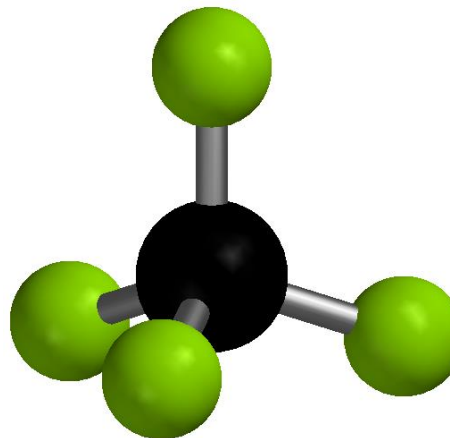
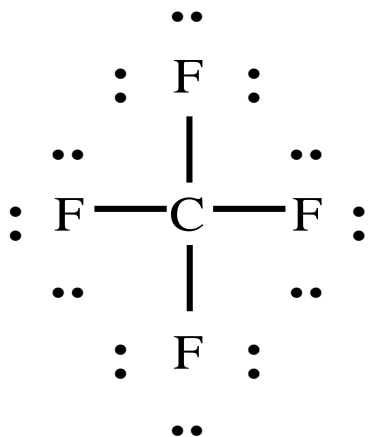
The angle between any two bonds is 109.5° .

Figure 7-5 Chemistry, 5/e
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Sketching a Molecule

- Because molecules are three-dimensional objects, our drawings should indicate their three-dimensional quality
- By convention:
 - A filled wedge indicates that the attached atom is coming out of the paper toward you.
 - A dashed wedge indicates that the attached atom is going behind the paper away from you.

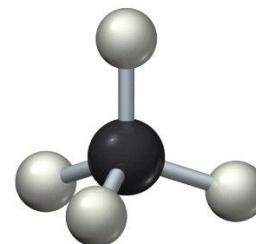
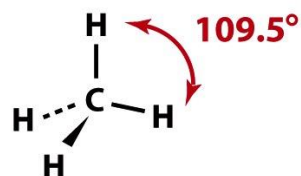
Sketching a Molecule, Continued



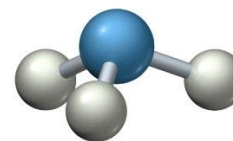
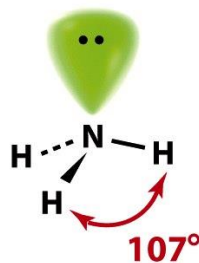
Molecular Shapes: the VSEPR Model

Four Charge Clouds

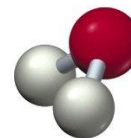
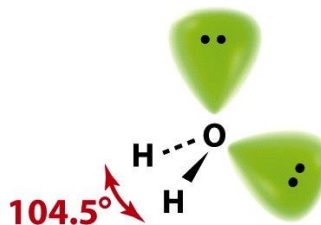
A methane molecule is tetrahedral, with bond angles of 109.5° .



An ammonia molecule is trigonal pyramidal, with bond angles of 107° .



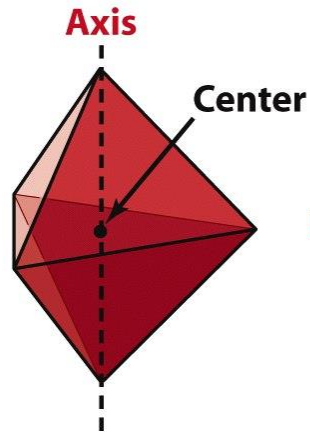
A water molecule is bent, with a bond angle of 104.5° .



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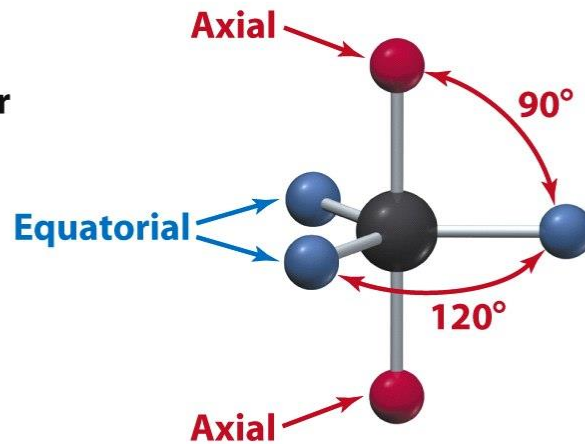
Molecular Shapes: the VSEPR Model

Five Charge Clouds

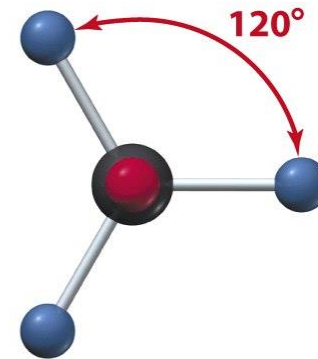


A trigonal bipyramid

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Side view

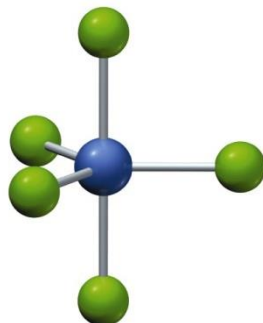
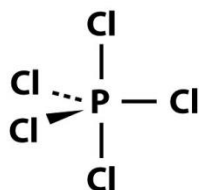


Top view

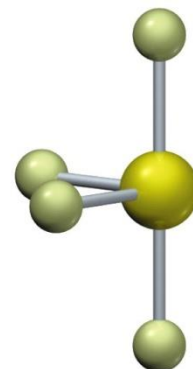
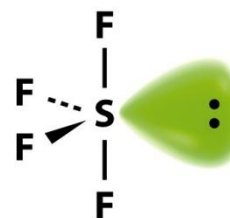
Molecular Shapes: the VSEPR Model

Five Charge Clouds

A PCl_5 molecule is trigonal bipyramidal.



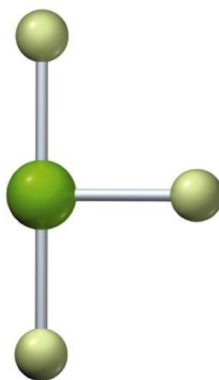
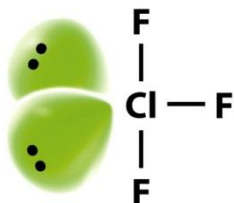
An SF_4 molecule is shaped like a seesaw (turn 90° to see it).



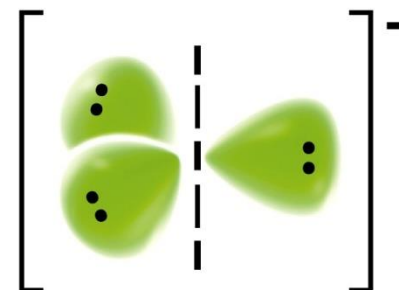
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Unnumbered 7 p246b Chemistry, 5/e

A ClF_3 molecule is T-shaped (turn 90° to see it).



An I_3^- ion is linear.

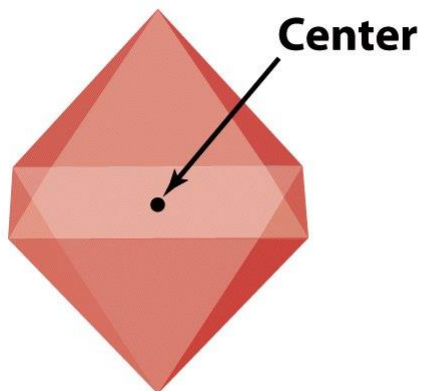


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Unnumbered 7 p246d Chemistry, 5/e
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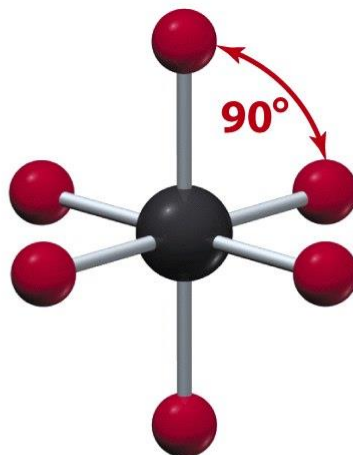
Molecular Shapes: the VSEPR Model

Six Charge Clouds

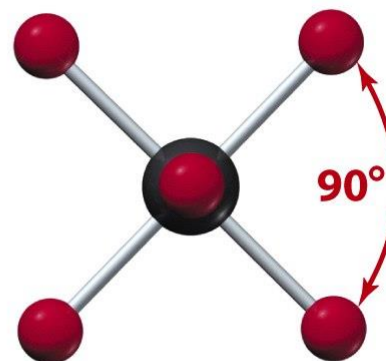


A regular octahedron

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Side view

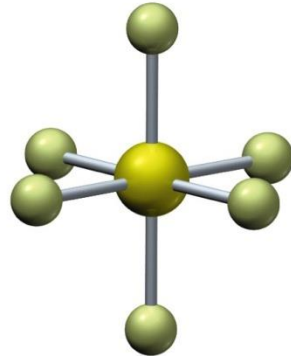
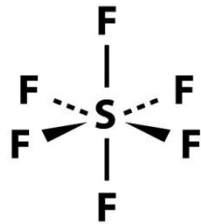


Top view

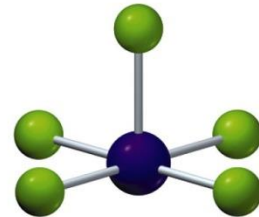
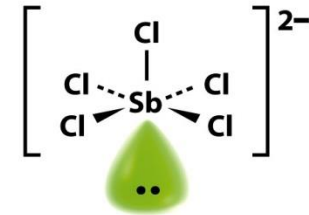
Molecular Shapes: the VSEPR Model

Six Charge Clouds

An SF_6 molecule is octahedral.

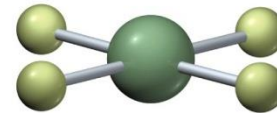
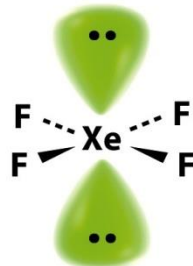


An SbCl_5^{2-} ion has a square pyramidal shape.



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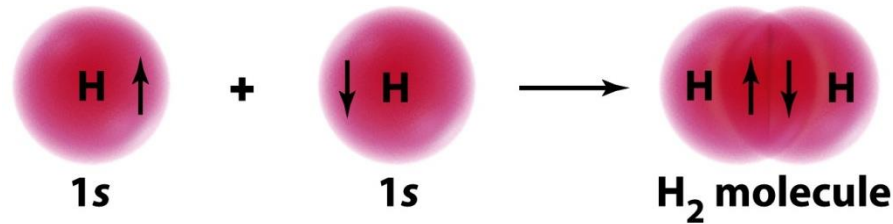
An XeF_4 molecule has a square planar shape.



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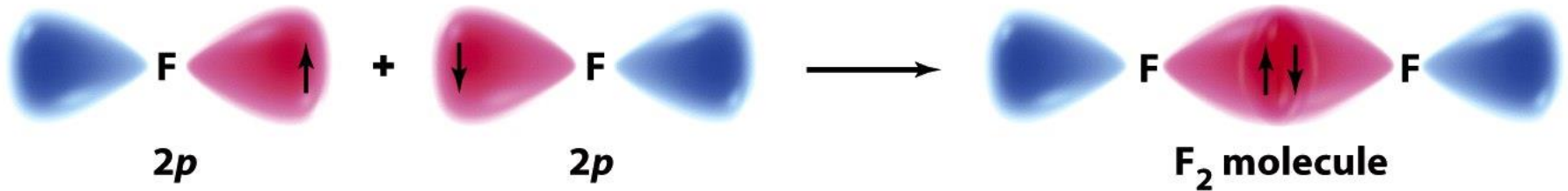
Valence Bond Theory

Valence Bond Theory: A quantum mechanical model which shows how electron pairs are shared in a covalent bond.



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sigma (σ) bonds



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Valence Bond Theory

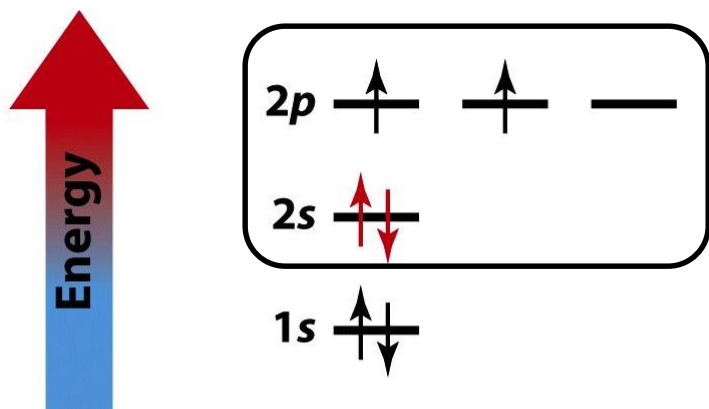
Valence Bond Theory: A quantum mechanical model which shows how electron pairs are shared in a covalent bond.

