Hybridization

- **When placing the electrons in shells, the lower energy orbitals are filled first before the higher energy orbitals are filled – recall Aufbau's principle**

- **Since the *s* orbital is of a lower energy level than the *p* orbital, it gets filled first**

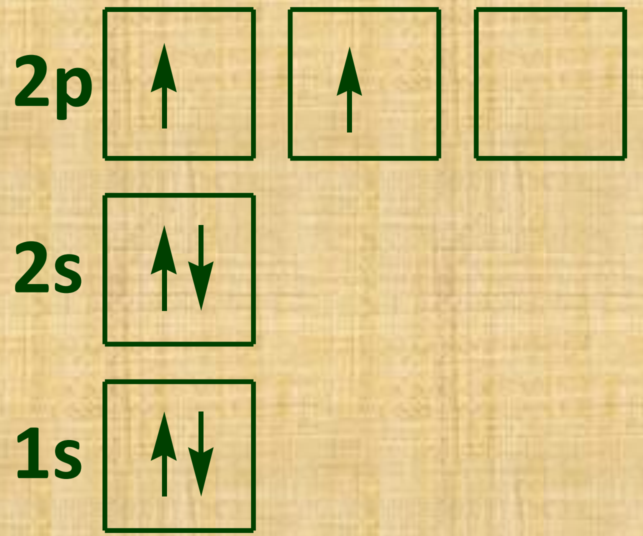
- **In carbon, this means that the *s* orbital in the second shell is filled first with 2 electrons and then the remaining 2 electrons are placed in the *p* orbitals – (remember there are three *p* orbitals)**

Hybridization

- **Carbon, therefore, has an electronic configuration of *1*s^2, *2*s^2, *2*p^2 and is said to be at the ground state**
- **Study this configuration and make sure you understand what it means**
- **The italicized number in front of the orbitals represents the energy levels so 2 being the highest level tells us that this particular element is in Period 2 of the Periodic Table**

Hybridization

- Carbon at ground state is therefore represented as follows:



Hybridization

- **When carbon is in this form, it is incapable of forming four covalent bonds (as seen in CH_4, CH_3Br, etc) because there are only 2 singly occupied orbitals**

- **If carbon was allowed to form covalent bonds in this form, it will only form two bonds**

- **So how come carbon forms four covalent bonds?**

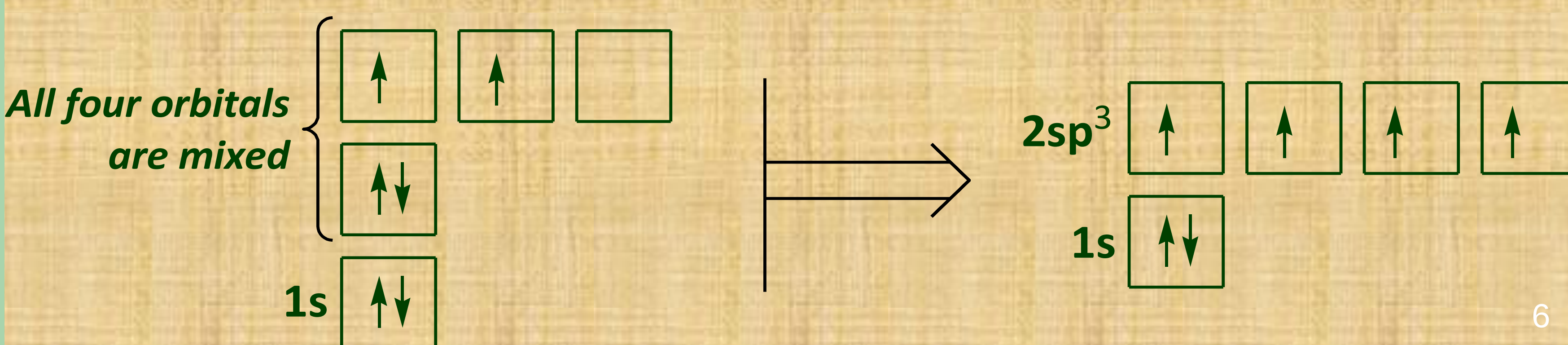
- **The answer to this question lies in what is called *hybridization***

Hybridization

- **What is *hybridization*?**
- **Hybridization is simply the mixing of the orbitals to form degenerate orbitals to satisfy the bonding needs**
- **So depending on the type of bond that is being formed, the valence shell electrons (i.e. the 2*s* and 2*p* orbitals) mix to form types of hybrid orbitals**
- **The three different types of hybrid orbitals that are formed are sp^1, sp^2, and sp^3 orbitals**

sp^3 Hybridization

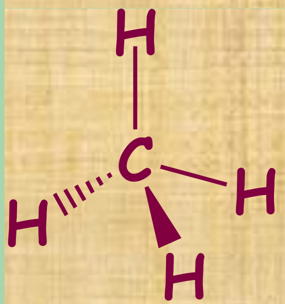
- **If the carbon is going to form 4 single bonds, then all valence shell orbitals will mix to form four degenerate hybrid orbitals**
- **The hybridization occurring here is known as sp^3 hybridization in which the 2*s* orbital mixes with the three 2*p* orbitals to form four sp^3 hybrid orbitals which all have the same energy**



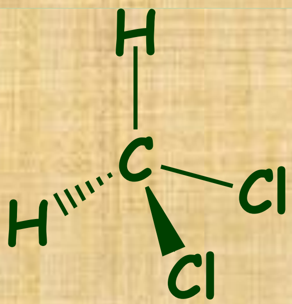
sp^3 Hybridization

- It can now be seen that there are now four orbitals that are singly occupied by an electron – i.e. 4 electrons in the level 2 energy

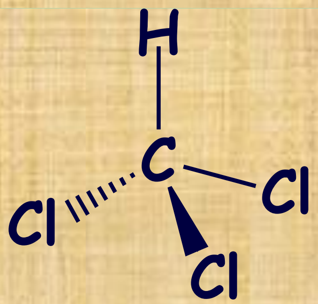
- This now allows for carbon to form four single bonds which will all be sigma bonds and the geometry around the carbon atom will be tetrahedral (bond angle 109°28')



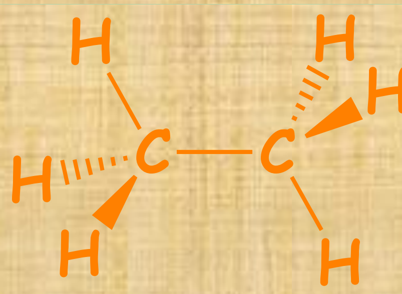
methane



dichloromethane



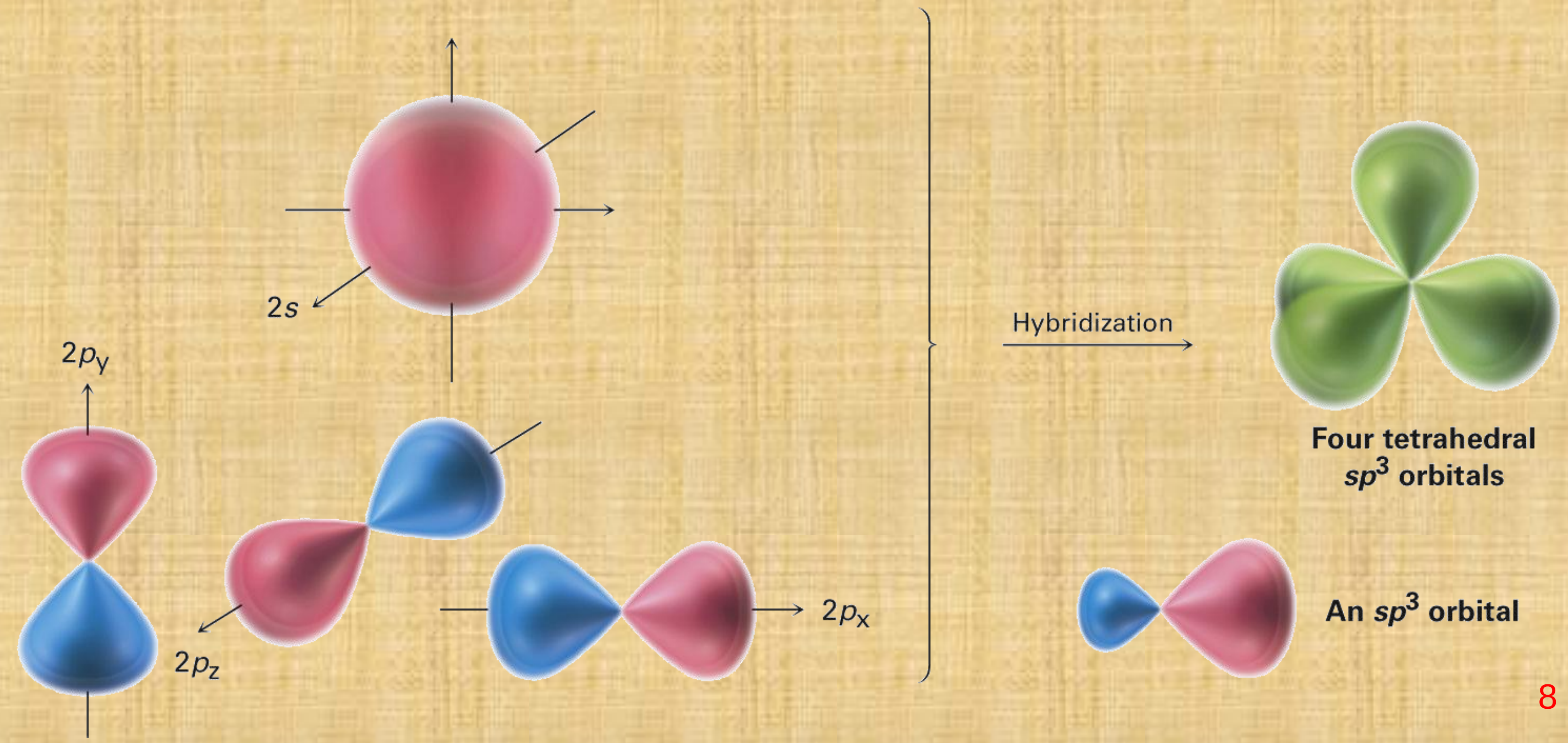
chloroform



ethane

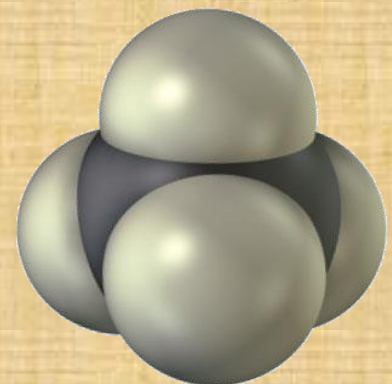
sp^3 Hybridization

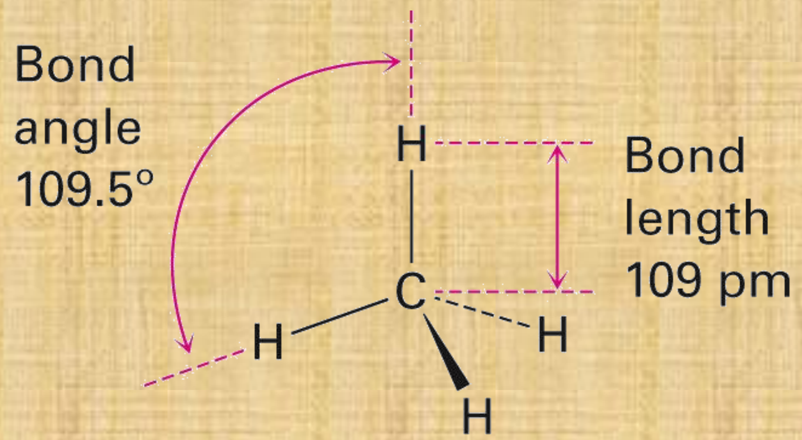
- ☞ **Figure below shows four (sp^3 = sppp), Pauling (1931) hybrid orbitals, oriented to the corners of a regular tetrahedron, *s* orbital (red) and three *p* orbitals (red/blue)**
- ☞ **The sp^3 orbitals have two lobes and are unsymmetrical about the nucleus, giving a directionality and allowing them to form strong bonds when they overlap an orbital from another atom**

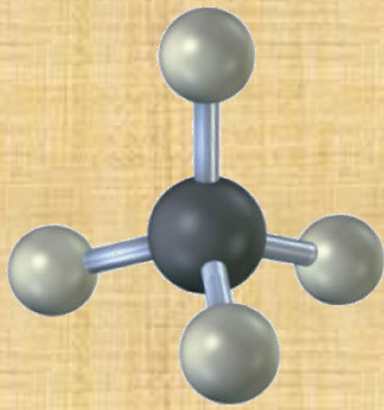


sp^3 Hybridization in the case of Methane

- The sp^3 orbitals on C atom overlap with 1*s* orbitals on 4 H atoms to form four identical C-H bonds
- Each C–H bond has a strength of (439) kJ/mol and a length of 109 pm
- Bond angle: each H–C–H is 109.5°, (*tetrahedral angle)*

