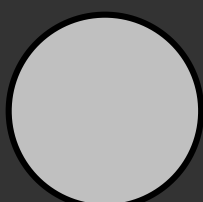
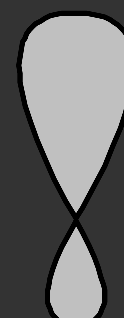
Covalent Bonding - Orbitals

Hybridization - The Blending of Orbitals

 +  = 

Poodle + Cocker Spaniel = Cockapoo

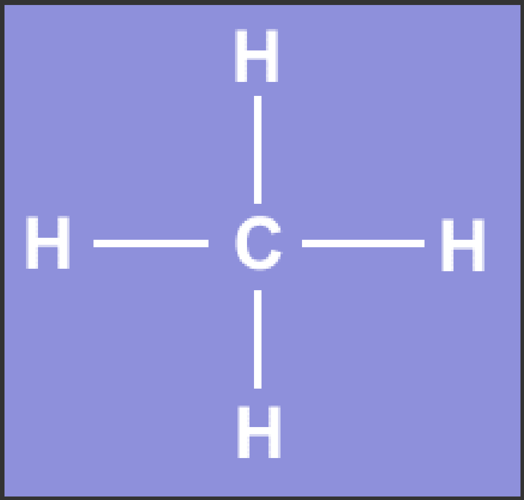
 +  = 

s orbital + *p* orbital = *sp* orbital

What Proof Exists for Hybridization?

We have studied electron configuration notation and the sharing of electrons in the formation of covalent bonds.

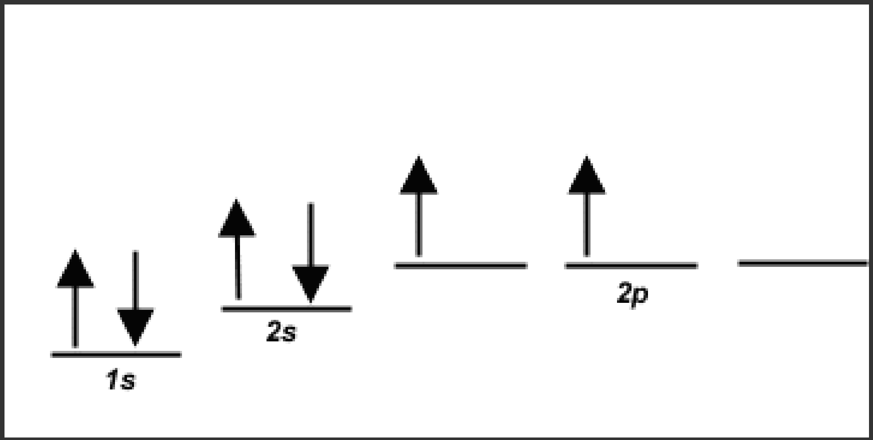
Lets look at a molecule of methane, CH_4.



Methane is a simple natural gas. Its molecule has a carbon atom at the center with four hydrogen atoms covalently bonded around it.

Carbon ground state configuration

What is the expected orbital notation of carbon in its ground state?

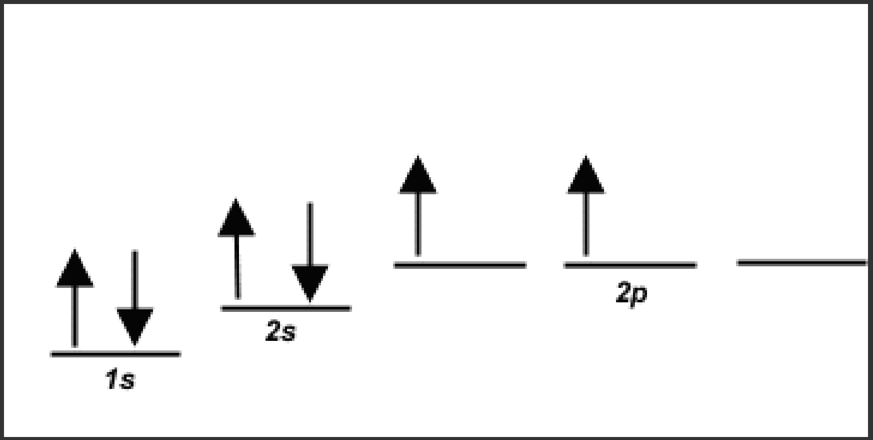


Can you see a problem with this?

(Hint: How many unpaired electrons does this carbon atom have available for bonding?)