- Covalent bonds are formed by overlap of atomic orbitals, each of which contains one electron of opposite spin.
- Each of the bonded atoms maintains its own atomic orbitals, but the electron pair in the overlapping orbitals is shared by both atoms.
- The greater the amount of overlap, the stronger the bond.

Hybridization and sp^3 Hybrid Orbitals

How can the bonding in CH_4 be explained?

4 valence electrons
2 unpaired electrons



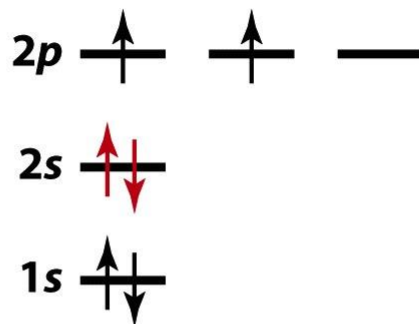
**Carbon:
ground-state electron
configuration**

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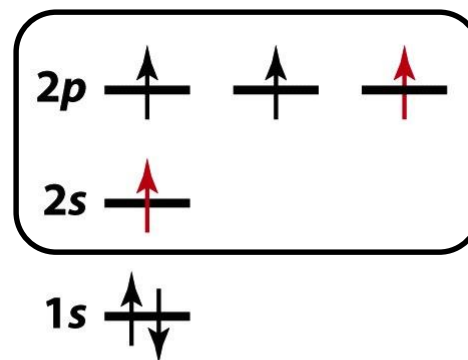
Hybridization and sp^3 Hybrid Orbitals

How can the bonding in CH_4 be explained?

4 valence electrons
4 unpaired electrons



Carbon:
ground-state electron
configuration

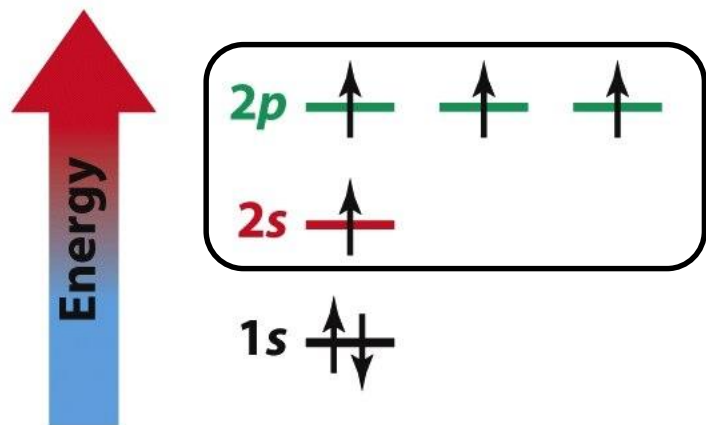


Carbon:
excited-state electron
configuration

Hybridization and sp^3 Hybrid Orbitals

How can the bonding in CH_4 be explained?

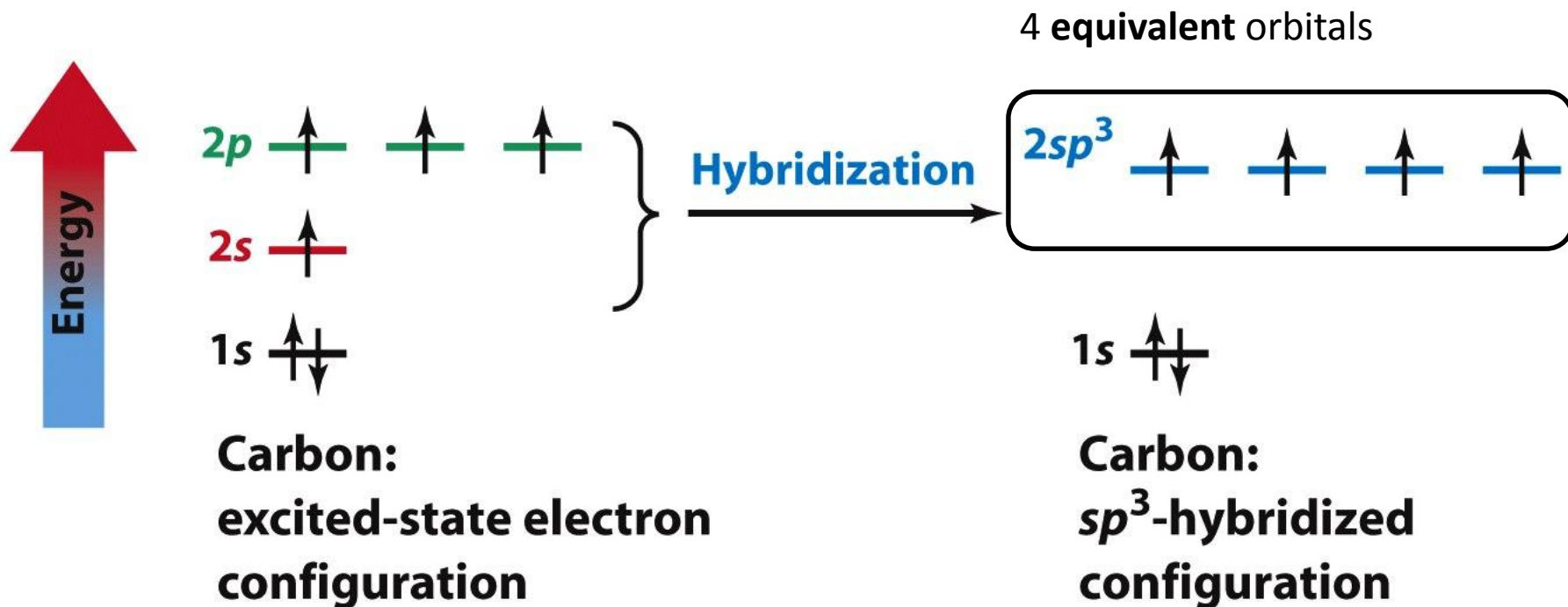
4 nonequivalent orbitals



**Carbon:
excited-state electron
configuration**

Hybridization and sp^3 Hybrid Orbitals

How can the bonding in CH_4 be explained?



Hybridization and sp^3 Hybrid Orbitals

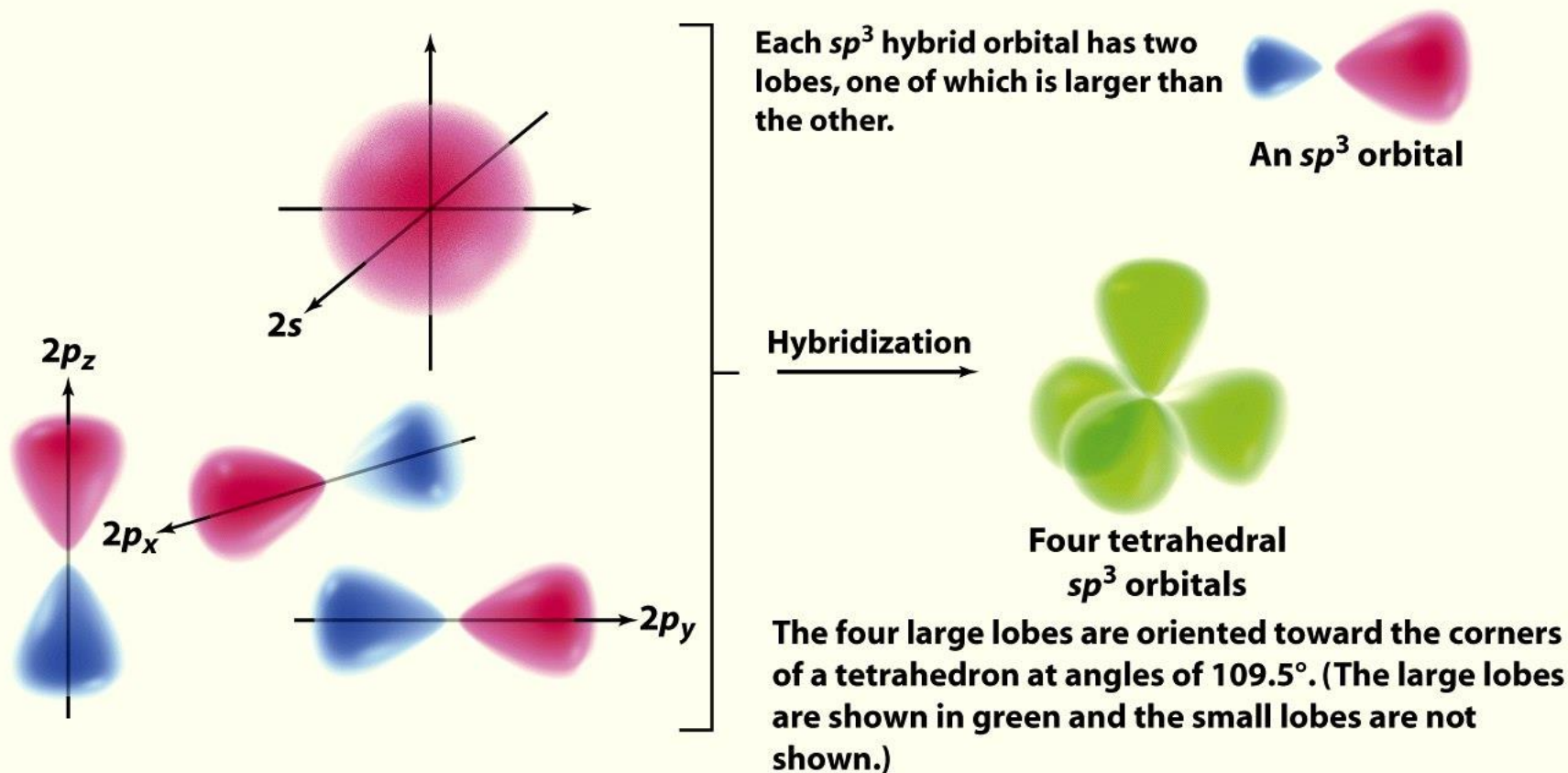


Figure 7-6 Chemistry, 5/e
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Hybridization and sp^3 Hybrid Orbitals

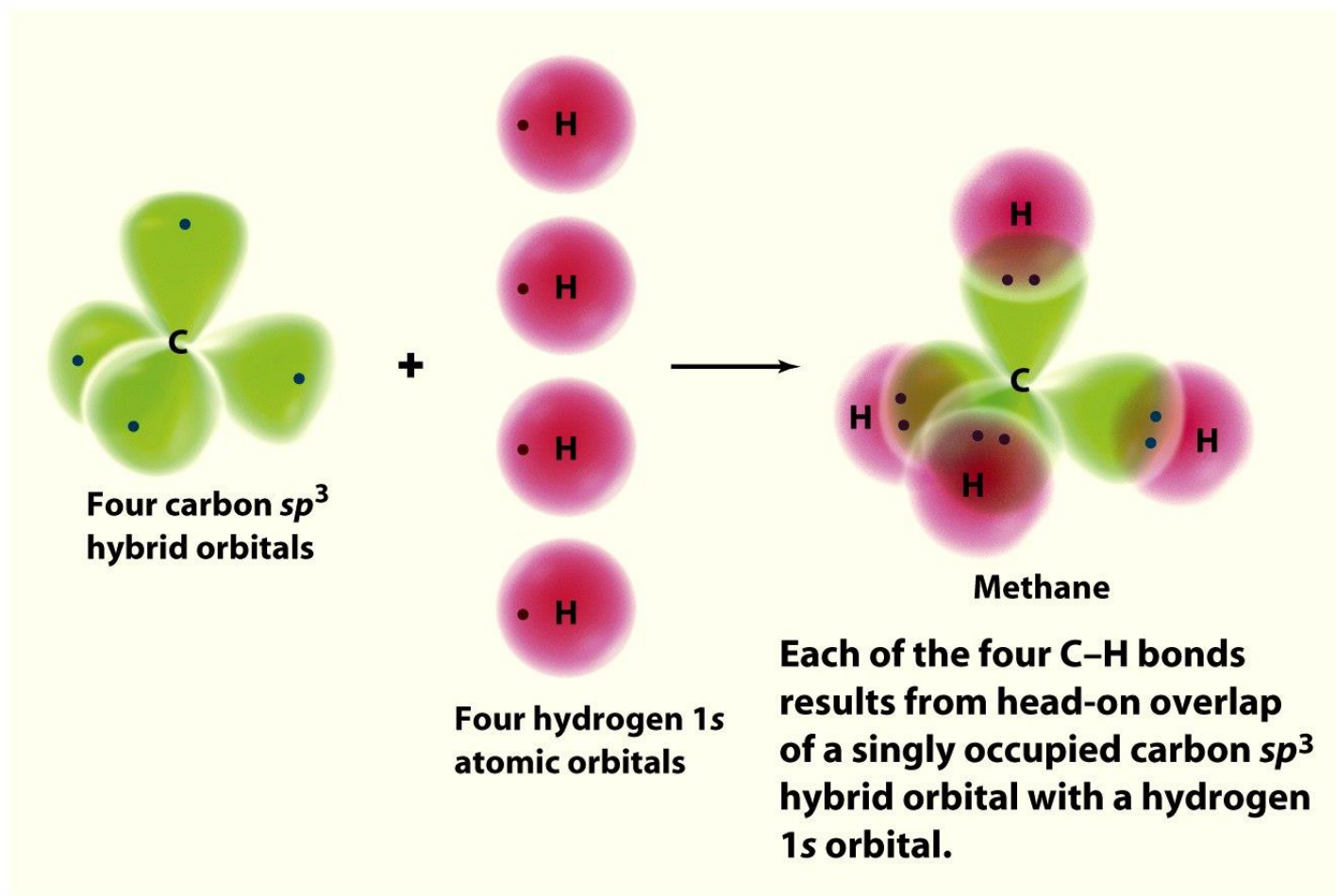


Figure 7-7 Chemistry, 5/e
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Other Kinds of Hybrid Orbitals

