Theories Covered

Valence Bond Theory (Hybridization) Topics

Concept Video

Formation of covalent bonds (single bonds/ sigma bonds)

Formation of covalent bonds (multiple bonds/ sigma and pi bonds)

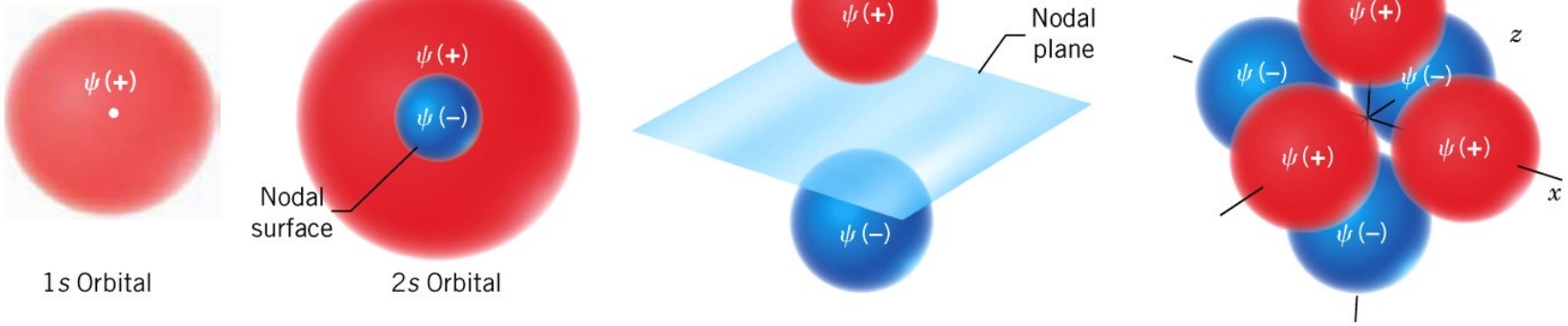
Concept Video

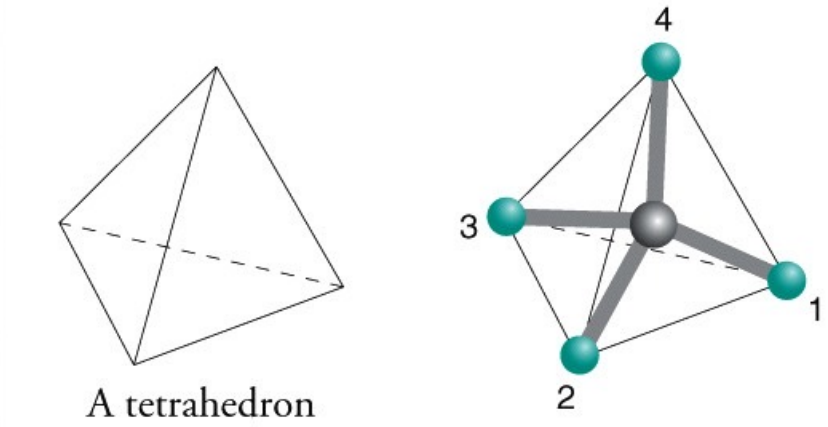
Hybridization of orbitals 1

Concept Video

Hybridization of orbitals 2

Limitations of Valence Bond Theory



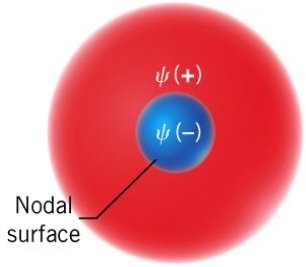


How can valence bond theory predict bond angles?

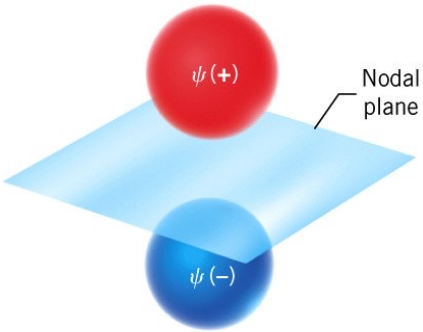
Valence bond theory cannot predict the geometry for all molecules