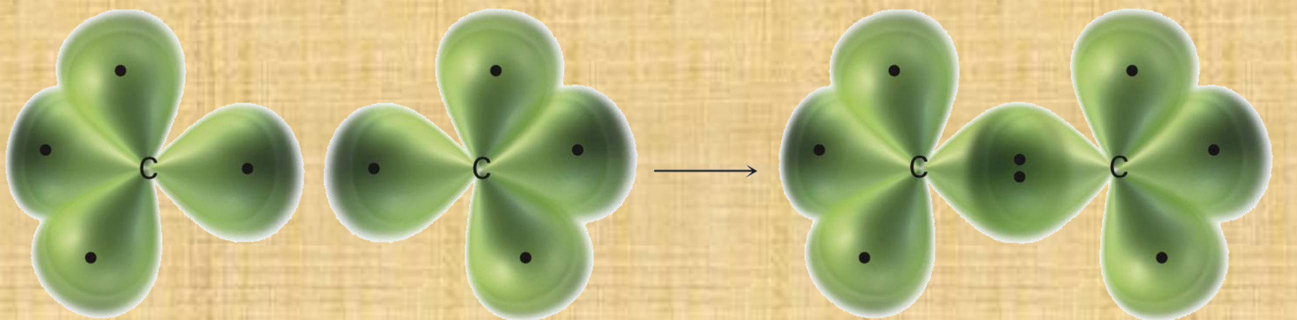




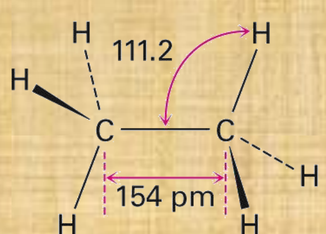


sp^3 Hybridization in the case of Ethane

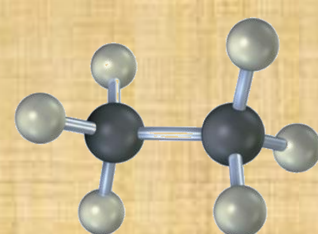
- Two C's bond to each other by σ overlap of an sp^3 orbital
- Three sp^3 orbitals on each C overlap with H 1*s* orbitals to form six C–H bonds; C–H bond strength in ethane 421 kJ/mol
- C–C bond is 154 pm long and strength is 377 kJ/mol
- All bond angles of ethane are also tetrahedral

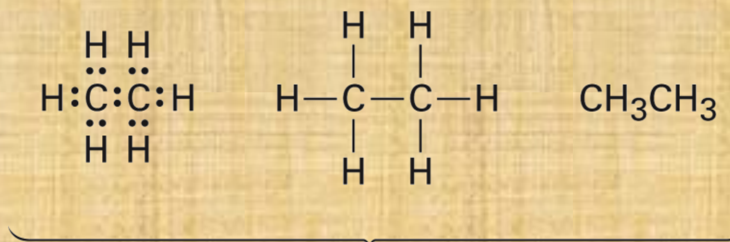


sp^3 carbon | *sp*^{3} carbon | *sp*^{3}–*sp*^{3} σ bond



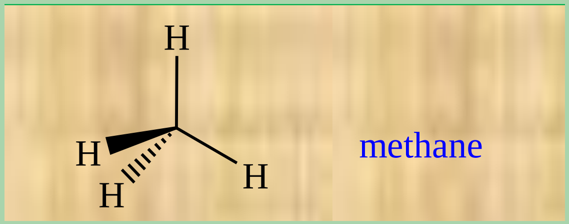
Ethane

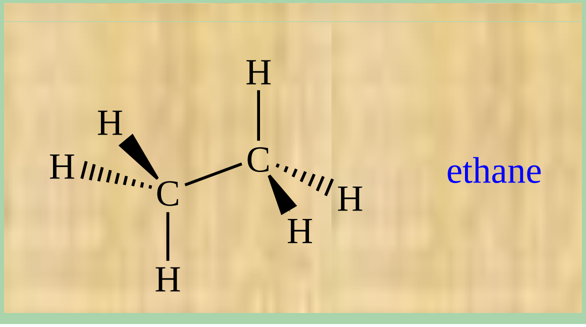


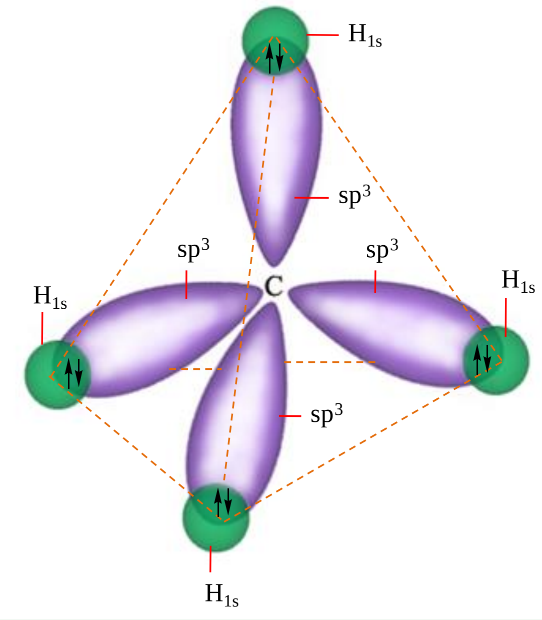


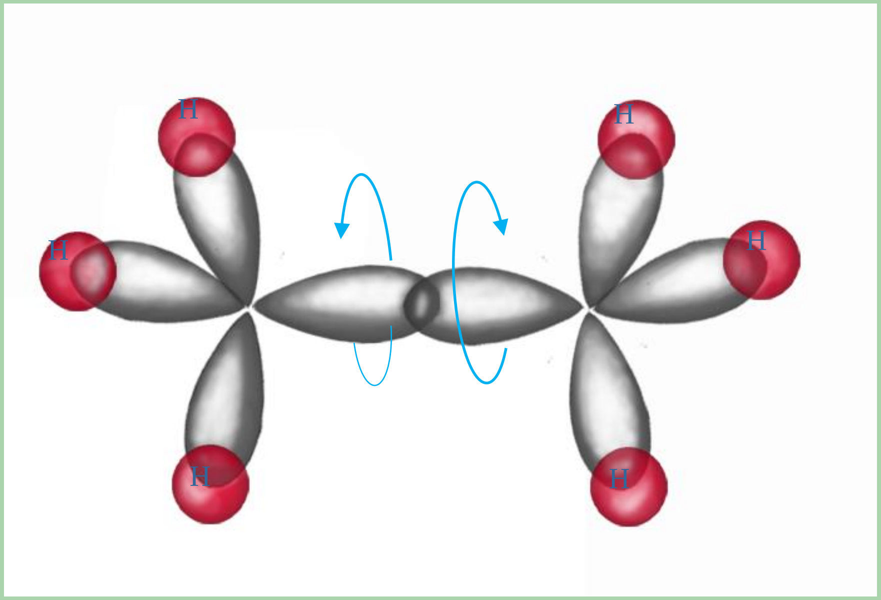
Some representations of ethane

sp^3 Hybridization





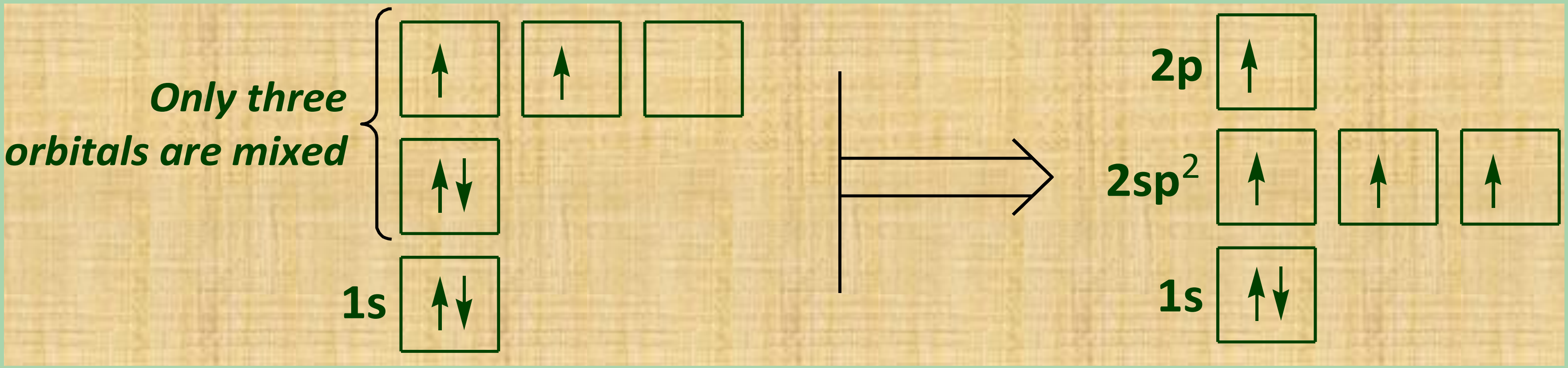




sp^2 Hybridization

- **The carbon can also form 2 single bonds and 1 double bond**
- **This can come about when the 2s orbital mixes with only two of the three 2p orbitals resulting in the formation of three (spp = sp^2) hybridized orbitals**
- **The other 2p orbital remains unaffected and the hybridization that occurs, as a result, is known as sp^2 hybridization**

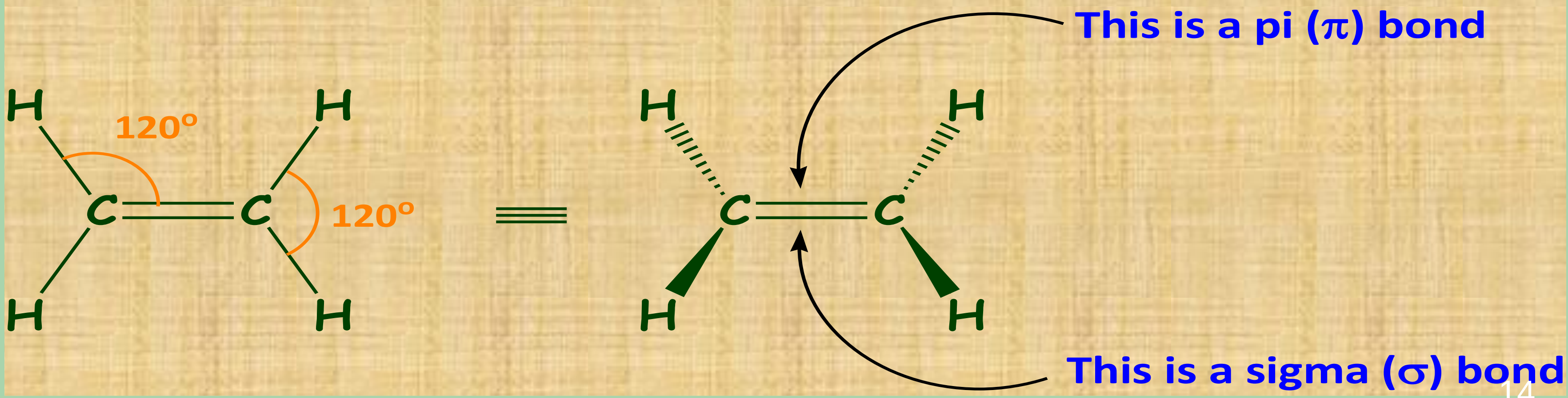
sp^2 Hybridization



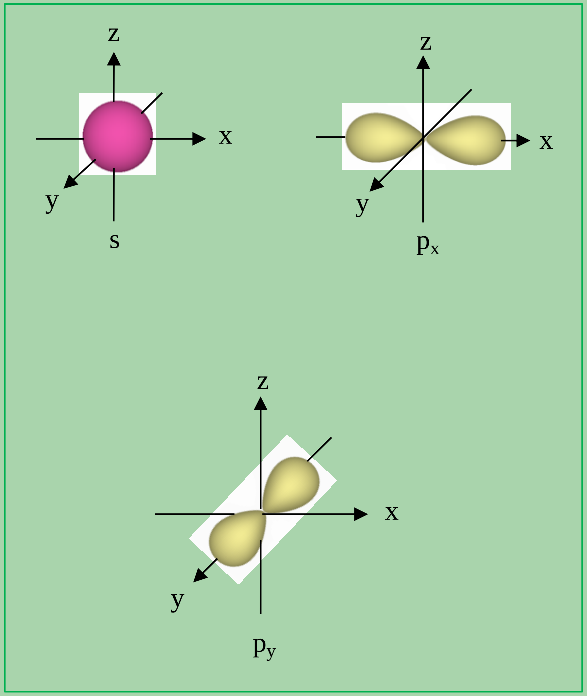
- **Here the *sp*^{2} hybridized carbon atom will form three sigma (σ) bonds and one pi (π) bond**
- **The molecular geometry observed here is that of a *trigonal planar***
- **The bond angle between the atoms is 120^o**

sp^2 Hybridization

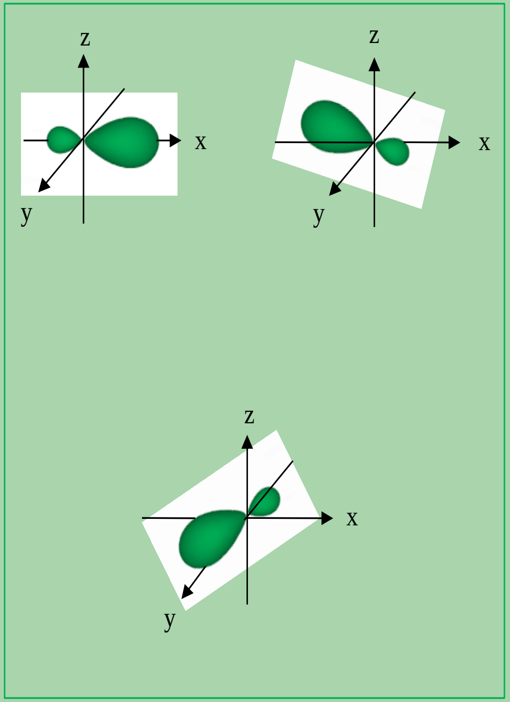
- All the sp^2 hybridized orbitals will form three sigma (σ) bonds while the unaffected *p* orbital will overlap sideways with another unaffected *p* orbital to form a pi (π) bond
- The double bond therefore is made up of a sigma bond and a pi bond

