

Covalent Bonding & Molecular Structure

I. Electronic Configuration and e^- sharing.

A. The Periodic Table's shape helps you understand outer- (and inner-) shell e^- configuration. Which e^- were of greatest interest to us in predicting ion formation?

These e^- also determine covalent bonding patterns.

B. Different elements show different tendencies to give, take, or share valence e^- . We use the term *electronegativity* to describe this.

1. Elements that tend to give up e^- have low electronegativity numbers. Metals tend to have low numbers. (My nephew is Cs.)
2. Elements that tend to take e^- have high electronegativity numbers. Non-metals have high numbers. (My sister is F, see below)

Electronegativity Table (Pauling scale)

1A																	8A
1 H 2.1																	2 He
	2A											3A	4A	5A	6A	7A	
3 Li 1.0	4 Be 1.5											5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0	10 Ne
11 Na 0.9	12 Mg 1.2	3B	4B	5B	6B	7B	8B		1B	2B	13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0	18 Ar	
19 K 0.8	20 Ca 1.0	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.9	28 Ni 1.9	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8	36 Kr
37 Rb 0.8	38 Sr 0.95	39 Y 1.0	40 Zr 1.1	41 Nb 1.2	42 Mo 1.3	43 Tc 1.4	44 Ru 1.5	45 Rh 1.6	46 Pd 1.7	47 Ag 1.8	48 Cd 1.9	49 In 1.9	50 Sn 2.0	51 Sb 2.1	52 Te 2.2	53 I 2.5	54 Xe
55 Cs 0.7	56 Ba 0.9	57 La 1.0	72 Hf 1.3	73 Ta 1.4	74 W 1.5	75 Re 1.6	76 Os 1.7	77 Ir 1.8	78 Pt 1.9	79 Au 2.0	80 Hg 2.1	81 Tl 2.0	82 Pb 2.1	83 Bi 2.2	84 Po 2.3	85 At 2.1	86 Rn
87 Fr (223)	88 Ra (226,025)	89 Ac (227)	104 Rf (261)	105 Ha (263)	106 Sg (263)	107 Ns (265)	108 Hs (265)	109 Mt (266)	110 - (269)	111 - (272)	112 - (277)						

C. Electronegativity lets us make predictions about bonding.

1. A metal bonded to a non-metal results in an ionic bond. (Electrons given and

taken; not shared.)

If electronegativity difference is > 2.1 , the bond is ionic. Comment re.

CuCl_2 (*Mostly ionic?*)

2. A bond between two non-metals results in a covalent bond. Electronegativity difference is < 1.9 (more below).

Examples: Indicate whether the compounds below form ionic or covalent.