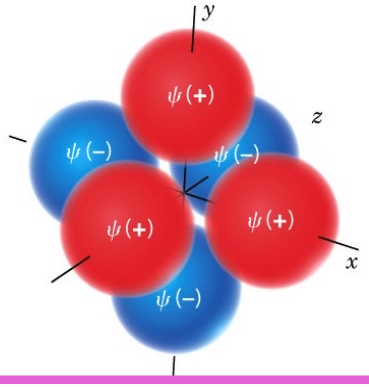
Combining Valence Bond Theory

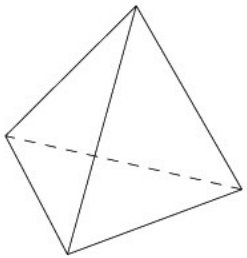
1*s* Orbital



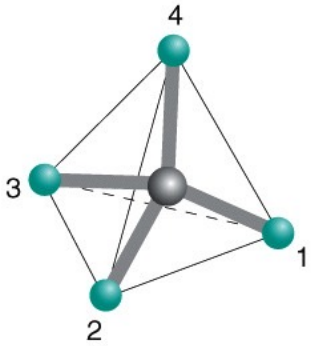
2*s* Orbital







A tetrahedron



Valence bond theory can predict orbitals involved but cannot predict the geometry for all molecules –
How are the bond angles in CH_4 109.5?

VSEPR theory can predict the geometry for molecules but not the orbitals involved in bonding
Which orbitals are involved in formation of CH_4 molecule?

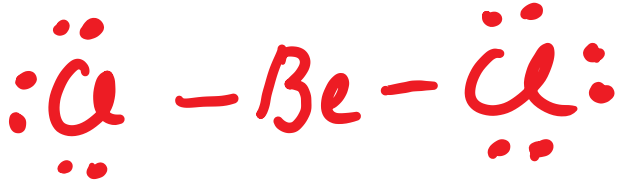
Combining VSEPR and Valence Bond Theory

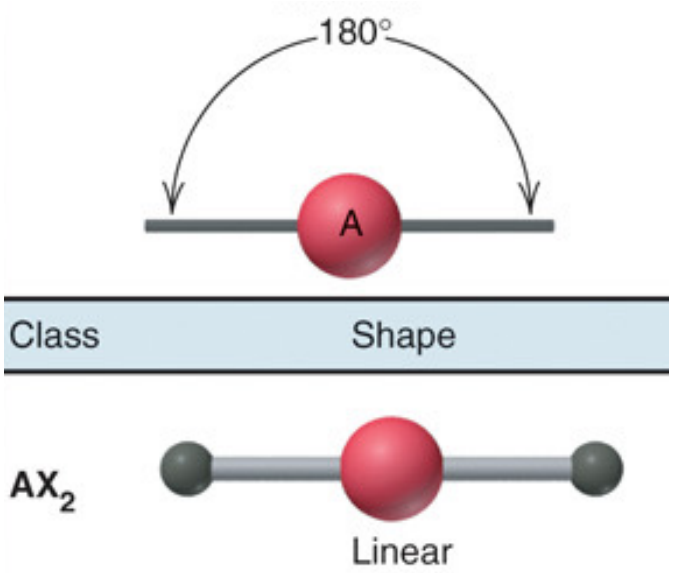
Linear Geometry (AX_2)

2 electron groups : 2 bonding groups (no lone pairs)