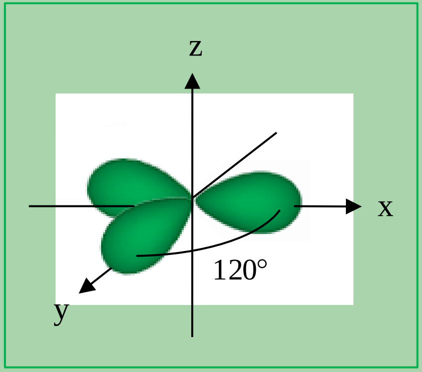


sp^2 Hybridization

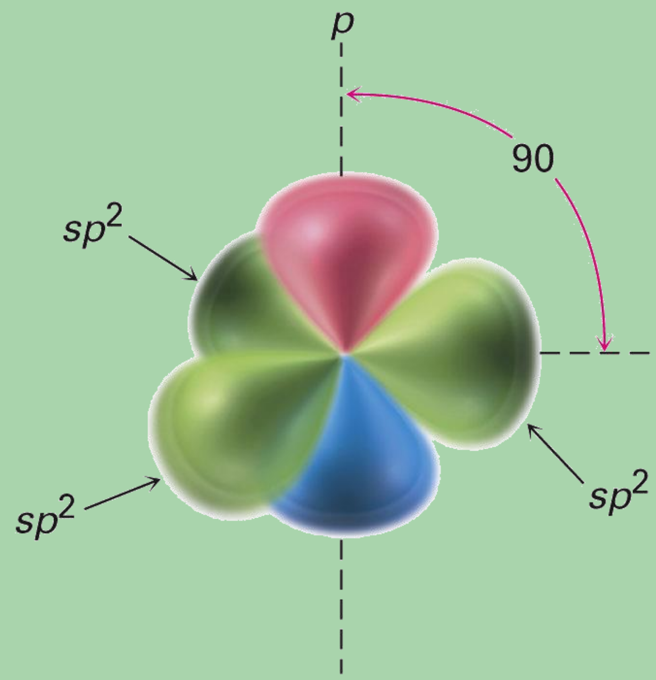


Hybridization

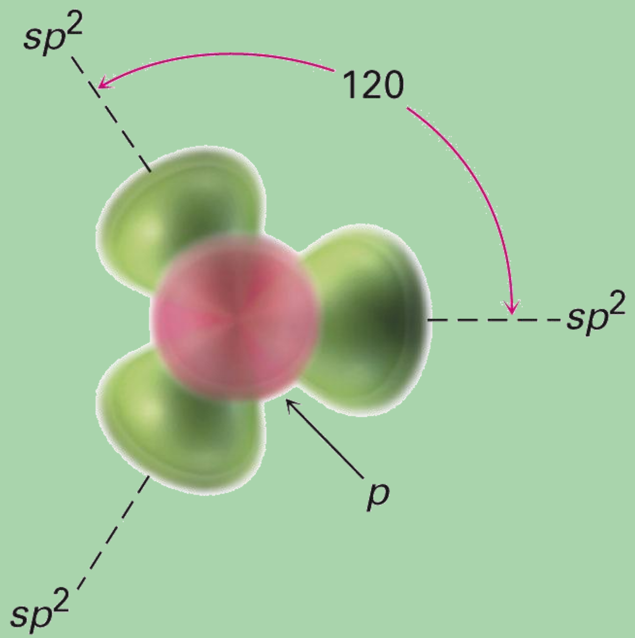




sp^2 Hybridization

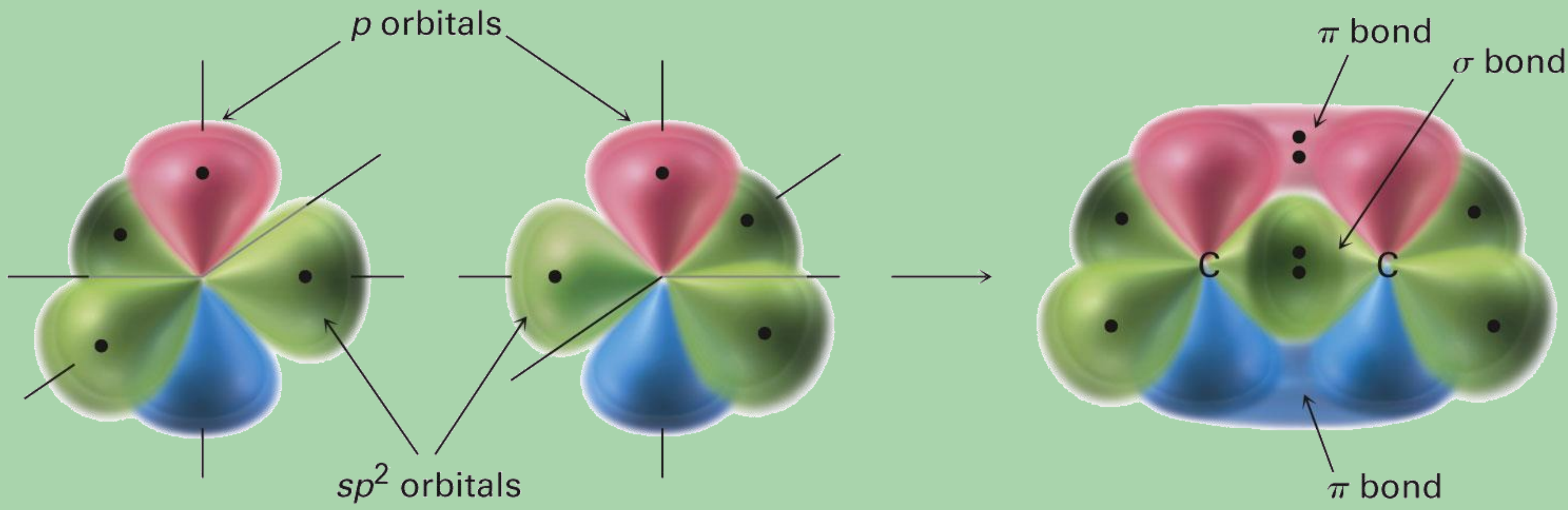


Side view

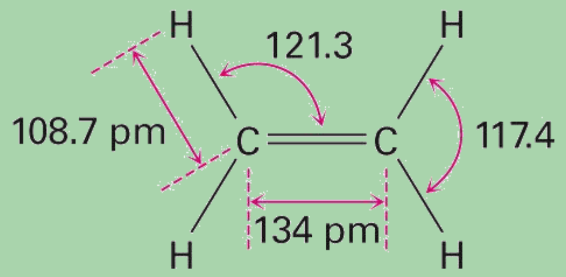


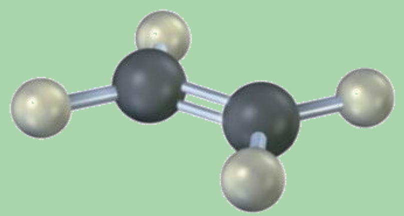
Top view

sp^2 Hybridization

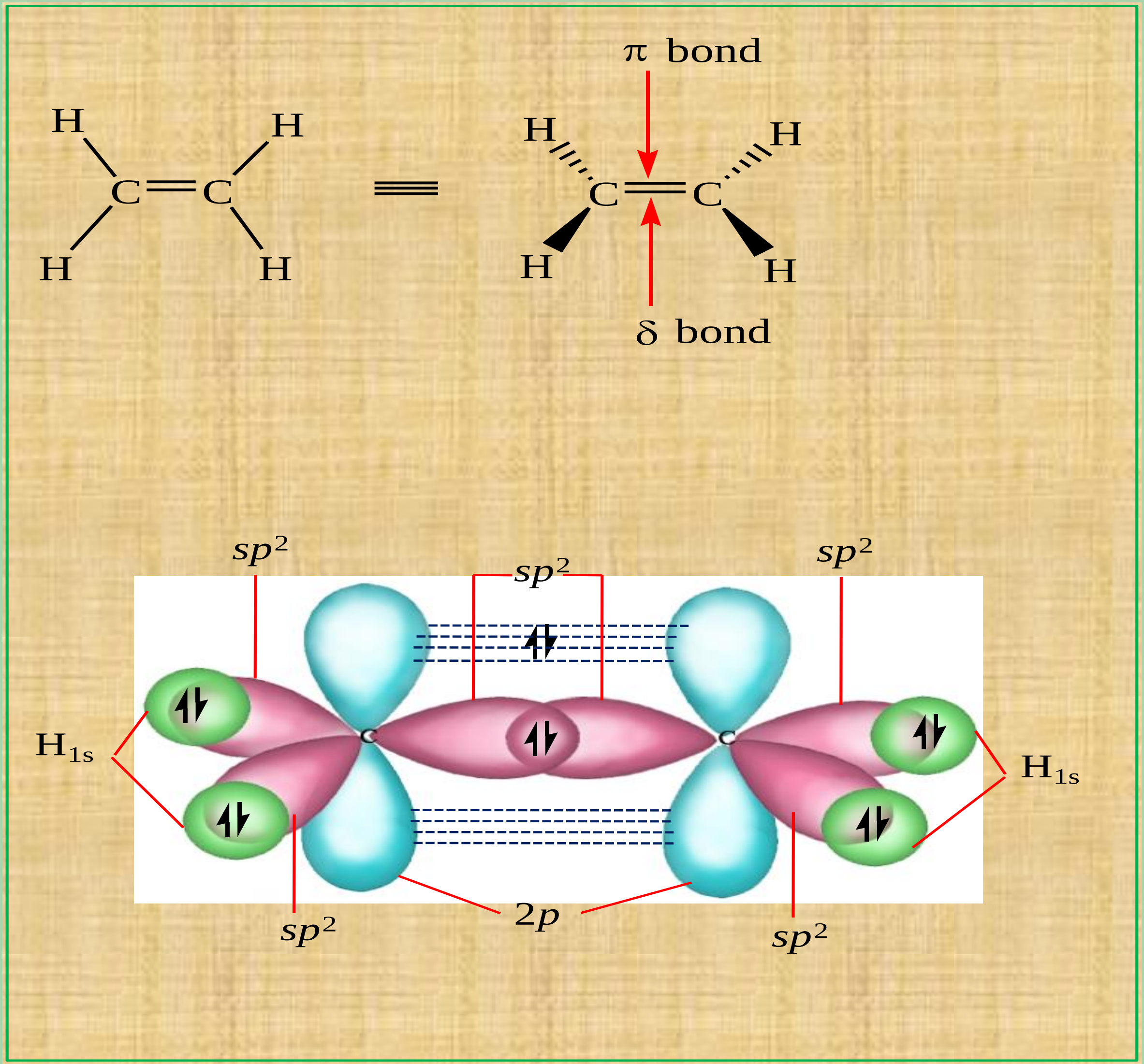


***sp*² carbon**   ***sp*² carbon**   **Carbon–carbon double bond**





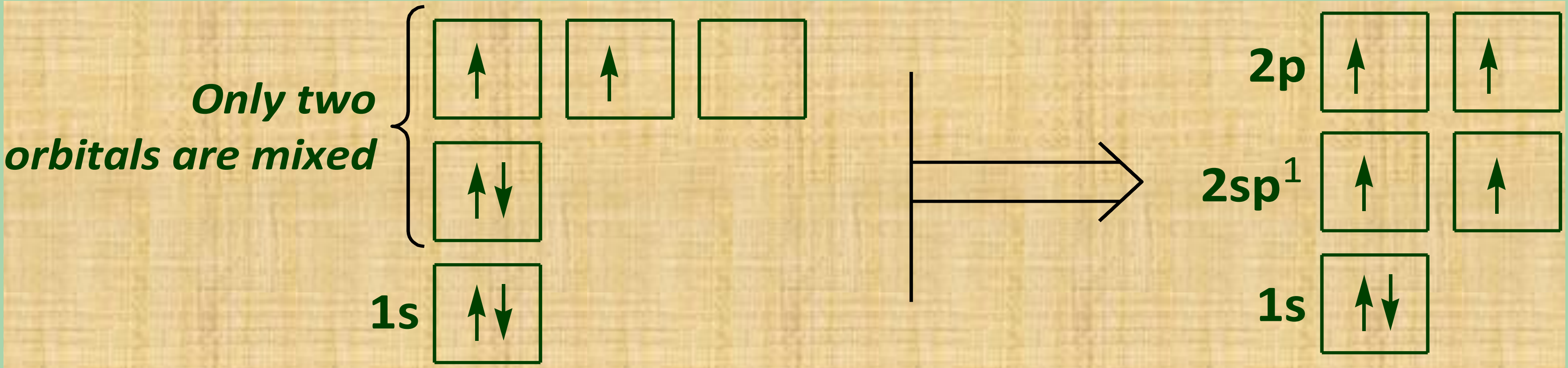
sp² Hybridization



sp^1 Hybridization

- The carbon can also form a triple bond and a single bond
- This can come about when the 2s orbital mixes with only one of the three 2p orbitals resulting in the formation of two (sp = *sp^1*) hybridized orbitals
- The other two 2p orbital remains unaffected and the hybridization that occurs as a result is know as sp^1 hybridization