NaCl

N_2

H_2O

K_3N

II. Lewis Structures of Atoms (*These help with e^- accounting.*)

A. Count valence e^- (these are in the outermost s & p e^-).

B. Arrange the e^- (dots) on the 4 sides of the elemental symbol.

C. Don't worry too much about transition metals.

D. Examples:

He

C

F

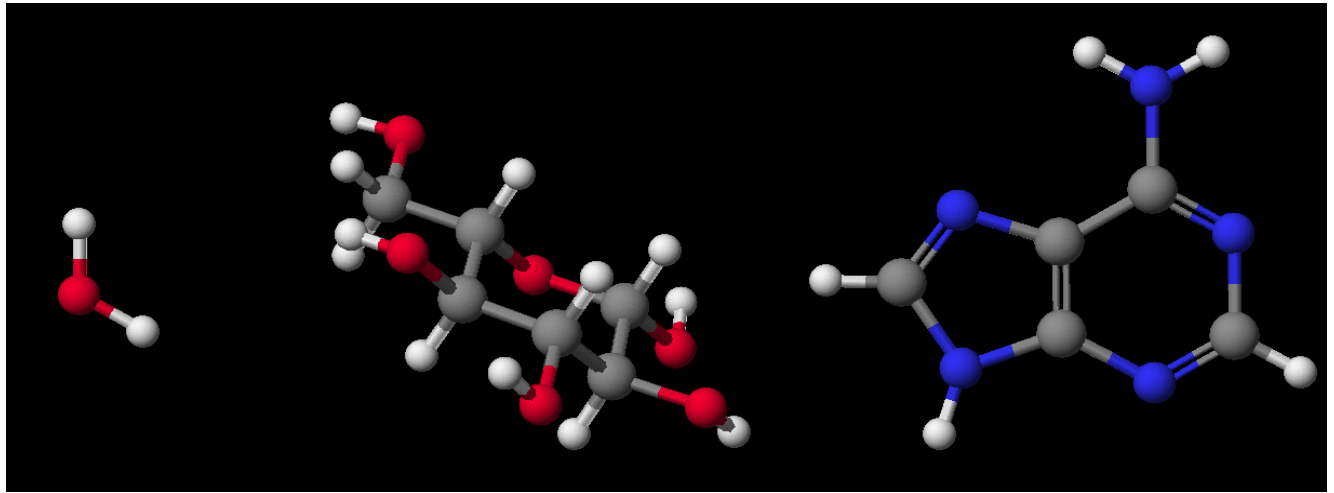
S

Xe

*Important: Inert gases are inert (non-reactive, stable) in the atomic state ($\# p^+ = \# e^-$) because these atoms have full valence shells. (**The Lewis Octet Principle**) More below.*

Although this seems very simple, you can do a lot of neat chemistry with the Lewis Octet Principle.

III. When (or more) two atoms join to form a covalent bond(s) we call the resulting entity a molecule. Examples:



water

β -D-glucose

adenine

IV. Patterns for combination of atoms to form molecules.

A. Atoms share electrons to fill their valence e^- shells. (*Why?*)

B. For valence e^- purposes, we count the shared e^- pair as belonging to both atoms. (Double dipping?)

Can we show the electron sharing in H_2 with a picture?

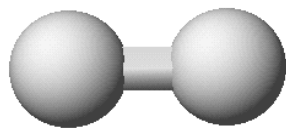
V. Electronegativity and Bond Polarity (view nuclei as reference points)

Covalent bonds involve e^- sharing, but how evenly is the negative charge arranged? How you decide? Electronegativity chart!

A. Non-polar covalent bonds have **completely even sharing**. These occur when:_____

Electronegativity:

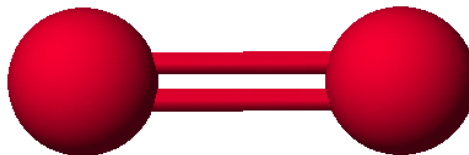
H 2.1 H 2.1



H₂

O 3.5

O 3.5



O₂

B. Polar covalent bonds occur when bonding atoms have different electronegativities. We will divide these into 2 groups:

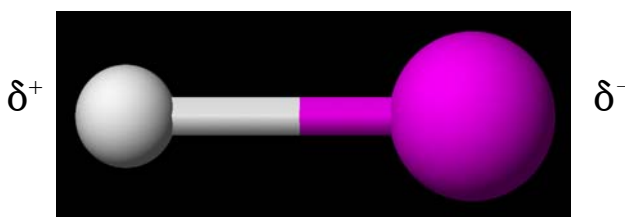
1. electronegativity difference < 0.9
2. electronegativity difference ≥ 0.9 (re. Hydrogen Bonds)

H 2.1

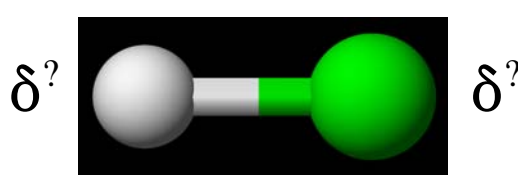
I 2.5

H 2.1

F 4.0



HI slightly polar bond.



HF exceedingly polar bond

Representing molecules & compound ions w/ Lewis Structures

Lewis Structures can be viewed as a visual bookkeeping device for valence electrons.

The Lewis Octet Principle tells us that atoms with full valence shells are more stable than atoms with unfilled valence shells. (Transition metal exceptions re. stability: Pt, Au, etc.)

Since only the inert gas (Group VIII) elements have full valence shells in their atomic state, all other elements must gain, lose, or share e⁻ to achieve full valence shells.

Gridlines to write Lewis Structures that you can't Zen:

1. Add up number of valence e^- (group #) for each atom
2. Make adjustments for non-zero net charge
 - a) Add one valence e^- for each negative charge
 - b) Subtract one valence e^- for each positive charge
3. Write elemental symbols (which atom is attached to which?)
4. Form single bonds to connect bonded atoms
5. Fill in non-bonding e^- pairs
6. If not enough e^- to go around, form double or triple bonds

Write Lewis structures for:

a Cl atom

a Cl^- ion

C H_4

N O_3^-

VI. Going from Lewis structures to Electron Pair Geometry, Molecular Shape, and Polarity

A. Polarity means *uneven distribution of charge*.

B. Since p^+ must stay in nucleus, uneven charge distribution refers to e^- distribution around specific nuclei or the molecule as a whole.

