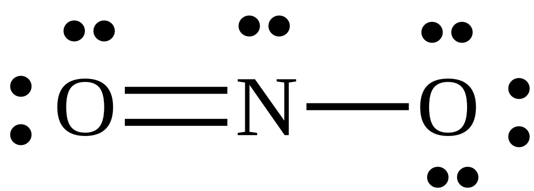
Molecular Shapes

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.



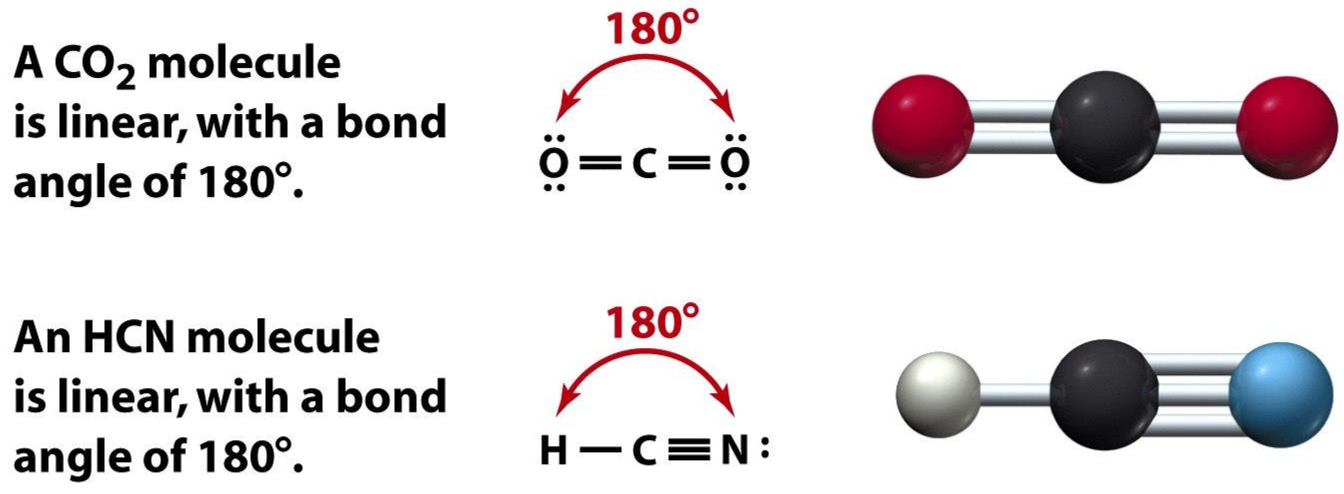
There are 3 electron groups on N.
1 lone pair.
1 single bond.
1 double bond.

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.

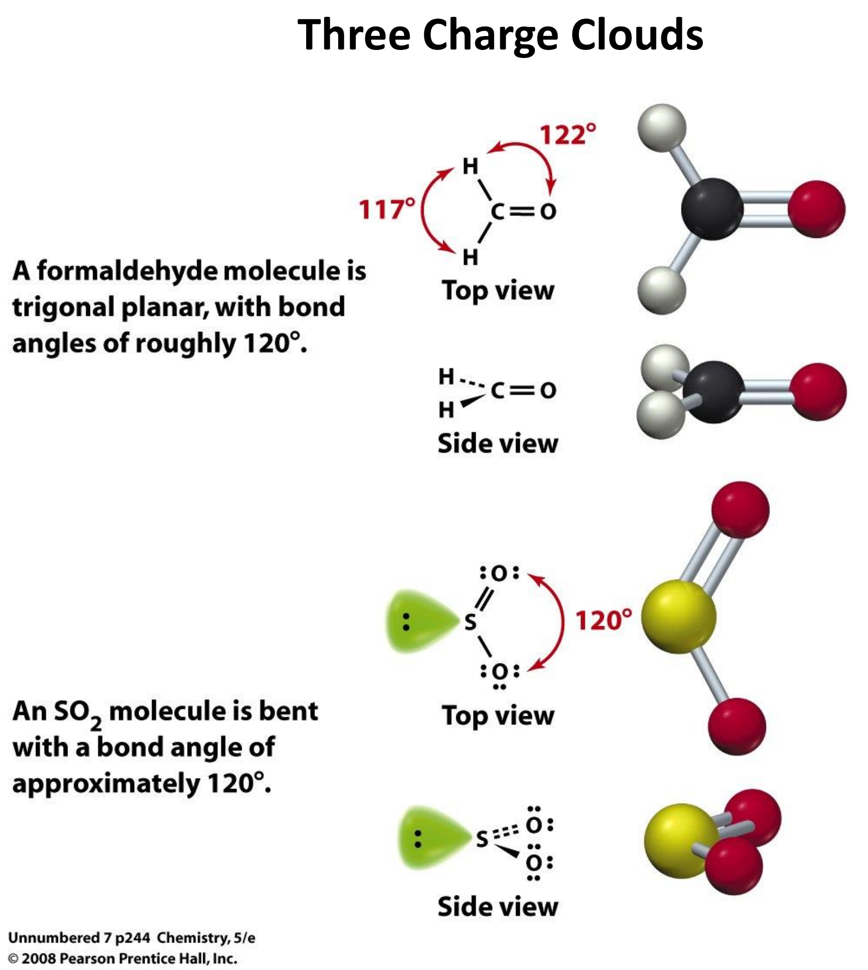
Molecular Shapes: the VSEPR Model

Two Charge Clouds



Unnumbered 7 p243b Chemistry, 5/e

Molecular Shapes: the VSEPR Model



Molecular Shapes: the VSEPR Model

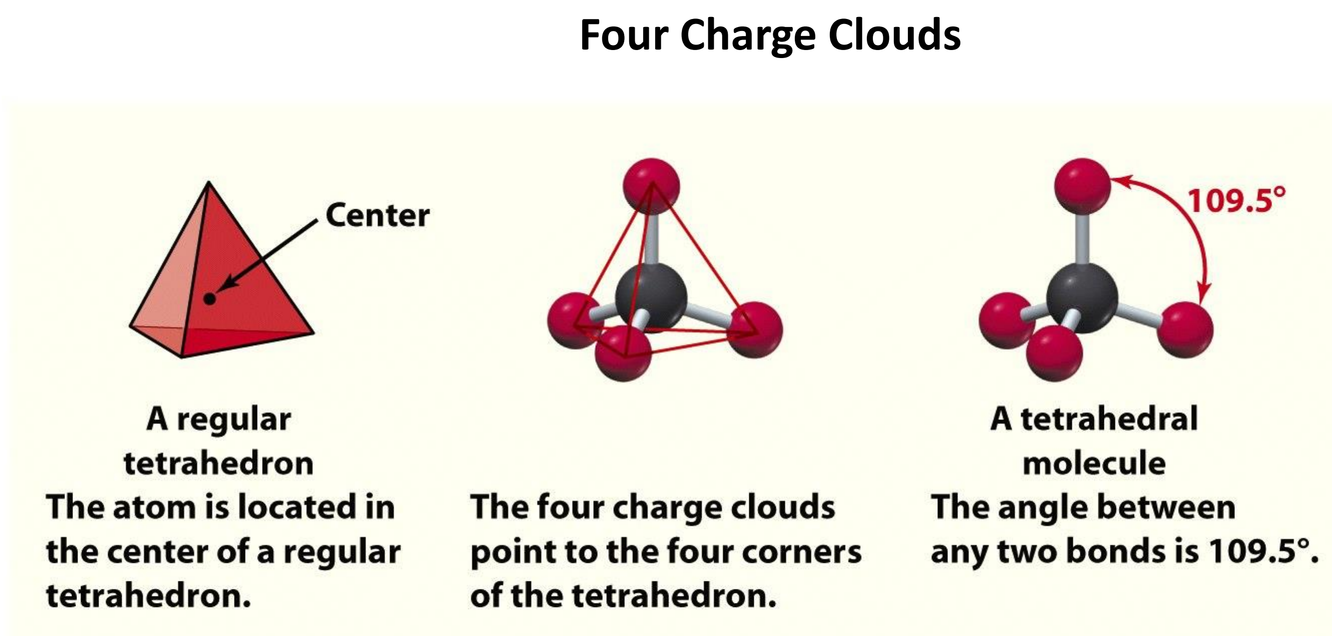
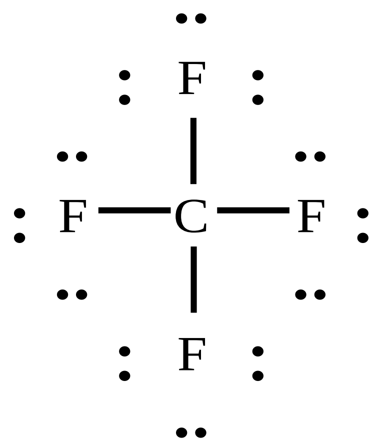


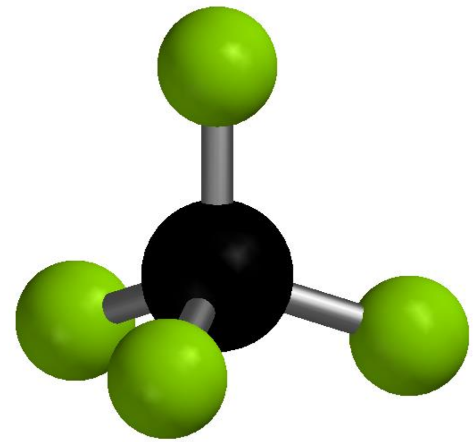
Figure 7-5 Chemistry, 5/e

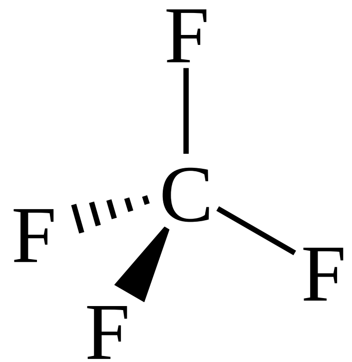
Sketching a Molecule

- 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.

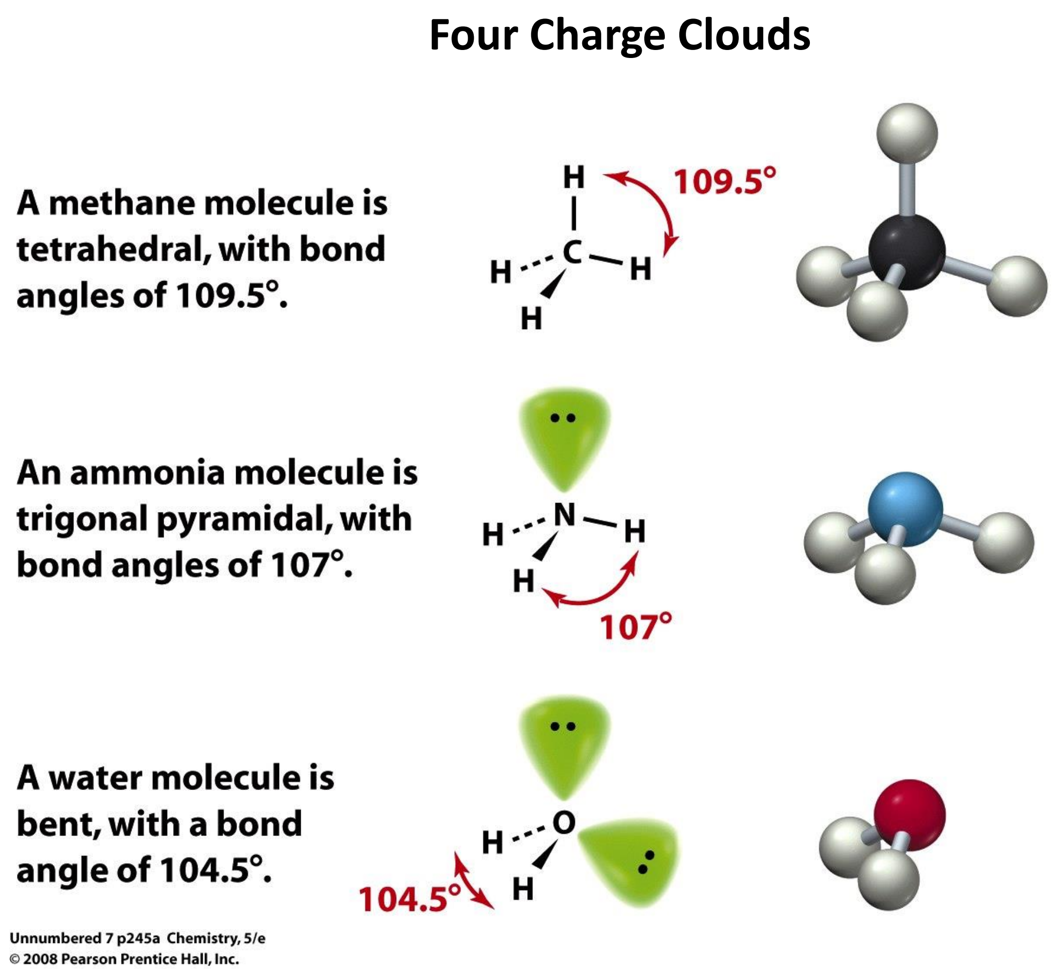
Sketching a Molecule, Continued



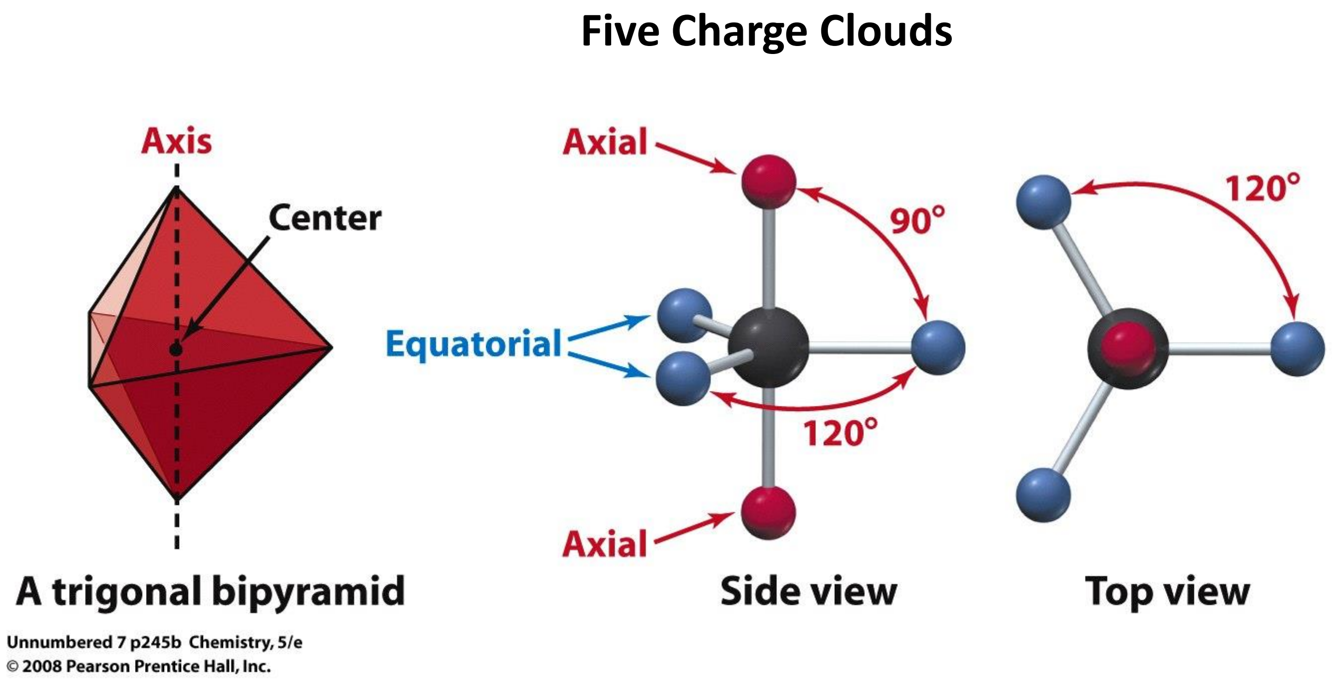




Molecular Shapes: the VSEPR Model



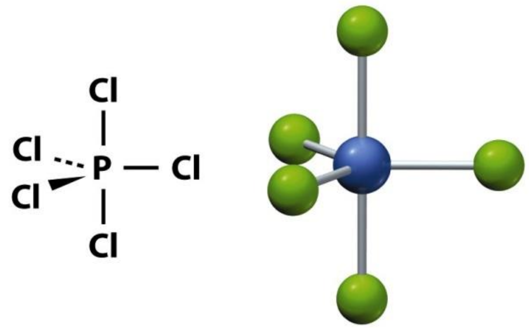
Molecular Shapes: the VSEPR Model



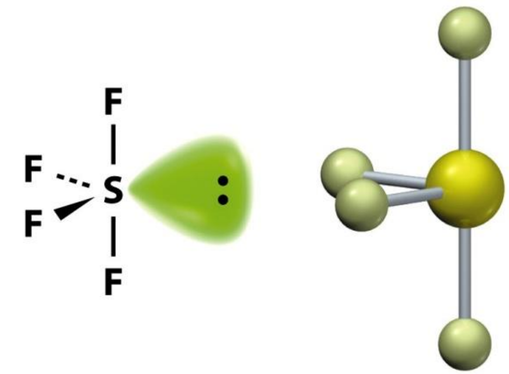
Molecular Shapes: the VSEPR Model

Five Charge Clouds

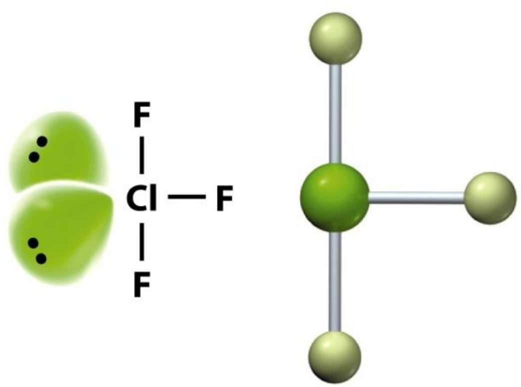
A PCl_5 molecule is trigonal bipyramidal.