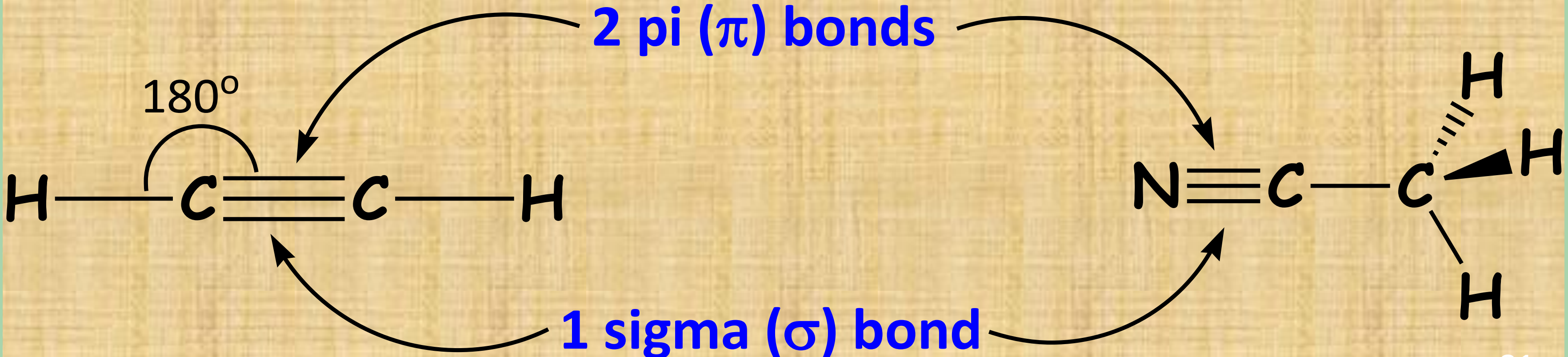
sp^1 Hybridization



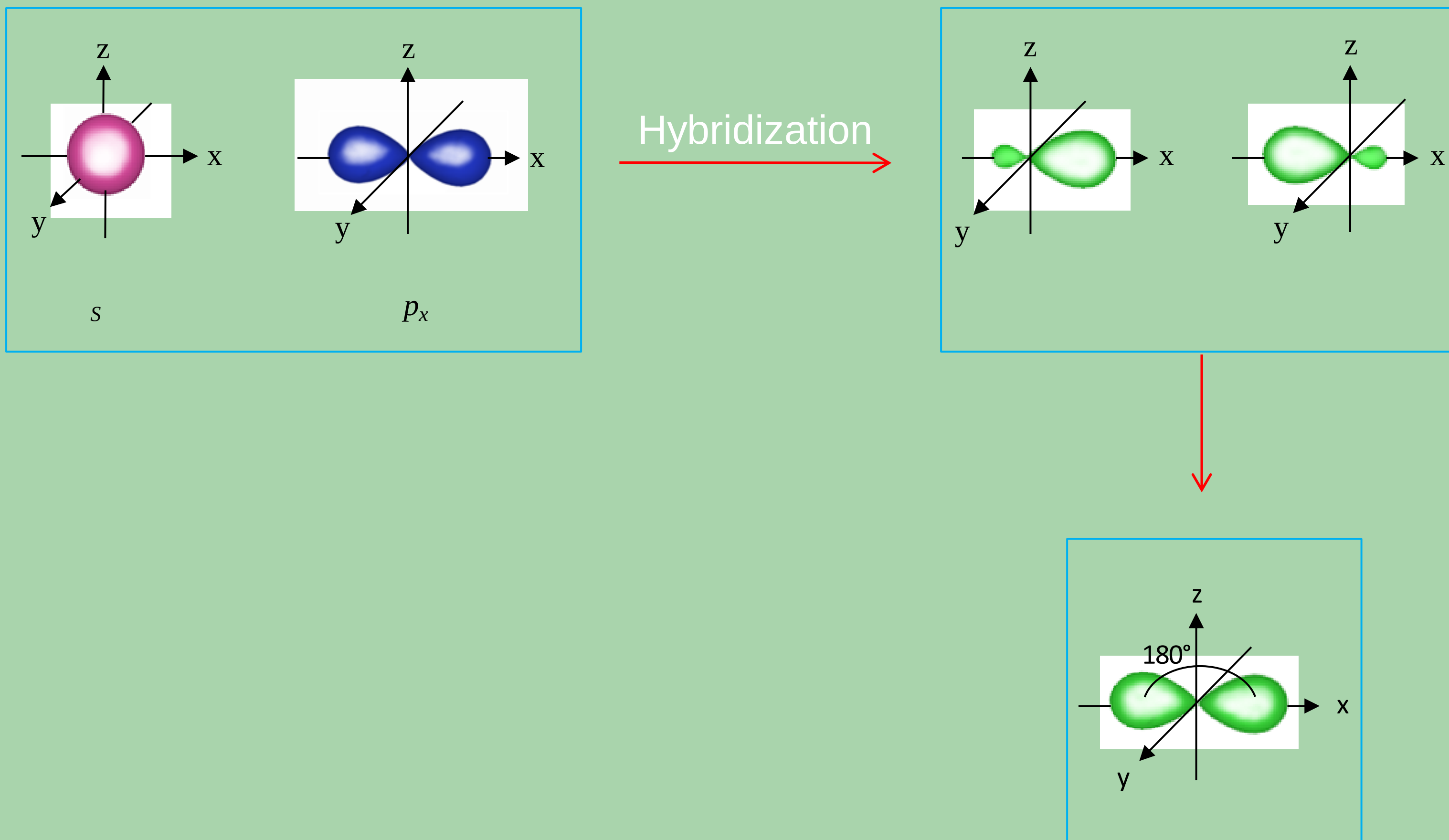
- Here the sp^1 hybridized carbon atom will form two sigma (σ) bonds and two pi (π) bonds
- The molecular geometry observed here is that of a *linear structure*
- The bond angle between the atoms is 180^o

sp^1 Hybridization

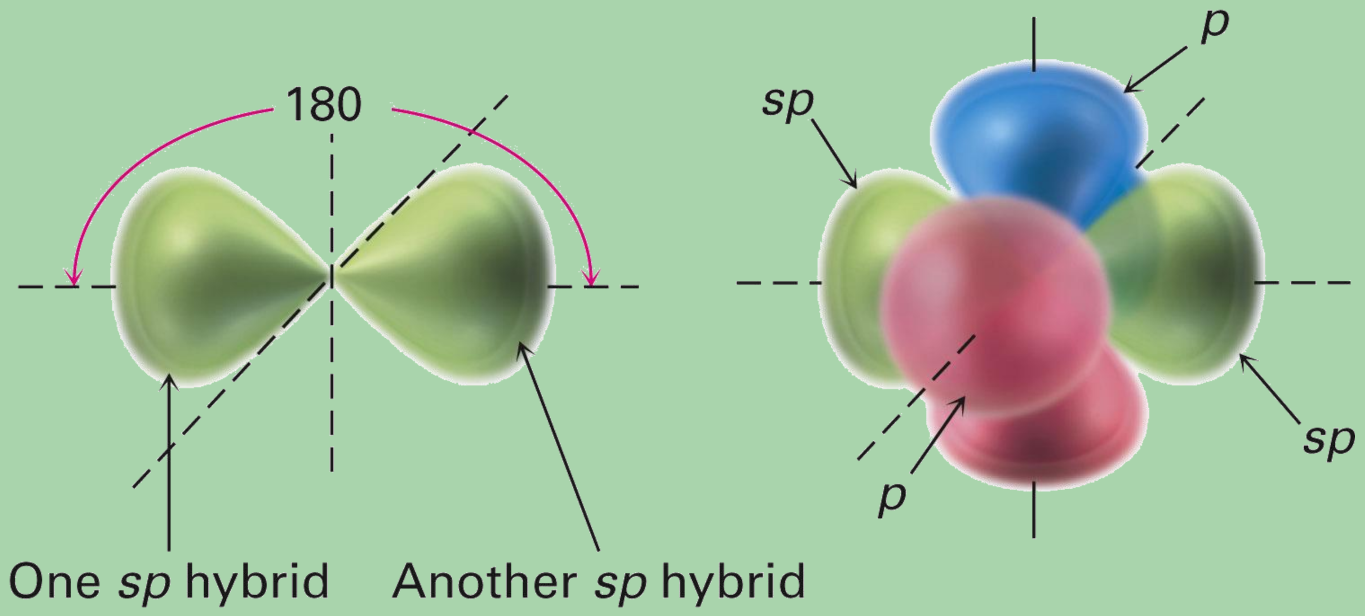
- The sp^1 hybridized carbon atom will form 2 sigma (σ) bonds while the two unaffected *p* orbitals will overlap sideways with two other unaffected *p* orbitals to form two pi (π) bonds
- This results in the formation of a single bond and a triple bond



