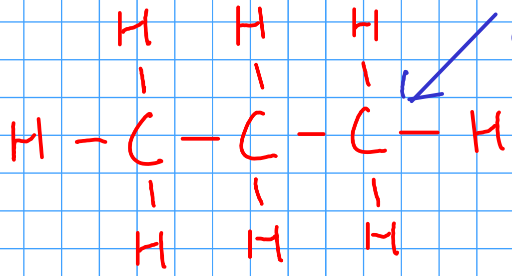
VSEPR and large molecules

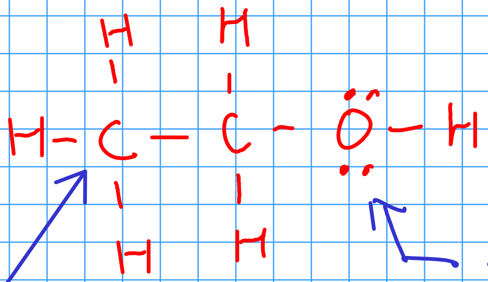
- Large molecules have more than one "center" atom
- Describe the molecule by describing the shape around each "center".

C_3H_8:



Each of the three carbon centers is TETRAHEDRAL, since each are surrounded by four groups.

CH_3CH_2OH:



The geometry around this oxygen atom is BENT.

These carbon atoms have TETRAHEDRAL geometry.

POLARITY and shape:

- A polar molecule has an uneven distribution of electron density, making it have ends (poles) that are slightly charged.

POLARITY influences several easily observable properties.

- Melting point. (Polar substances have higher melting points than nonpolar substances of similar molecular weight.)
- Boiling point. (Polar substances have higher boiling points than nonpolar substances of similar molecular weight.)
- Solubility. (Polar substances tend to dissolve in other polar substances, while being insoluble in nonpolar substances. Nonpolar substances dissove other nonpolar substances, and generally have poor solubility in polar solvents.)

- Polar molecules contain POLAR BONDS arranged in such a way that they do not cancel each other out.

... but how can we tell whether or not a bond will be POLAR? Use experimental data on ELECTRONEGATIVITY!

ELECTRONEGATIVITY:

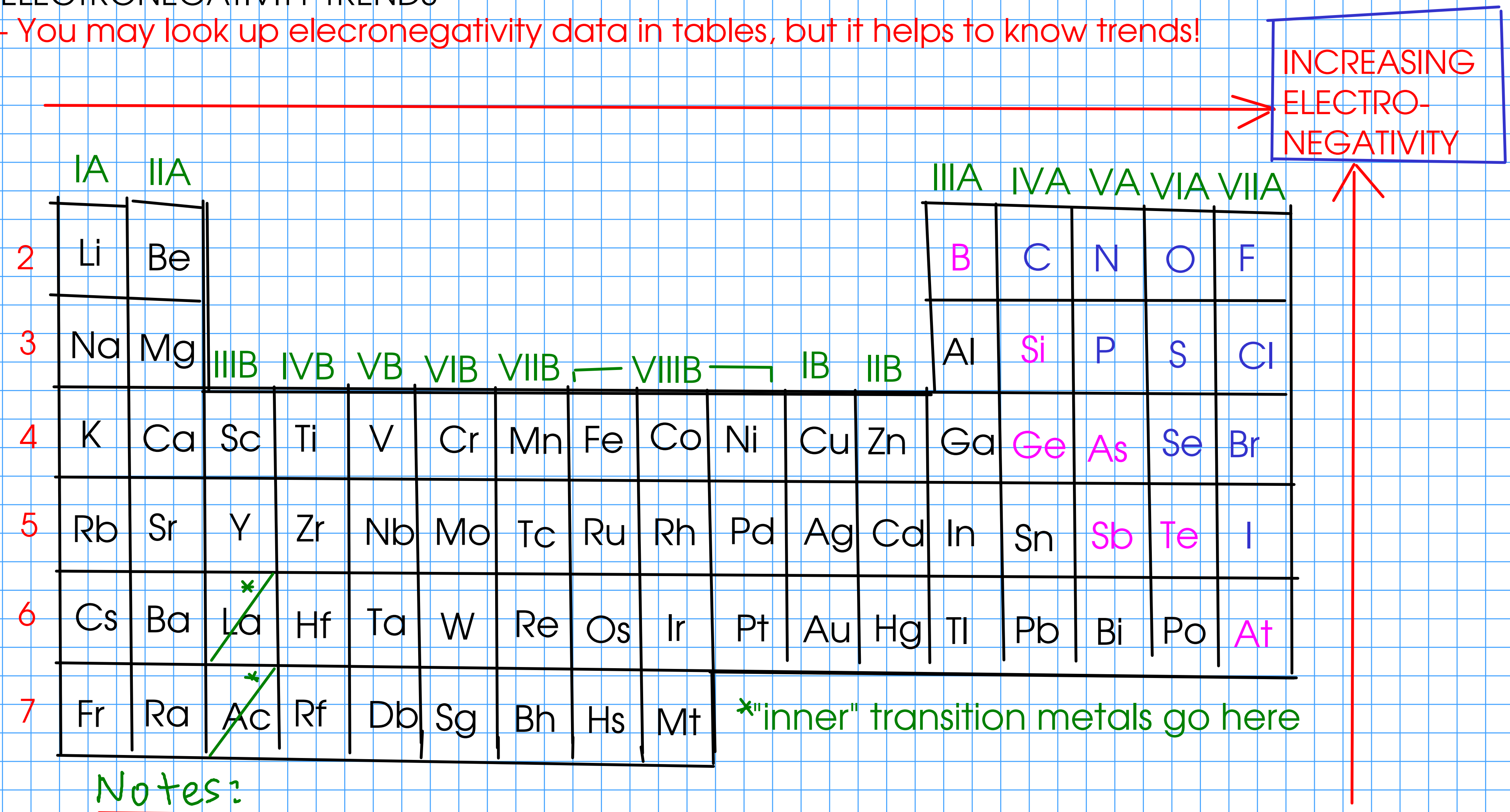
-A measure of how closely to itself an atom will hold shared electrons