C. You *must* look at e^- pair geometry (molecular symmetry) to determine molecular polarity.

D. VSEPR stands for valence shell electron pair repulsion.

The situation is a bit more complicated for molecules with polar bonds:

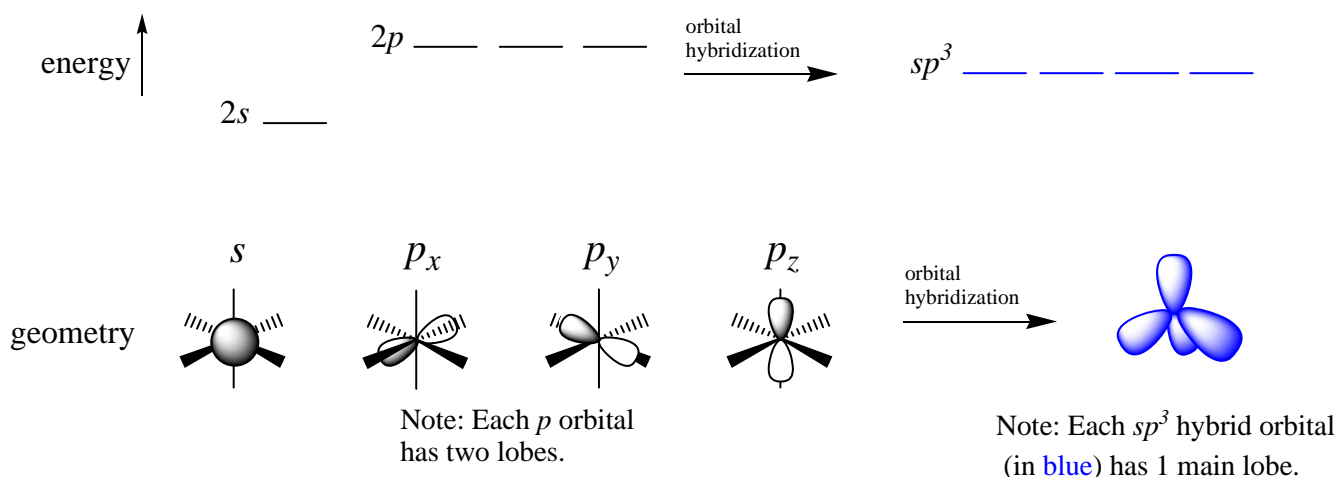
1. Some are polar. Example: H_2O
2. Some are non-polar (comment on symmetry, tractor pulls?)
Example: CH_4

What about CH_3Cl ?

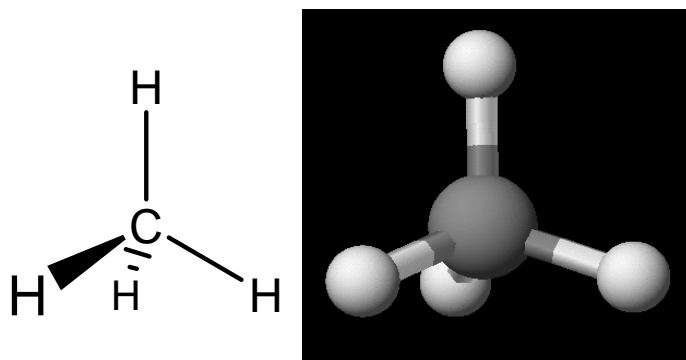
Appendix A: Orbital hybridization

Have you wondered yet how the electron pair geometries and molecular shapes discussed in the VSEPR modeling lab you worked on relate to the atomic orbitals ($1s$, $2s$, $2p$, $3s$, $3p$, $3d$, etc.)? Bonding and geometry patterns of the Period 2 elements C, N, and O that are so important biochemistry can be usefully described by the concept of *orbital hybridization*. I view orbital hybridization like an orbital food processor. We put a $2s$ orbital with the appropriate number of $2p$ orbitals and after blending obtain a set of hybrid orbitals. The number of hybrid orbitals obtained is equal to the sum of the s and p orbitals added together. Unlike p orbitals that have two lobes per orbital, sp , sp^2 , and sp^3 hybrid orbitals have just one main lobe (but see Dr. Winter's Orbitron at <http://winter.group.shef.ac.uk/orbitron/>) per orbital. See examples below and on the following page. Note that the geometries of the hybrid orbitals match the patterns predicted from VSEPR theory. Further, the two lobed pi bonds that are part of double and triple bonds accurately predict the limited rotation that is observed with these types of bonds.