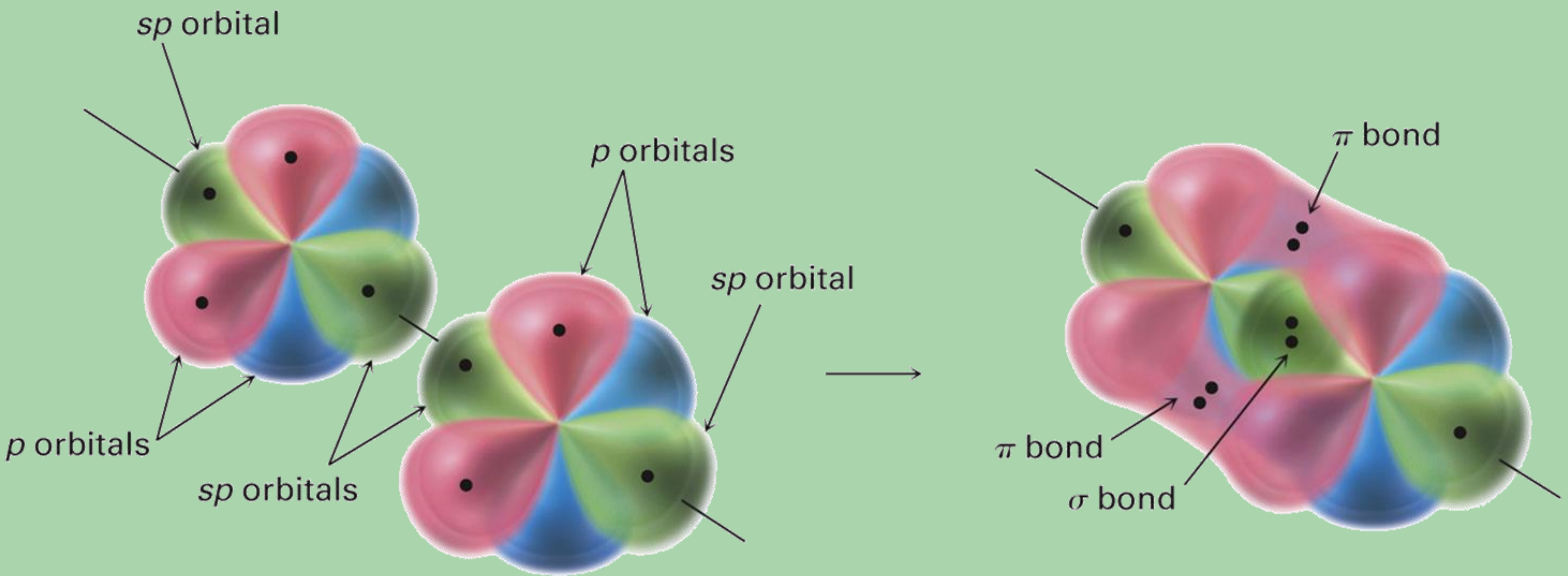
sp¹ Hybridization



sp^1 Hybridization

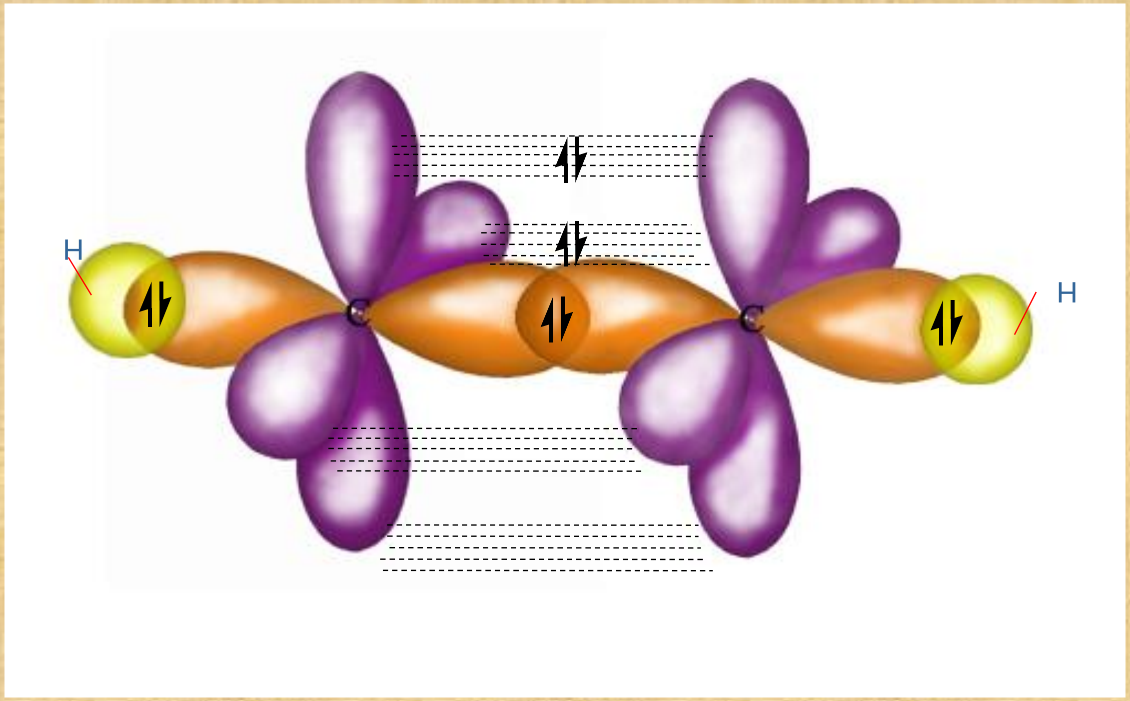


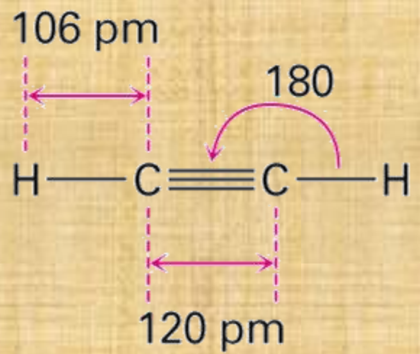
sp^1 Hybridization

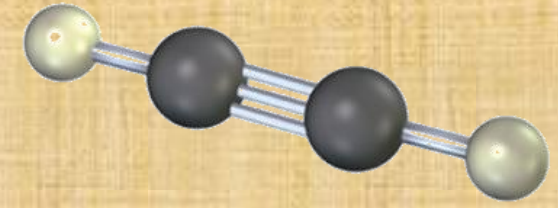


Carbon–carbon triple bond

sp¹ Hybridization



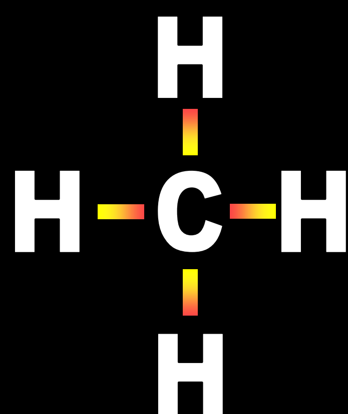


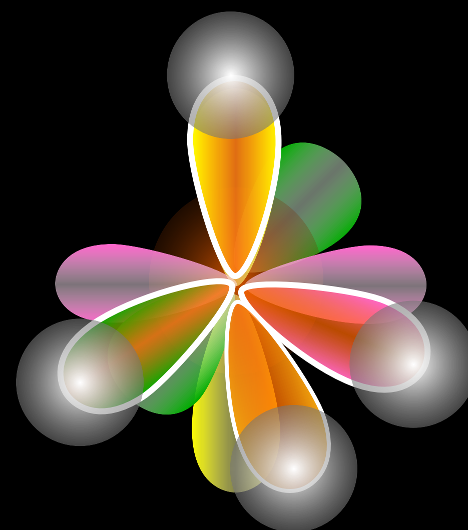


Organic compounds

- **All the bonds that are contained in organic compounds that you will encounter have one of these three hybridizations in them**
- **When all the bonds in a compound are single bonds (sigma bonds), then that compound is said to be saturated**
- **When they contain a double bond or a triple bond, then the compound is said to be unsaturated**