- A bond where there is a LARGE electronegativity difference between atoms will be either POLAR or (for very large differences) IONIC!

- A bond with little or no electronegativity difference between atoms will be NONPOLAR

ELECTRONEGATIVITY TRENDS

- You may look up elecronegativity data in tables, but it helps to know trends!



	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA
2	Li	Be											B	C	N	O	F
3	Na	Mg											Al	Si	P	S	Cl
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I
6	Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At
7	Fr	Ra	Ac*	Rf	Db	Sg	Bh	Hs	Mt								

*"inner" transition metals go here

Notes:

① - FLUORINE is the most elecronegative element, while FRANCIUM is the least!

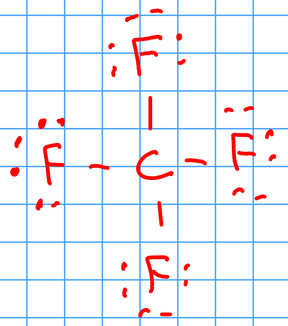
② - All the METALS have low electronegativity, and metal/nonmetal combinations form IONIC bonds

③ - HYDROGEN is similar in electronegativity to CARBON, so C-H bonds are considered NONPOLAR

Examples:

CF_4:

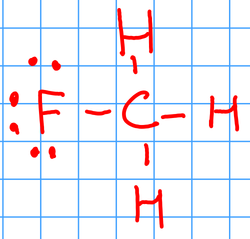
C: 4
F: 7 x4
32



Polar or nonpolar?
* Polar bonds? YES. C-F should be polar
* Geometry? C-F bonds are arranged symmetrically.
They cancel each other, so the molecule is NONPOLAR!

CH_3F

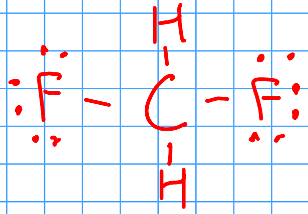
C: 4
H: 1x3
F: 7
14



Polar or nonpolar?
* Polar bonds? C-F is polar, C-H isn't
* Geometry? Electrons are pulled towards the fluorine atom, making the fluorine side negative and the other side of the molecule positive. So we expect a POLAR molecule.

CH_2F_2.

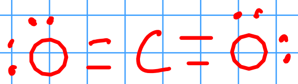
C 4
H 1 x2
F: 7 x2
20



Polar or nonpolar?
* Polar bonds? C-F is polar, C-H isn't
* Geometry? In 3D, this molecule has a hydrogen "side" and a fluorine "side", so it will be a POLAR molecule.

CO_2

C: 4
O: 6x2
16



Polar or nonpolar?
* Polar bonds? C=O bonds should be polar.
* Geometry? In this linear molecule, the two C=O bonds cancel each other out, making carbon dioxide nonpolar.