Carbon's Bonding Problem

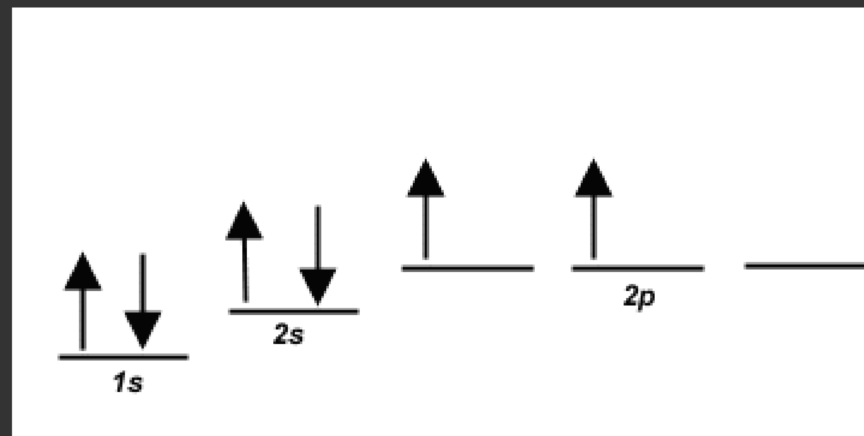
You should conclude that carbon only has <u>TWO</u> electrons available for bonding. That is not enough!



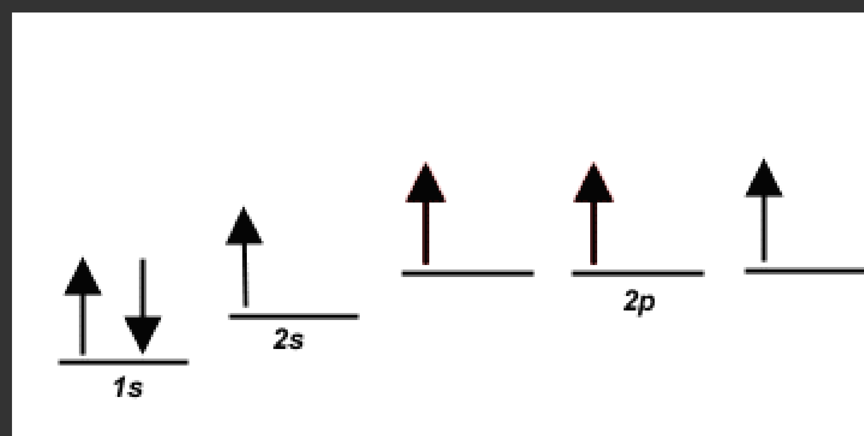
How does carbon overcome this problem so that it may form four bonds?

Carbon's Empty Orbital

The first thought that chemists had was that carbon promotes one of its *2s* electrons…

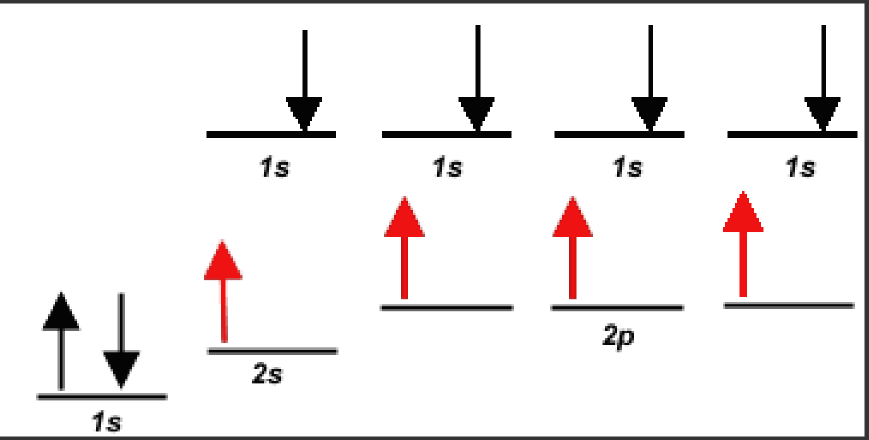


…to the empty *2p* orbital.



A Problem Arises…

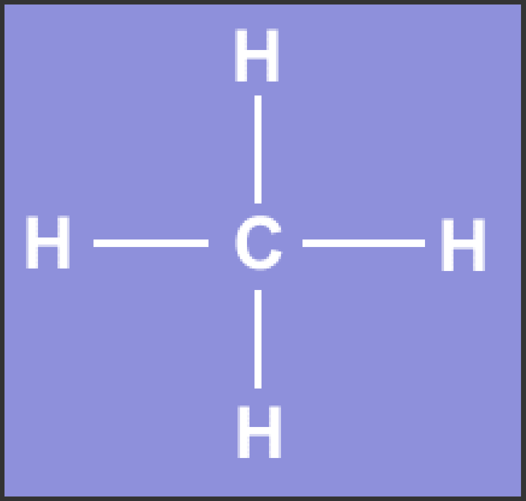
However, they quickly recognized a problem with such an arrangement…



Three of the carbon-hydrogen bonds would involve an electron pair in which the carbon electron was a *2p*, matched with the lone *1s* electron from a hydrogen atom.