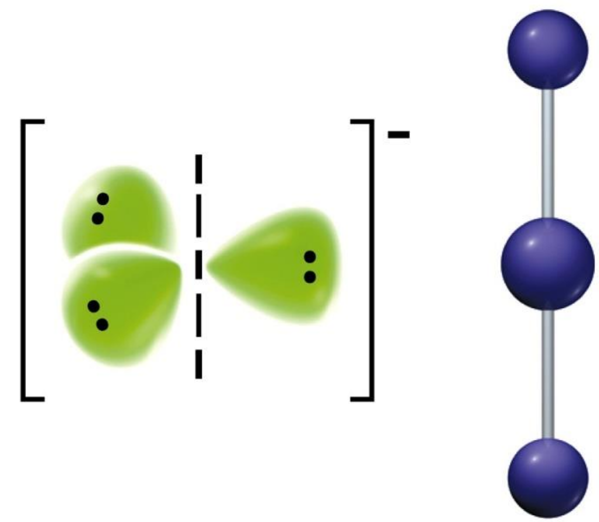
An SF_4 molecule is shaped like a seesaw (turn 90° to see it).



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

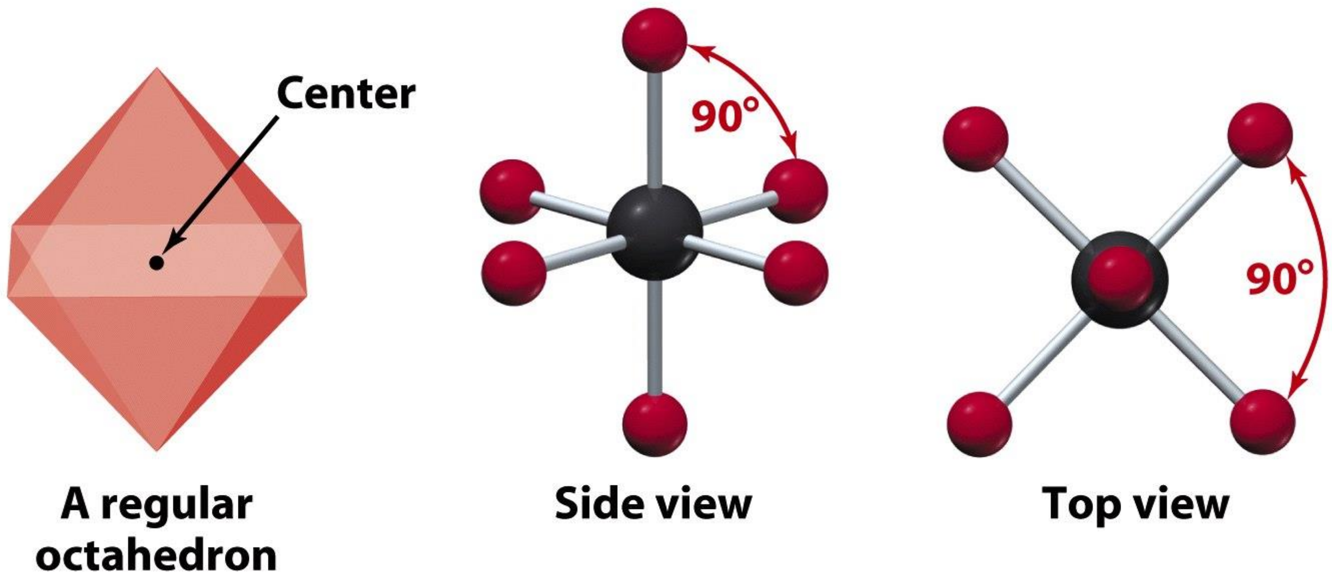


An I_3^- ion is linear.



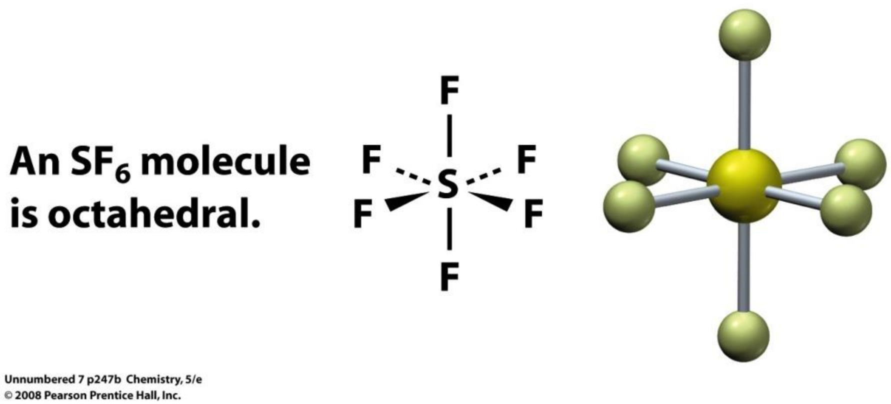
Molecular Shapes: the VSEPR Model

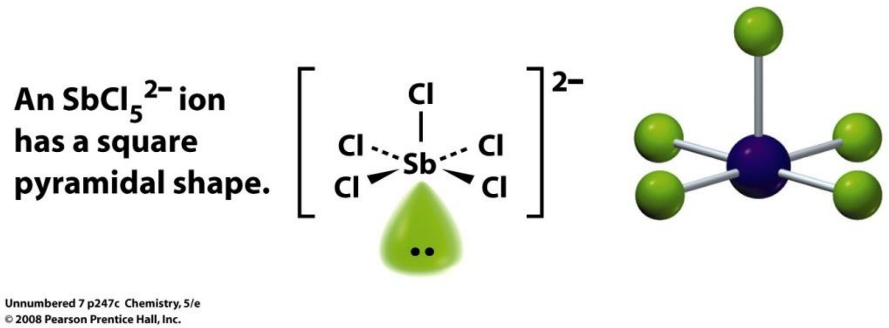
Six Charge Clouds

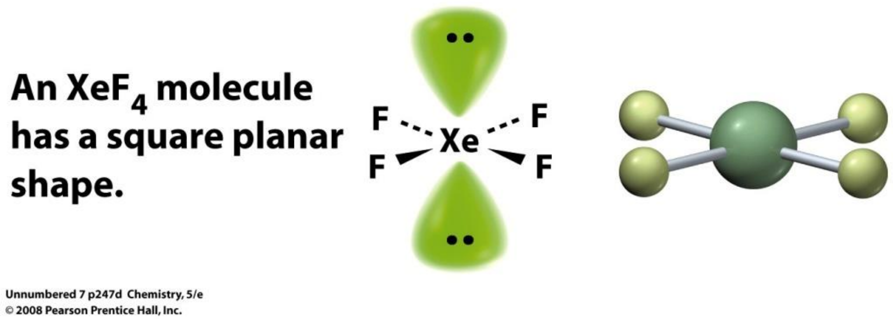


Molecular Shapes: the VSEPR Model

Six Charge Clouds

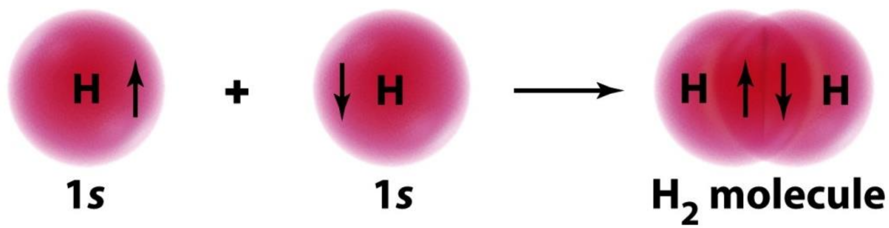




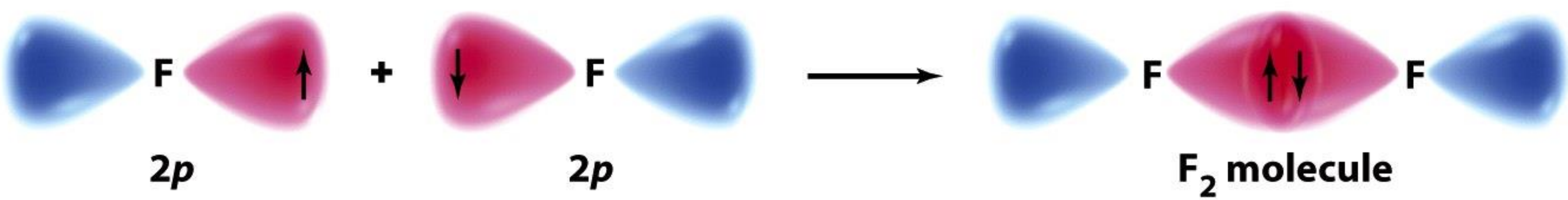


Valence Bond Theory

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



sigma (σ) bonds



Valence Bond Theory

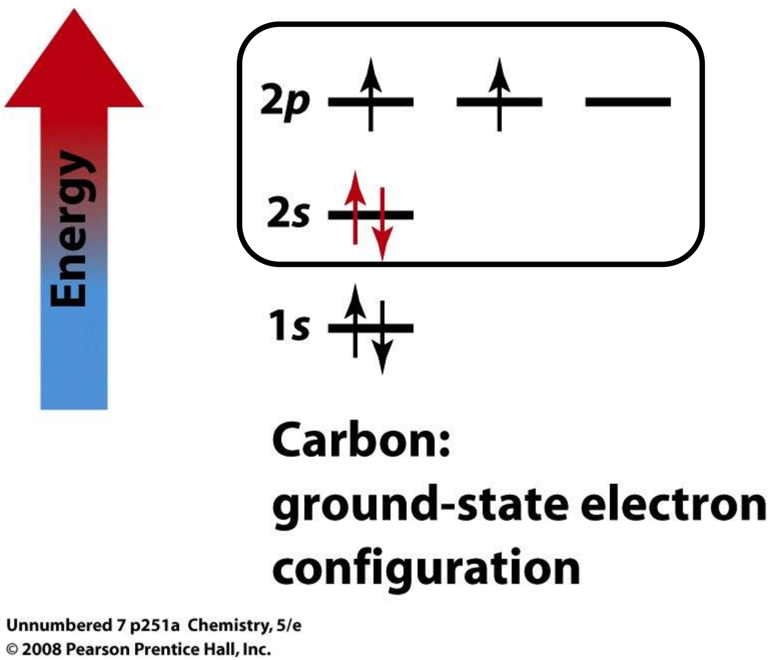
Valence Bond Theory: A quantum mechanical model which shows how electron pairs are shared in a covalent bond.

- 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?

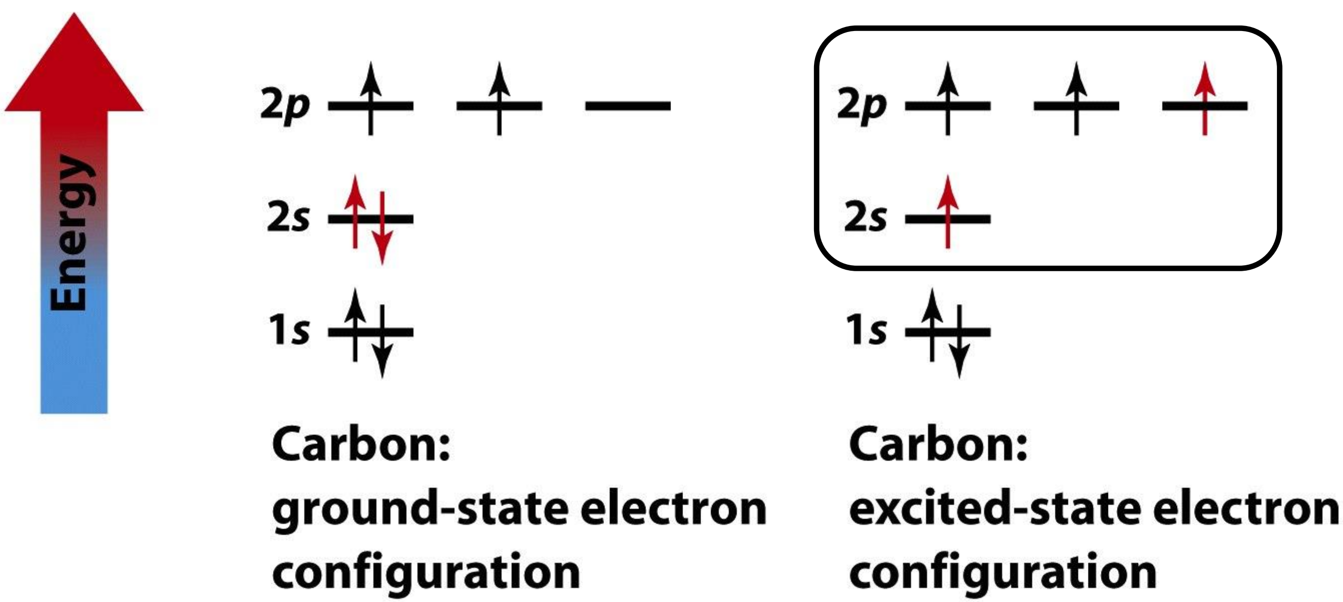
4 valence electrons
2 unpaired electrons



Hybridization and sp^3 Hybrid Orbitals

How can the bonding in CH_4 be explained?