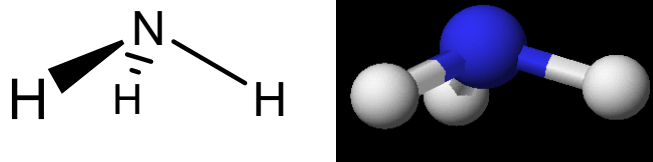
Formation of 4 sp^3 hybrid orbitals from 1 s and 3 p orbitals



Molecules that contain sp^3 hybridized Period 2 atoms



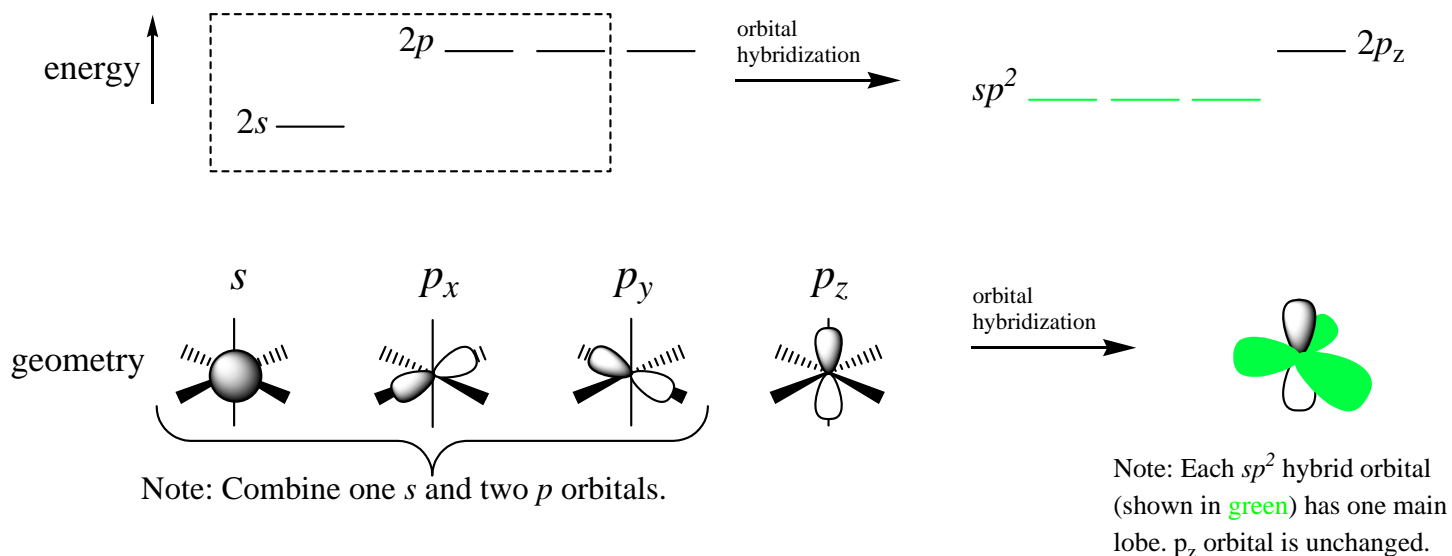
CH_4 , methane



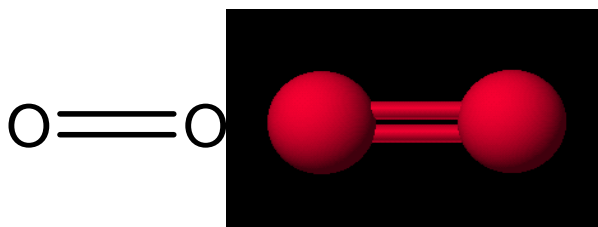
NH_3 , ammonia

Atoms involved in forming one double bond exhibit sp^2 orbital hybridization patterns:

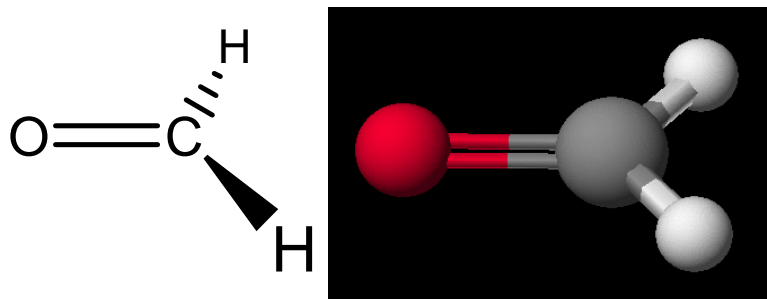
Formation of 3 sp^2 hybrid orbitals from 1 s and 2 p orbitals



Molecules that contain sp^2 hybridized Period 2 atoms



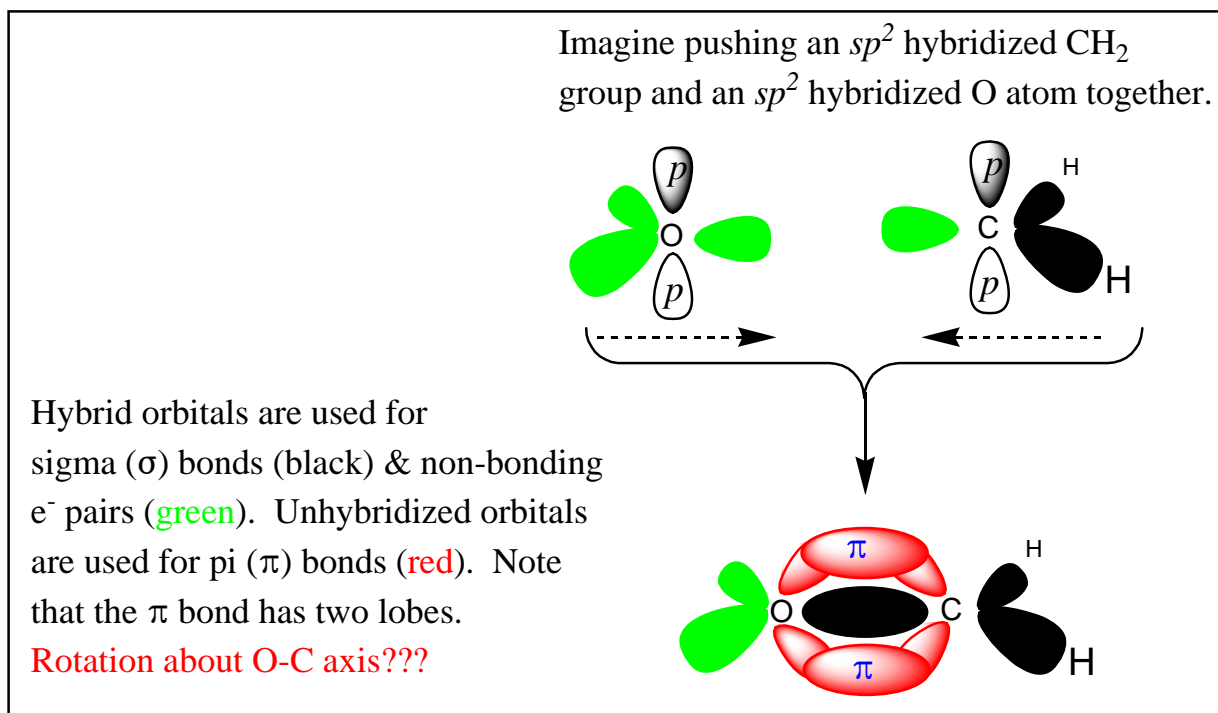
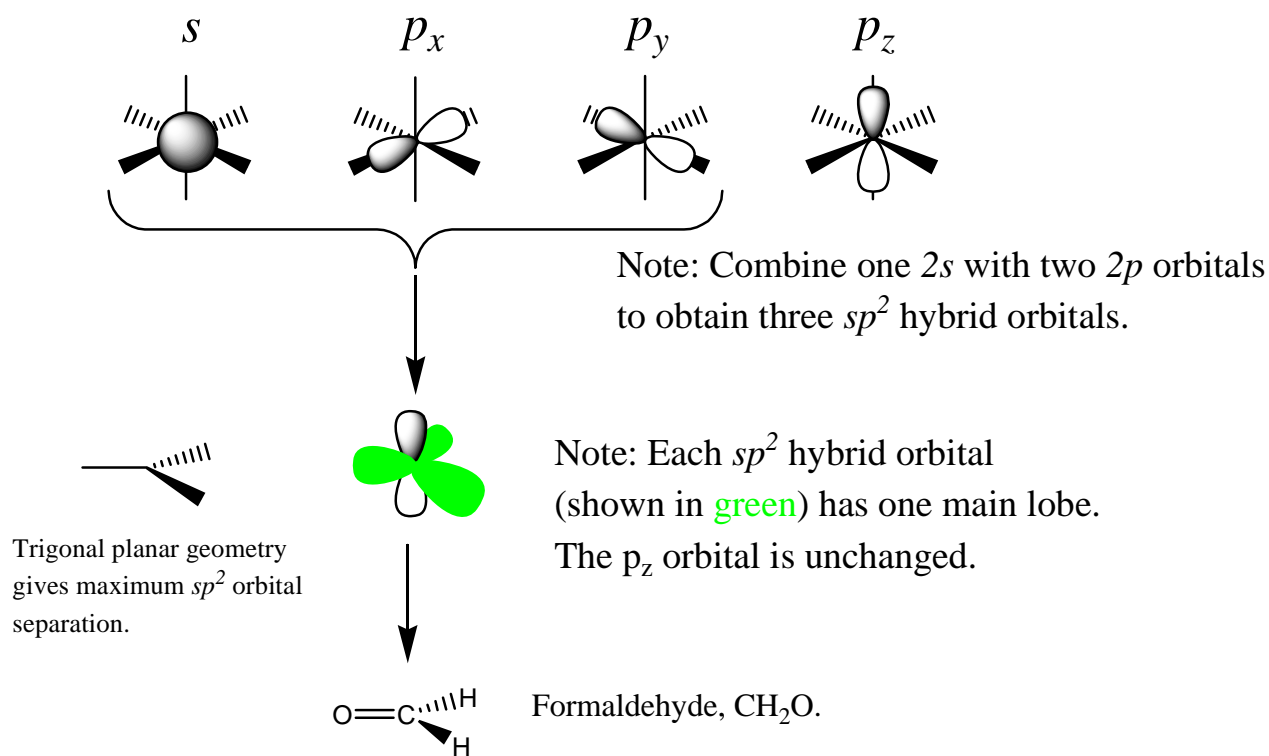
O_2 , elemental oxygen