Unequal bond energy

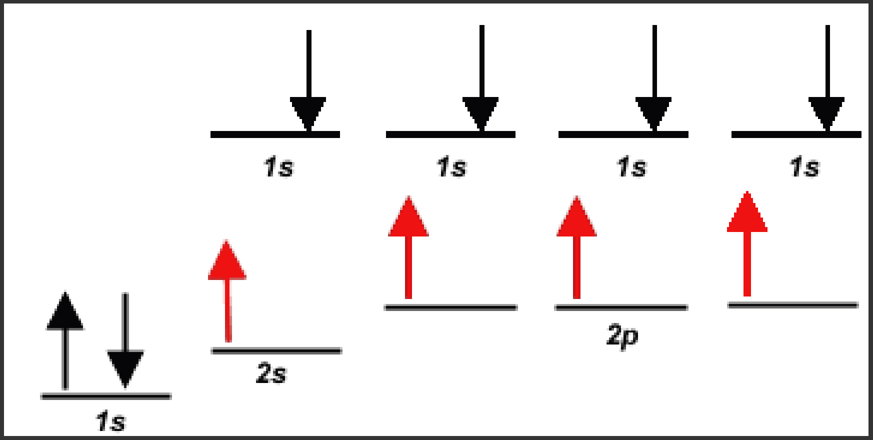
This would mean that three of the bonds in a methane molecule would be identical, because they would involve electron pairs of equal energy.



But what about the fourth bond…?

Unequal bond energy

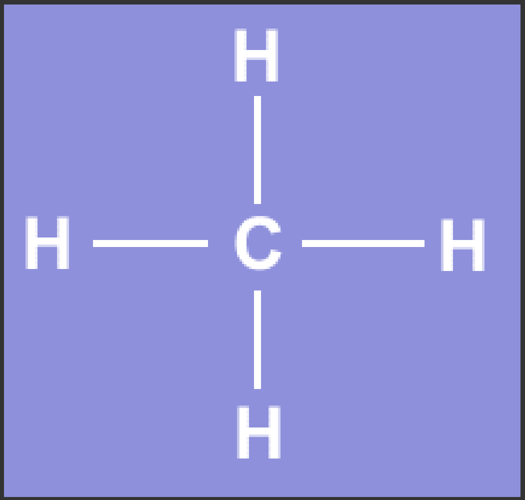
The fourth bond is between a *2s* electron from the carbon and the lone *1s* hydrogen electron.



Such a bond would have slightly less energy than the other bonds in a methane molecule.

Unequal bond energy

This bond would be slightly different in character than the other three bonds in methane.



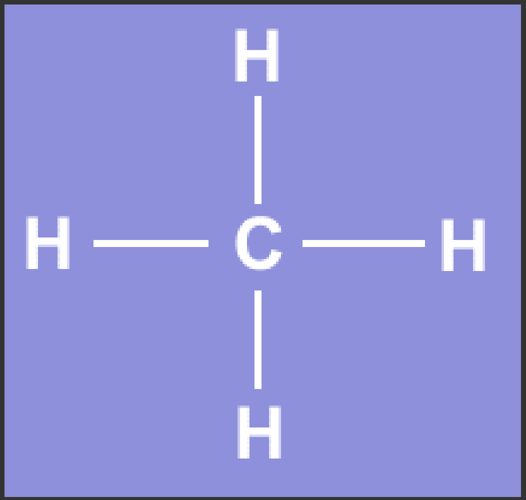
This difference would be measurable to a chemist by determining the bond length and bond energy.

<u>But is this what they observe?</u>

Enter Hybridization:

The simple answer is, "No".