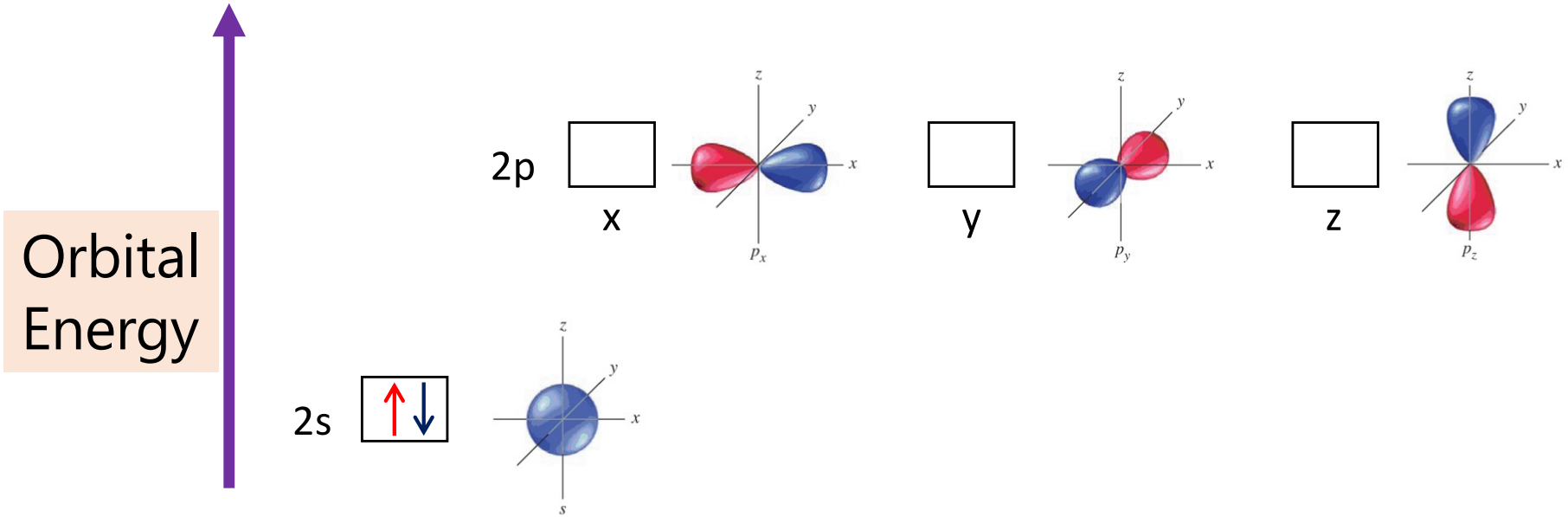
Bond Angle (XAX): 180˚

e.g. $BeCl_2$



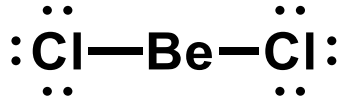


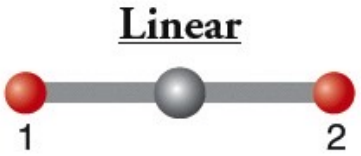
Orbitals for Linear Geometry in AX_2



1. Need the electrons to be unpaired to share with the unpaired electron in Cl atoms
2. The bond lengths are equal – this implies that the orbitals forming the sigma bonds are equivalent.

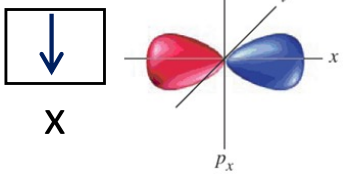
Orbitals for Linear Geometry in AX_2



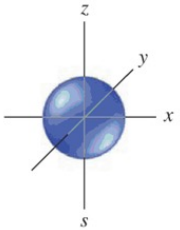


Orbital Energy

2p



2s



1. Need the electrons to be unpaired to share with the unpaired electron in Cl atoms - excite an electron from 2s orbital of Be
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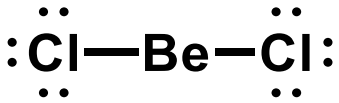
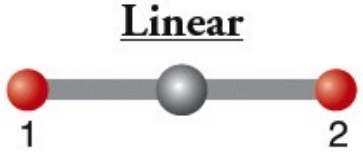
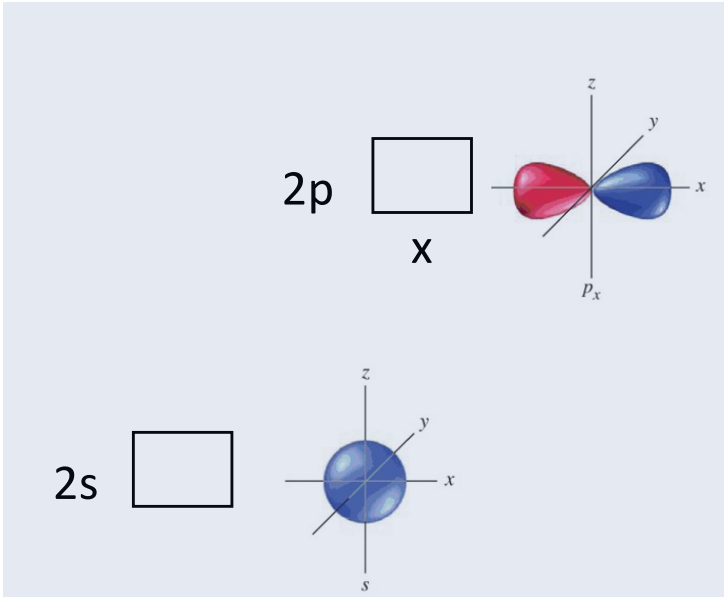
Orbitals for Linear Geometry in AX_2





Mix <u>two</u> valence orbitals to get two equivalent orbitals

Orbital Energy



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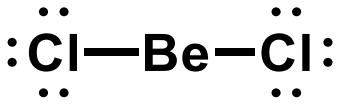
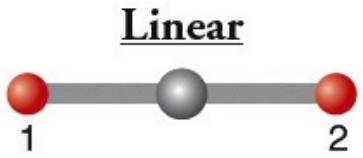