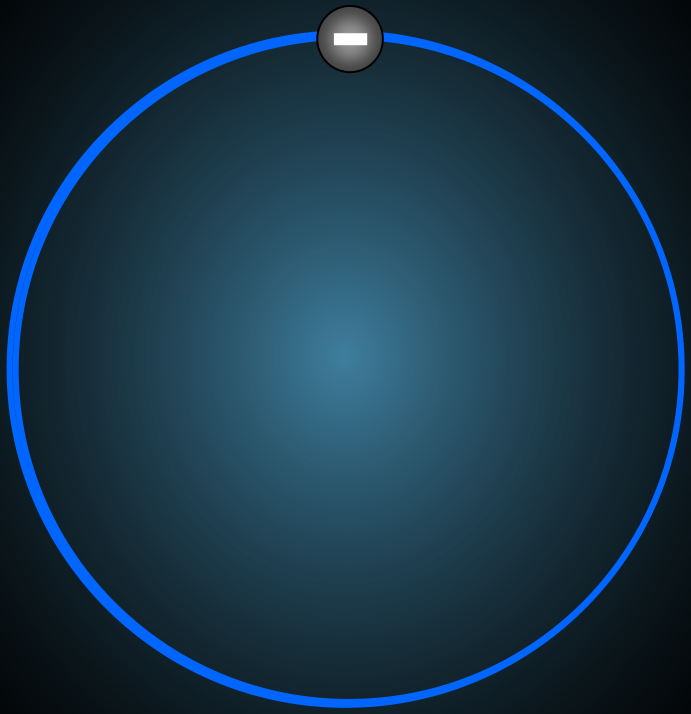
UNDERSTANDING MOLECULAR GEOMETRIES PREDICTED BY VSEPR



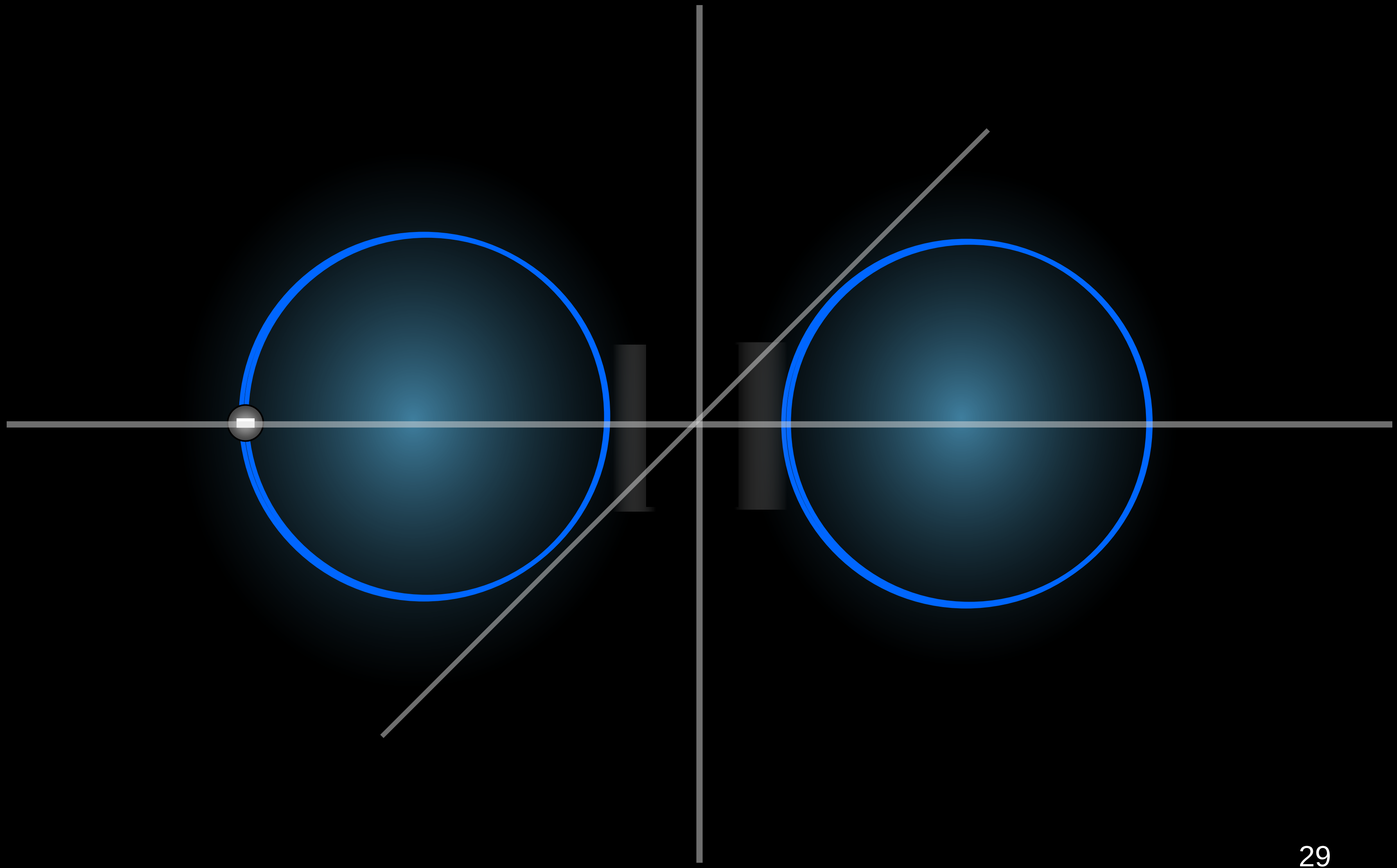


FROM THE PERSPECTIVE OF HYBRIDIZATION OF ATOMIC ORBITALS

Electron: Both wave and particle

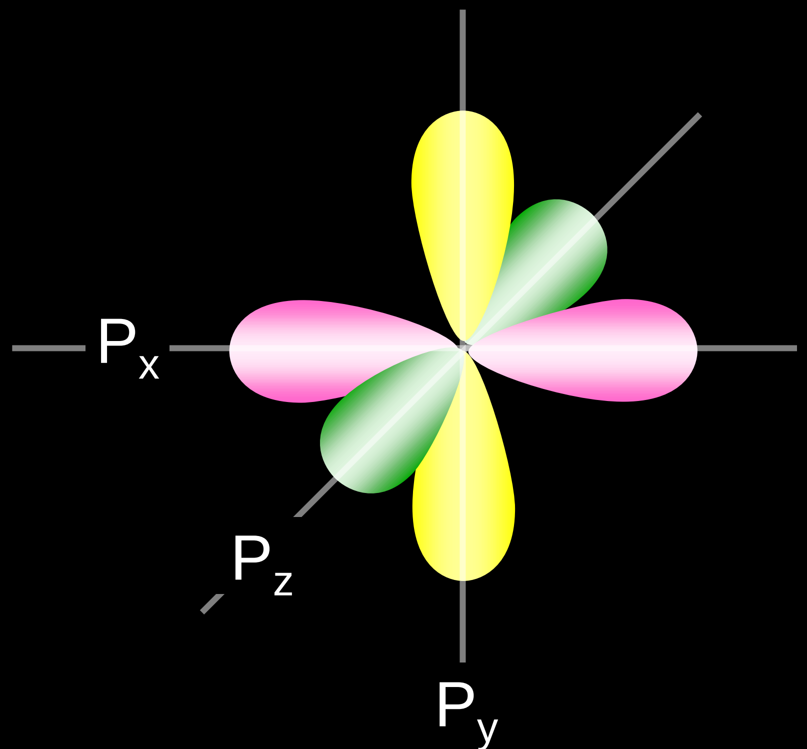


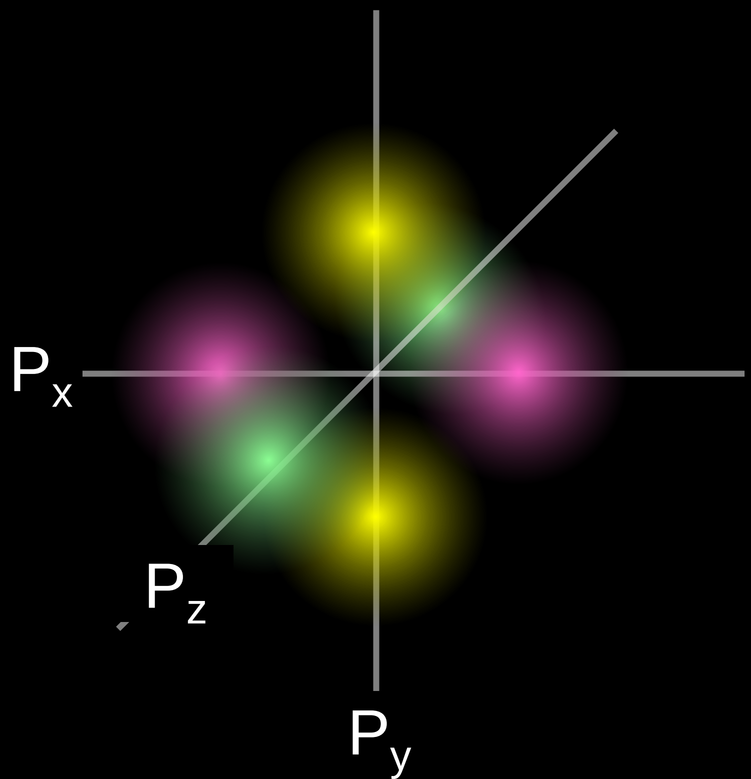
Electron: Both wave and particle



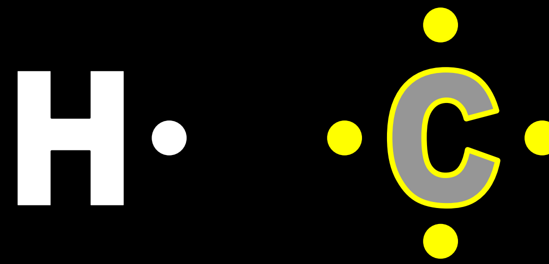
s, p, & d Orbitals

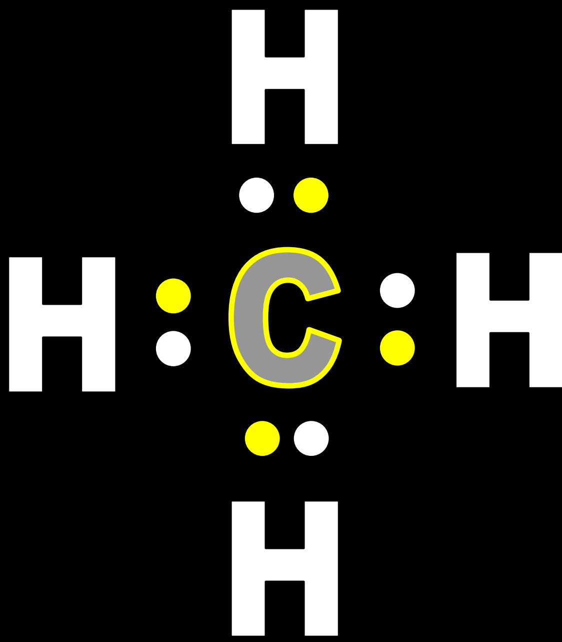
p Orbitals



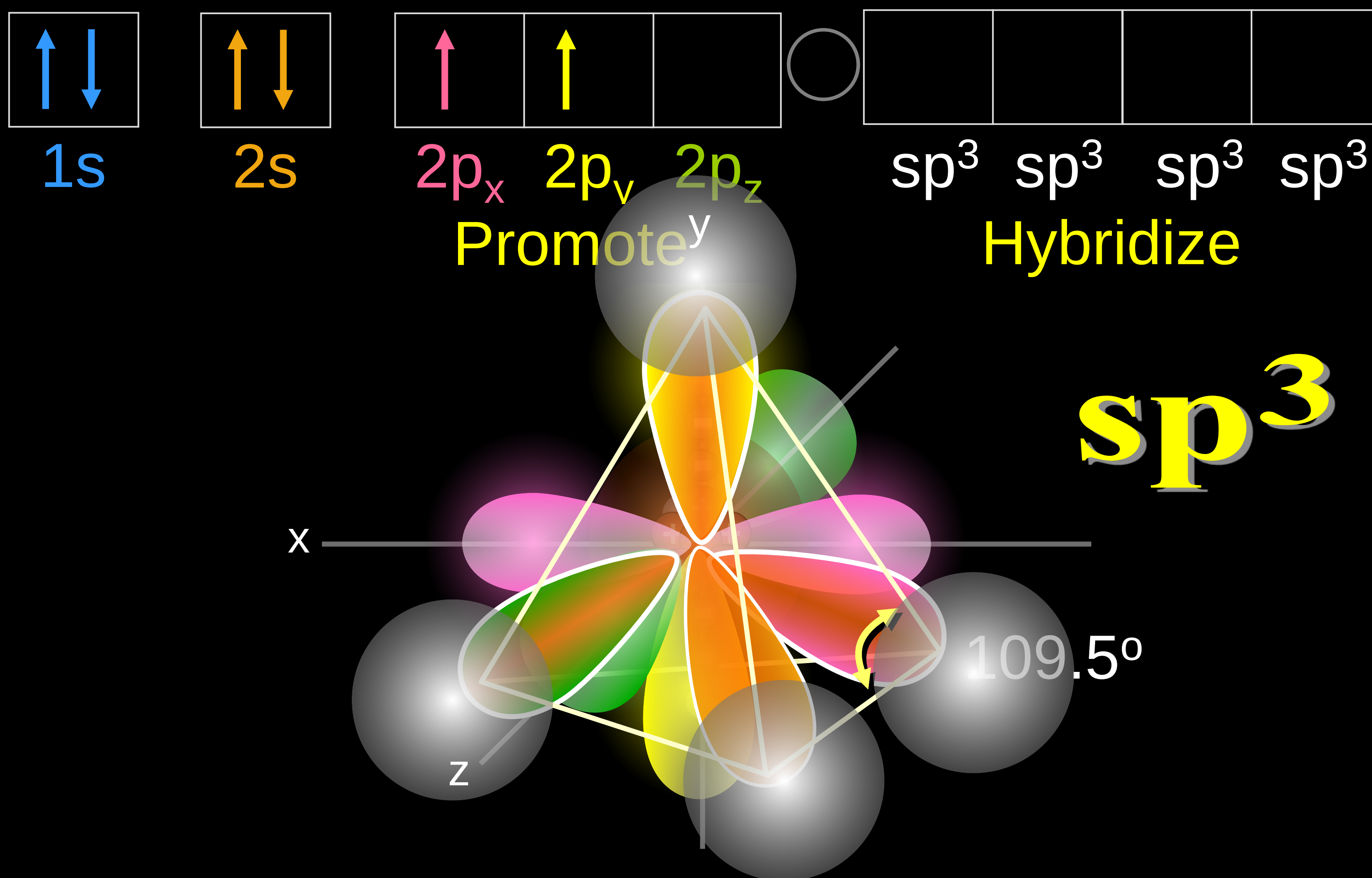


Methane building blocks



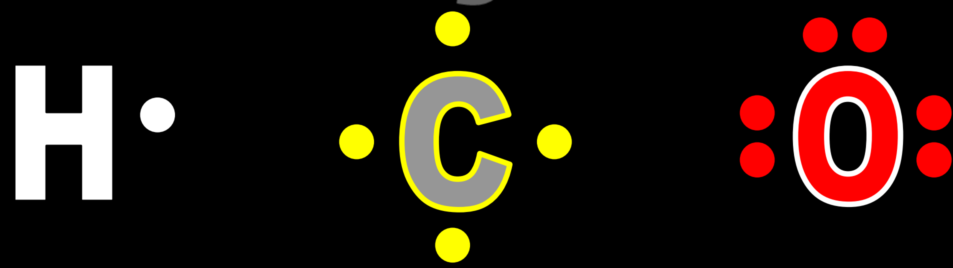


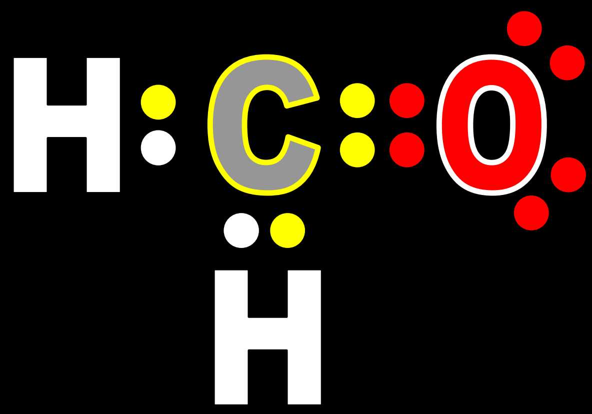
VSEPR



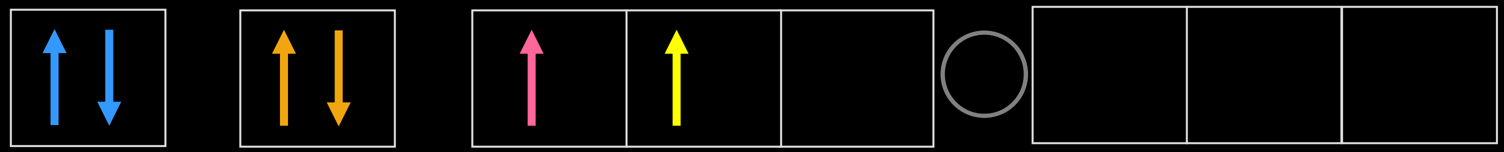
Methane: Carbon