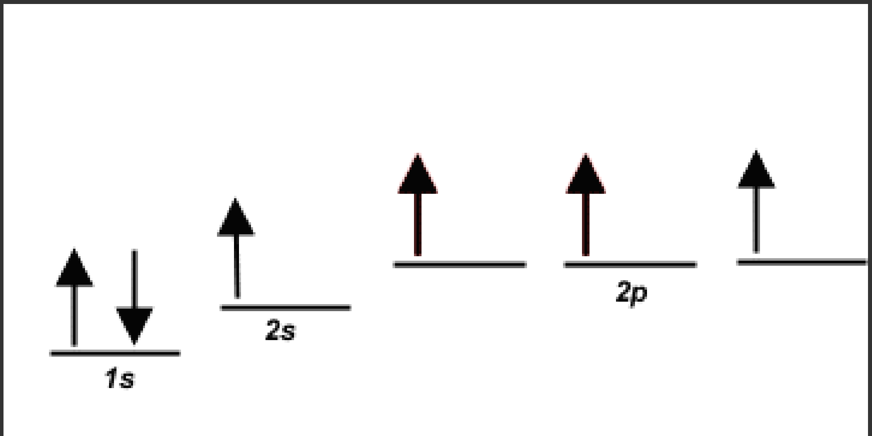
Measurements show that all four bonds in methane are equal. Thus, we need a new explanation for the bonding in methane.



Chemists have proposed an explanation – they call it Hybridization.

Hybridization is the combining of two or more orbitals of nearly equal energy within the same atom into orbitals of equal energy.

In the case of methane, they call the hybridization ***sp*³**, meaning that an *s* orbital is combined with three *p* orbitals to create four equal hybrid orbitals.



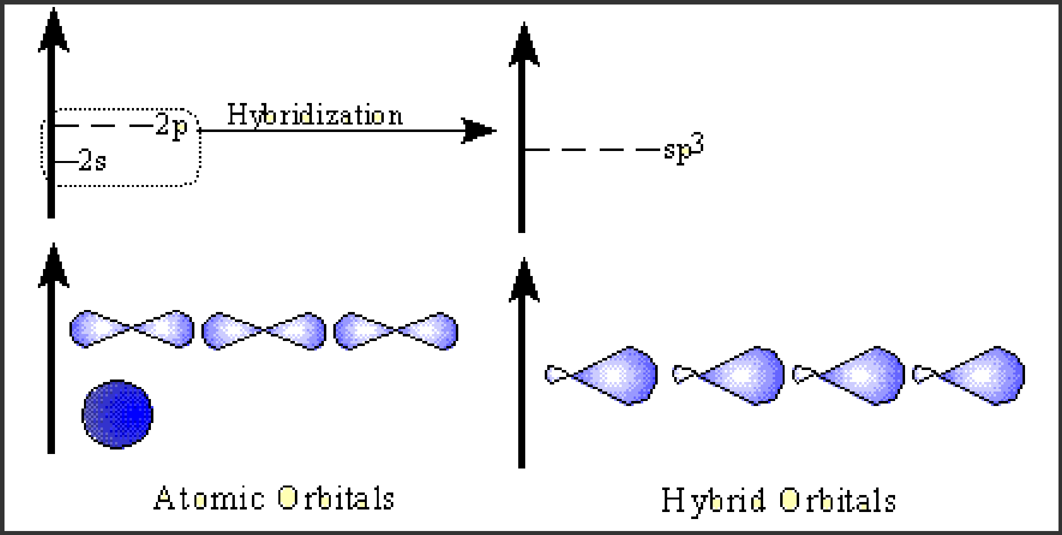
These new orbitals have slightly MORE energy than the *2s* orbital...

... and slightly LESS energy than the *2p* orbitals.

sp³ Hybrid Orbitals

sp^3 Hybrid Orbitals

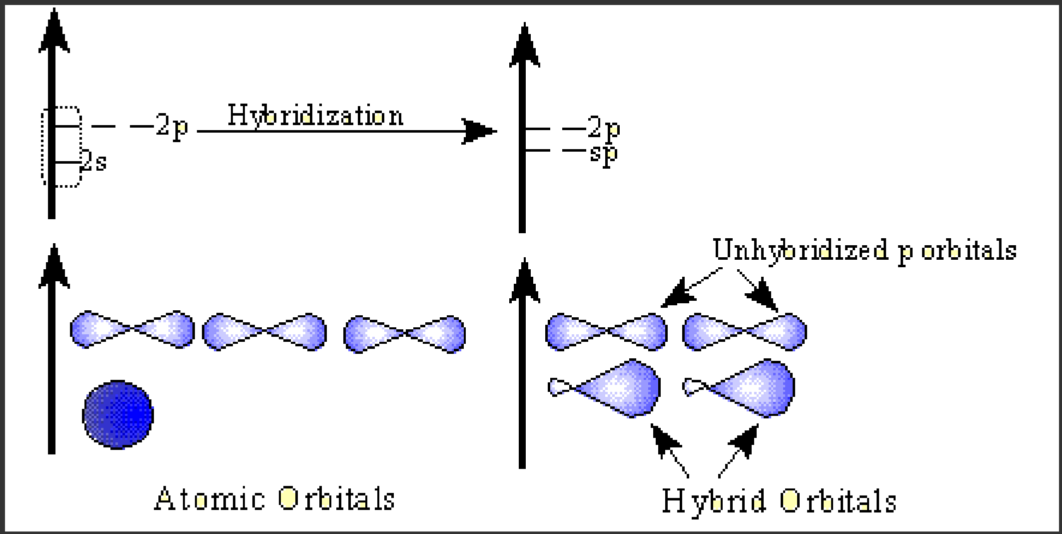
Here is another way to look at the sp^3 hybridization and energy profile…



sp Hybrid Orbitals

While sp^3 is the hybridization observed in methane, there are other types of hybridization that atoms undergo.