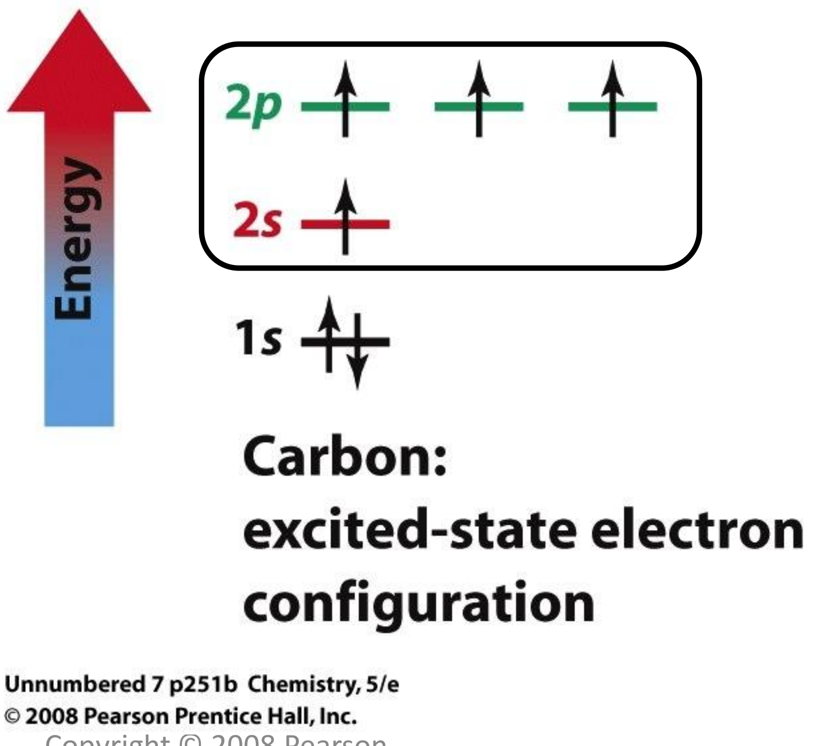
4 valence electrons
4 unpaired electrons



Hybridization and *sp*^{3} Hybrid Orbitals

How can the bonding in CH_4 be explained?

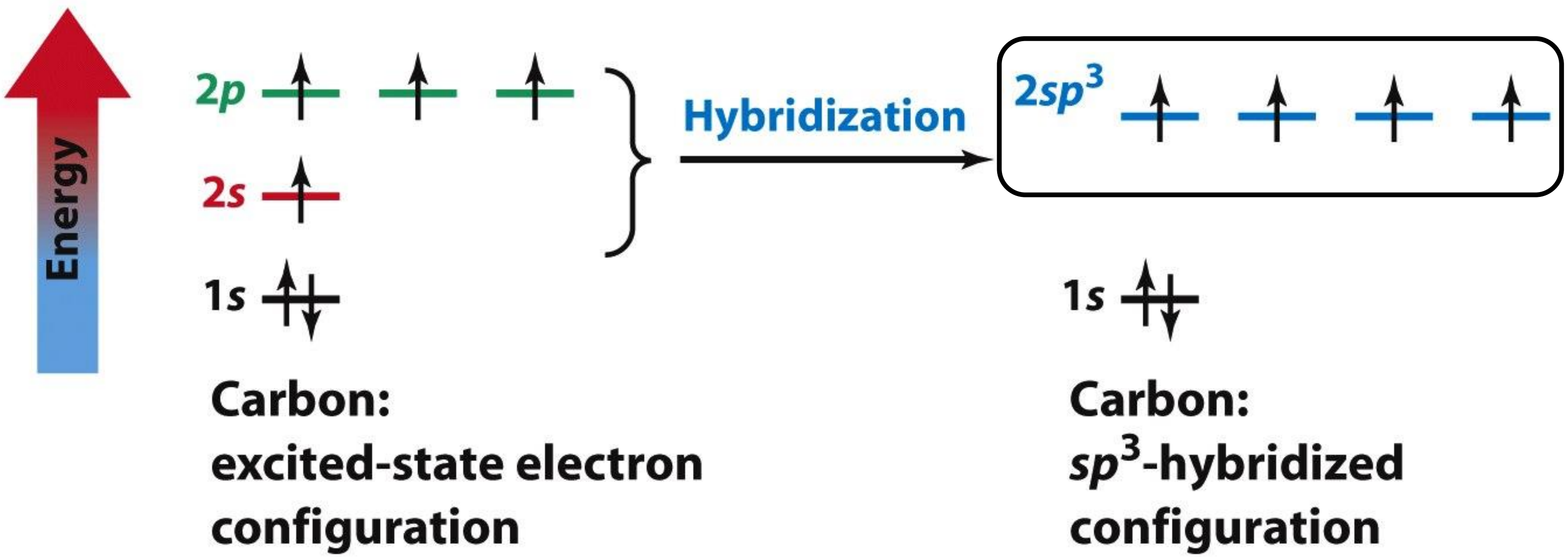
4 **nonequivalent** orbitals



Hybridization and *sp*^{3} Hybrid Orbitals

How can the bonding in CH_4 be explained?