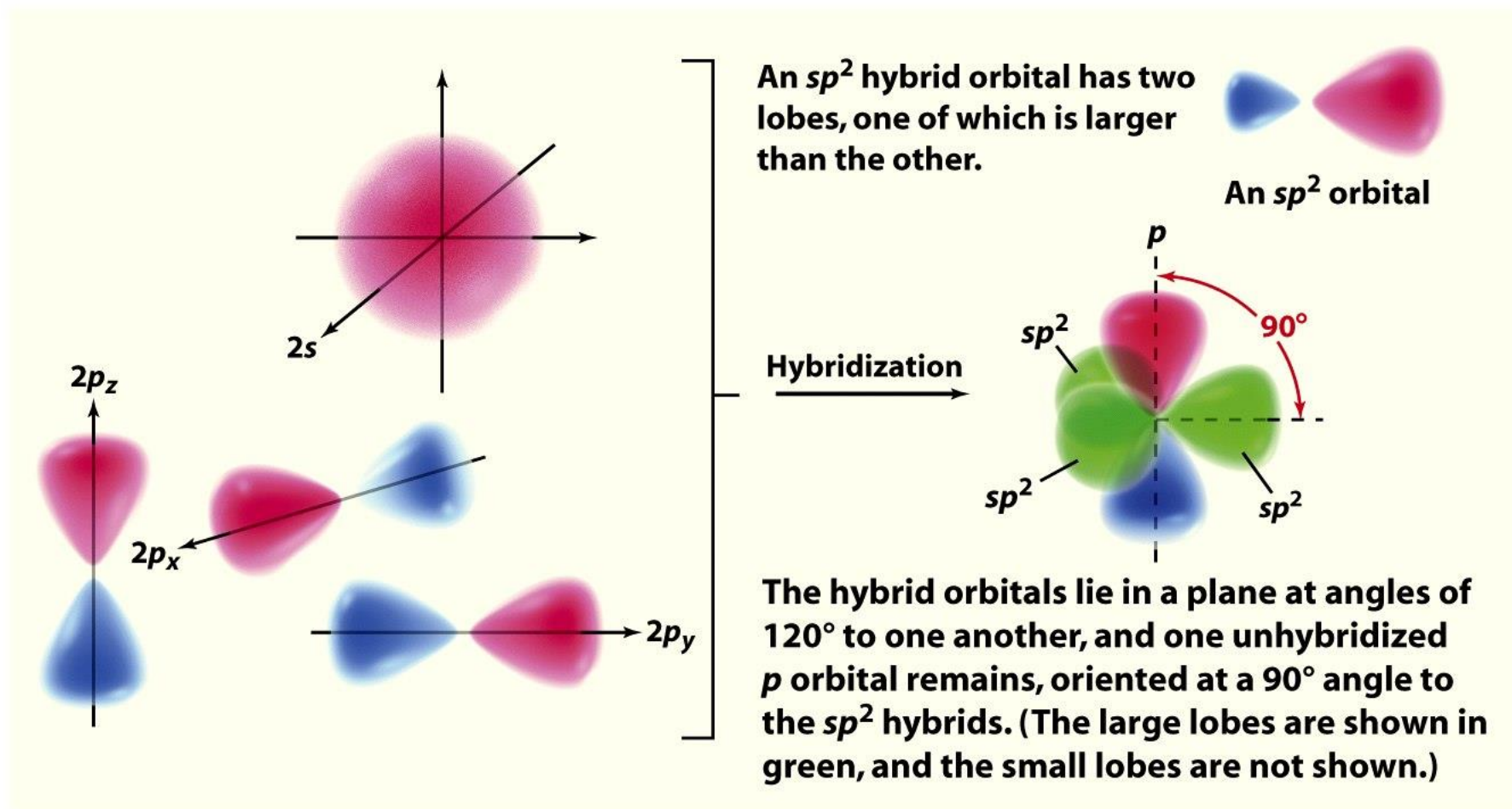


Figure 7-8 Chemistry, 5/e

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Other Kinds of Hybrid Orbitals

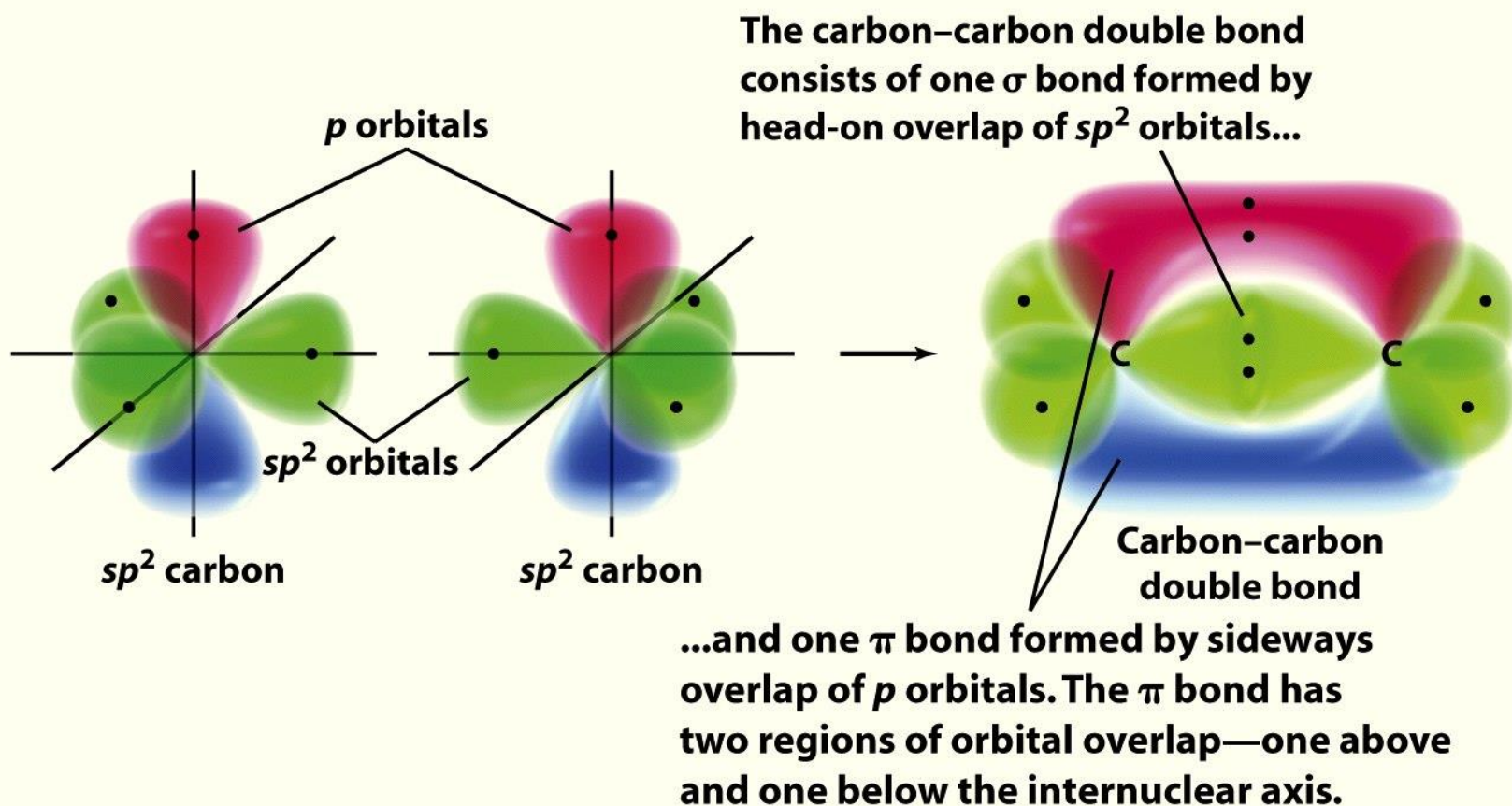
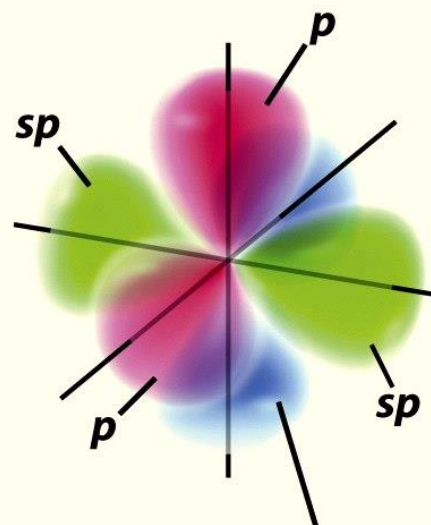
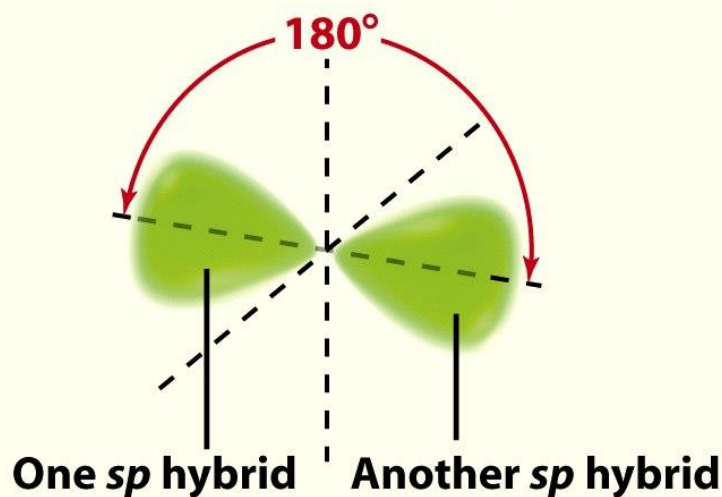


Figure 7-9 Chemistry, 5/e
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Other Kinds of Hybrid Orbitals

The combination of one s and one p orbital gives two sp hybrid orbitals oriented 180° apart.



In addition, two unhybridized p orbitals remain, oriented at 90° angles to the sp hybrids.