Formaldehyde CH_2O



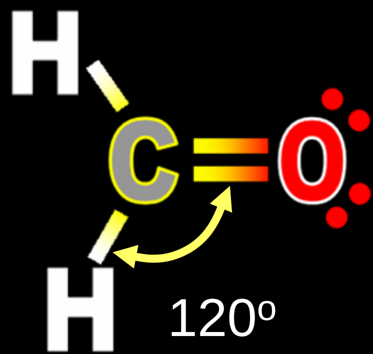


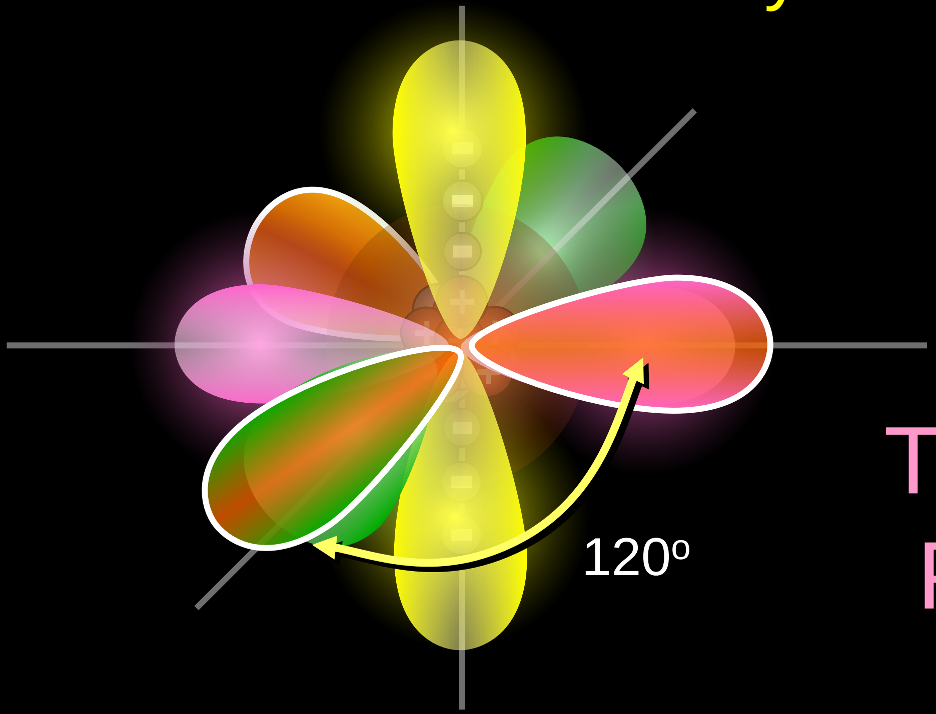
VSEPR



1s 2s $2p_x$ $2p_y$ $2p_z$ sp^2 sp^2 sp^2

Promoted Hybridized



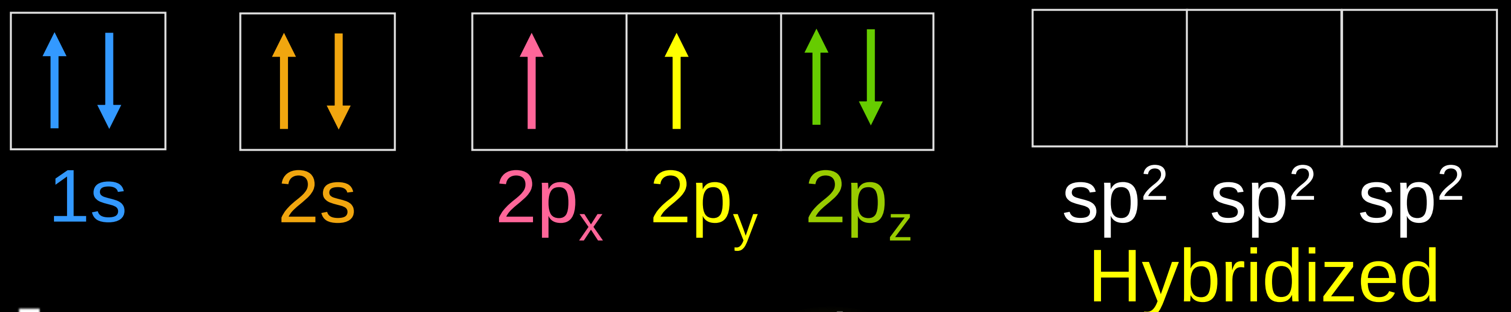


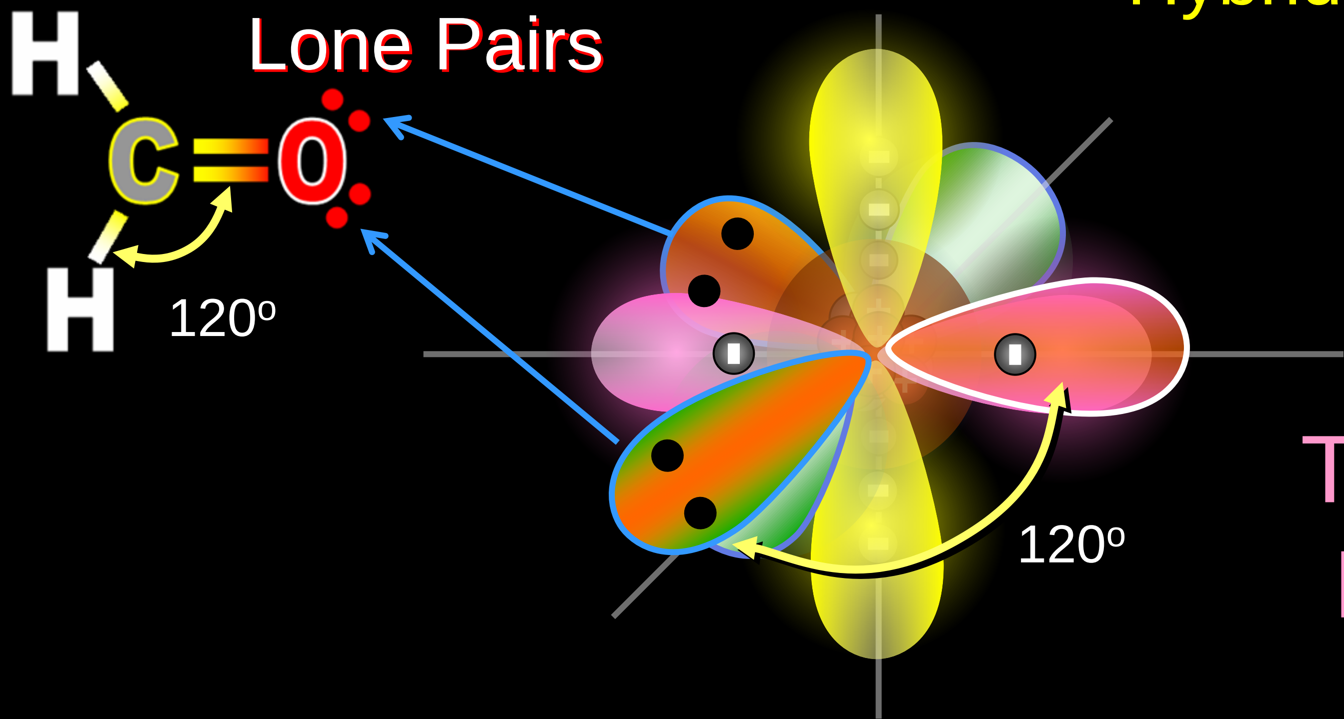
sp^2

Trigonal Planar

$2s + 2p_x + 2p_z$

Formaldehyde: Carbon



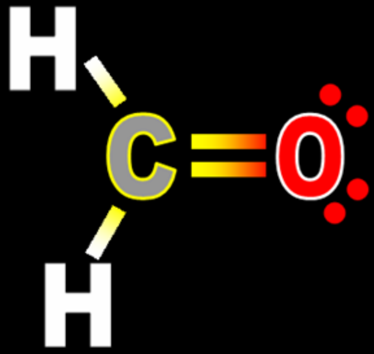


sp^2

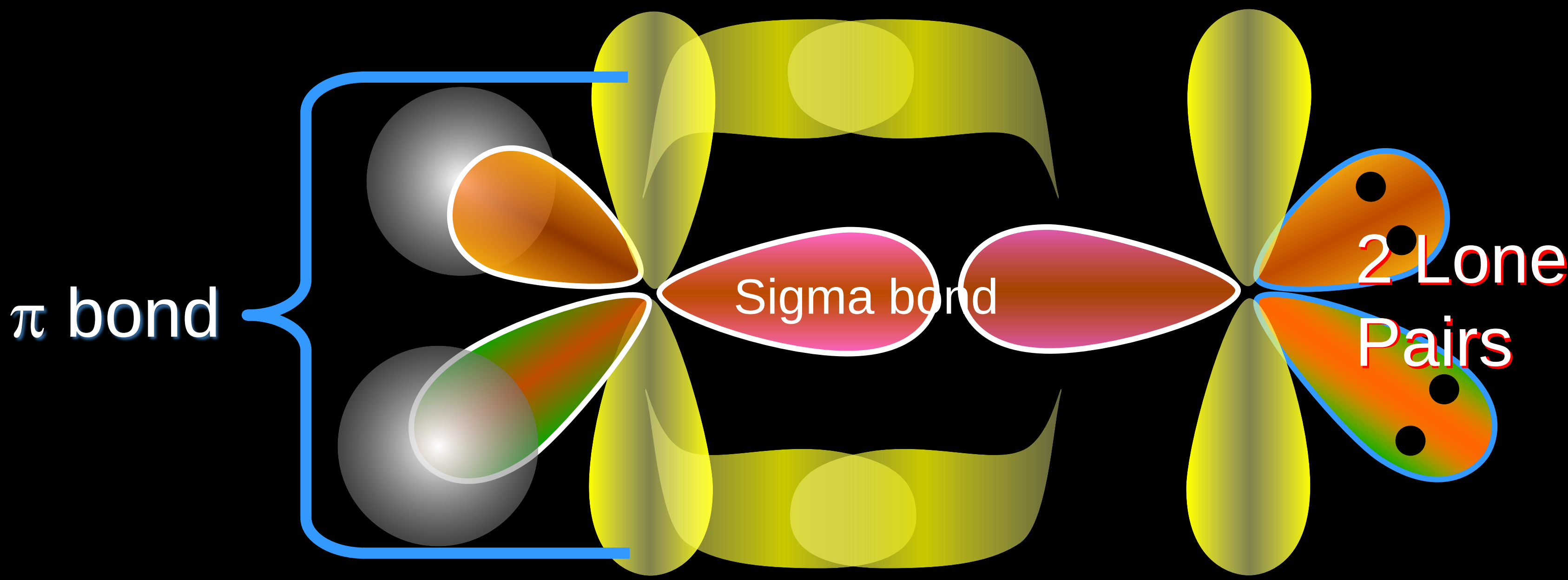
Trigonal Planar

$2s + 2p_x + 2p_z$

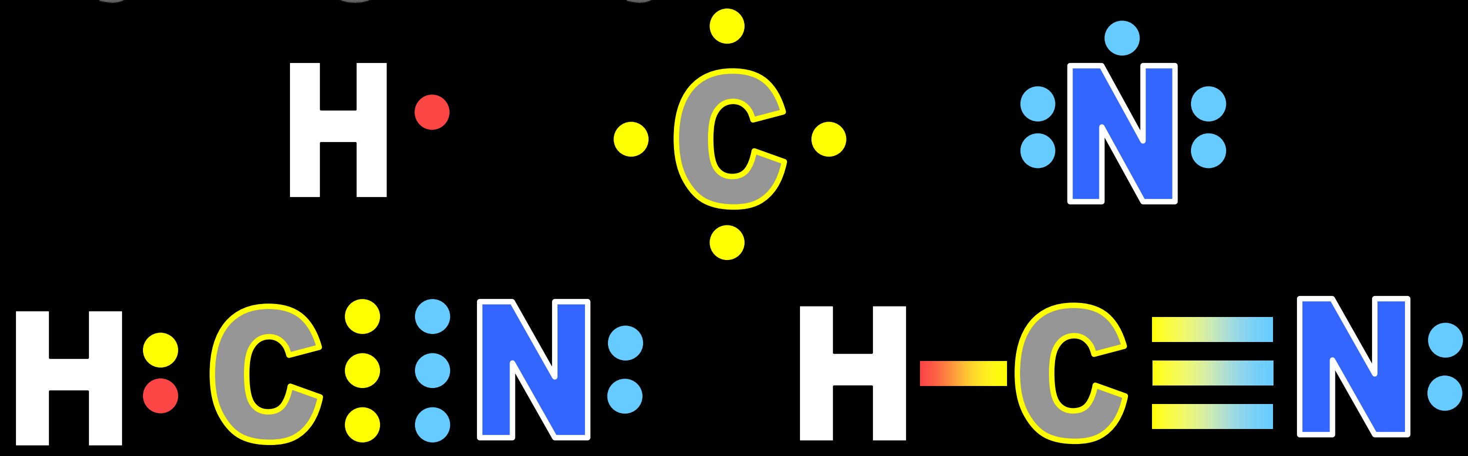
Formaldehyde: Oxygen



Formaldehyde

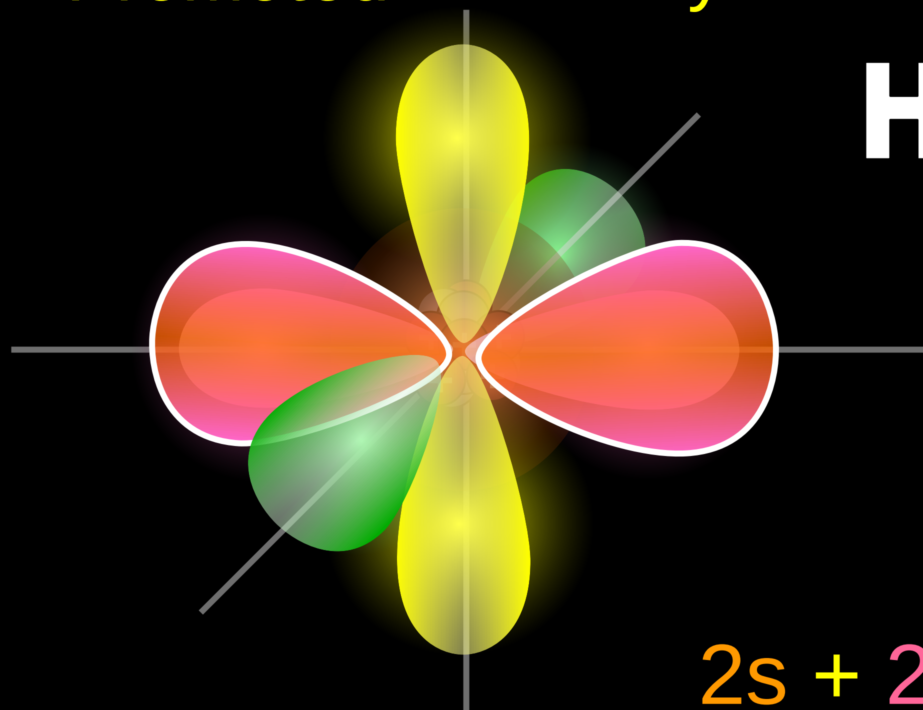


Hydrogen Cyanide HCN



1s 2s $2p_x$ $2p_y$ $2p_z$ sp sp

Promoted Hybridized



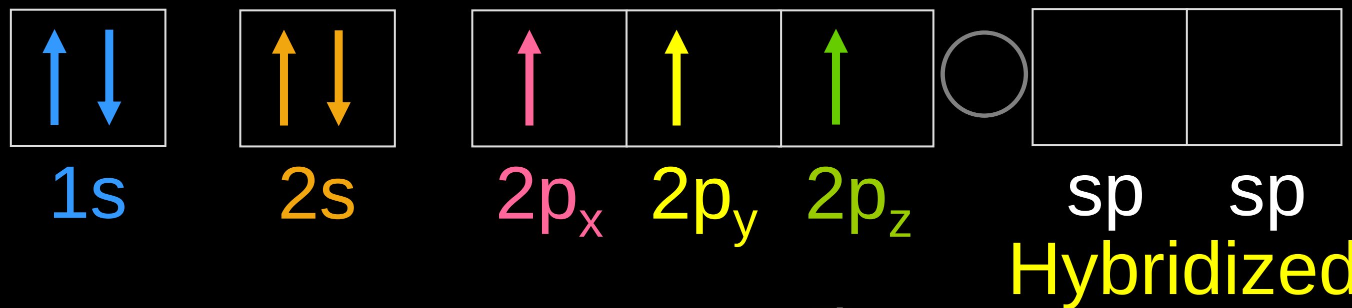
H–C≡N:

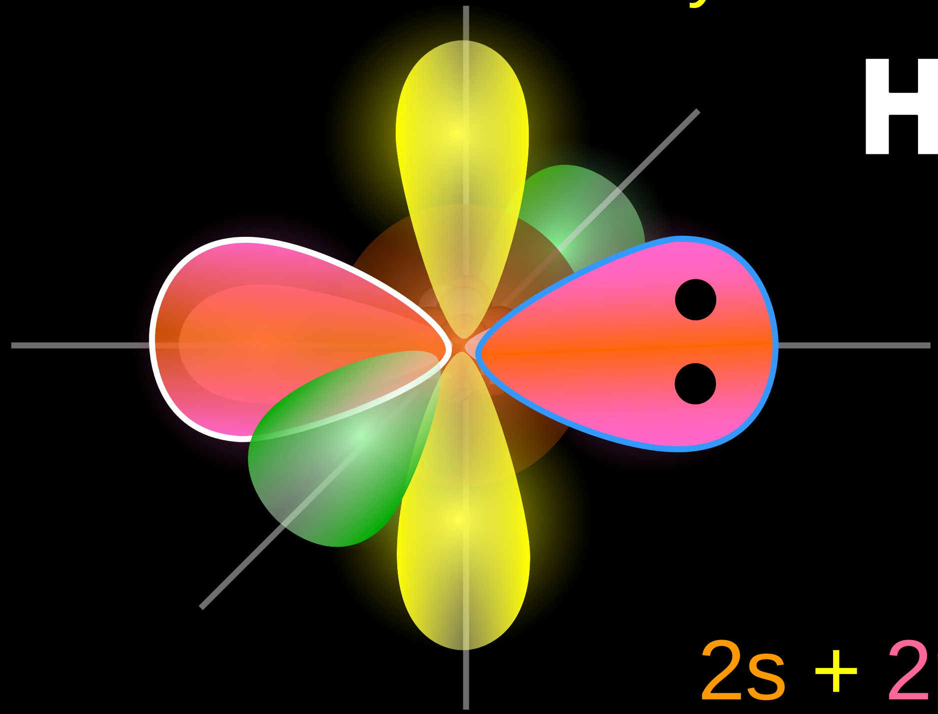
sp

Linear

$2s + 2p_x$

Hydrogen Cyanide: Carbon





$H{-}C{\equiv}N{:}$

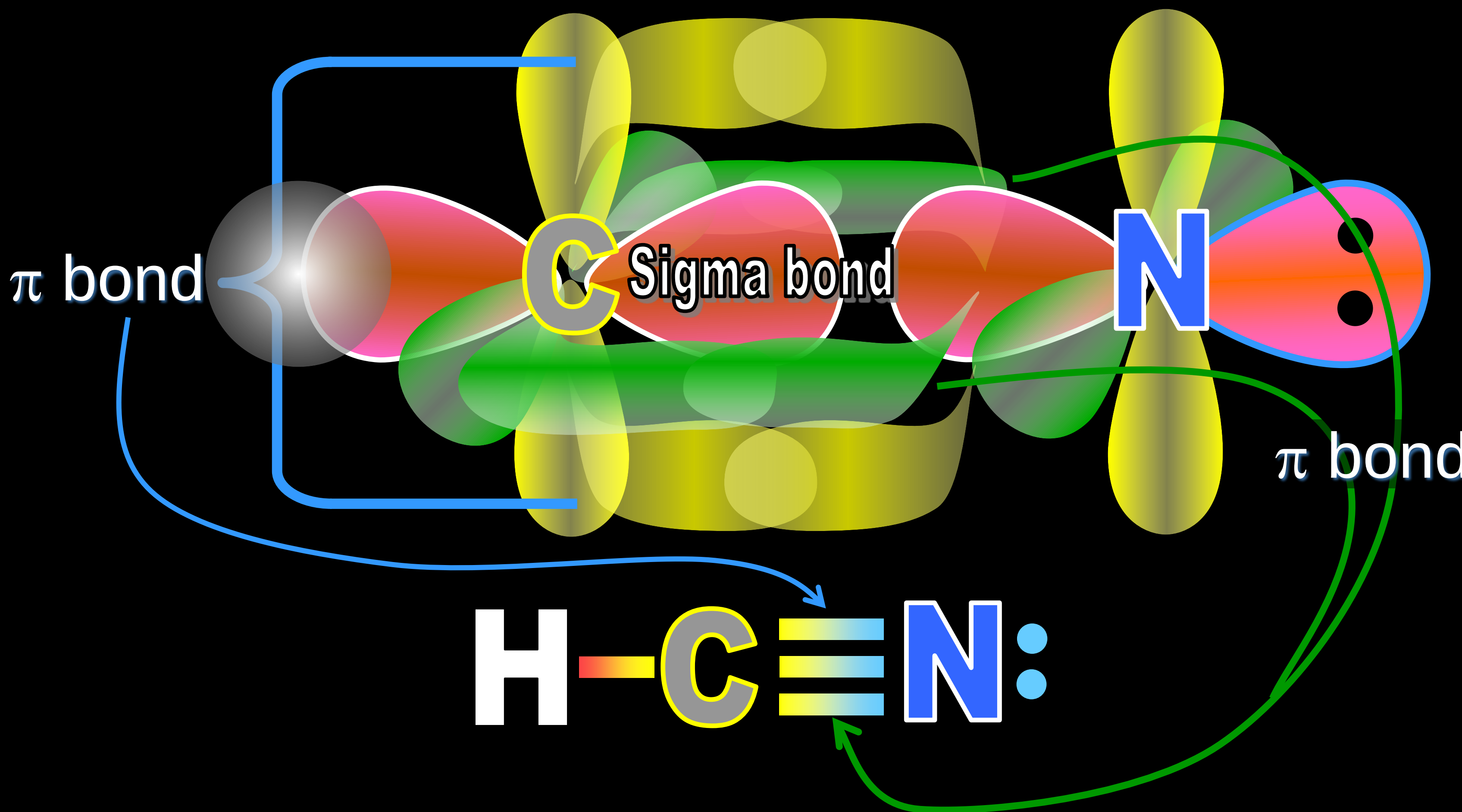
sp

Linear

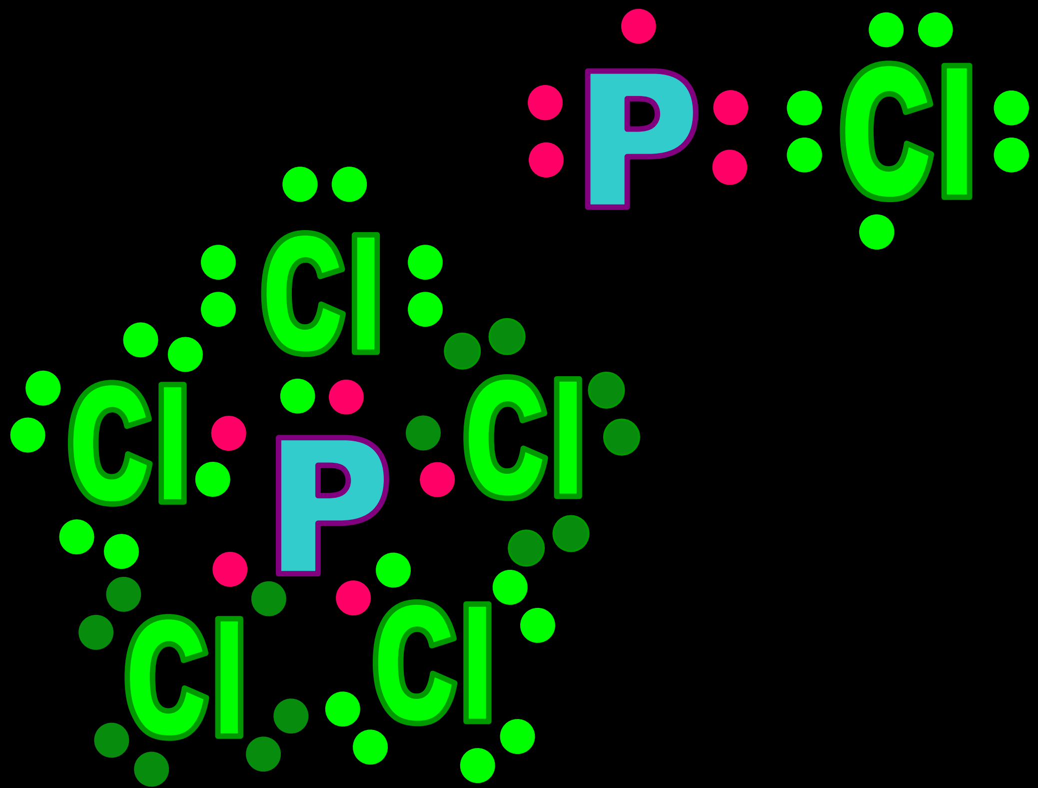
$2s + 2p_x$

Hydrogen Cyanide: Nitrogen

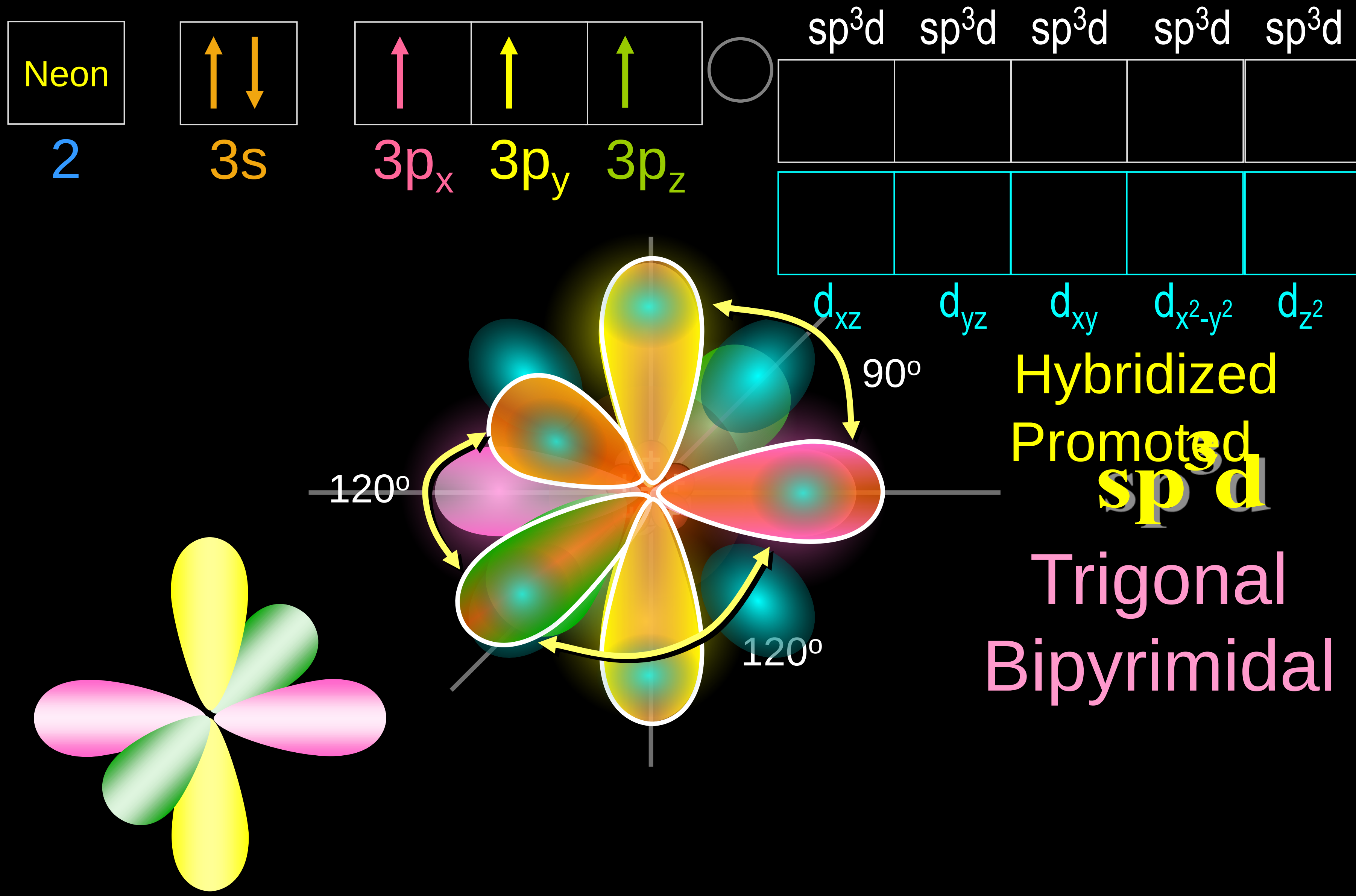
Hydrogen Cyanide HCN



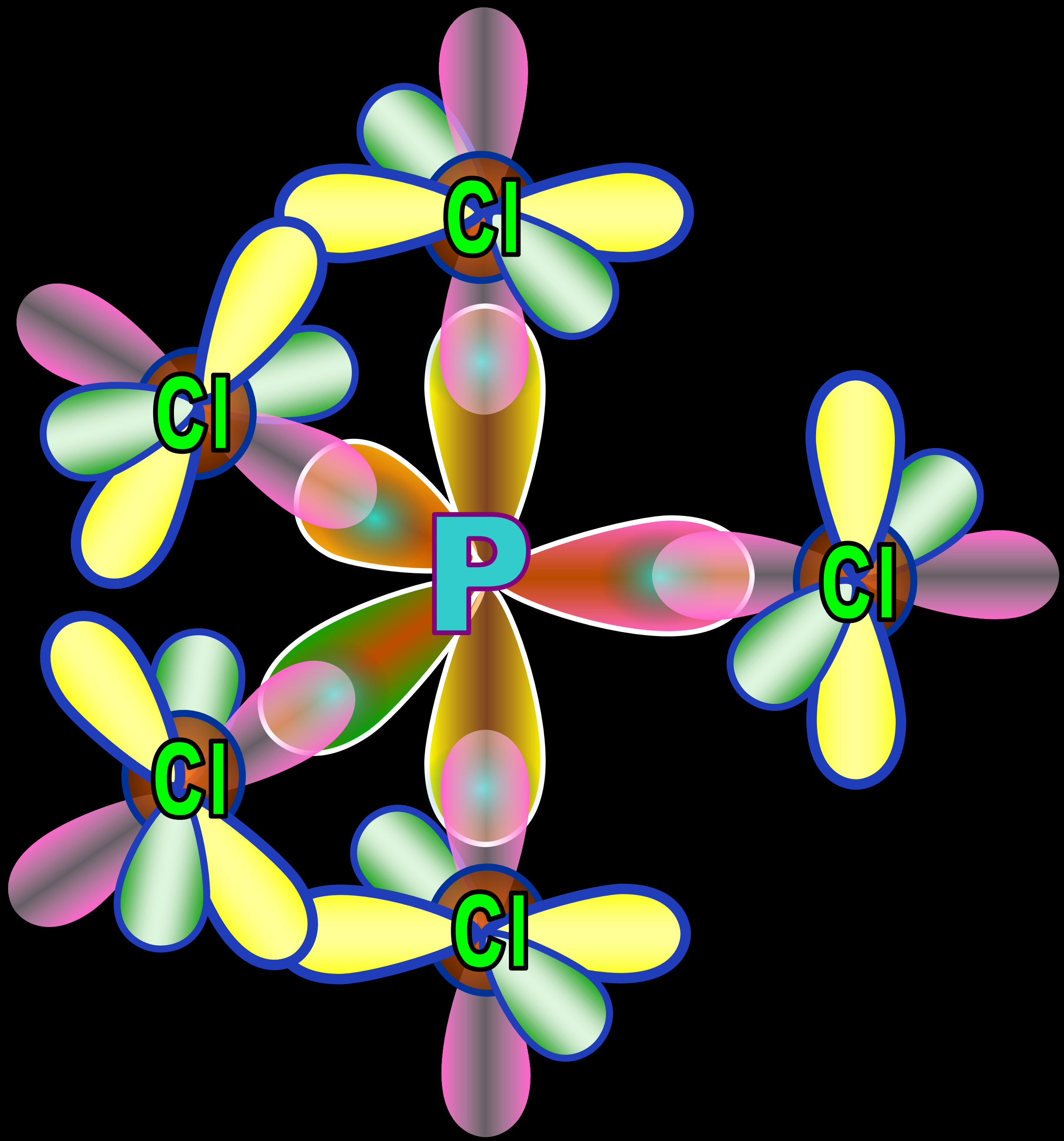
Phosphorus Pentachloride PCl_5



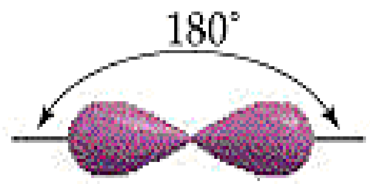
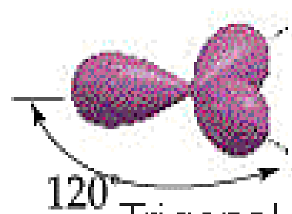
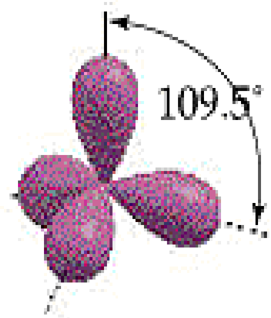
VSEPR



Phosphorus Pentachloride: Phosphorus


Cl
Cl
P
Cl
Cl
Cl

Geometrical Arrangements Characteristic of Hybrid Orbital Sets

Atomic Orbital Set	Hybrid Orbital Set	Geometry	Examples
sp	Two *sp*	 Linear	BeF_2, $HgCl_2$
spp	Three sp^2	 Trigonal planar	BF_3, SO_3
sppp	Four sp^3	 Tetrahedral	CH_4, NH_3, H_2O, NH_4^+