4 **equivalent** orbitals



Hybridization and *sp*^{3} Hybrid Orbitals

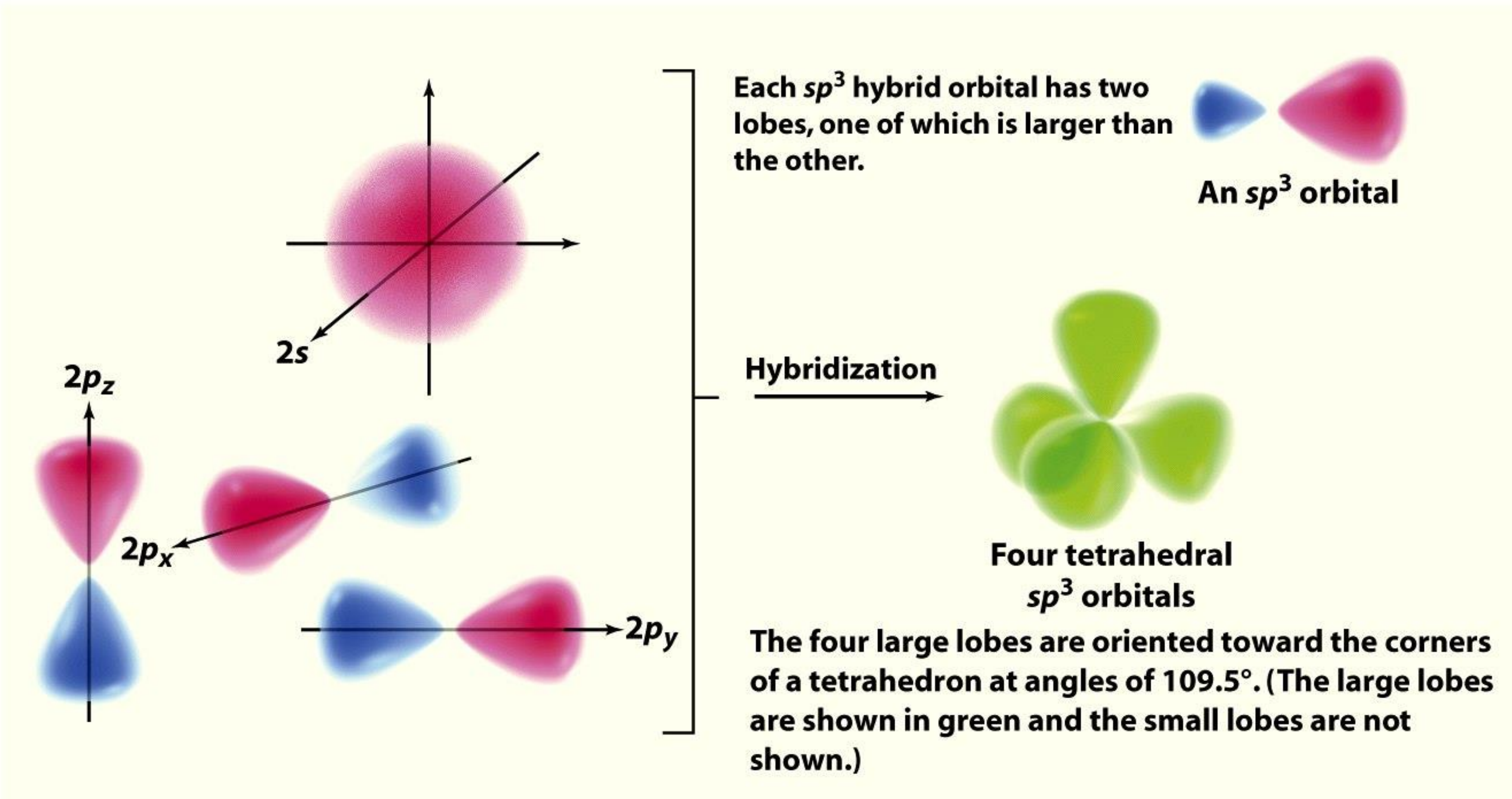


Figure 7-6 Chemistry, 5/e

Hybridization and *sp*^{3} Hybrid Orbitals

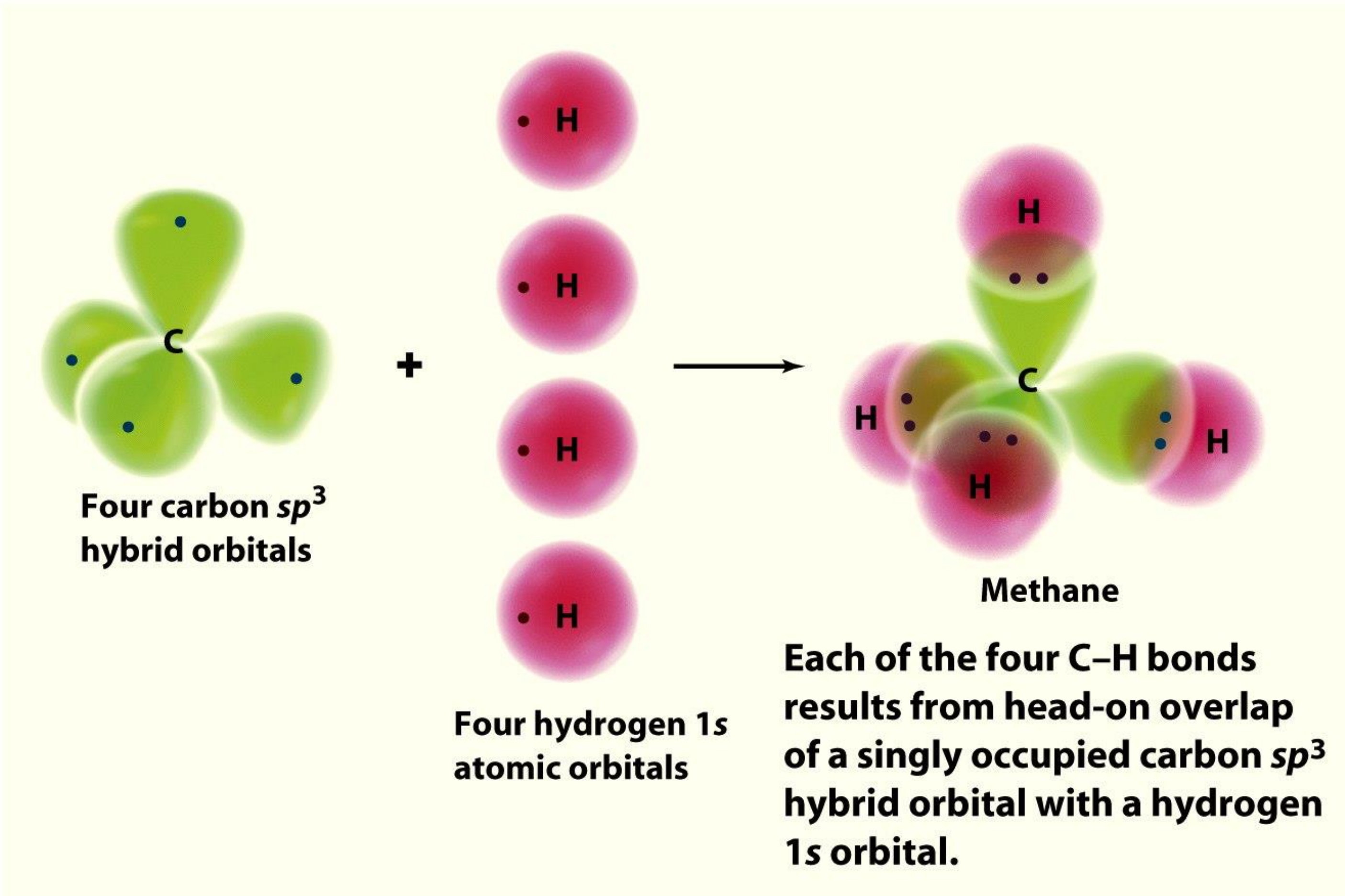


Figure 7-7 Chemistry, 5/e

Other Kinds of Hybrid Orbitals

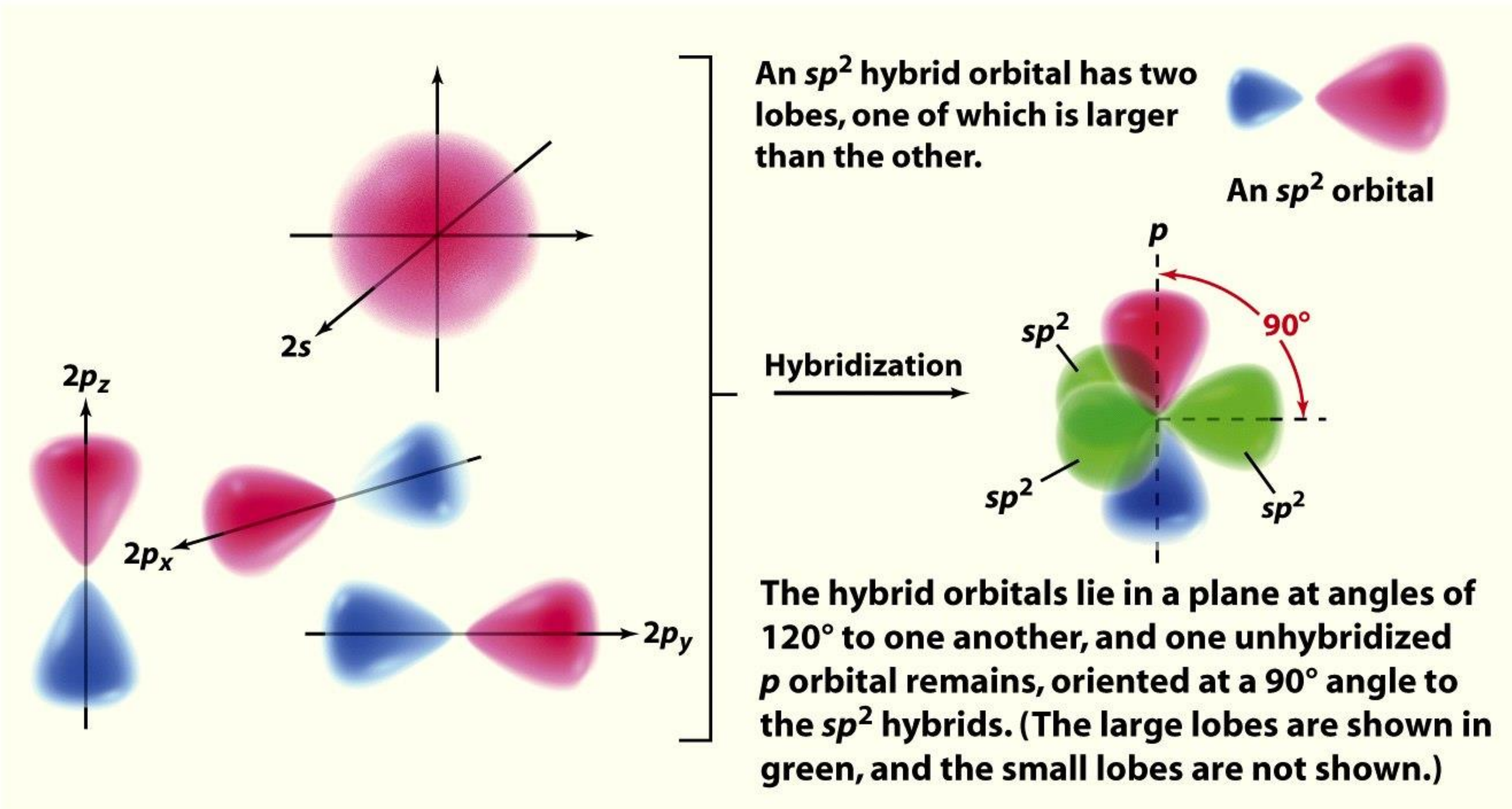


Figure 7-8 Chemistry, 5/e

Other Kinds of Hybrid Orbitals

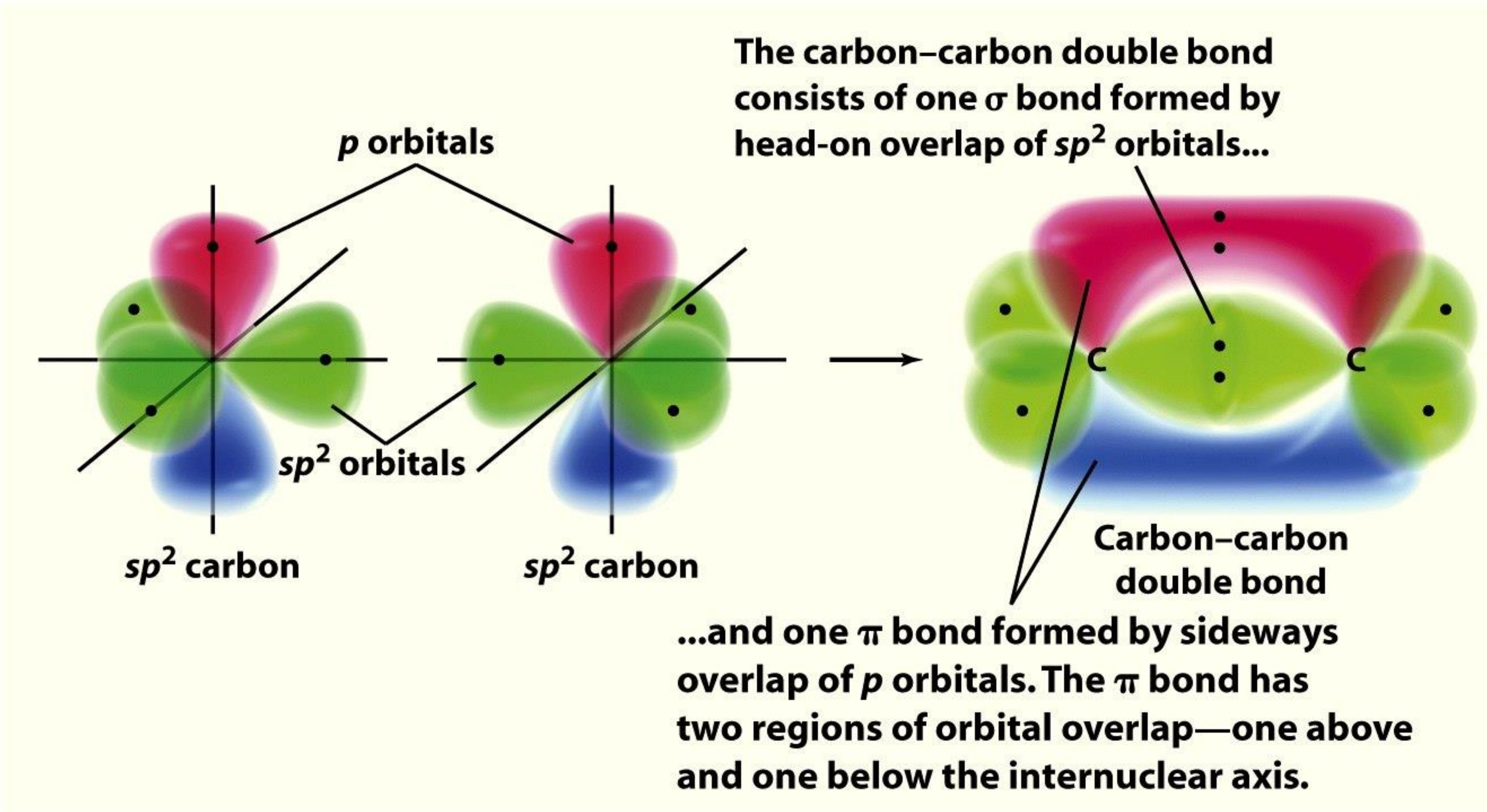


Figure 7-9 Chemistry, 5/e

Other Kinds of Hybrid Orbitals