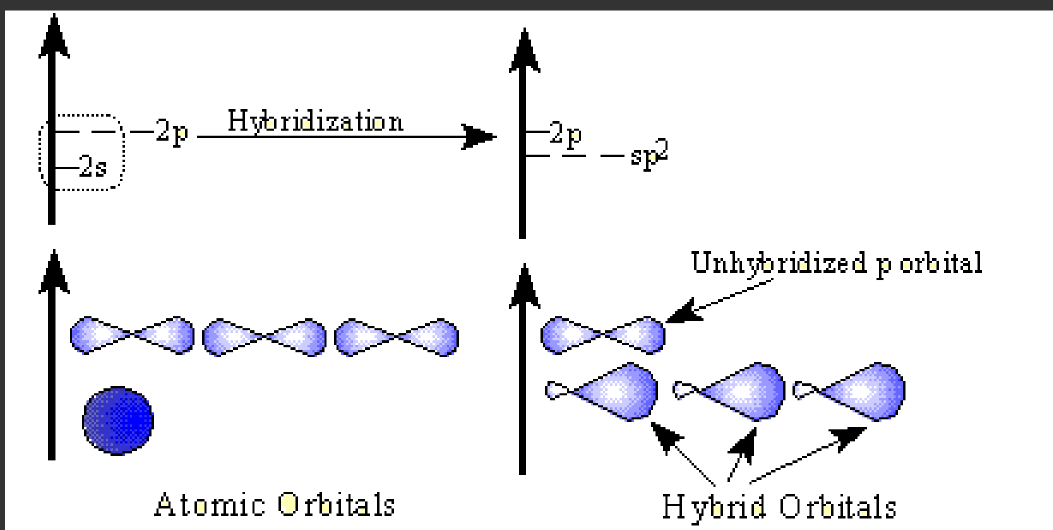
These include **sp hybridization**, in which one *s* orbital combines with a single *p* orbital.



This produces two hybrid orbitals, while leaving two normal *p* orbitals

sp^2 Hybrid Orbitals

Another hybrid is the sp^2, which combines two orbitals from a *p* sublevel with one orbital from an s sublevel.

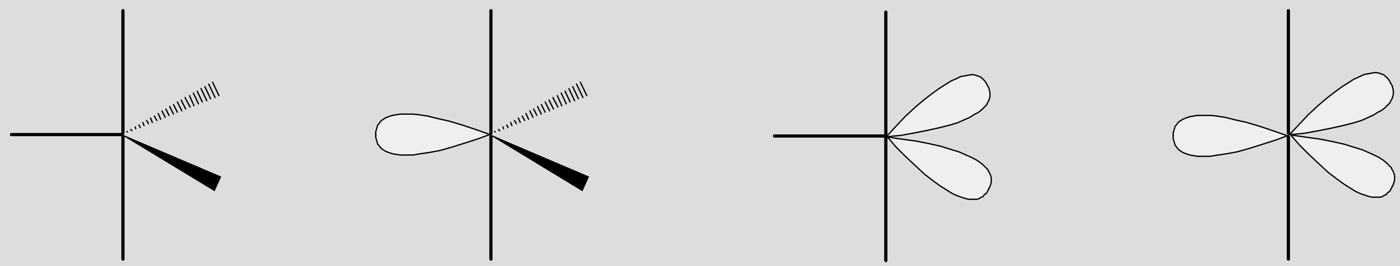


One *p* orbital remains unchanged.