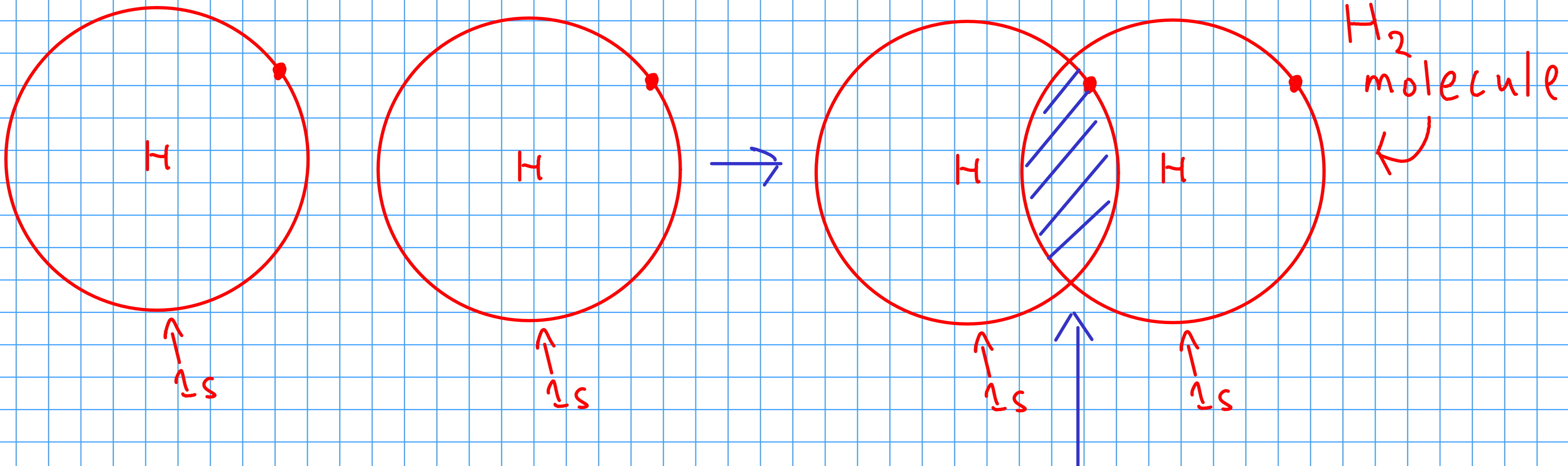
VALENCE BOND THEORY

- an attempt to explain why molecules behave in the way that the VSEPR model predicts.

- Describes the formation of bonds in terms of the OVERLAP of ORBITALS from the bonding atoms.

① Bonds are formed when two atoms are close enough together so that their ORBITALS OVERLAP (share the same space).

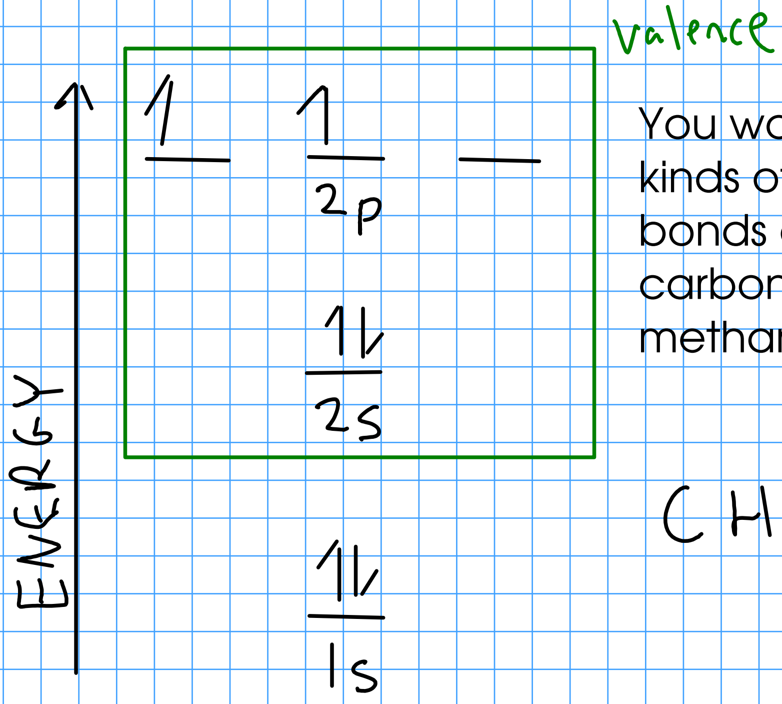
② Each SET of overlapping orbitals can contain at most a total of TWO electrons. So, two orbitals with one electron each may bond. An orbital with two electrons can only bond with an EMPTY orbital (This is called a COORDINATE COVALENT BOND.) * Ag^+ with $:NH_3$ ... the cleanup in the AgCl lab



These 1s orbitals overlap to form what we call a "sigma bond" with overlap BETWEEN the two atomic nuclei.