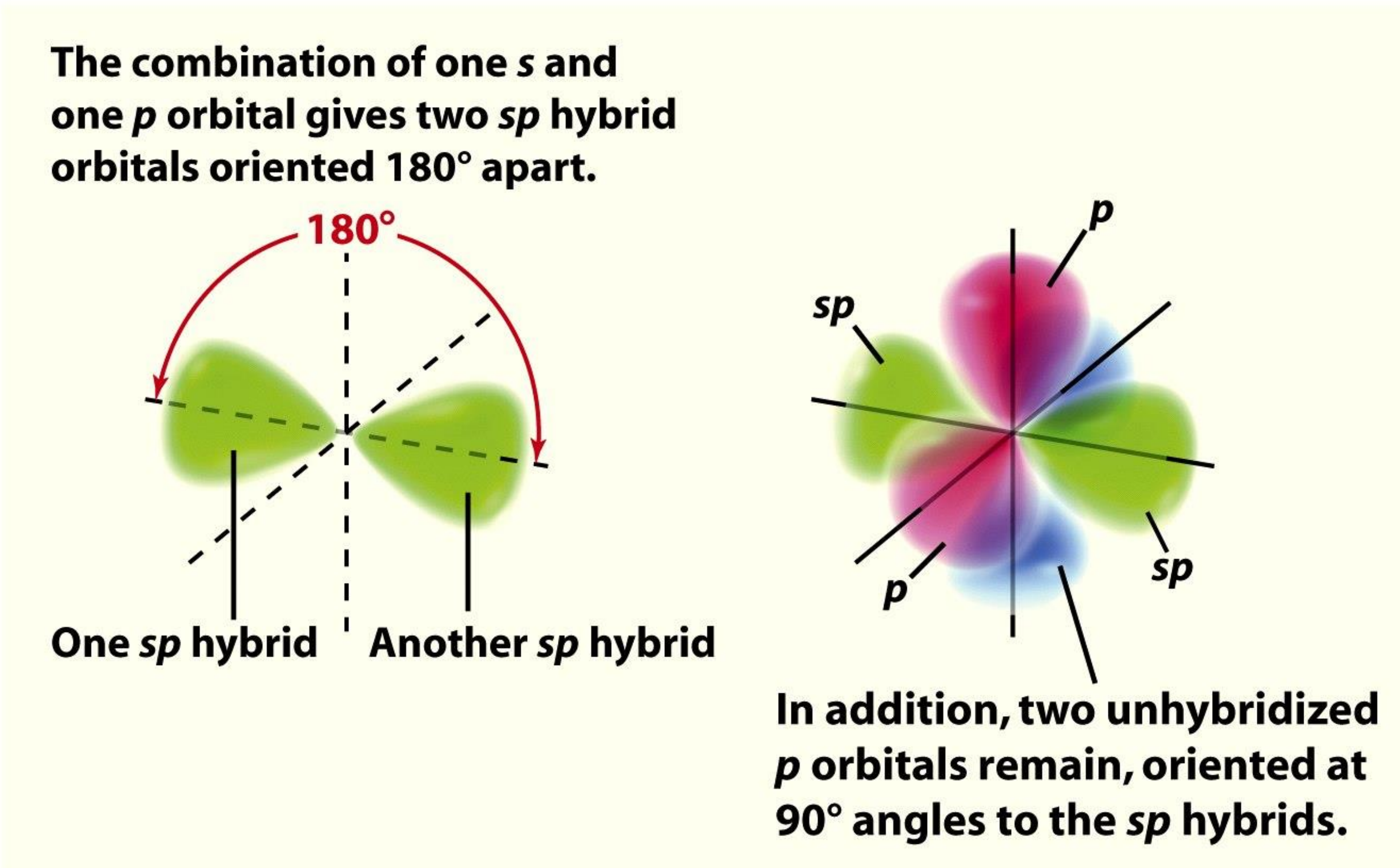


Figure 7-10 Chemistry, 5/e

Other Kinds of Hybrid Orbitals

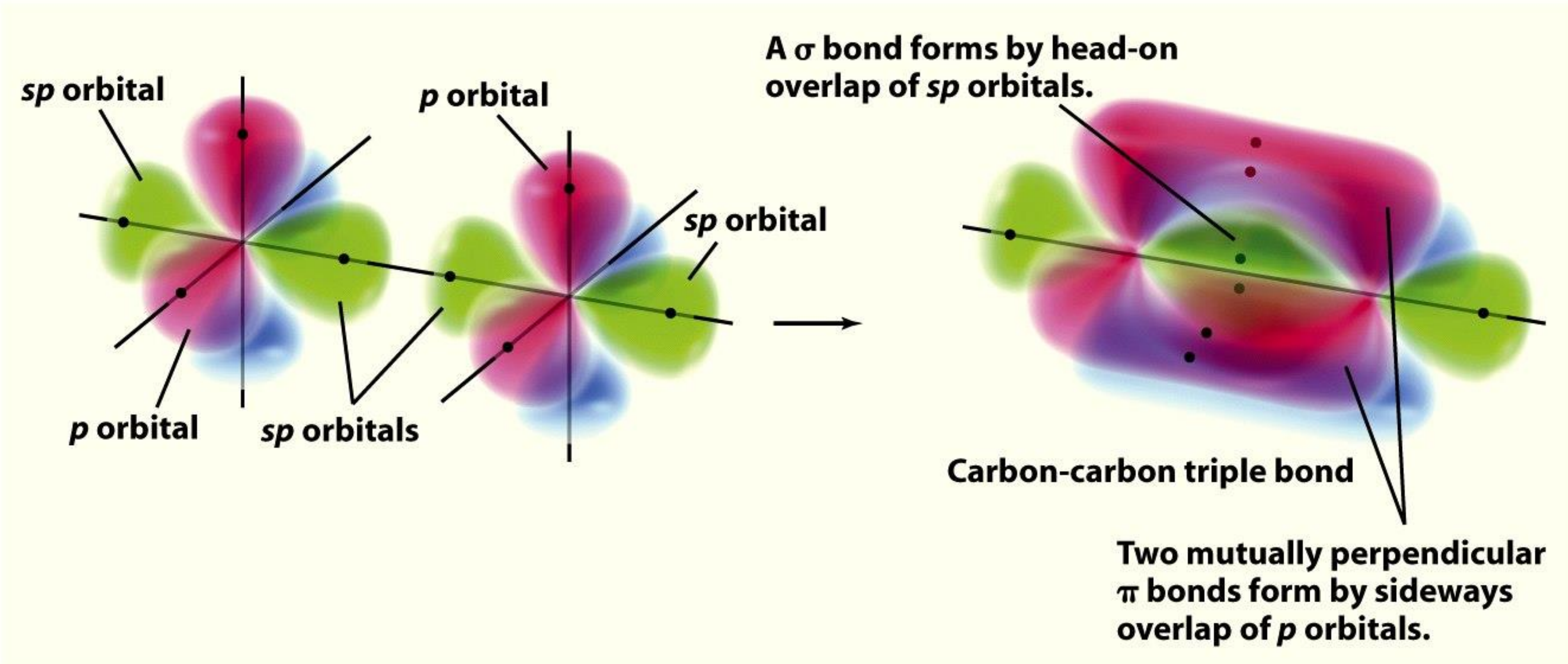


Figure 7-11 Chemistry, 5/e

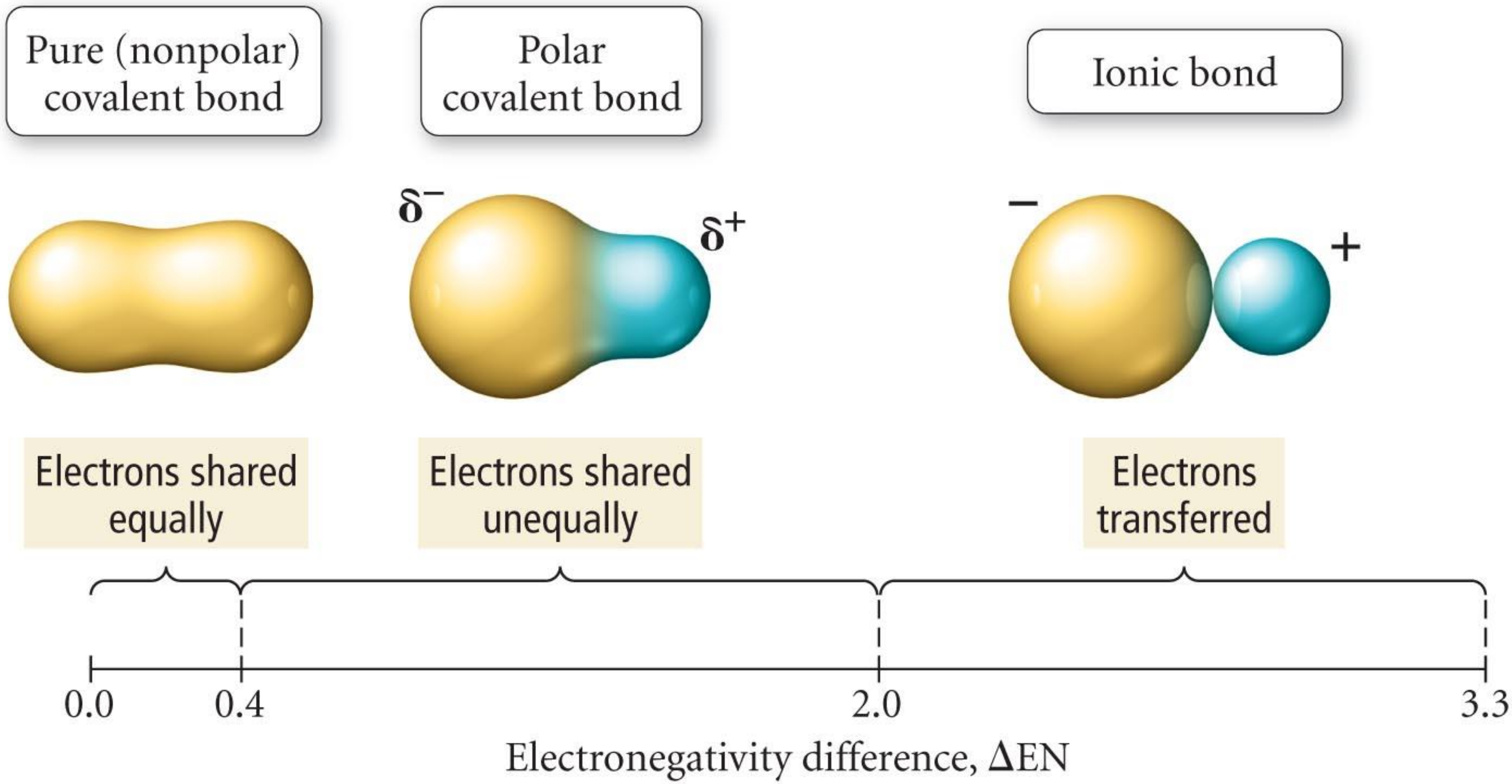
Other Kinds of Hybrid Orbitals

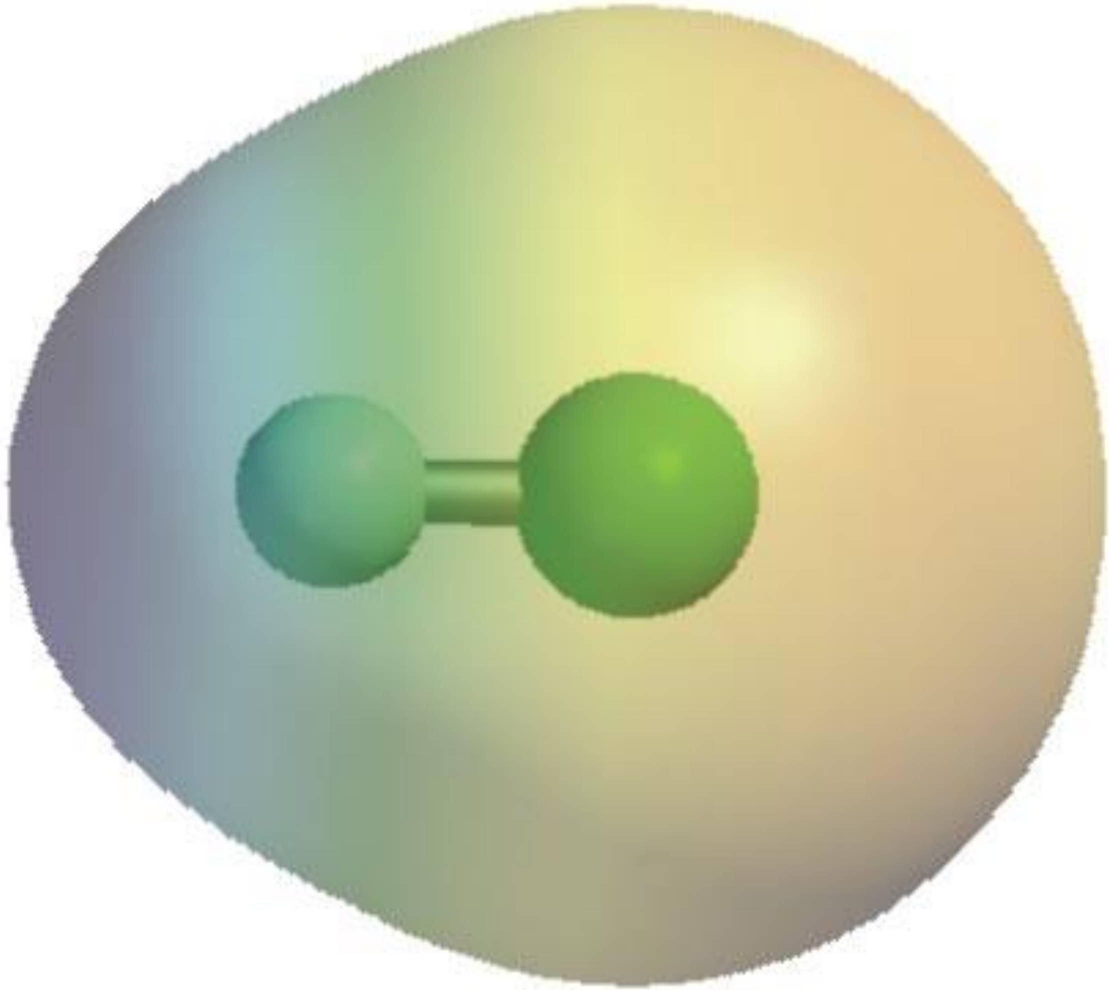
TABLE 7.5 Hybrid Orbitals and Their Geometry

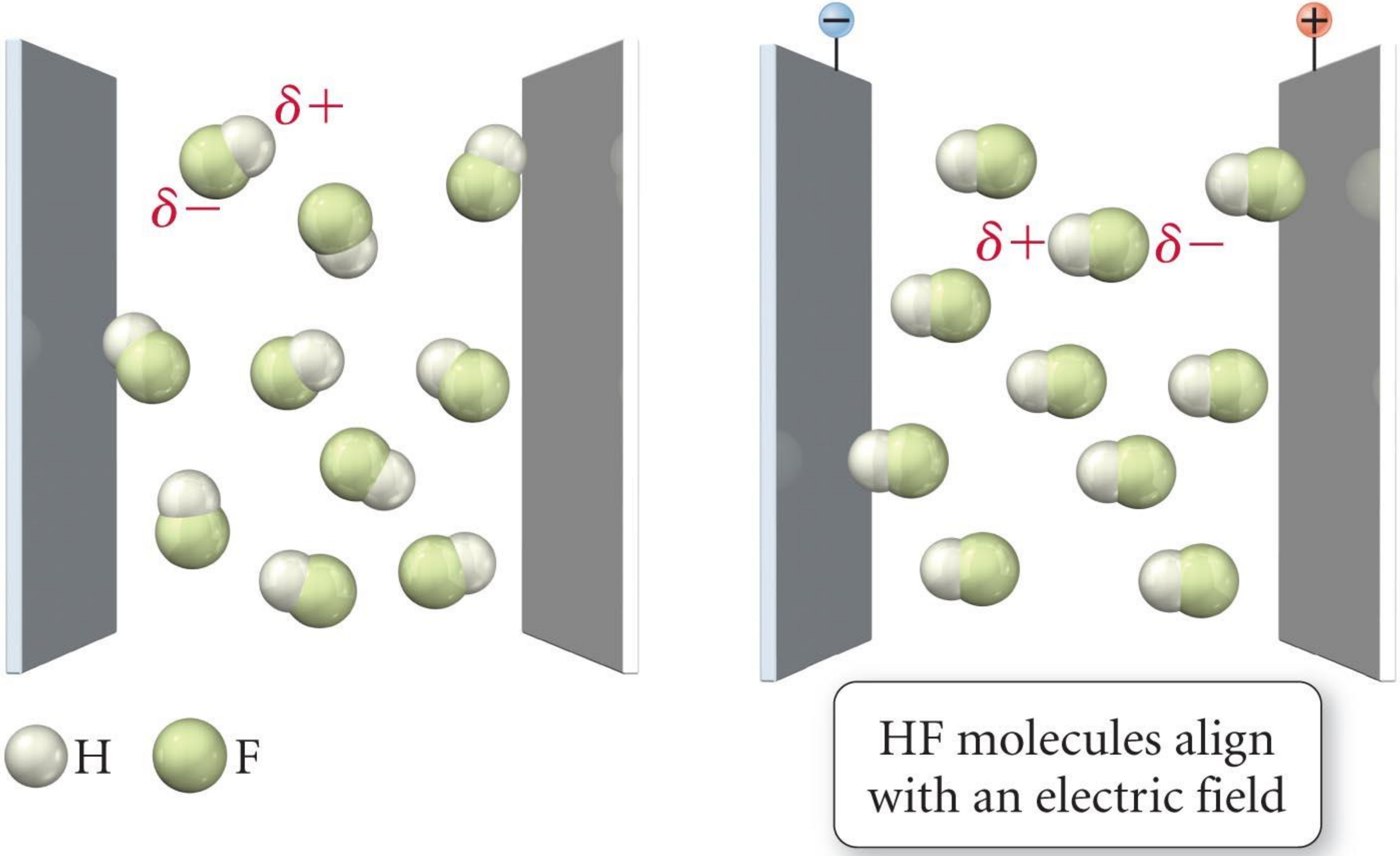
Number of Charge Clouds	Geometry of Charge Clouds	Hybridization
2	Linear	*sp*
3	Trigonal planar	sp^2
4	Tetrahedral	sp^3