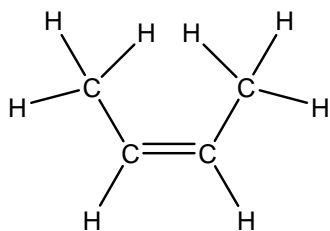
CH_2O , formaldehyde (a.k.a., ethanal)

Although you might conclude from the structures shown above that the two bonds that make up a double bond are identical, that is not the case. (See next page.) Formation of a double bond has the important consequence of eliminating freedom of rotation about the bonding axis that does exist for singly bonded atoms..

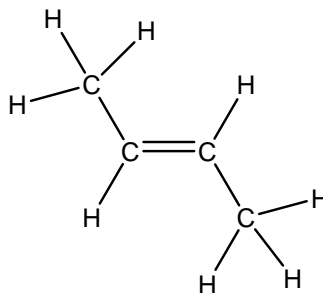
Orbital hybridization: Building CH₂O from sp^2 hybridized CH₂ and O



Your instructor will perform a short demonstration with molecular models to show how the pi bond component of double (and triple) bonds limits rotation about these bonds. Contrast this with the relatively free rotation about the C-C single bond in ethane. This limited rotation in double bonds is responsible for another group of *cis/trans* isomers. The structures of the *cis* and *trans* isomers of 2-butene are shown below. The “-ene” ending indicates that there is a double bond, and the “2” indicates the position of the double bond.

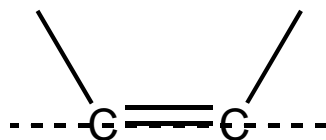


cis-2-butene

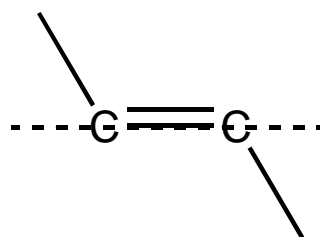


trans-2-butene

In general terms, a compound is *cis* if its higher ranking groups are on the same side of a line running through the C atoms involved in the double bond, and *trans* if they are on opposite sides of the line.



cis



trans

Biological relevance? The first biochemical step in the visual process:

Cis- to *trans*-retinal in Rhodopsin, The 1st biochemical step in the visual process