Figure 7-10 Chemistry, 5/e
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Other Kinds of Hybrid Orbitals

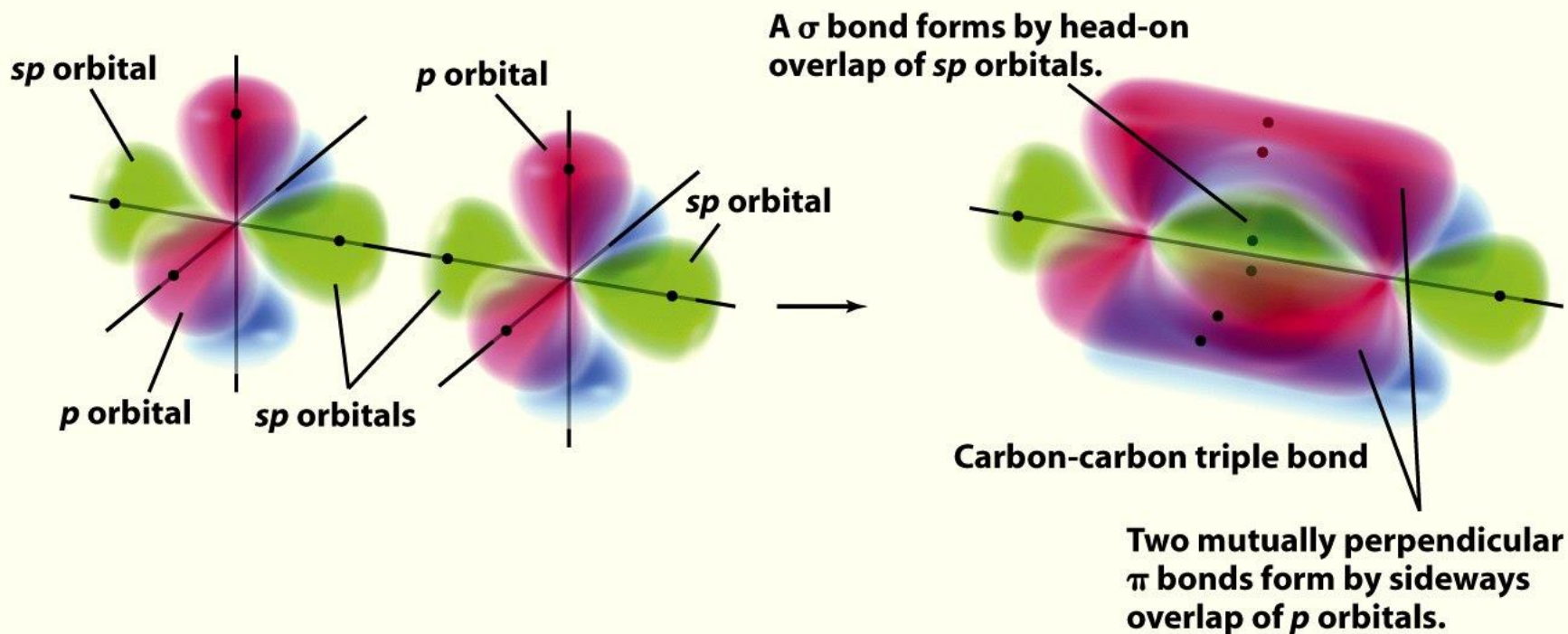


Figure 7-11 Chemistry, 5/e
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Other Kinds of Hybrid Orbitals

TABLE 7.5 Hybrid Orbitals and Their Geometry

Number of Charge Clouds	Geometry of Charge Clouds	Hybridization
2	Linear	sp
3	Trigonal planar	sp^2
4	Tetrahedral	sp^3

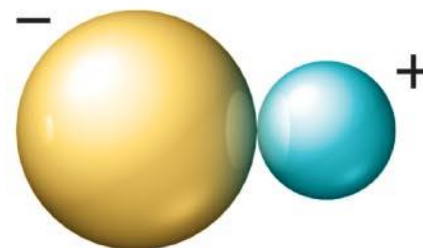
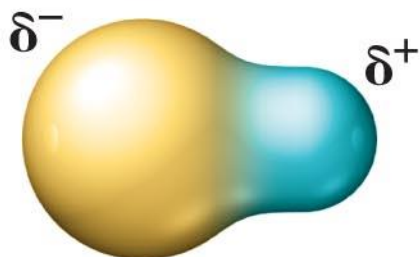
Table 7-5 Chemistry, 5/e
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The Continuum of Bond Types

Pure (nonpolar)
covalent bond

Polar
covalent bond

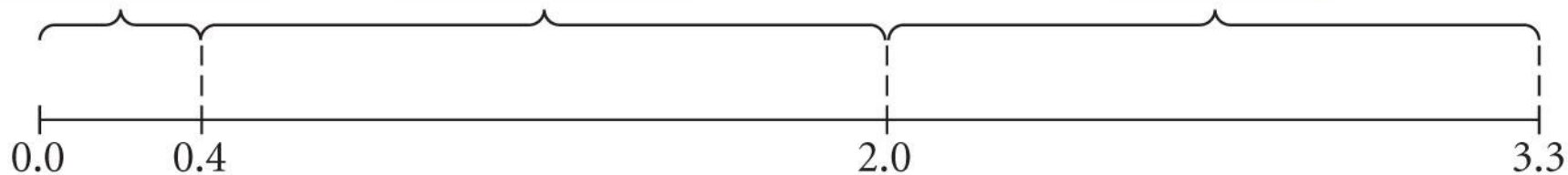
Ionic bond



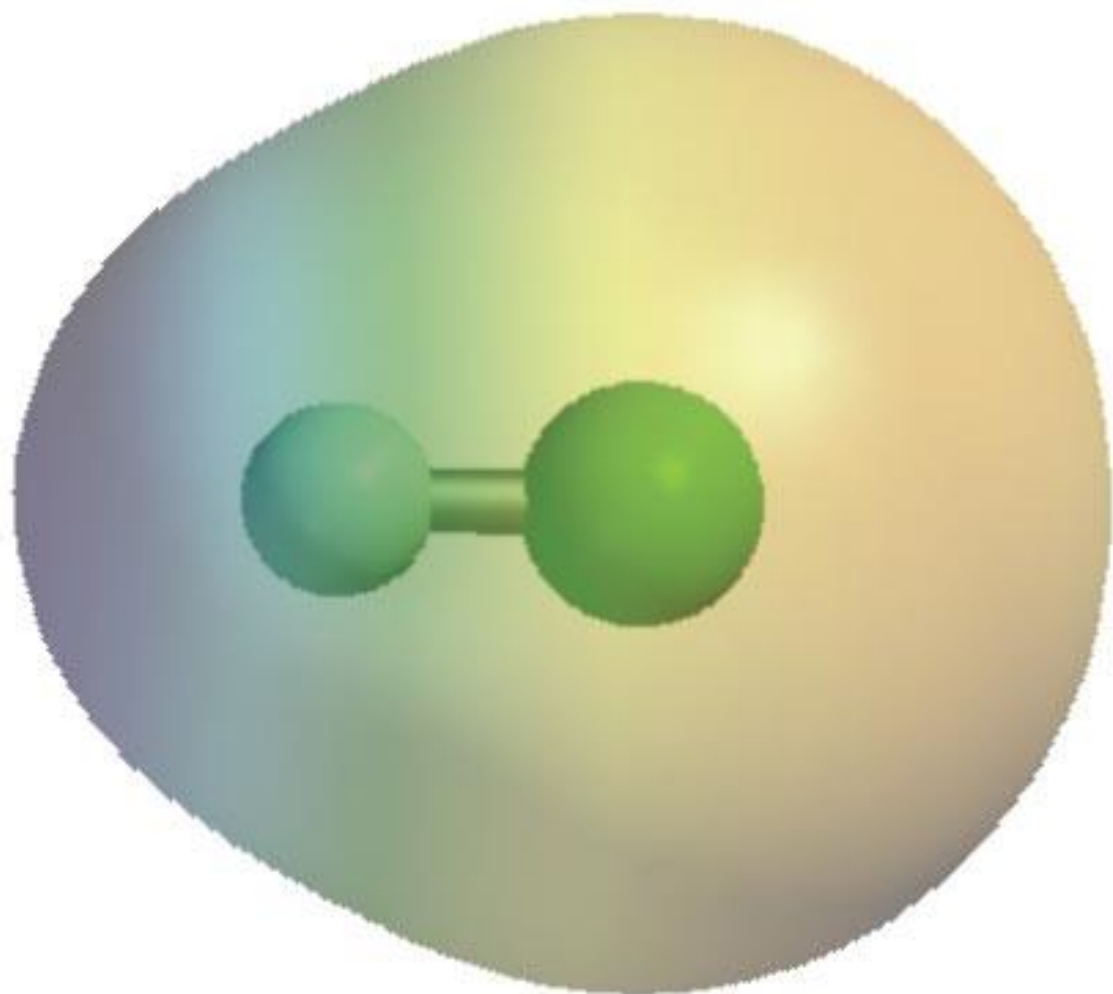
Electrons shared
equally

Electrons shared
unequally

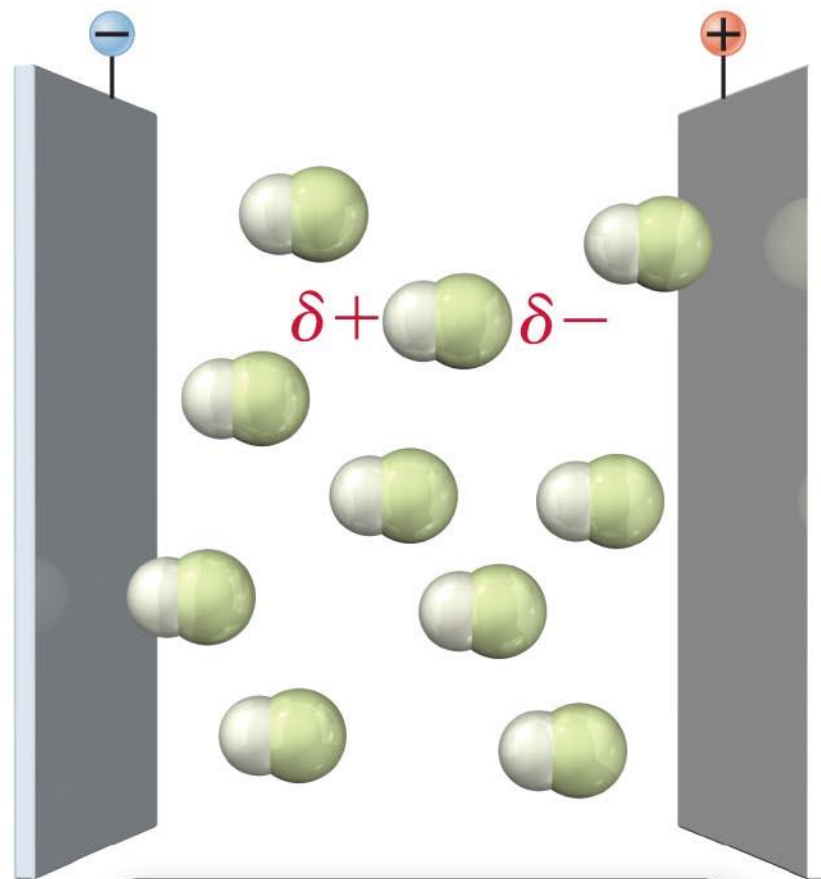
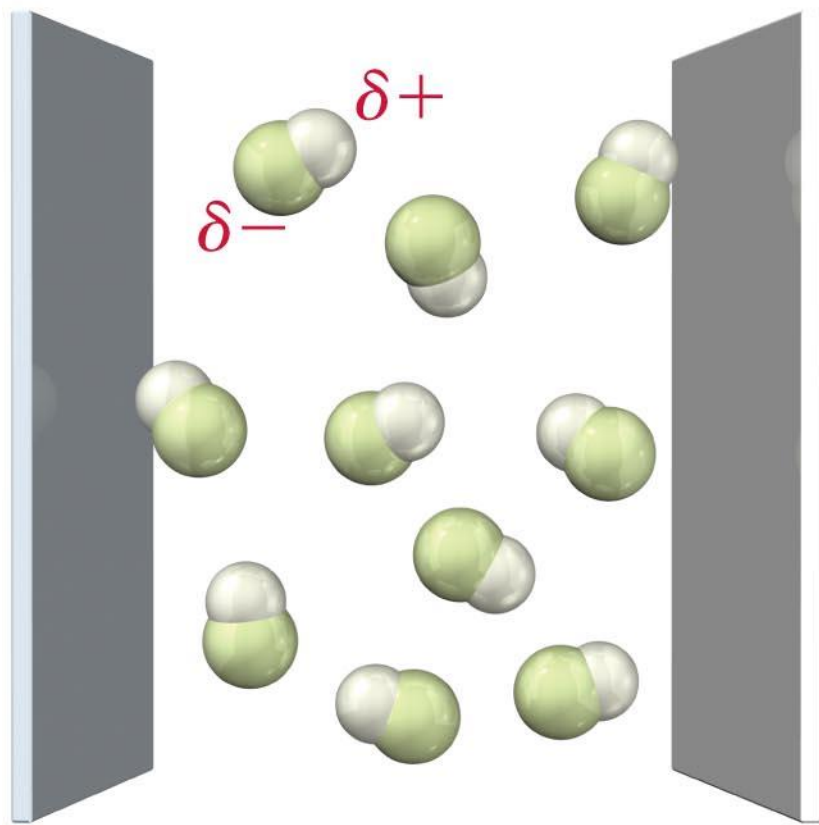
Electrons
transferred