Table 7-5 Chemistry, 5/e

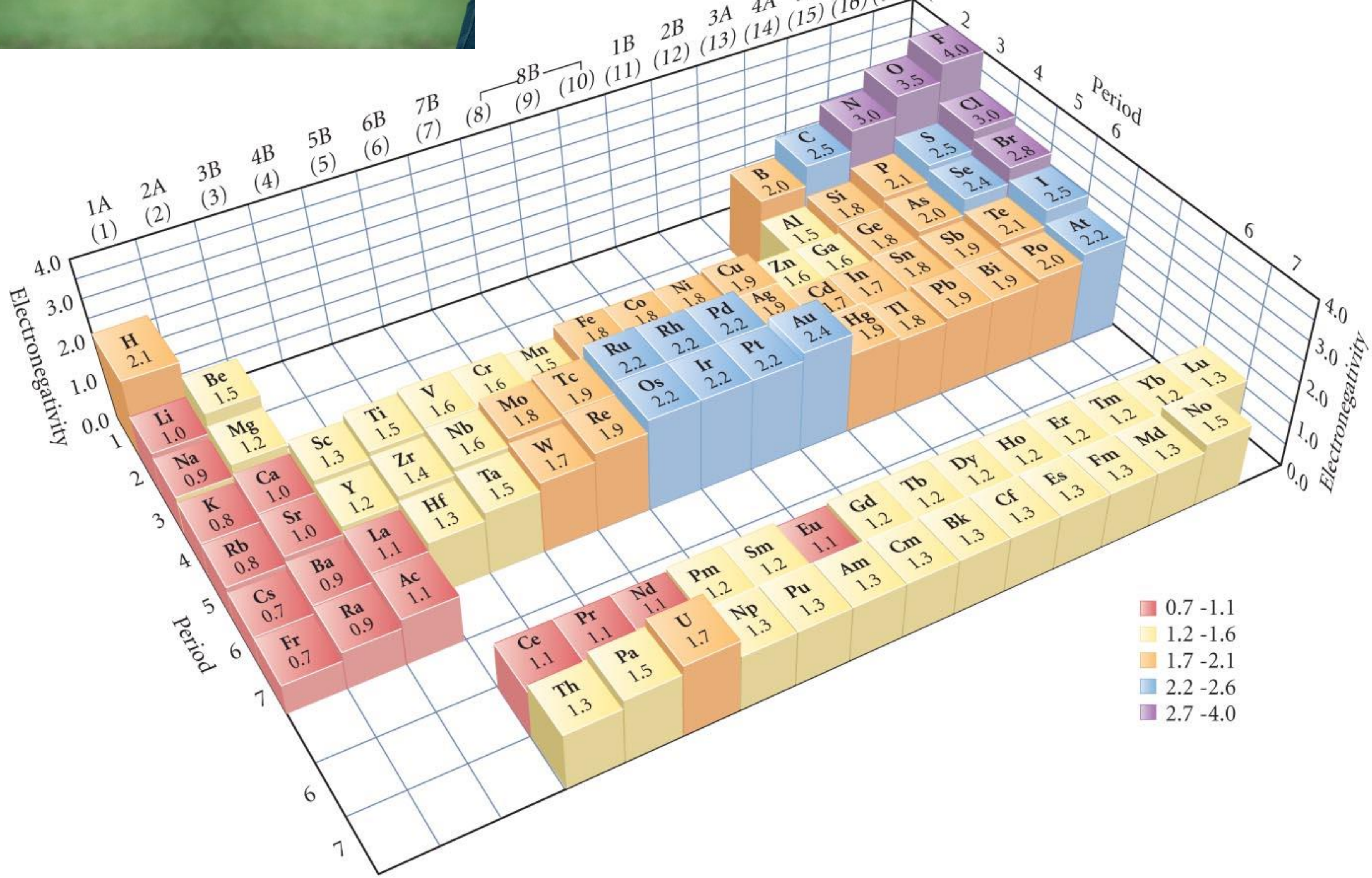
The Continuum of Bond Types



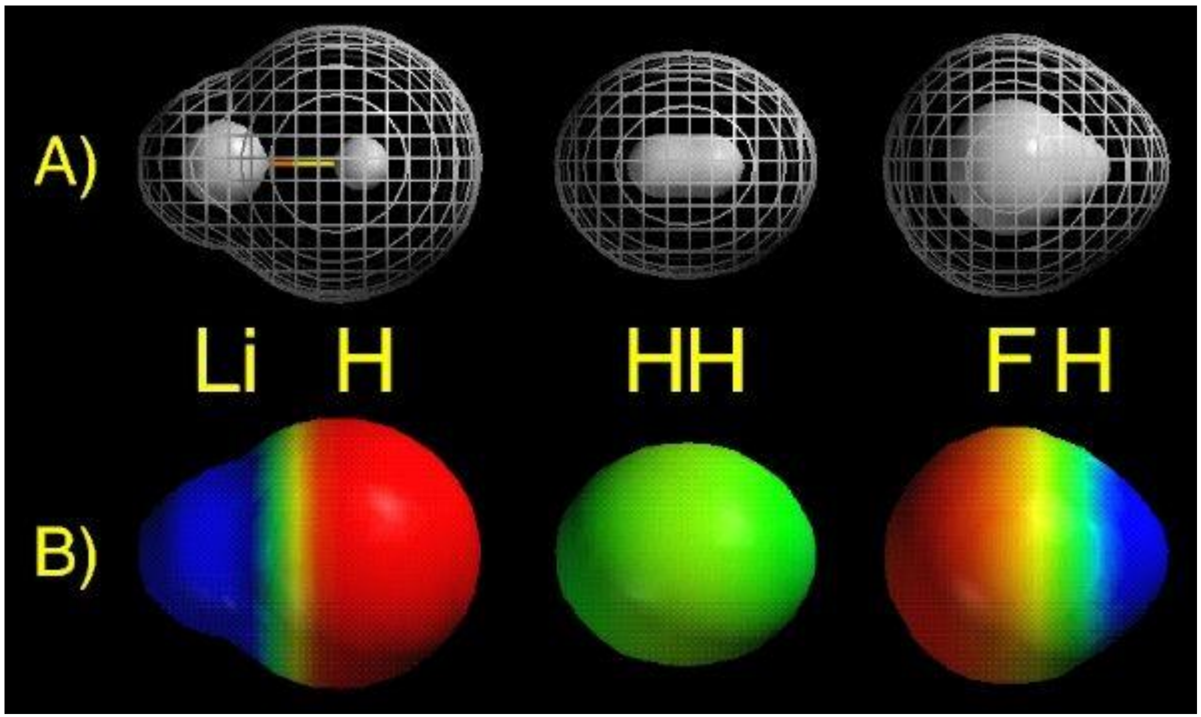


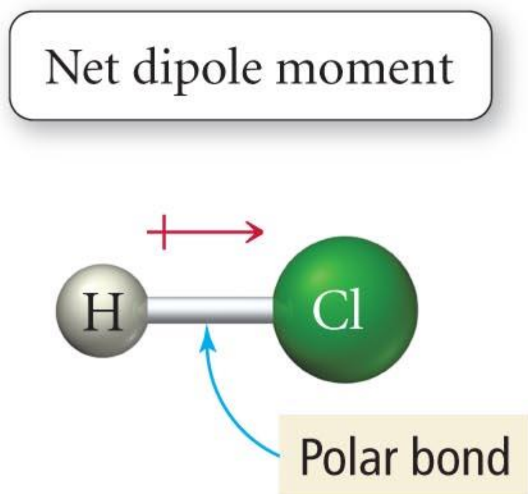

δ+
δ−
δ+
δ−
H
F
HF molecules align
with an electric field

Trends in Electronegativity



Bond Polarity




Net dipole moment
H
Cl
Polar bond

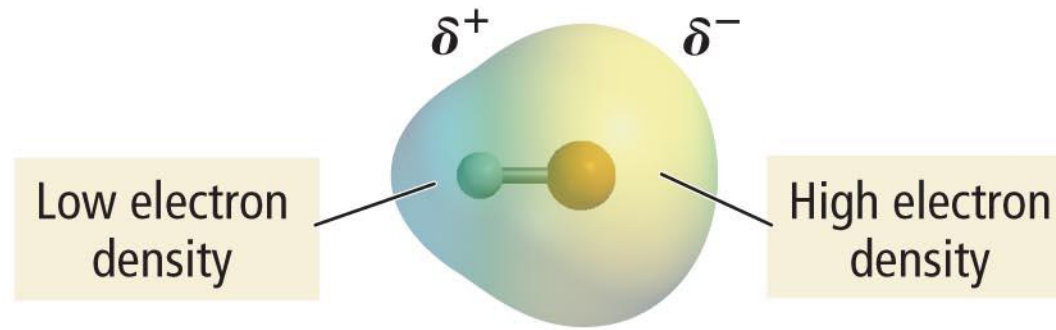
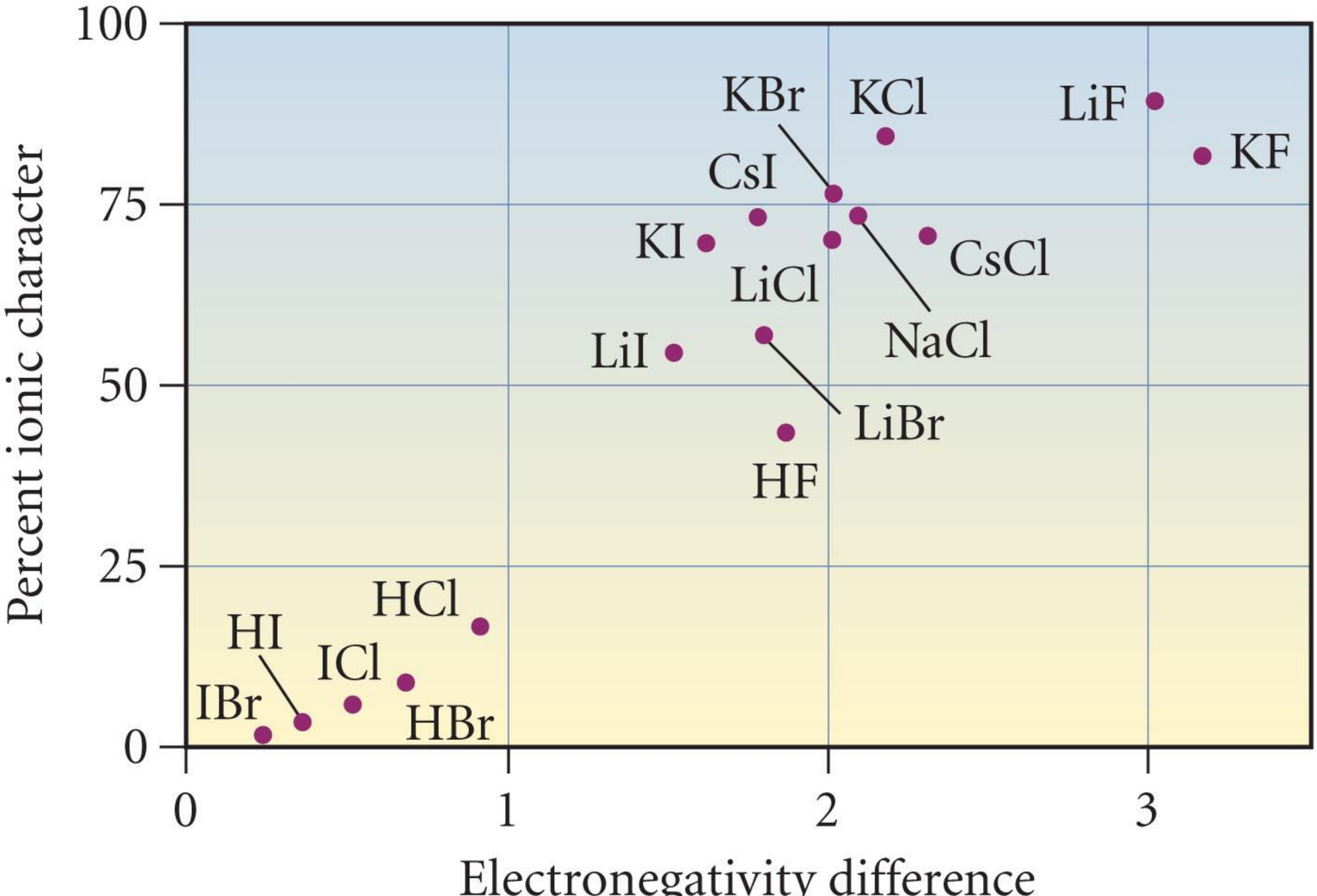

δ+
δ−
Low electron density
High electron density

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


Percent ionic character
100
75
50
25
0
KBr
KCl
LiF
KF
CsI
KI
CsCl
LiCl
NaCl
LiI
LiBr
HF
HCl
HI
ICl
IBr
HBr
0
1
2
3
Electronegativity difference

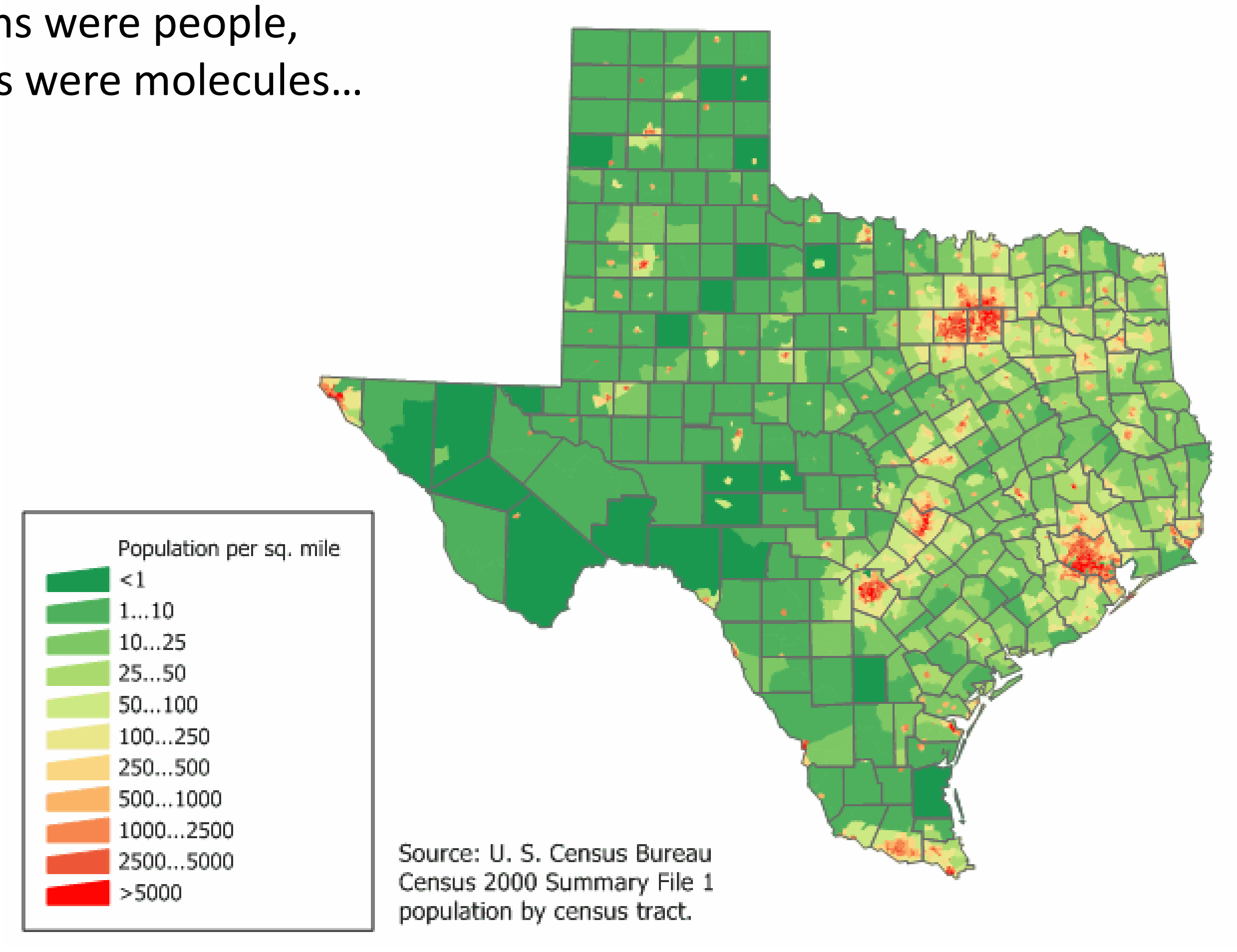
Molecular Polarity

- 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.

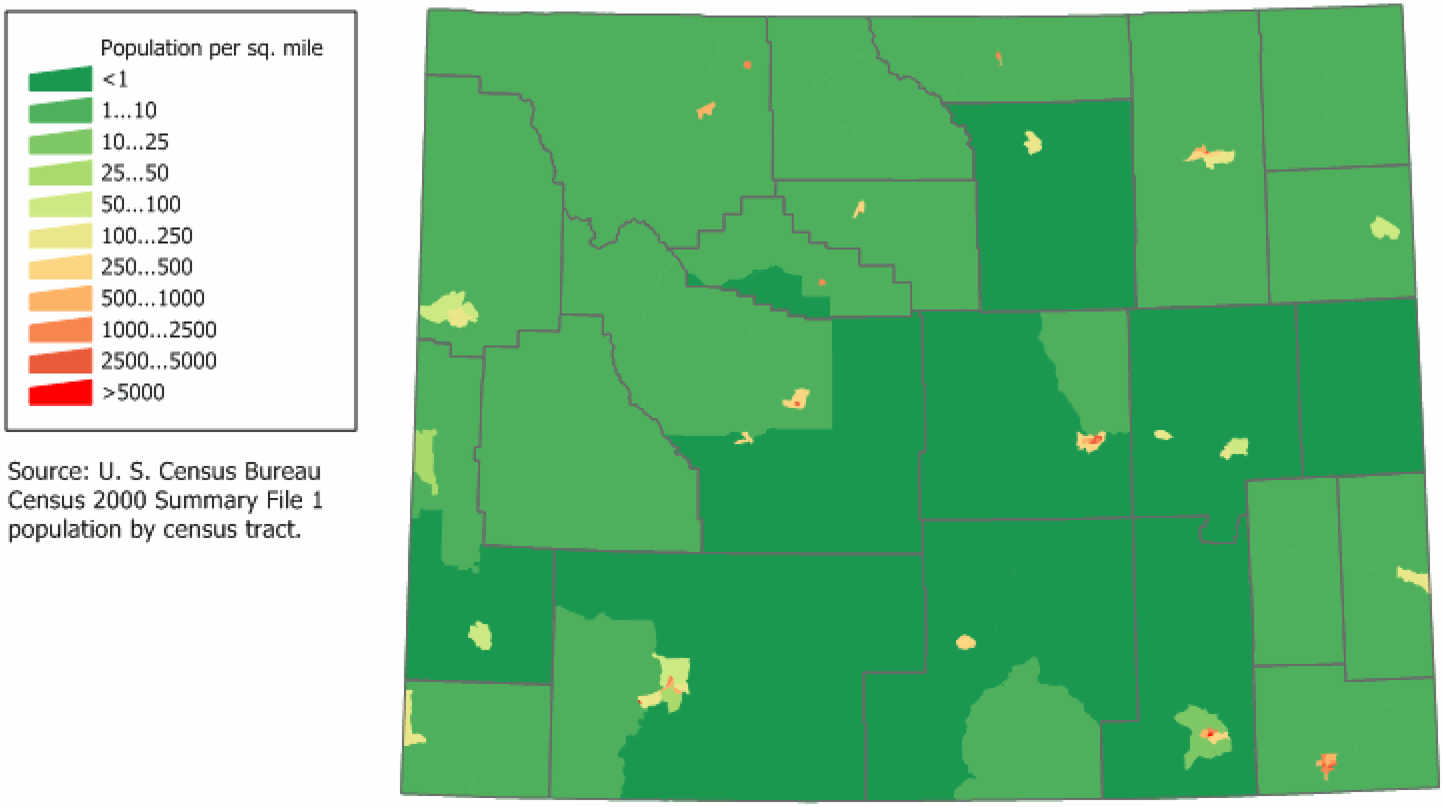
THINK SYMMETRY!!!

Population Density: Texas

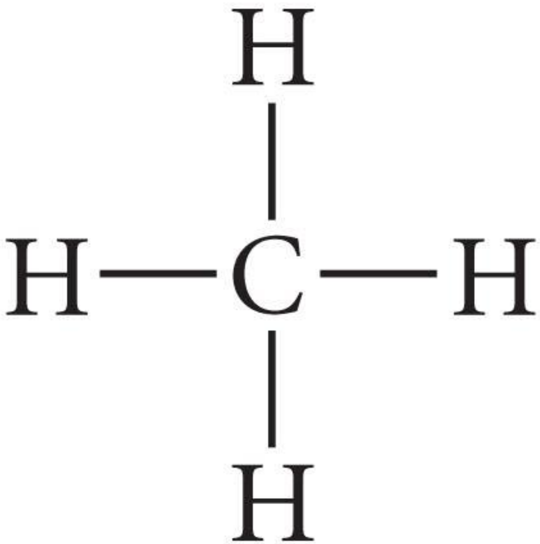
If electrons were people,
and states were molecules…

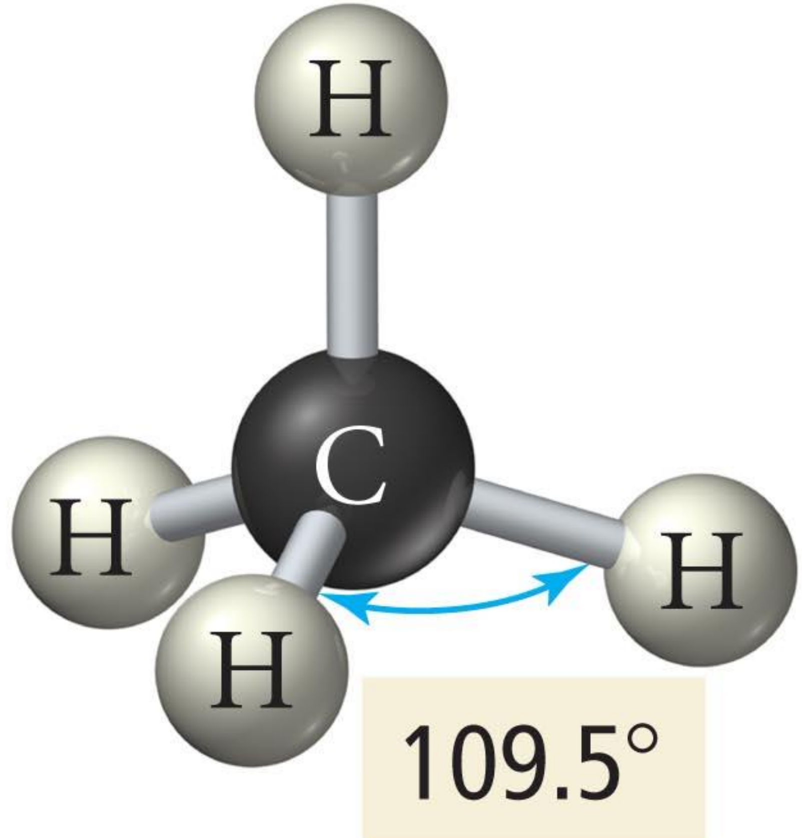


Population Density: Wyoming



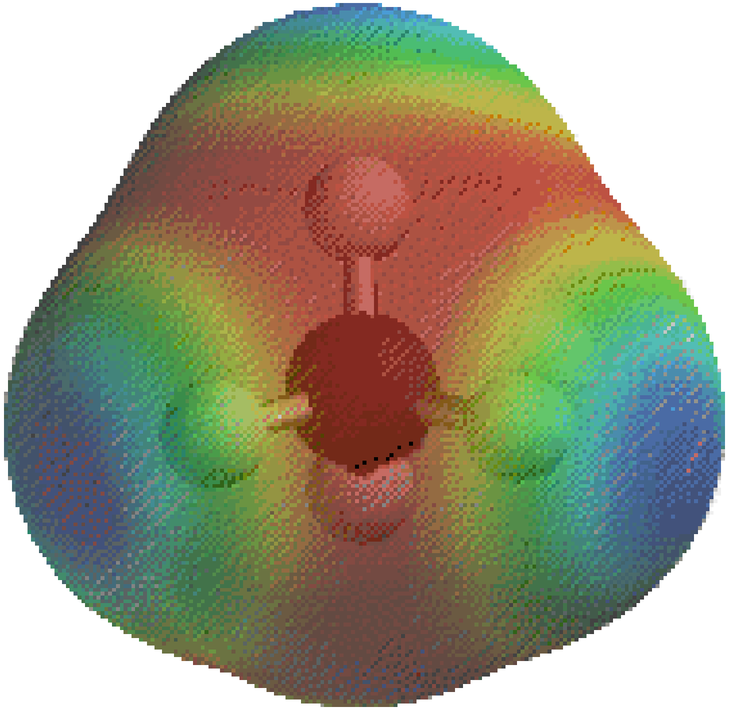
Source: U. S. Census Bureau
Census 2000 Summary File 1
population by census tract.