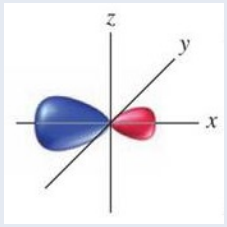


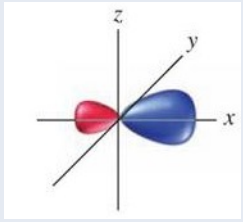
Mix <u>two</u> valence orbitals to get two equivalent orbitals

Orbital Energy

$1s^2 2(sp)^2 2p^0$

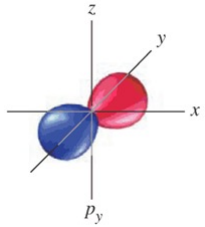
sp ↑ sp ↑



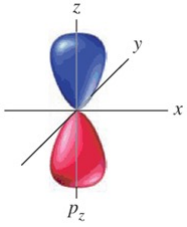


(s:p = 1:1 = "sp")

y



z



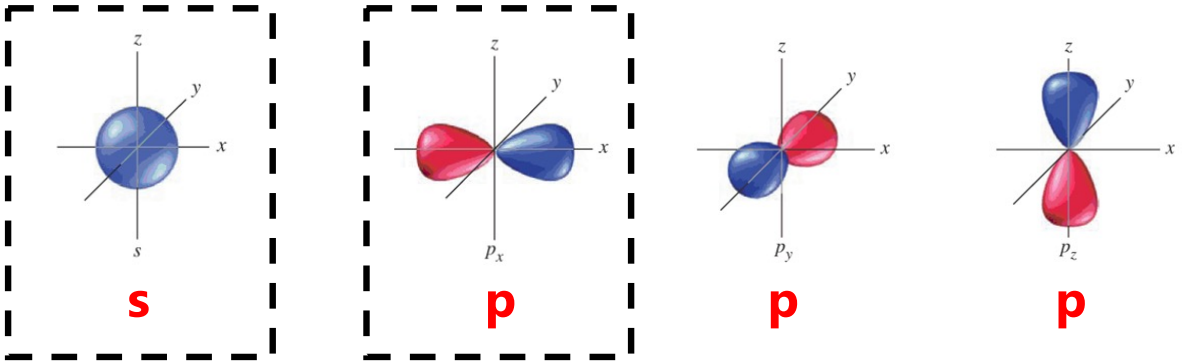
Obtain two new atomic hybrid orbitals!

1. Need the electrons to be unpaired to share with the unpaired electron in Cl atoms - excite an electron from 2s orbital of Be
2. The bond lengths are equal – this implies that the orbitals forming the sigma bonds are equivalent.

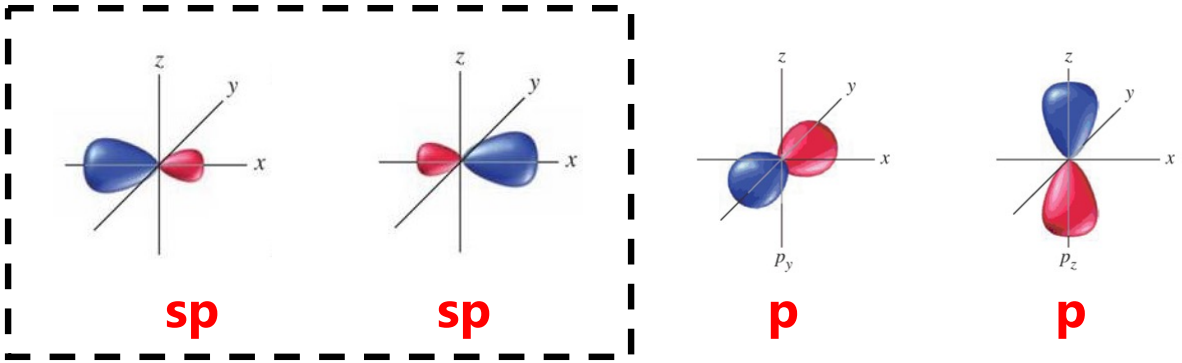
Hybridization

Mixing of valence orbitals in an element to obtain orbitals with appropriate geometry

Atomic Be
Valence Orbitals:



Be atoms in $BeCl_2$
Valence Orbitals:



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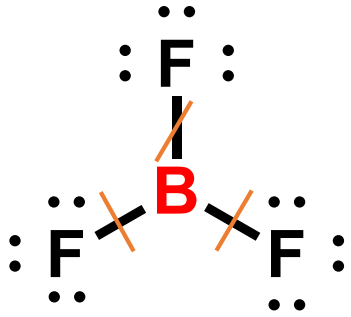
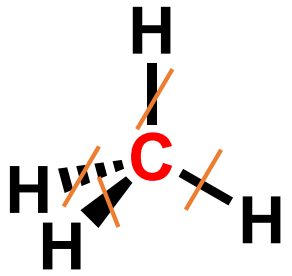
Hybridization

Mixing of valence orbitals in an element to obtain orbitals with appropriate geometry

Number of electron groups = number of hybrid orbitals





Electron groups	2	3	4
Hybrid Orbitals	2	3	4

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What about hybridization when there are multiple bonds?

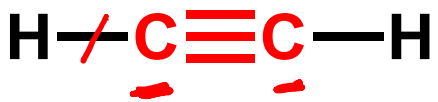
Linear Geometry

2 electron groups : 2 bonding groups (no lone pairs)

Bond Angle (XAX): 180˚

e.g. C_2H_2 (ethyne)

Number of electron groups = number of hybrid orbitals



2 hybrid orbitals: sp hybridization

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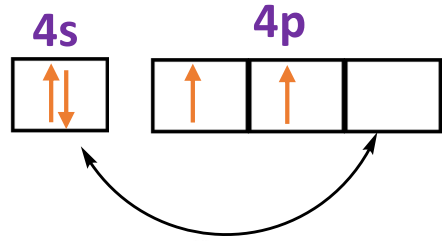
Depicting orbitals for C_2H_2 (ethyne)

H—C≡C—H

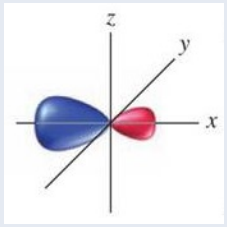
C $1s^2\ 2s^2\ 2p^2$

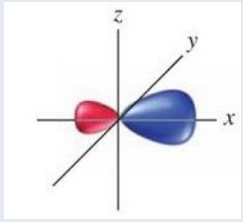


Orbital Energy

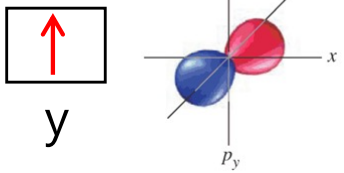
$1s^2 2(sp)^2 2p^2$

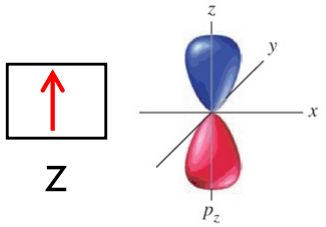
sp sp





(s:p = 1:1 = "sp")





Obtain two new atomic hybrid orbitals!

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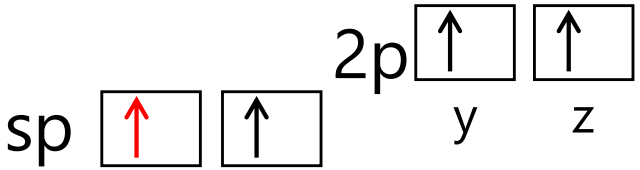
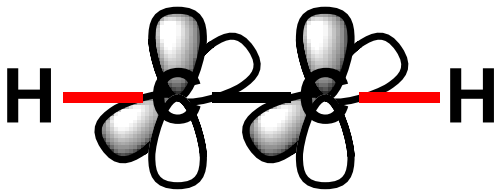
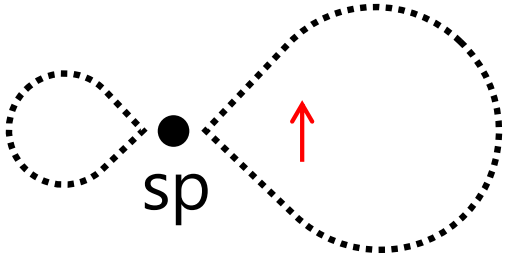
C-H bonds in ethyne (sigma bond)