Electronegativity difference, ΔEN



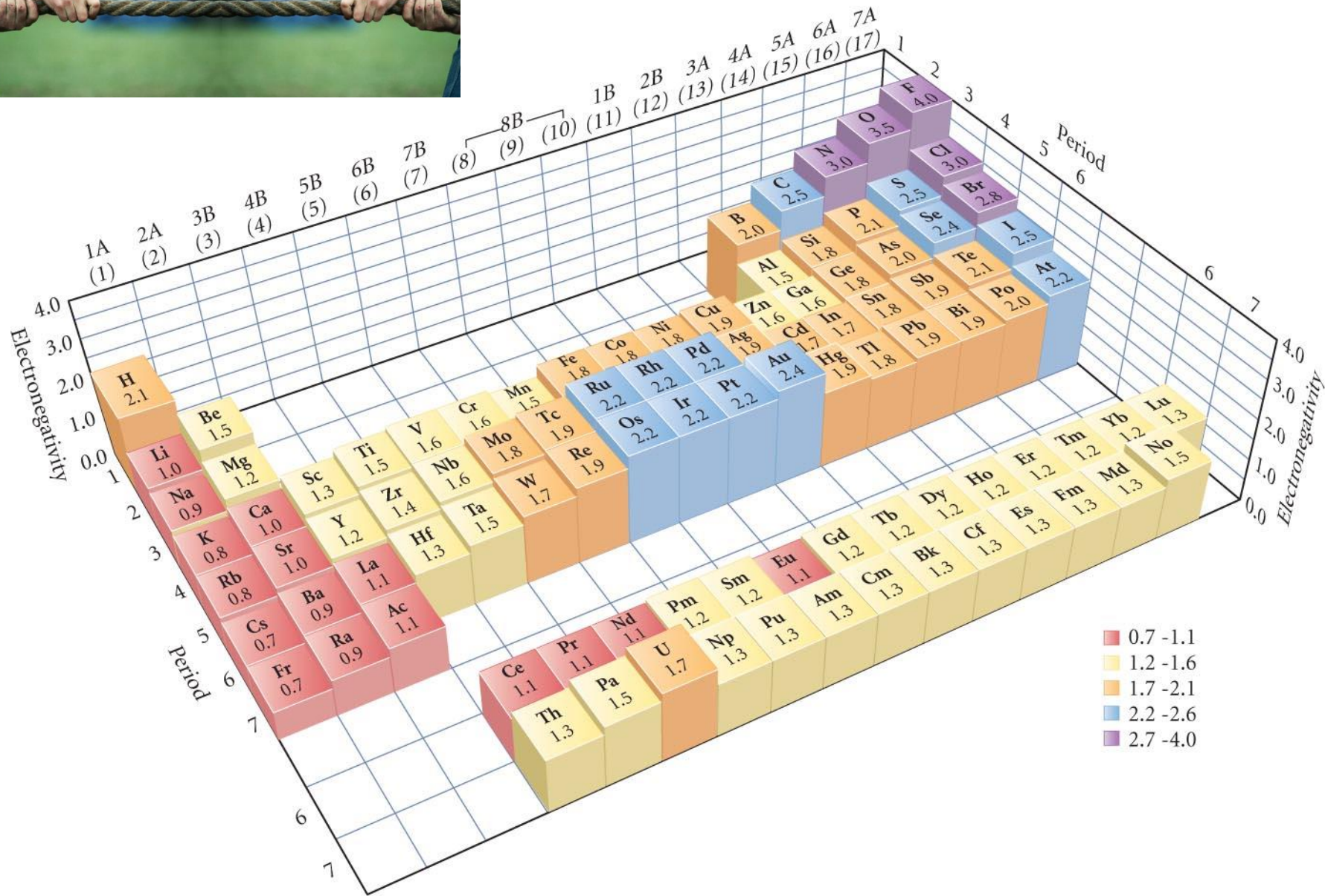
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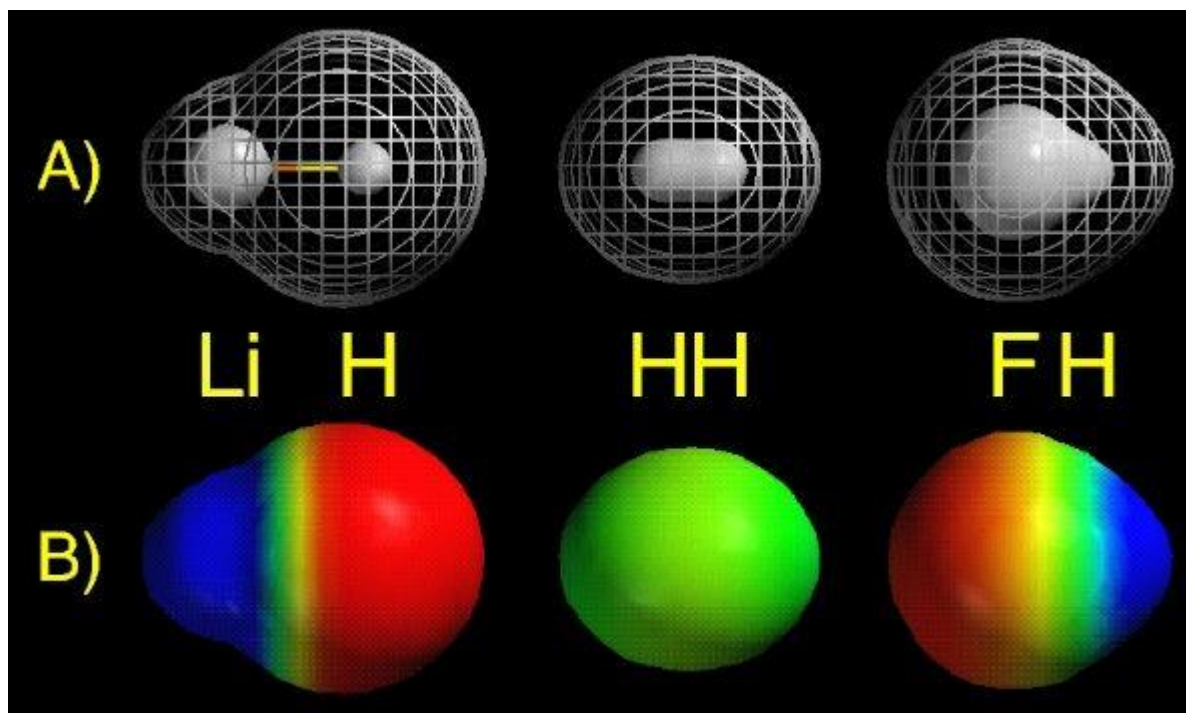
HF molecules align with an electric field



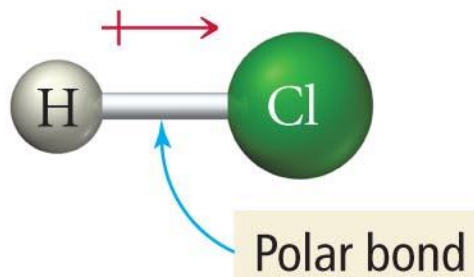
Trends in Electronegativity



Bond Polarity



Net dipole moment



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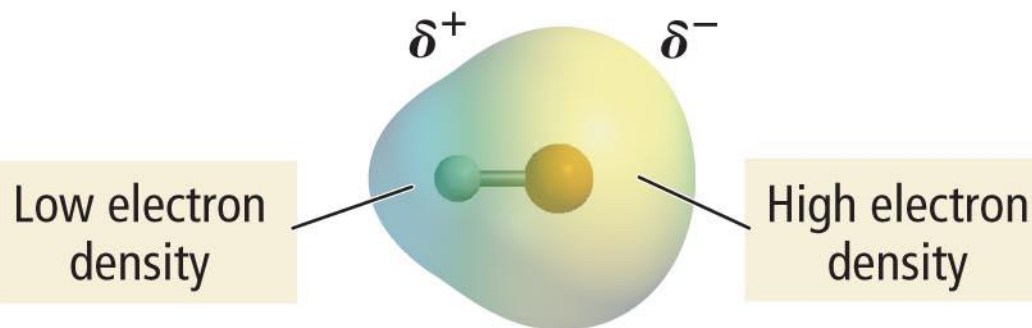
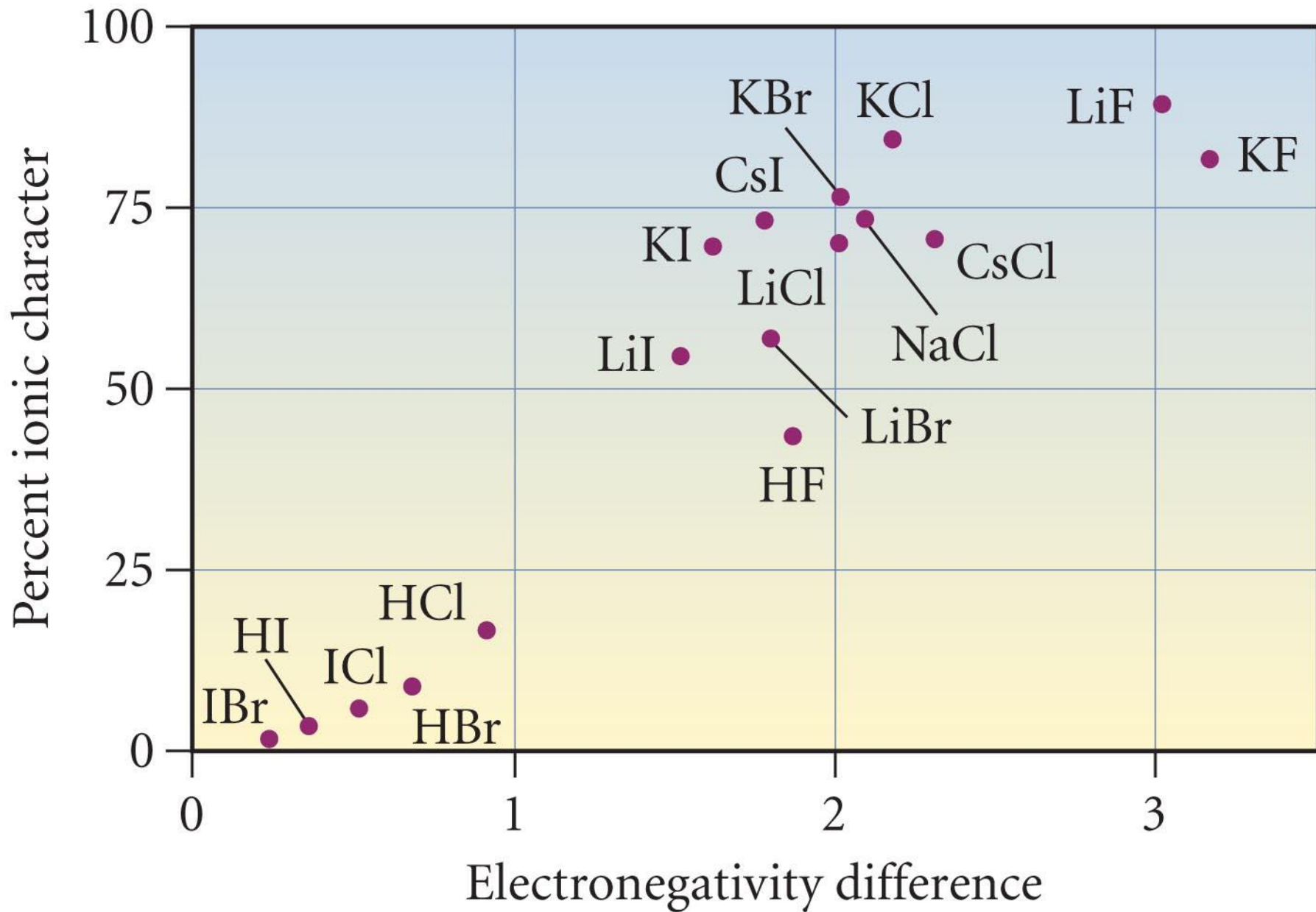