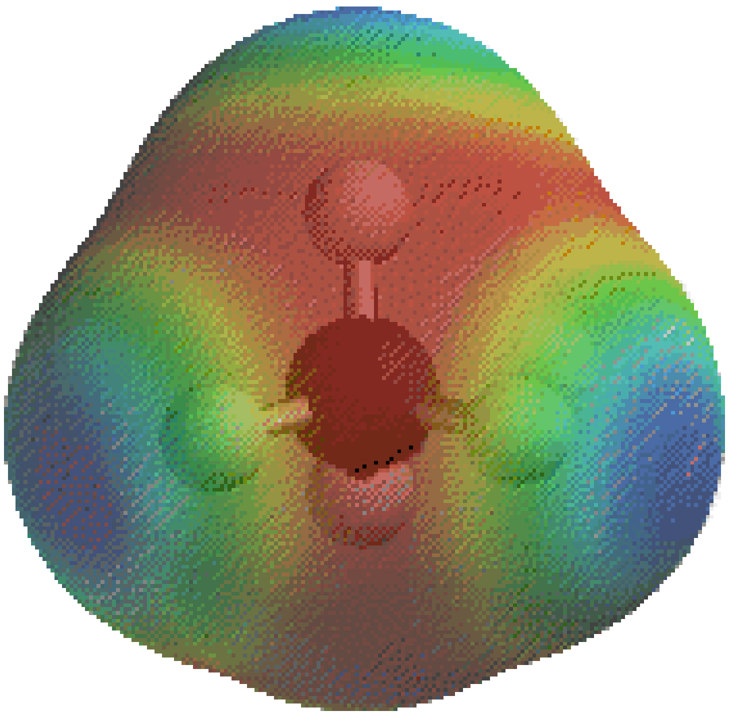
Tetrahedral geometry

Electron Density Maps

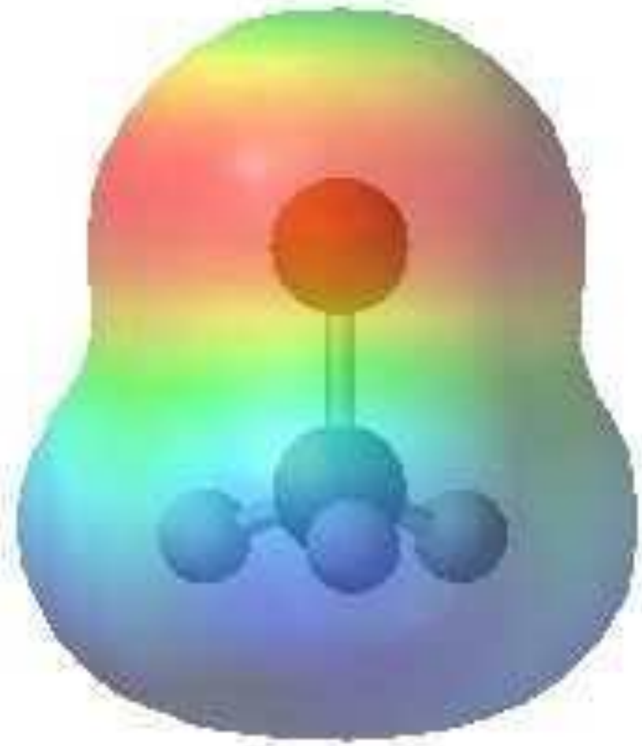


CH_4

Electron Density Maps

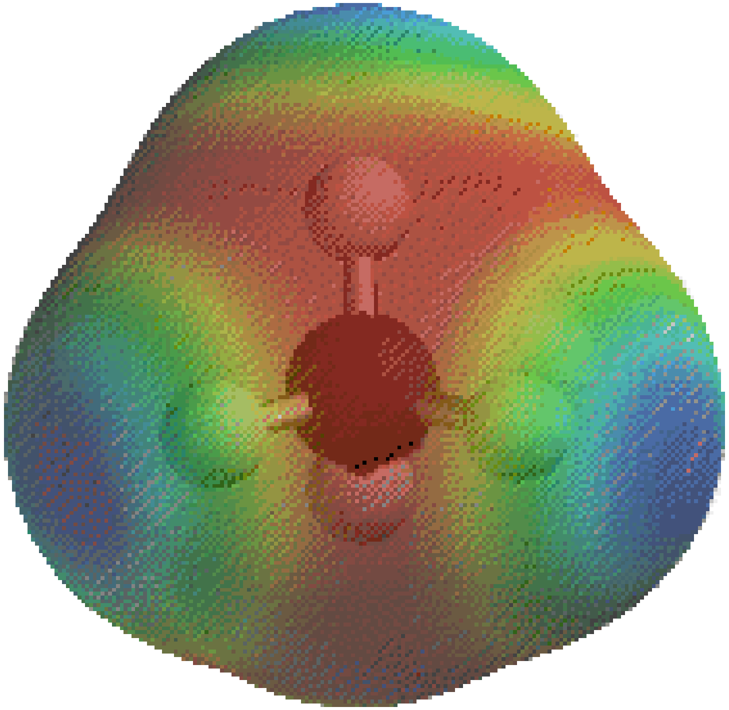


CH_4

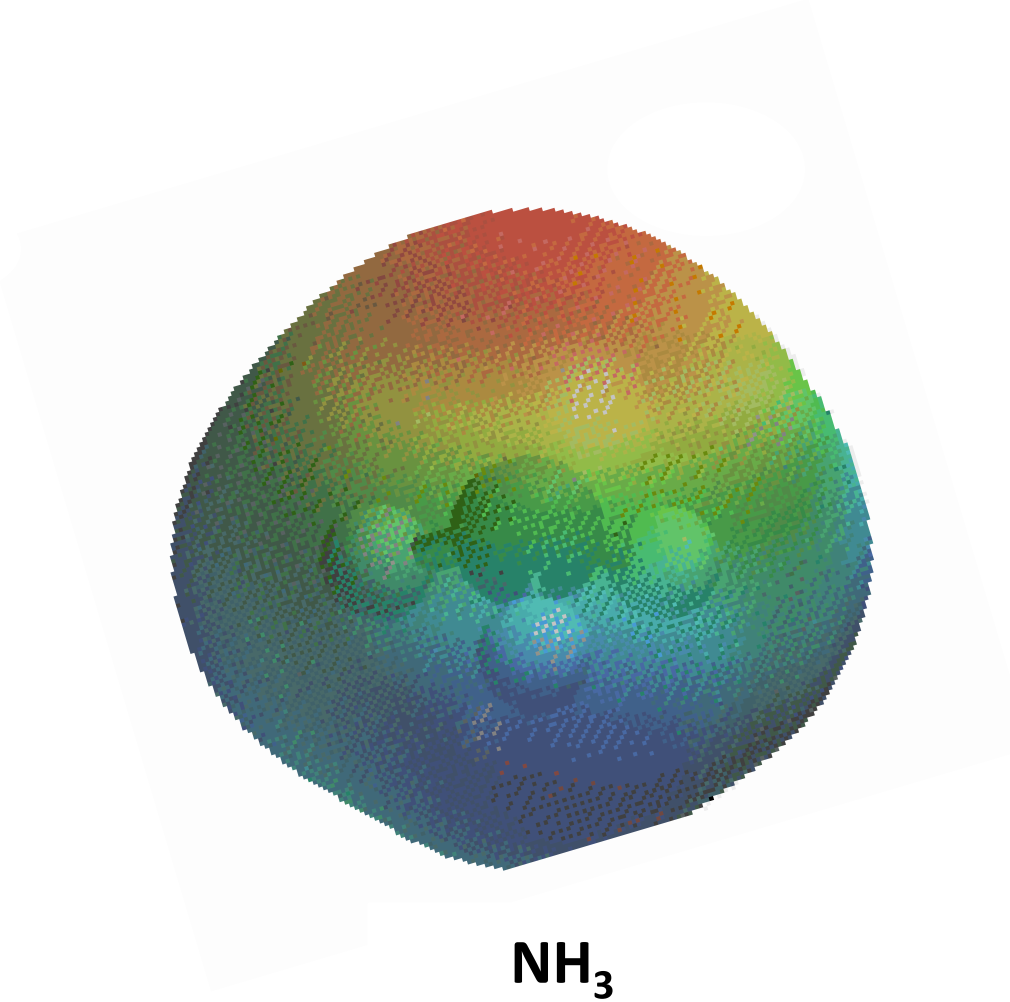


CH_3Br

Electron Density Maps

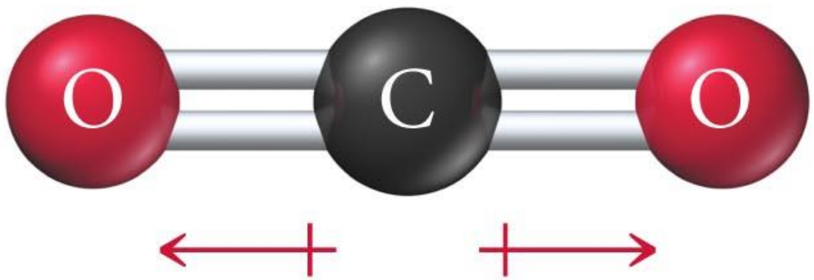


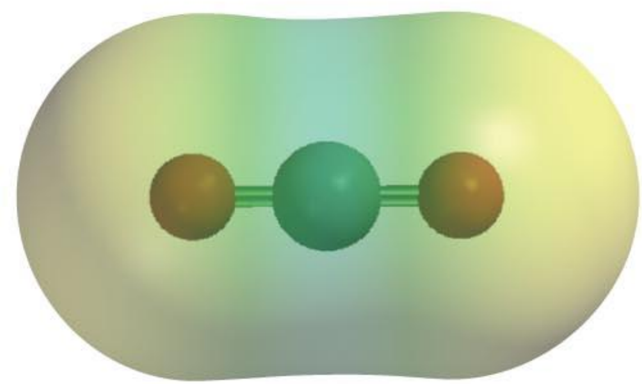
CH_4



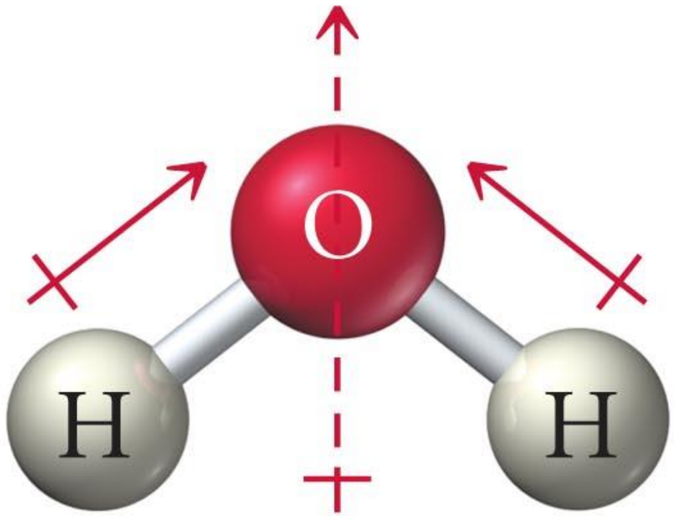
NH_3

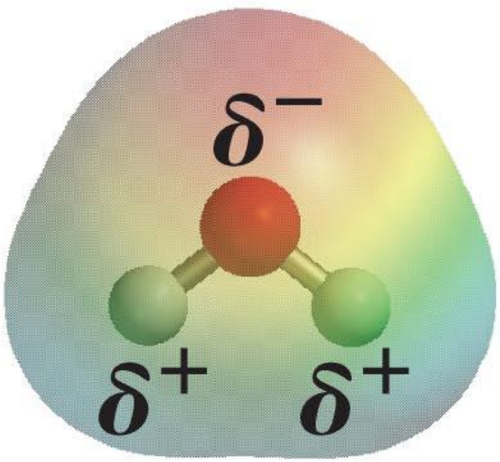
No net dipole moment



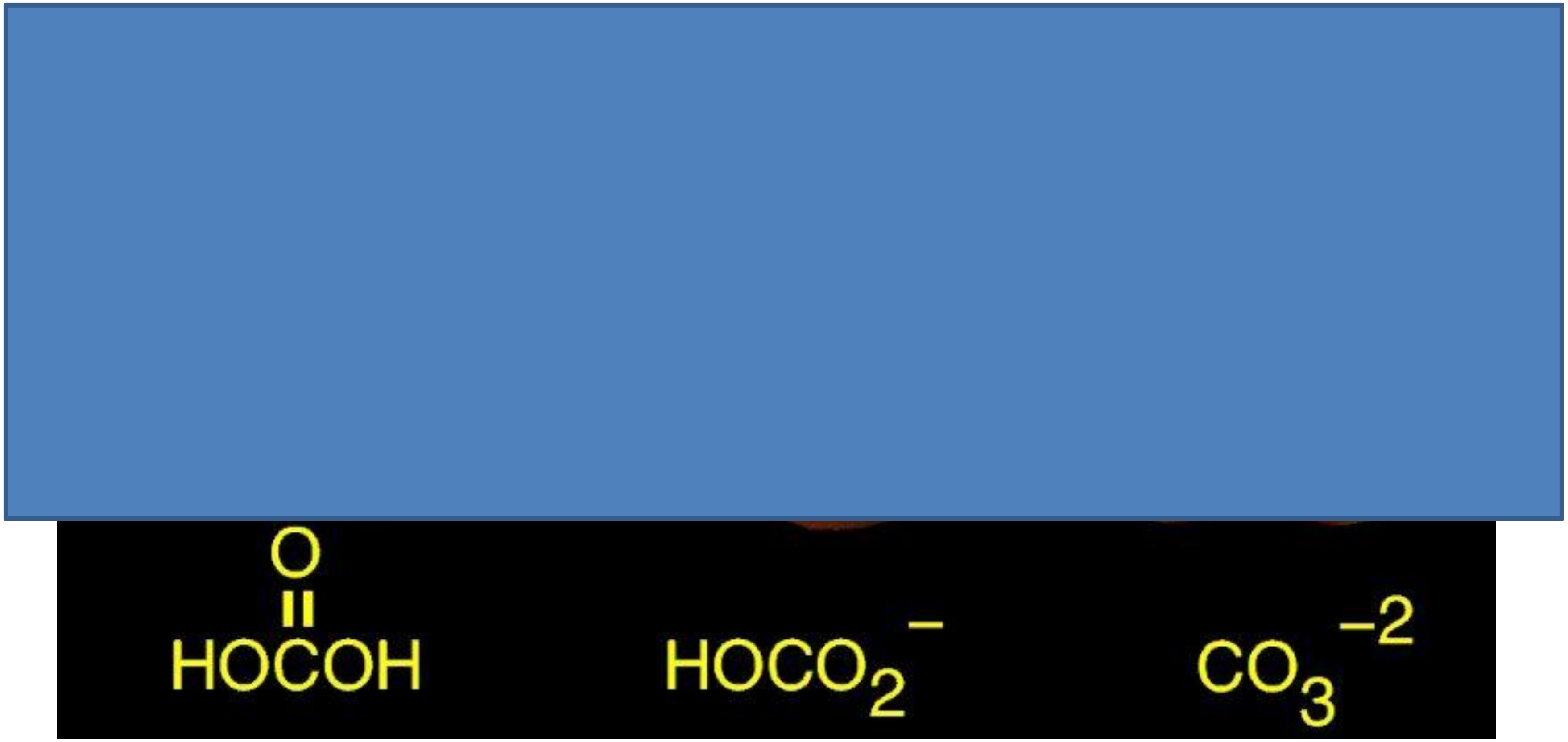


Net dipole moment