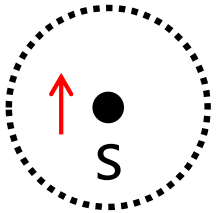
Hydrogen atom

Carbon atom



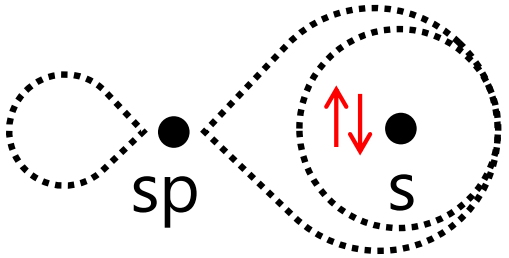






<u>ONE</u> C-H Single Bond:

sp-s σ-bond



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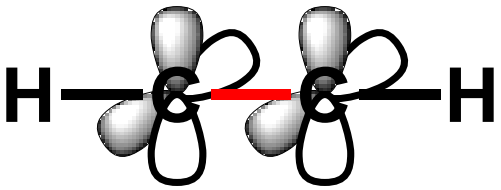
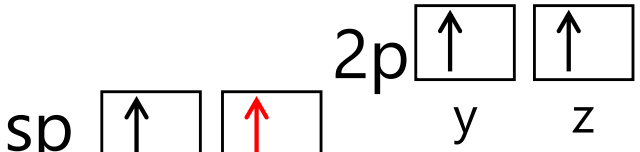
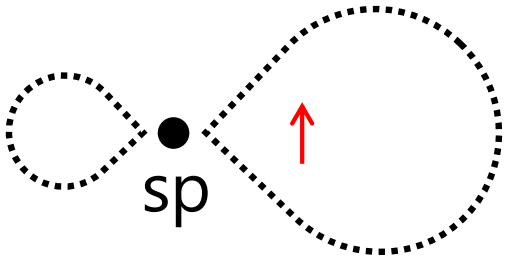
C-C bonds in ethyne (sigma bond)

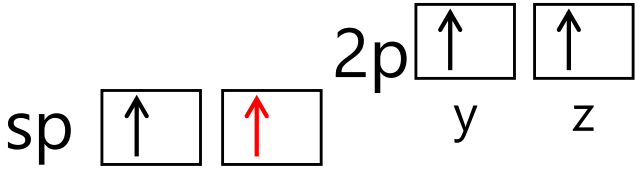


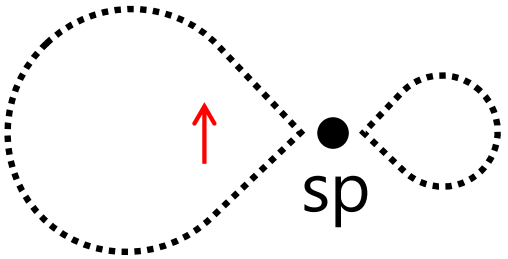
Carbon atom





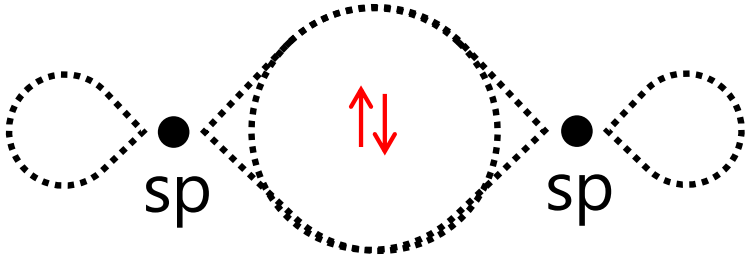
Carbon atom



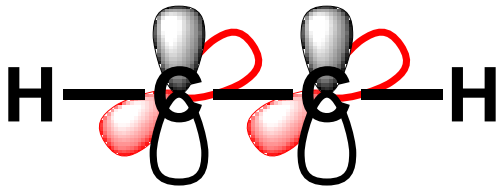


<u>ONE</u> C-C Single Bond:

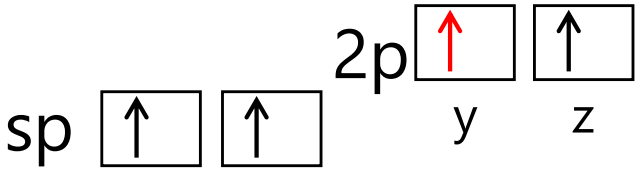
sp-sp σ-bond

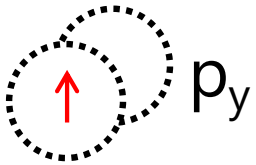


C-C bonds in ethyne (pi bond)