TABLE 9.2 Dipole Moments of Several Molecules in the Gas Phase

Molecule	ΔEN	Dipole Moment (D)
Cl ₂	0	0
ClF	1.0	0.88
HF	1.9	1.82
LiF	3.0	6.33



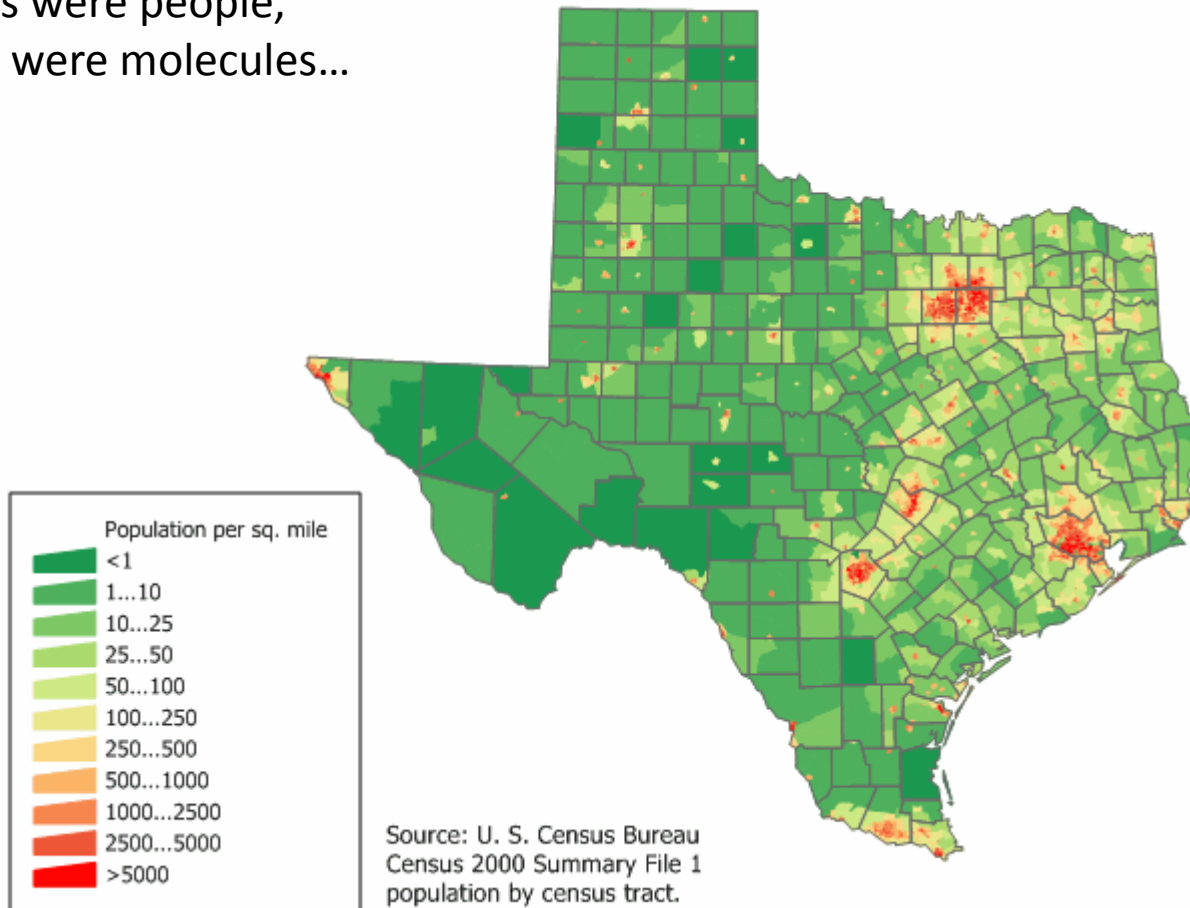
Molecular Polarity

- Diatomic: Same as bond polarity
- 3 or more atoms:
 - Depends on two things:
 - Individual bond polarities
 - 3D Shape of molecule
 - If a molecule is nonpolar, the bond polarities must be the same (not necessarily nonpolar), AND the shape must be symmetric.

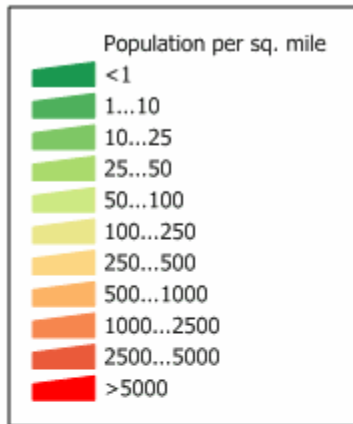
THINK SYMMETRY!!!

Population Density: Texas

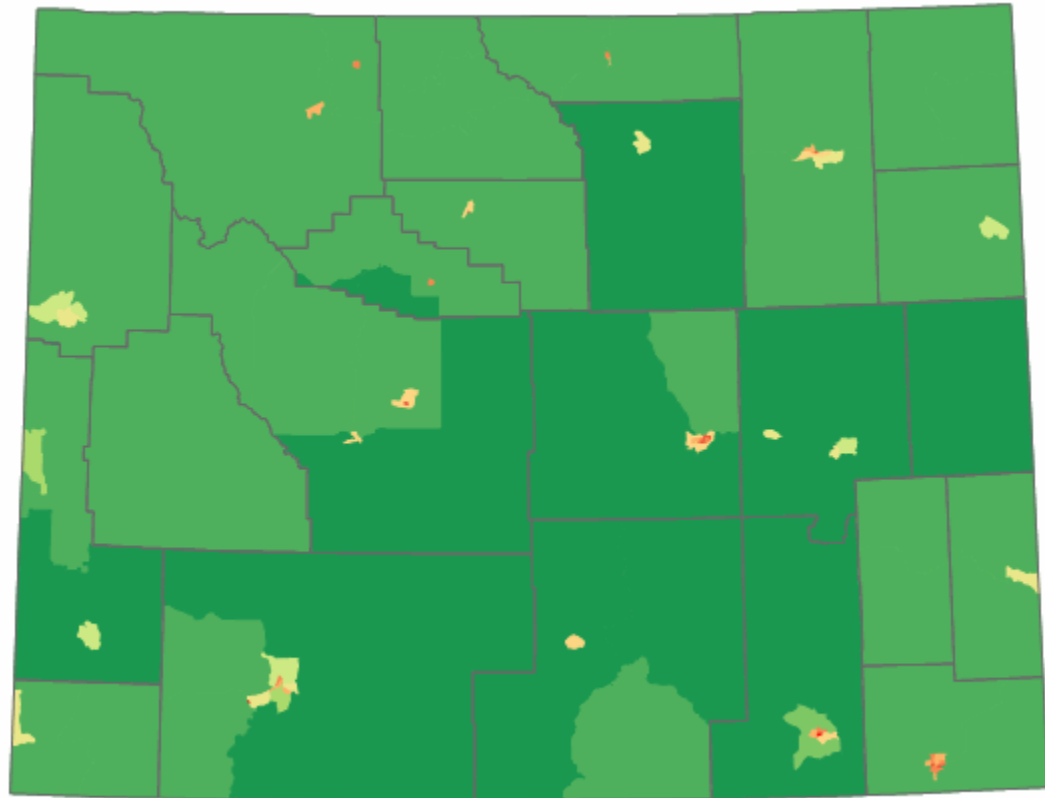
If electrons were people,
and states were molecules...

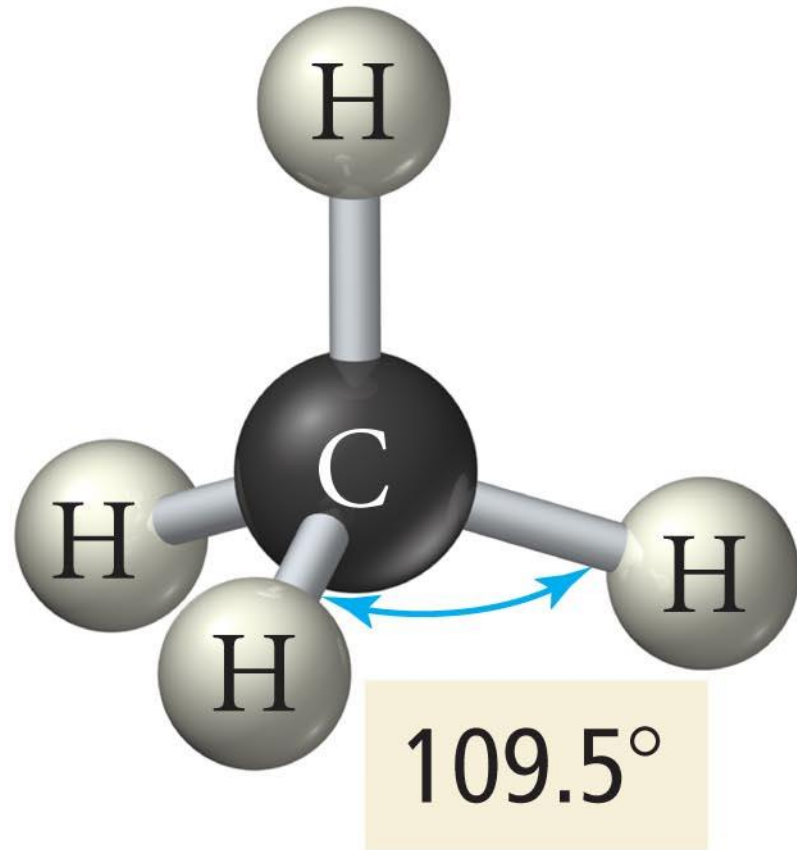
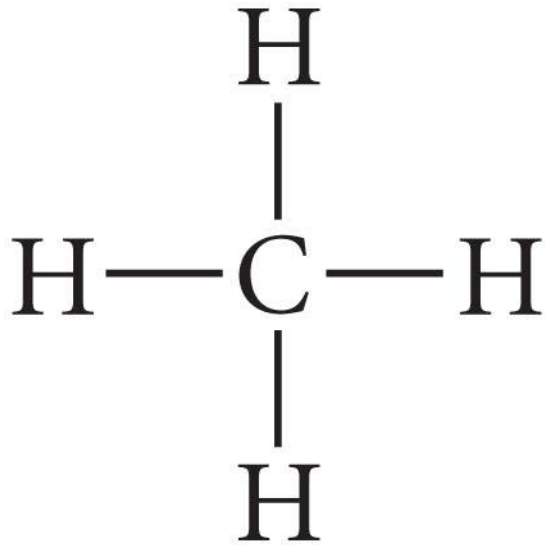


Population Density: Wyoming



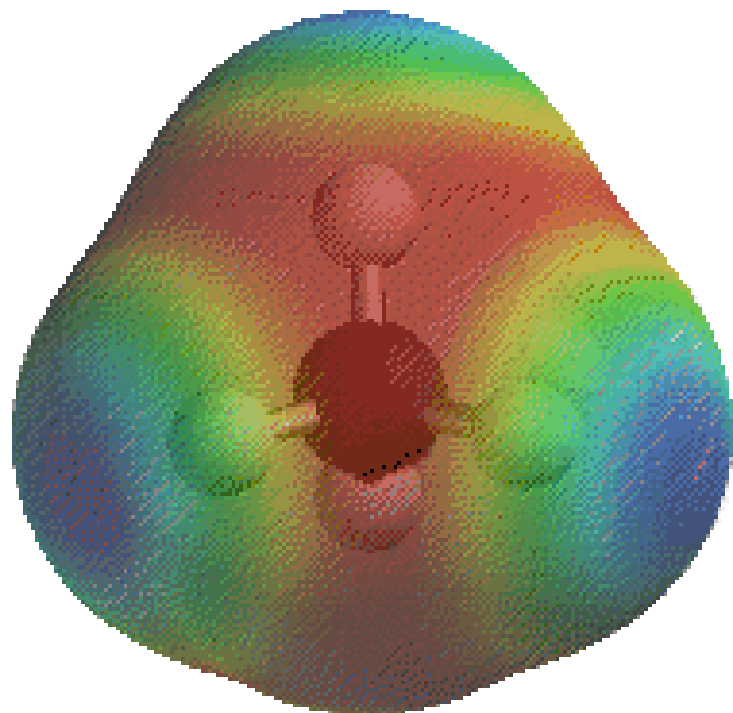
Source: U. S. Census Bureau
Census 2000 Summary File 1
population by census tract.