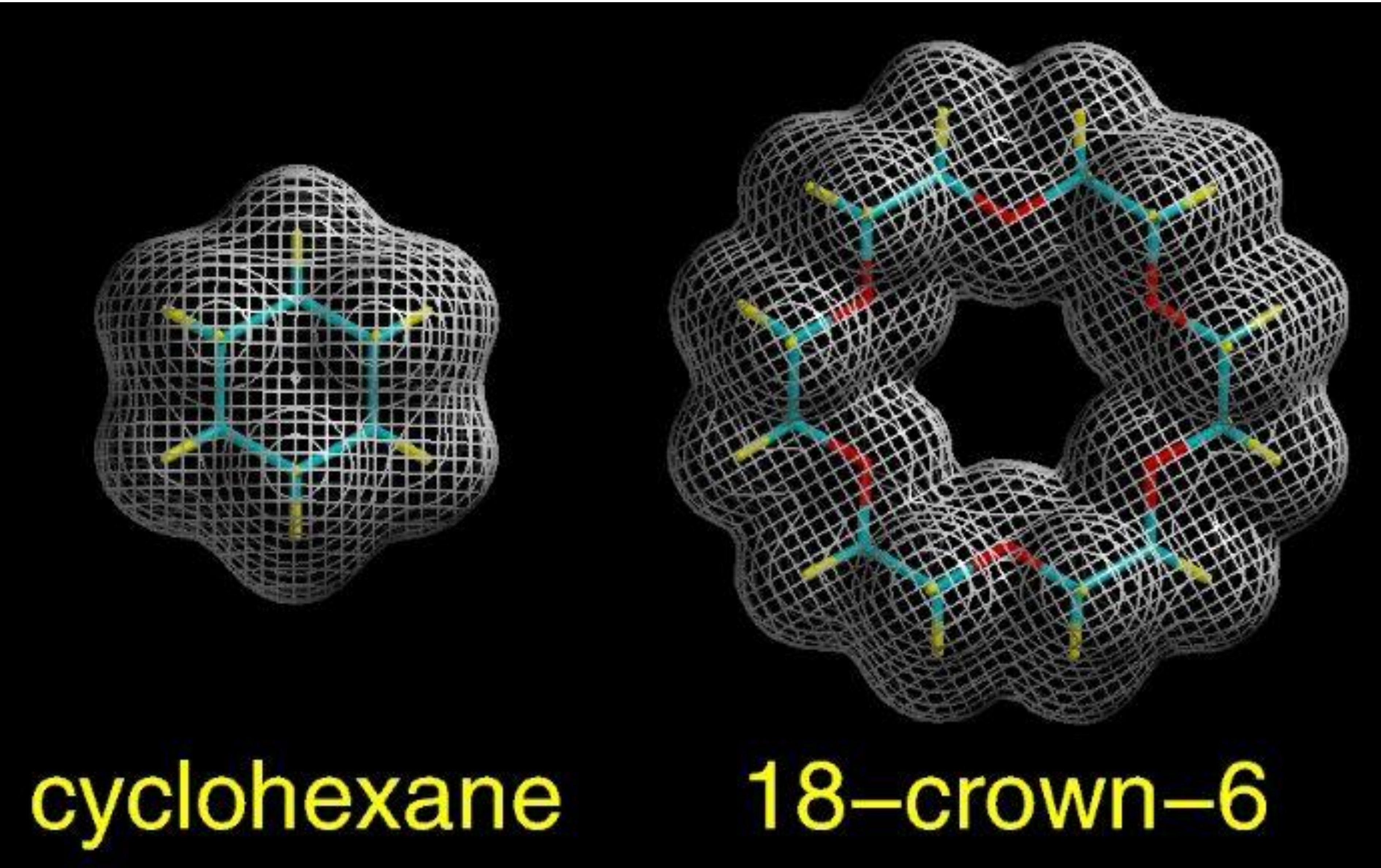




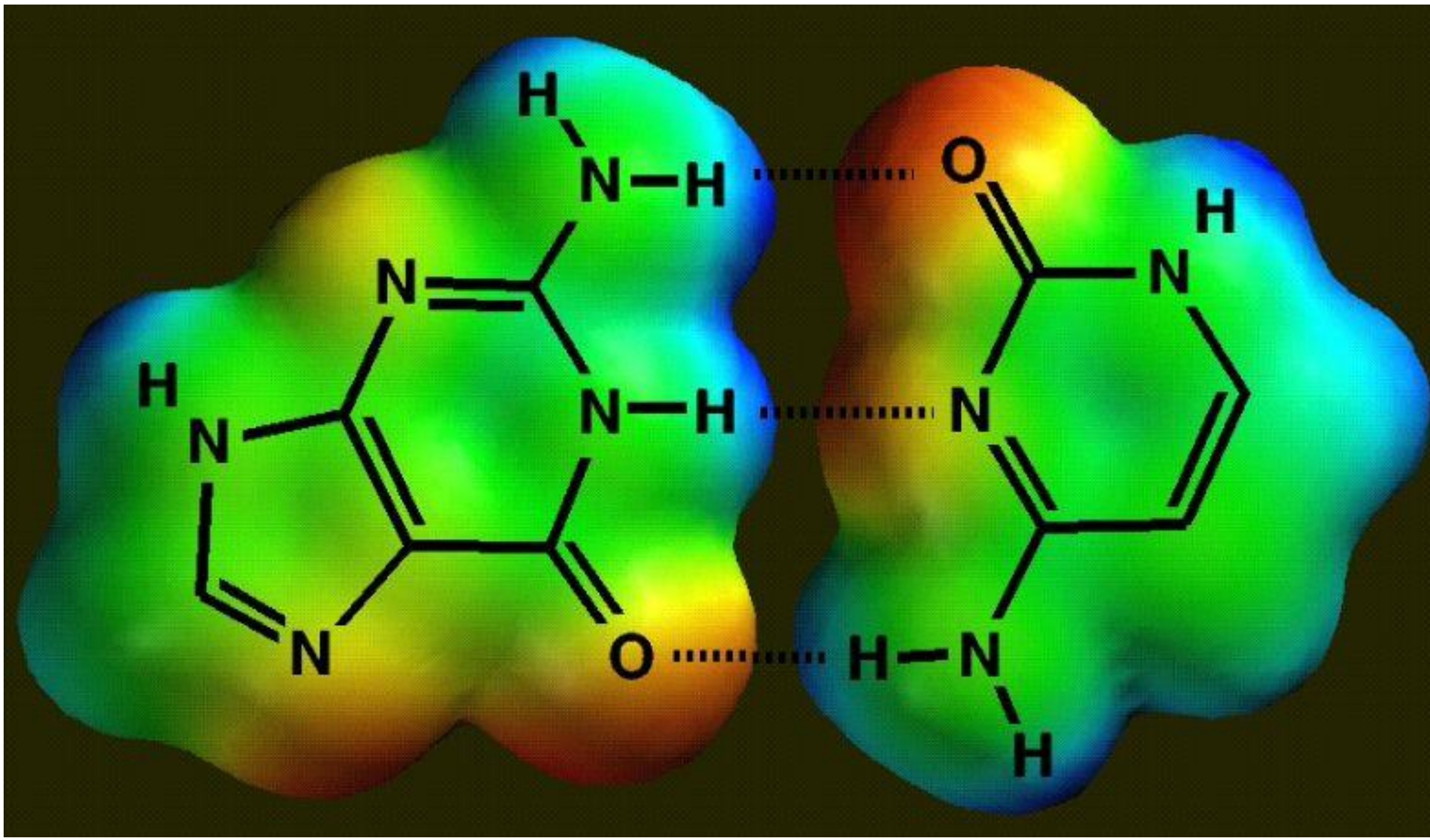
Polar or Non?



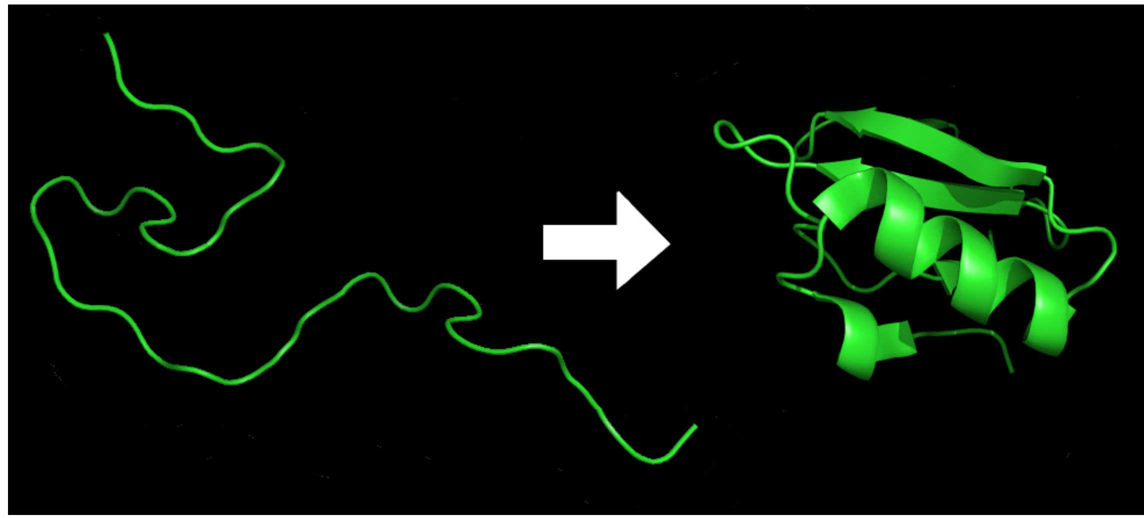
Larger Molecules: Nonpolar

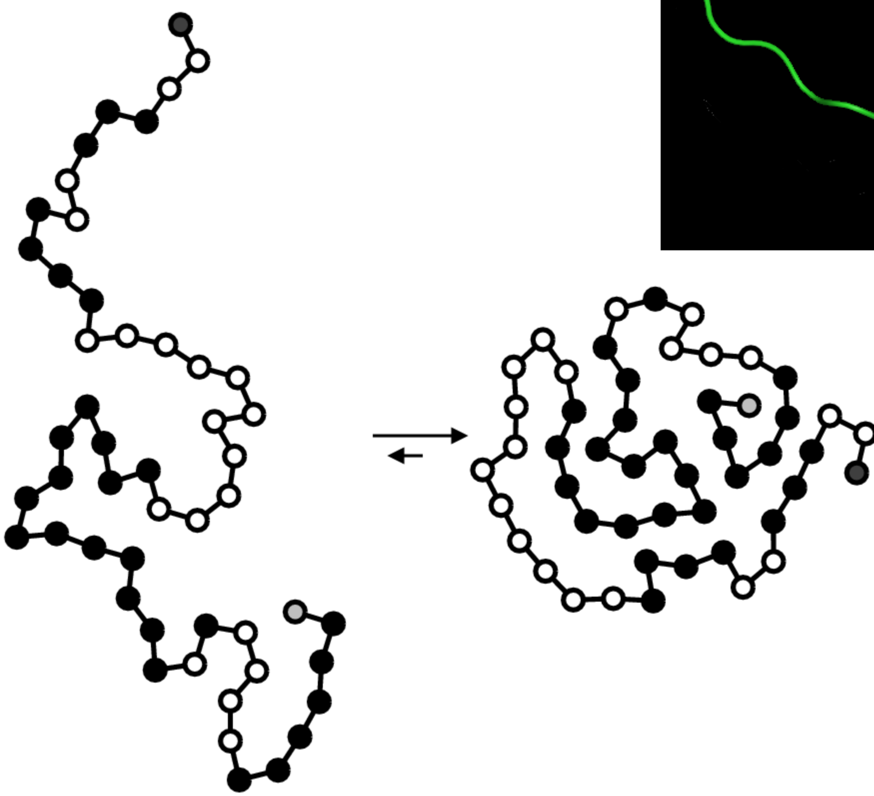


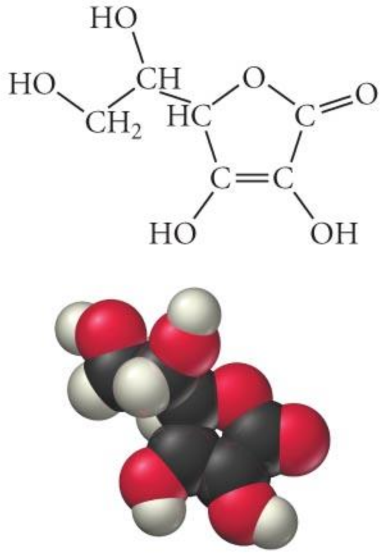
The Bigger Picture: Guanine and Cytosine



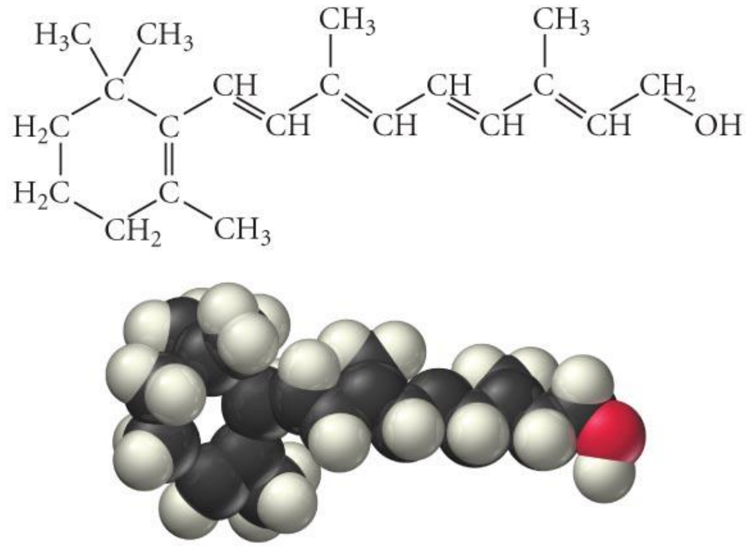
Protein Folding



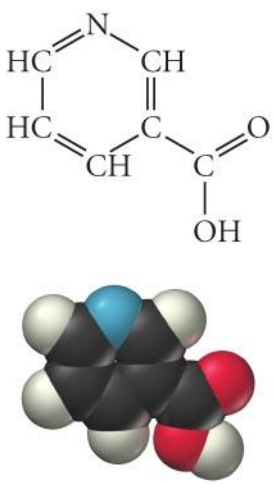




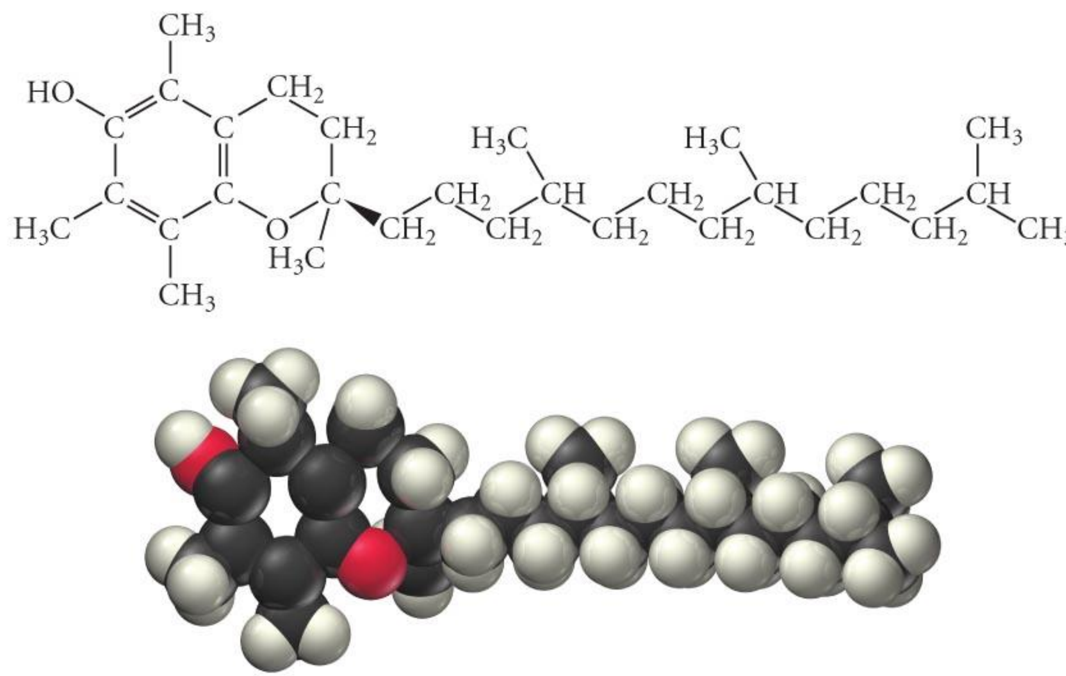
(**a**) vitamin C



(**b**) vitamin A



(**c**) niacin (vitamin B_3)



(**d**) vitamin E