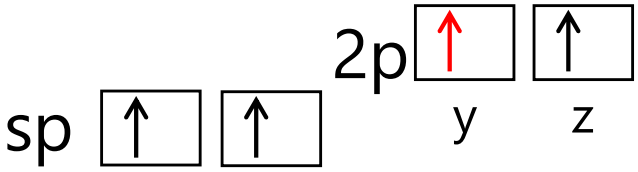


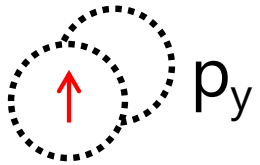
Carbon atom





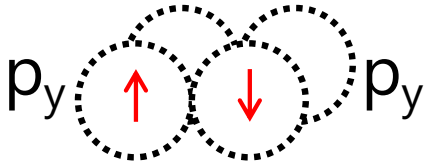
Carbon atom



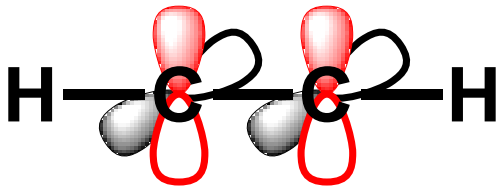


ONE C-C π Bond:

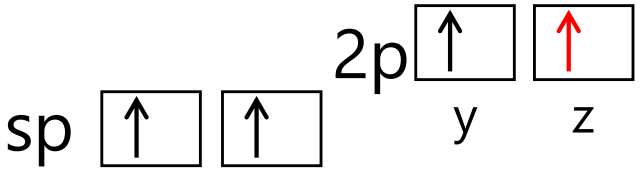
p_y-p_y π-bond

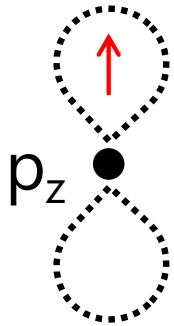


C-C bonds in ethyne (pi bond)

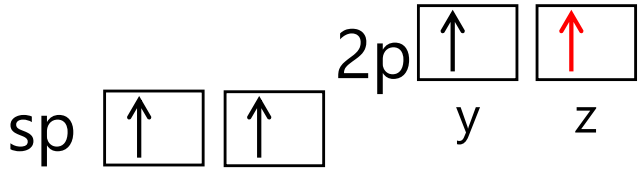


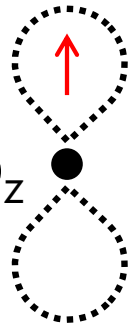
Carbon atom





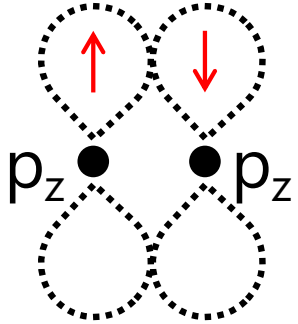
Carbon atom





ONE C-C π Bond:

p_z-p_z π-bond



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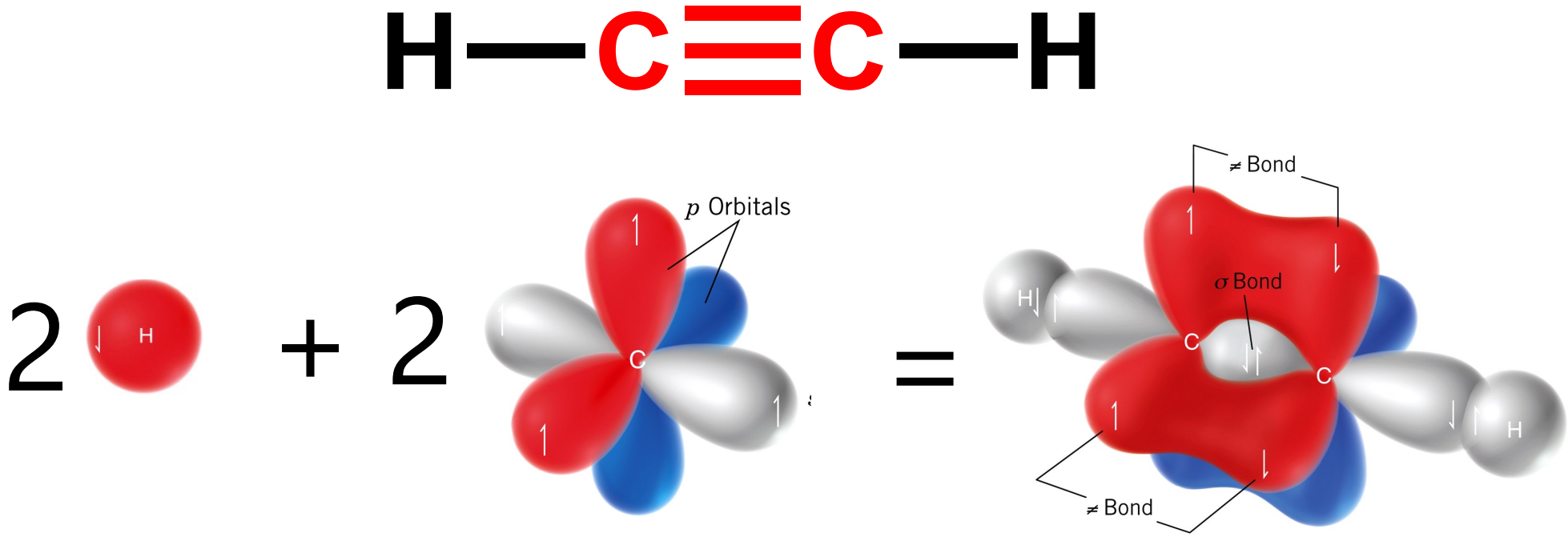
Depicting orbitals for C_2H_2