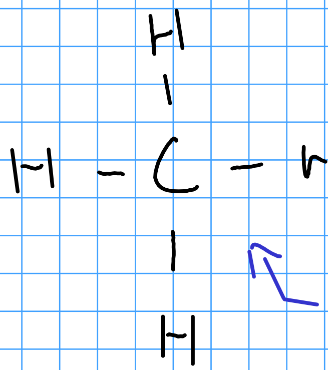
Hybridization

- Look at carbon's electron configuration:



You would expect that carbon would form several different kinds of bonds in a molecule like methane. But, methane's bonds are experimentally all identical. How does carbon form the four equivalent C-H bonds we see in methane?

CH_4 :



We observe that these bonds are IDENTICAL! Same bond energy, distance, and angle.

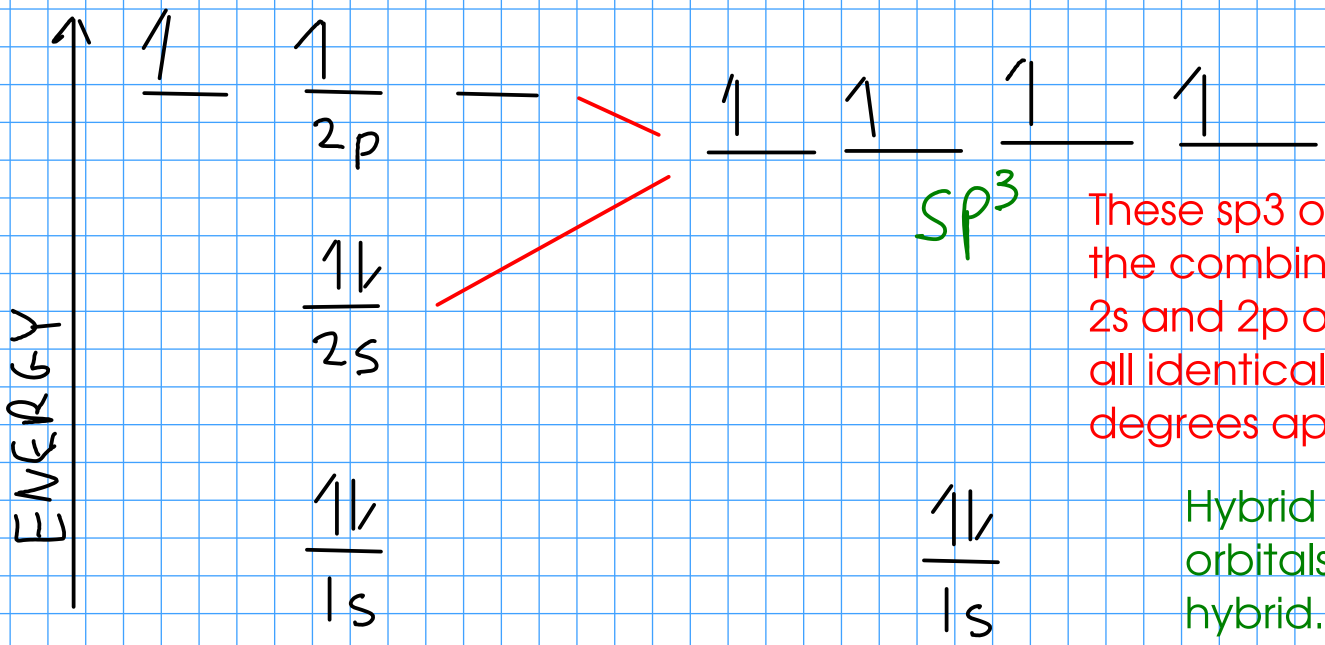
- In valence bond theory, atomic orbitals can COMBINE to make new orbitals that can then go on to bond with other molecules.

- When orbitals combine to make HYBRID ORBITALS, ...