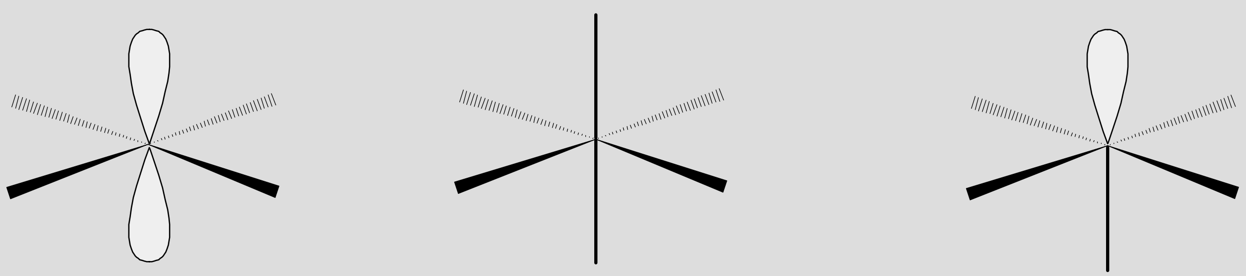
Hybridization Involving "*d*" Orbitals

Beginning with elements in the third row, "*d*" orbitals may also hybridize

dsp^3 = five hybrid orbitals of equal energy



d^2sp^3 = six hybrid orbitals of equal energy



Hybridization and Molecular Geometry

Forms	Overall Structure	Hybridization of "A"
AX_2	Linear	*sp*
AX_3, AX_2E	Trigonal Planar	sp^2
AX_4, AX_3E, AX_2E_2	Tetrahedral	sp^3
AX_5, AX_4E, AX_3E_2, AX_2E_3	Trigonal bipyramidal	dsp^3
AX_6, AX_5E, AX_4E_2	Octahedral	d^2sp^3

A = central atom

X = atoms bonded to A

E = nonbonding electron pairs on A

Sigma and Pi Bonds

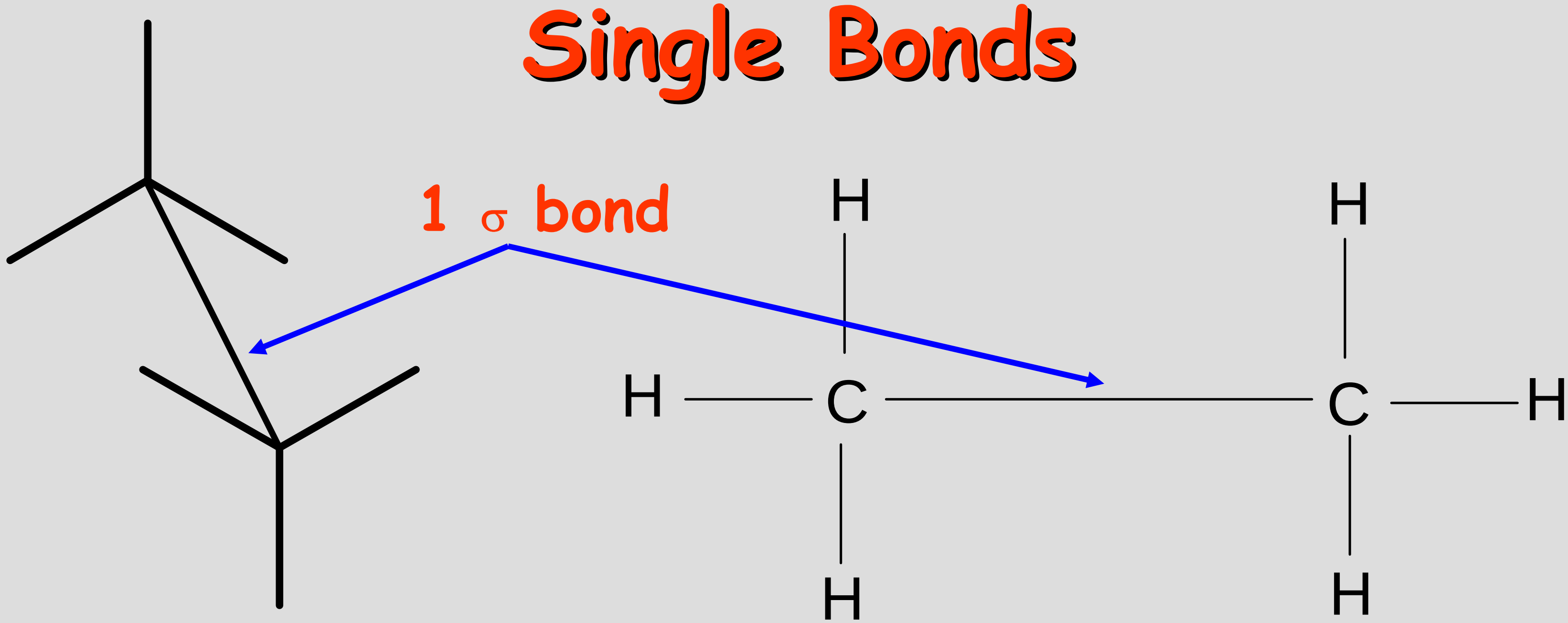
Sigma (σ) bonds exist in the region directly between two bonded atoms.

Pi (π) bonds exist in the region above and below a line drawn between two bonded atoms.