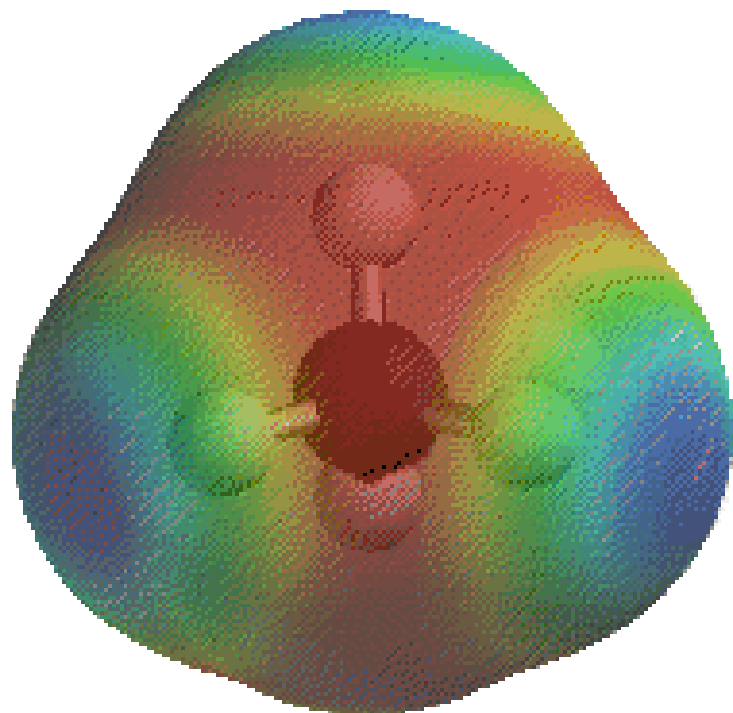
Tetrahedral geometry

Electron Density Maps

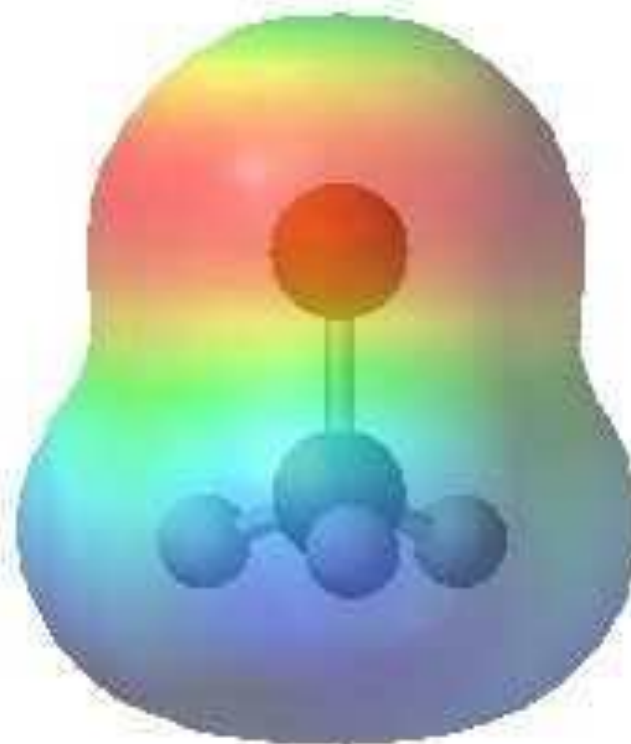


CH₄

Electron Density Maps

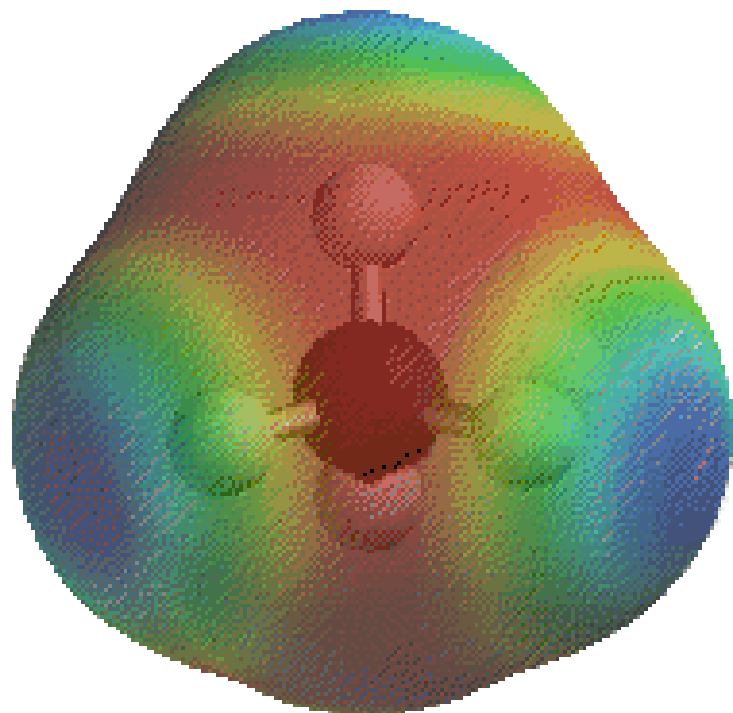


CH₄

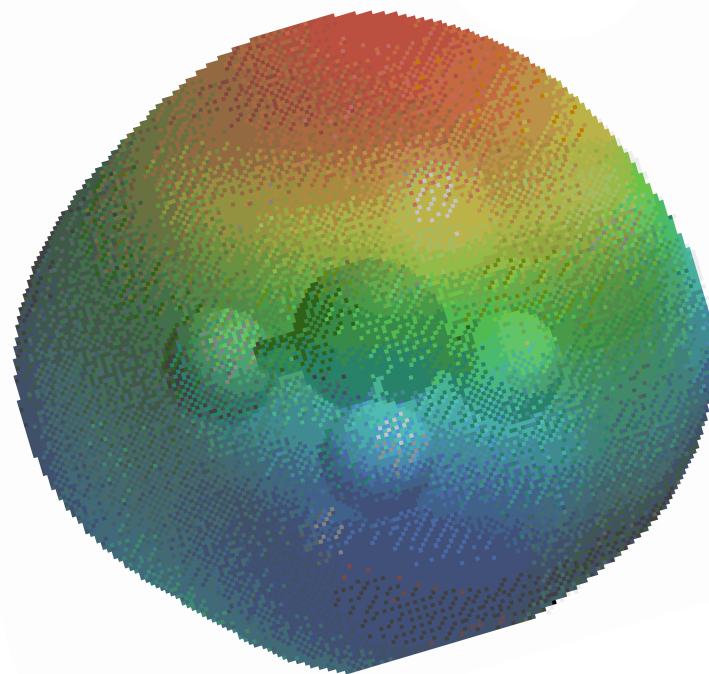


CH₃Br

Electron Density Maps

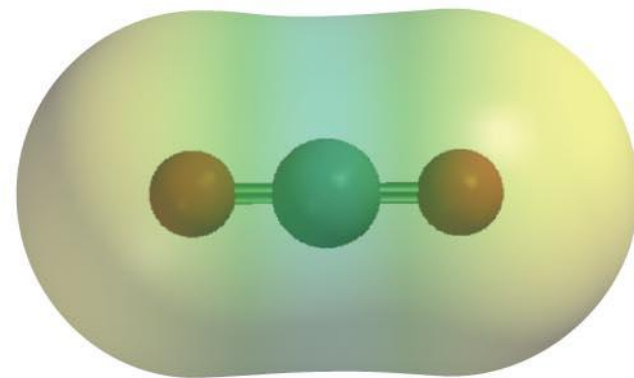
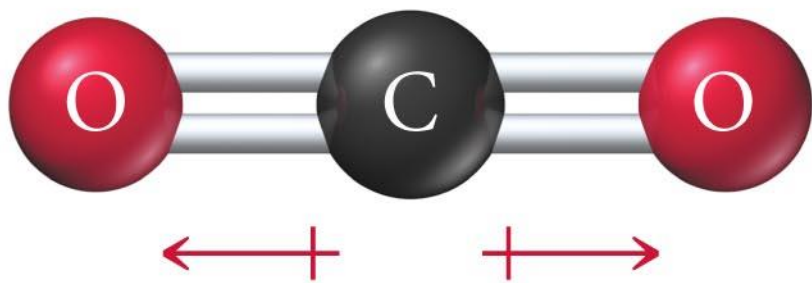


CH₄

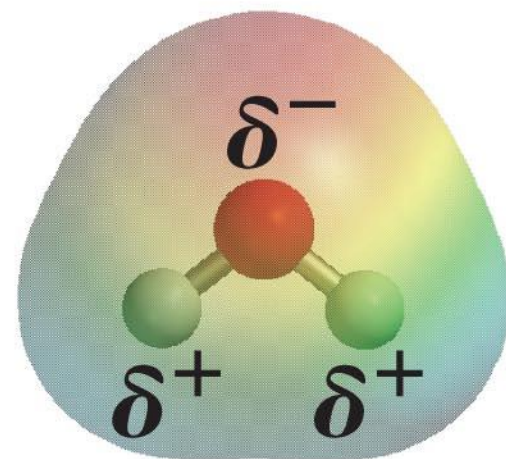
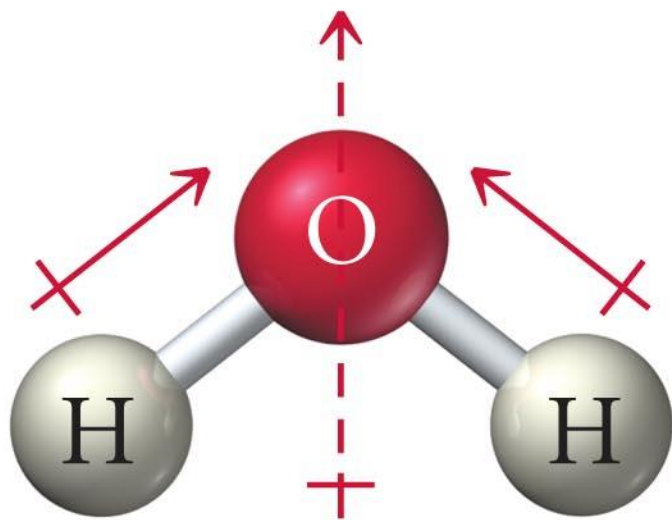


NH₃

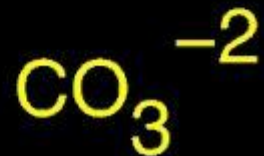
No net dipole moment



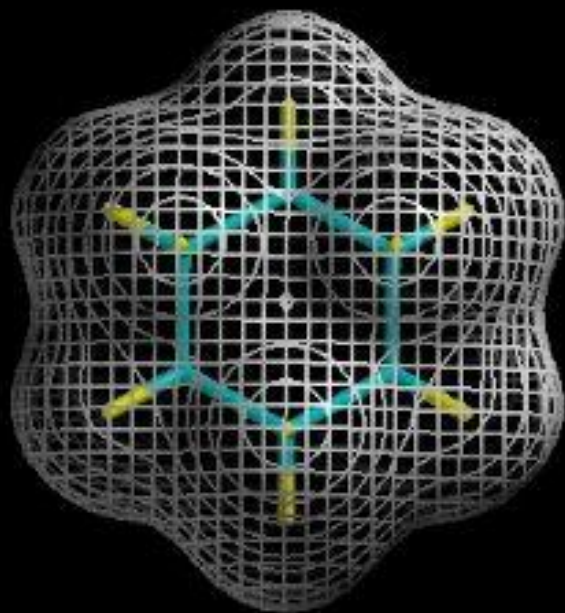
Net dipole moment



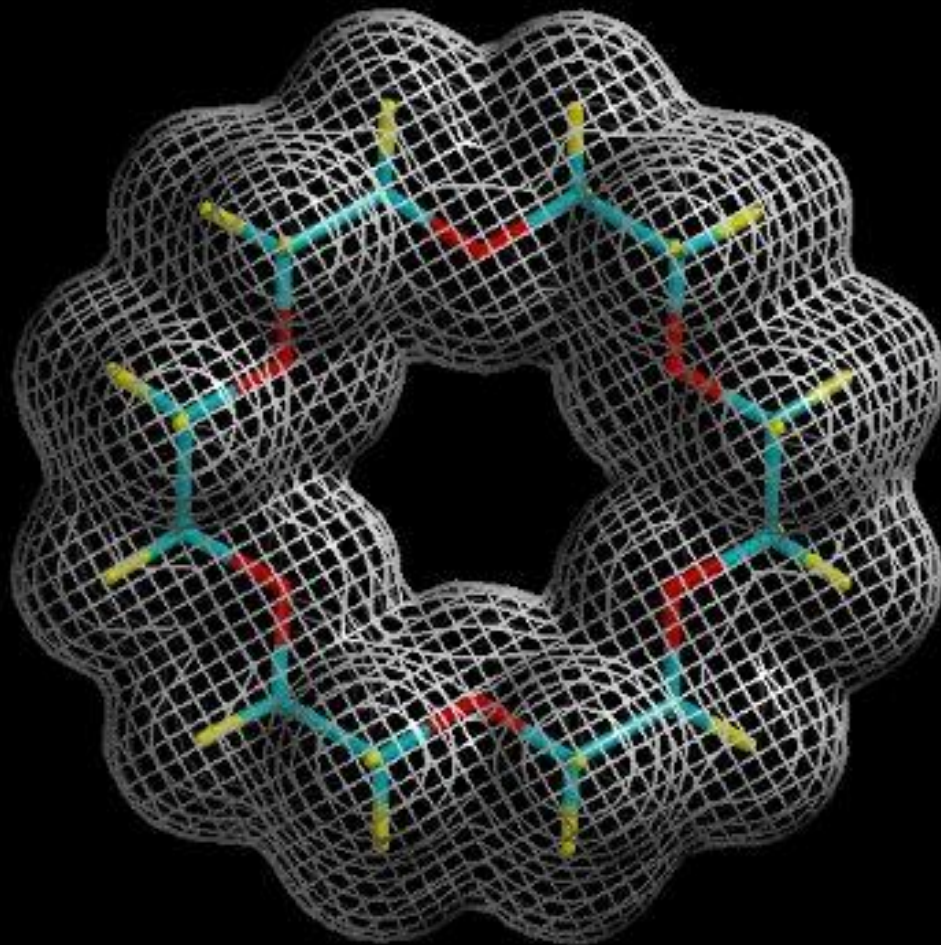
Polar or Non?