① The overall NUMBER OF ORBITALS does not change.

② The overall NUMBER OF ELECTRONS around the atom does not change

③ The energy of the orbitals is between the energies of the orbitals that combine.



These sp3 orbitals were formed from the combination of carbon's original 2s and 2p orbitals. These orbitals are all identical, and are spread 109.5 degrees apart from one another.

Hybrid orbitals are named from the orbitals that go into making the hybrid. 2s + 3 2p orbitals = "sp3"!

Types of hybrid orbitals:

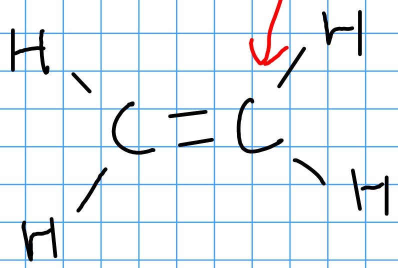
Hybrid type	Number of orbitals	Molecular shape
sp	2	linear
sp2	3	trigonal planar
sp3	4	tetrahedral (or derivatives)
sp3d	5	trigonal bipyramidal (or derivatives)
sp3d2	6	octahedral (or derivatives)

MULTIPLE BONDS and VALENCE BOND THEORY

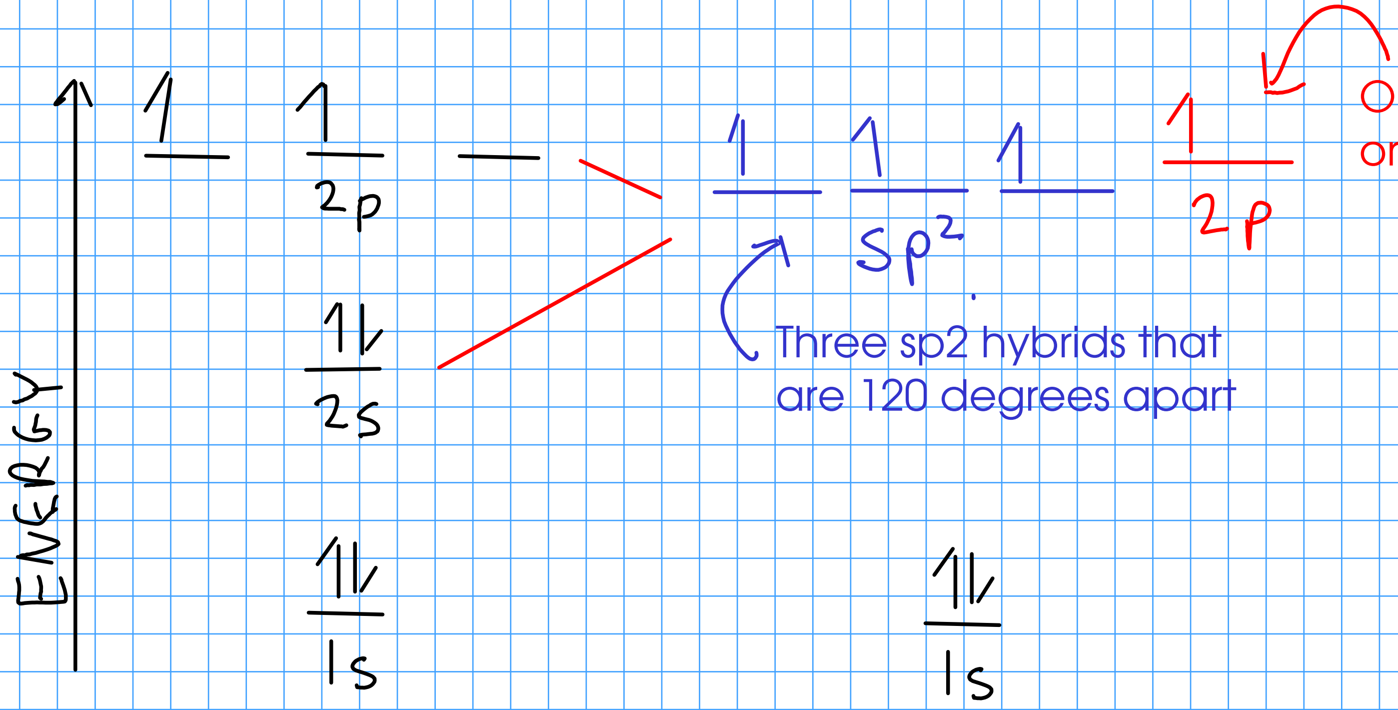
- Valence bond theory provides an explanation of multiple (double and triple) bonding that explains some interesting observations about these kinds of bonds.