Single bond	1 sigma bond
Double Bond	1 sigma, 1 pi bond
Triple Bond	1 sigma, 2 pi bonds

Sigma and Pi Bonds

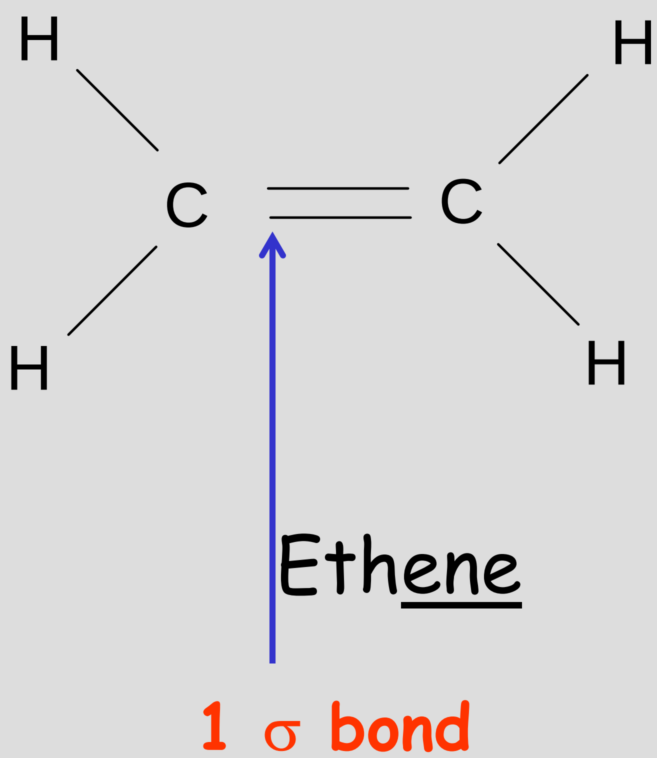
Single Bonds

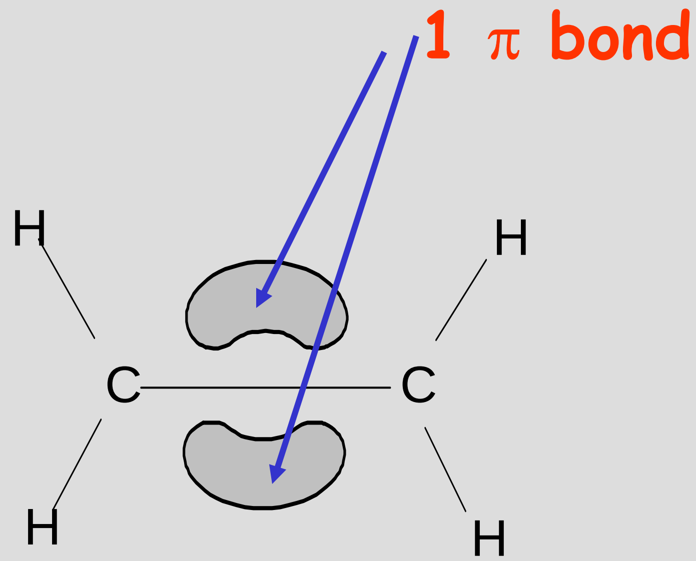


Ethane

Sigma and Pi Bonds:

Double bonds

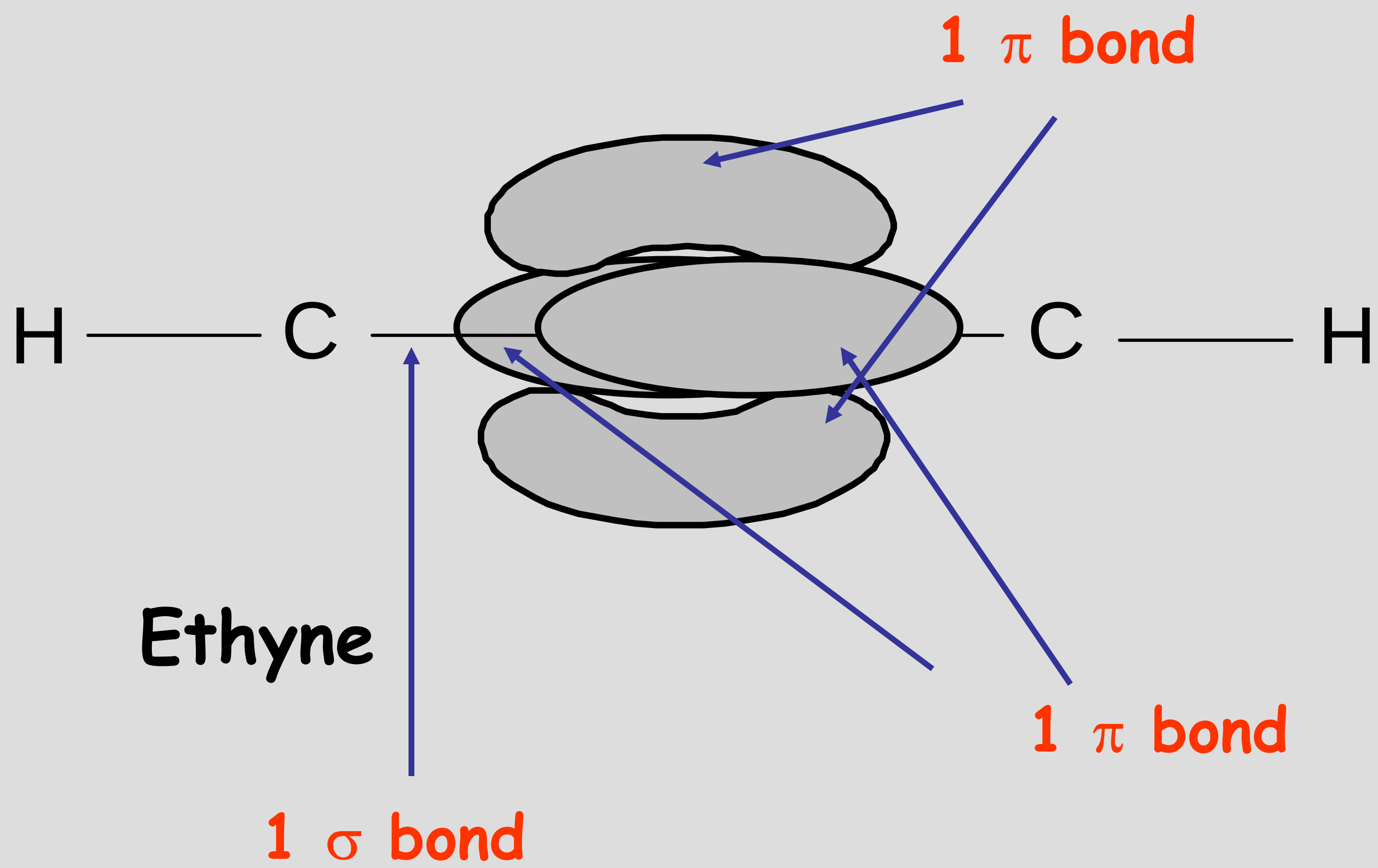




Sigma and Pi Bonds

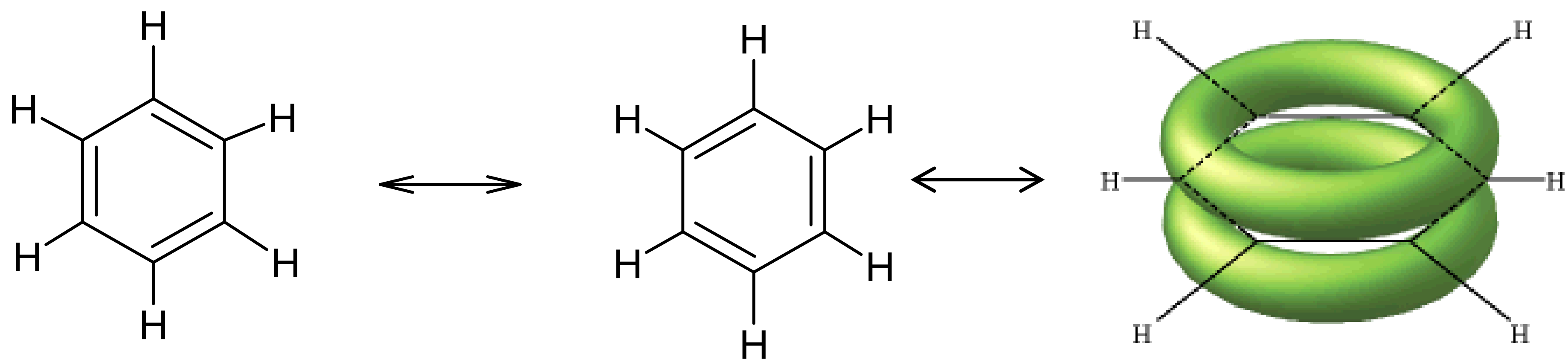
Triple Bonds

$H - C \equiv C - H$



The De-Localized Electron Model

Pi bonds (π) contribute to the delocalized model of electrons in bonding, and help explain resonance



Electron density from π bonds can be distributed symmetrically all around the ring, above and below the plane.