Larger Molecules: Nonpolar

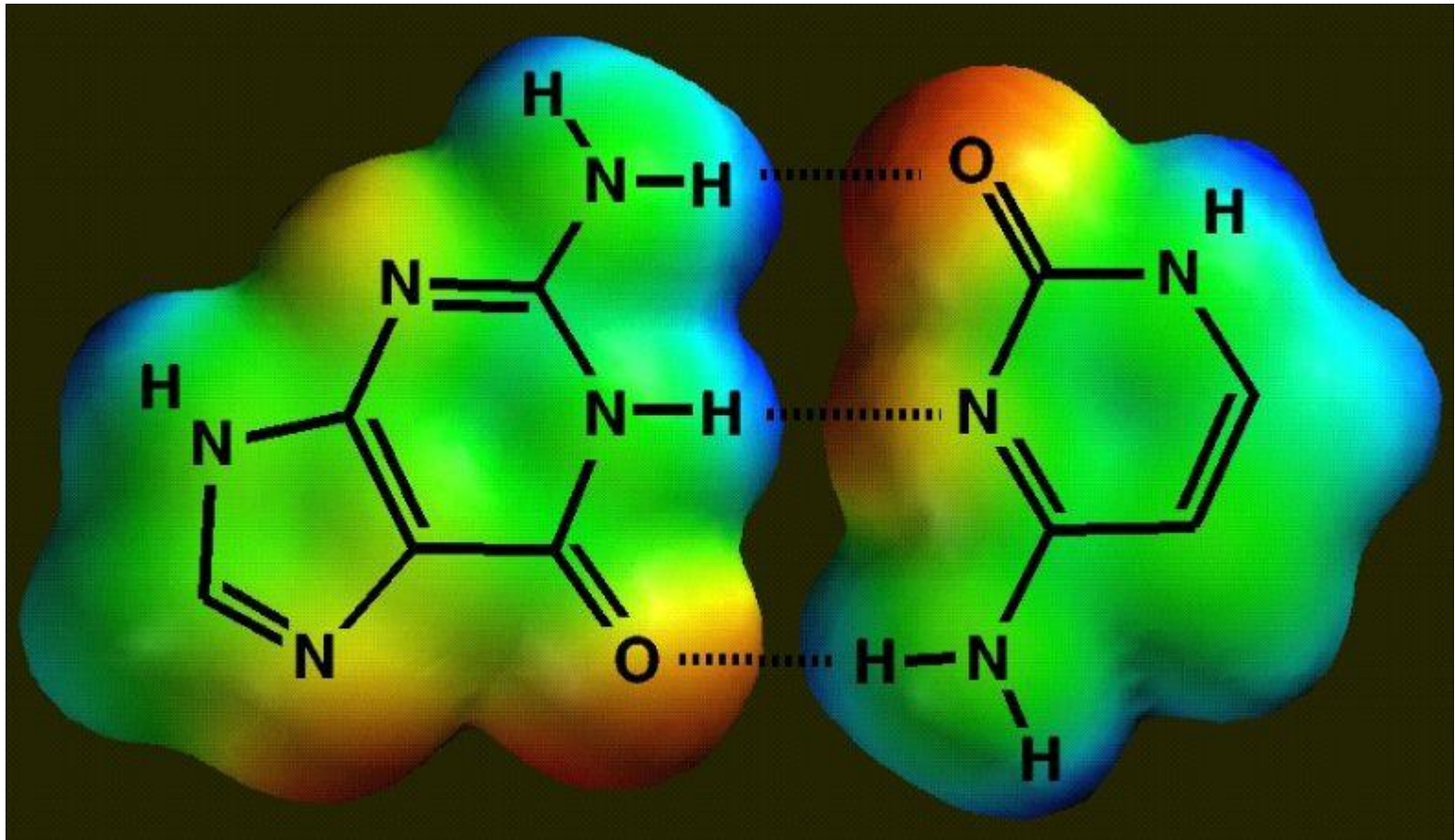


cyclohexane

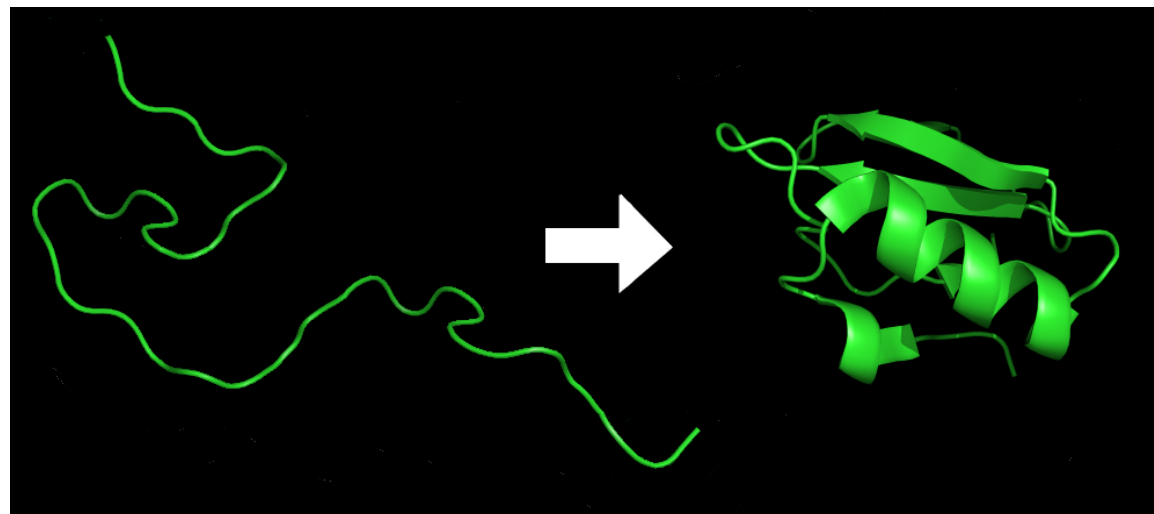
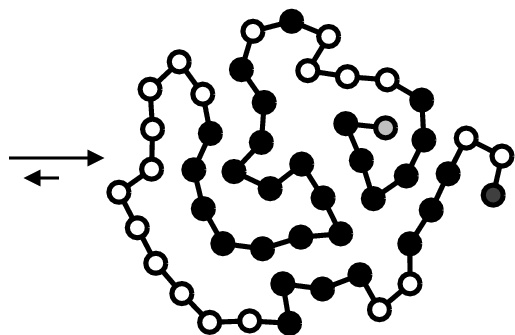
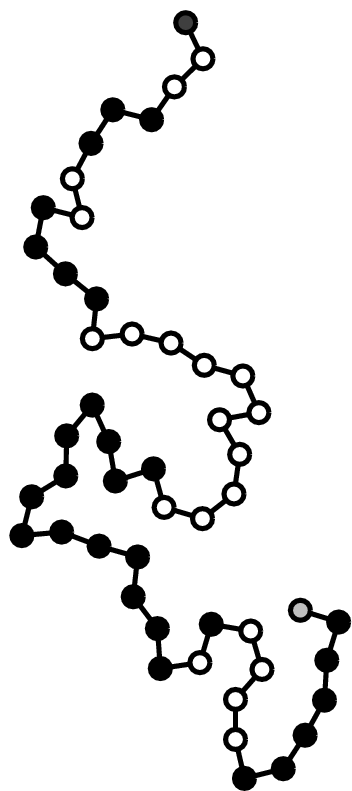


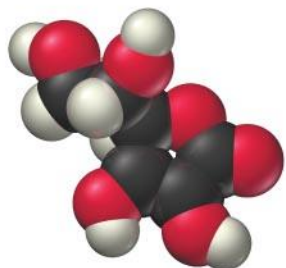
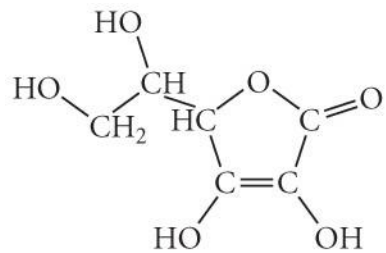
18-crown-6

The Bigger Picture: Guanine and Cytosine

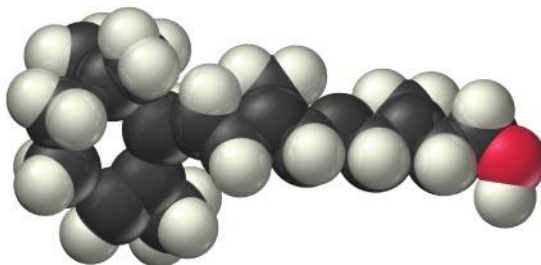
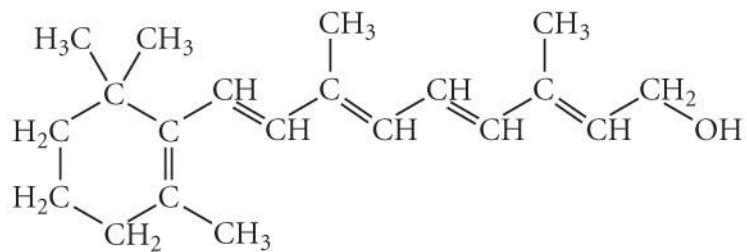


Protein Folding

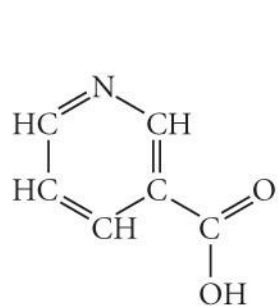




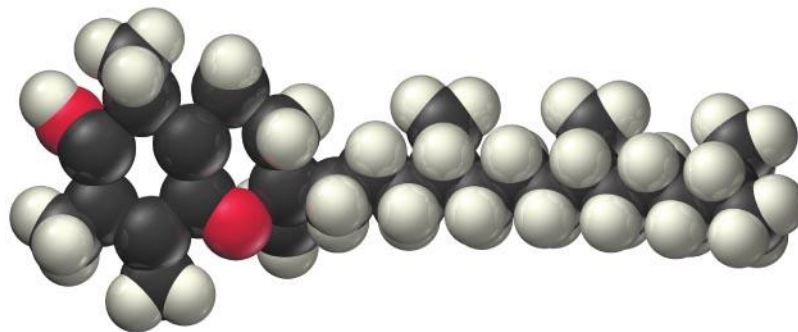
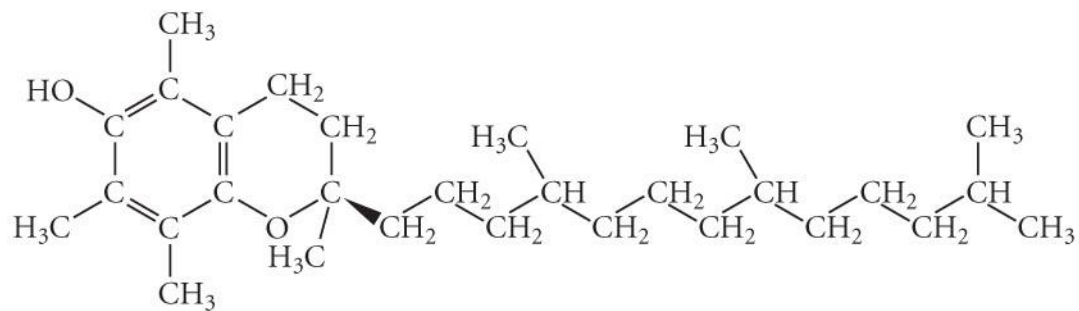
(a) vitamin C



(b) vitamin A



(c) niacin (vitamin B₃)



(d) vitamin E