C_2H_4:

ethylene

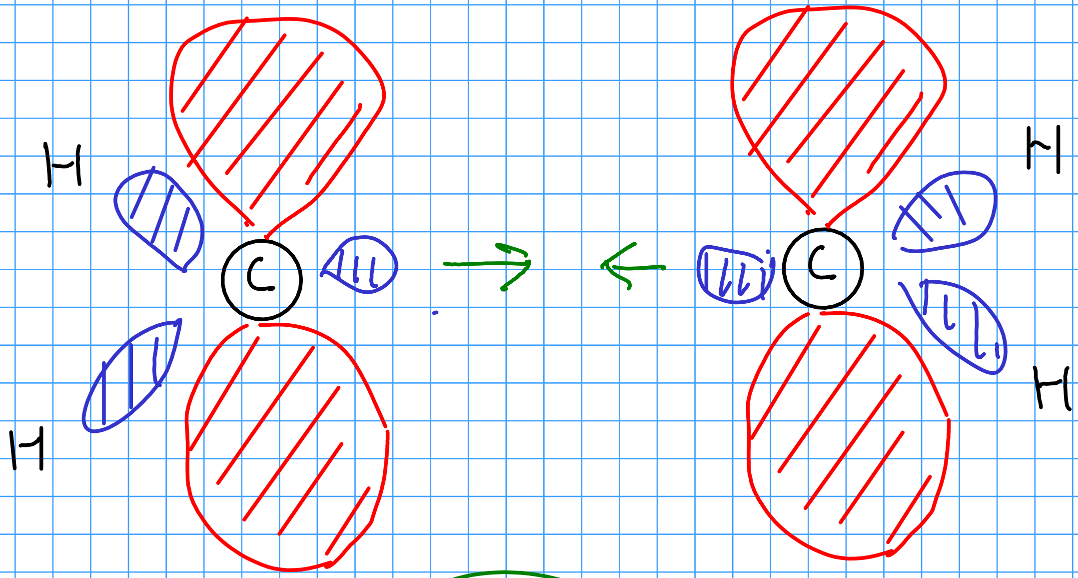


Each carbon has a TRIGONAL PLANAR geometry. This suggests that the carbons are "sp2 hybridized".



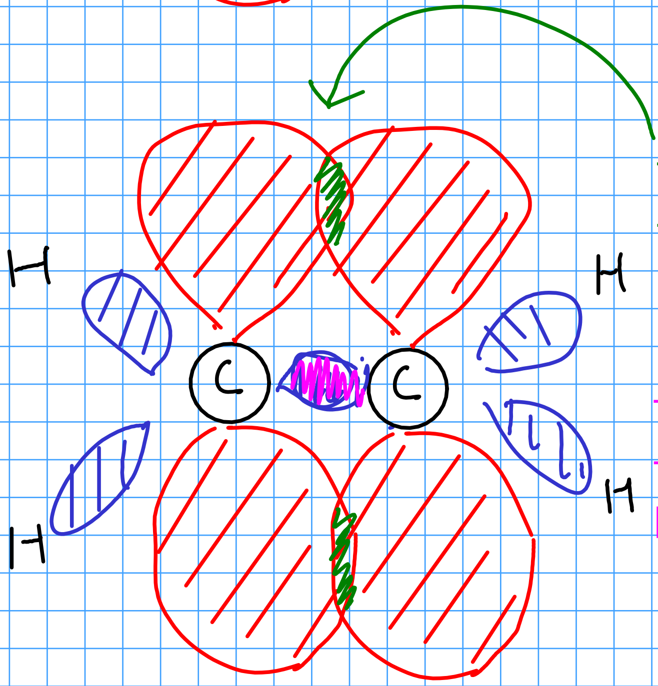
Three sp2 hybrids that are 120 degrees apart

One unchanged 2p orbital



sp2 hybrid orbitals in BLUE

2p orbital in RED



The 2p orbitals overlap above and below the axis between the two carbon atoms. This OFF-AXIS overlap is called a PI BOND.

The sp2 hybrid orbitals overlap ON THE AXIS between the two carbon atoms. This bond is called a SIGMA BOND.

As you can see, the carbon-carbon double bond in ethylene is made up of TWO DIFFERENT KINDS OF BONDS!