TWO σ-bonds per C
sp-s (between C and H) , sp-sp (between C and C)

TWO π bonds total
p-p (between C and C)

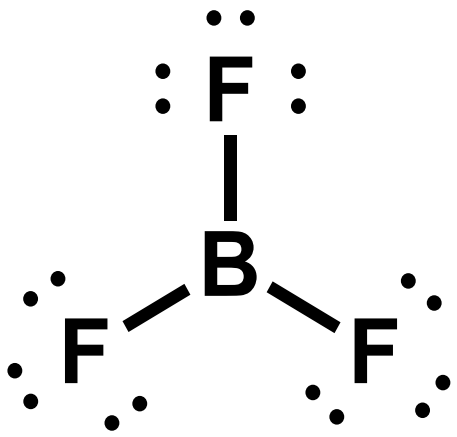
Trigonal Planar Geometry

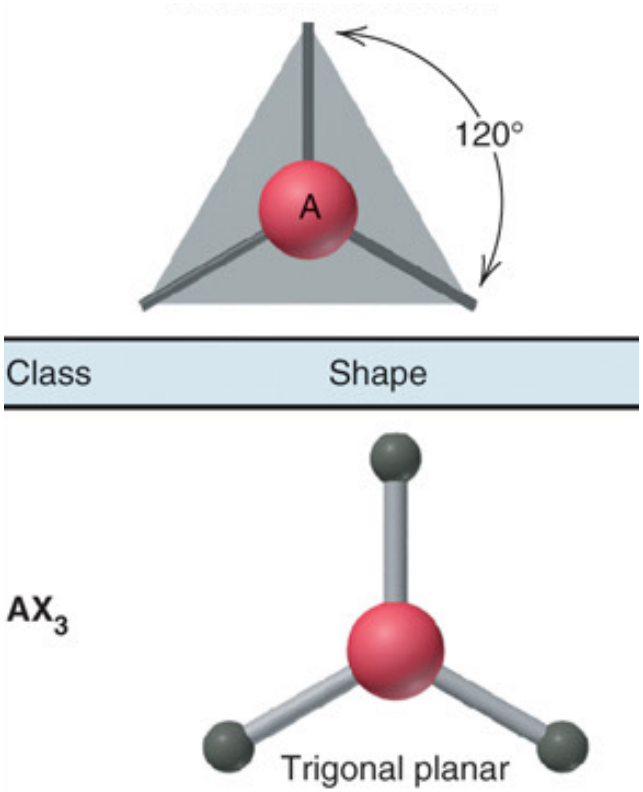
Trigonal Planar Geometry (AX_3)

3 electron groups : 3 bonding groups (no lone pairs)

Bond Angle (XAX): 120˚

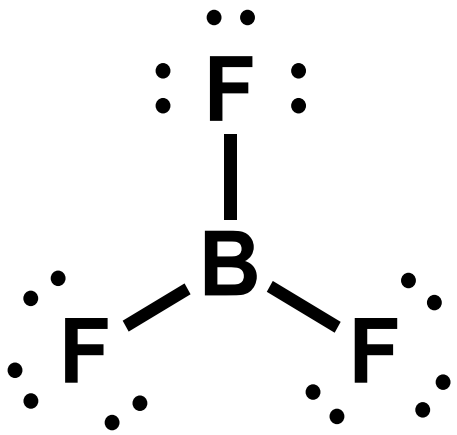
e.g. BF_3





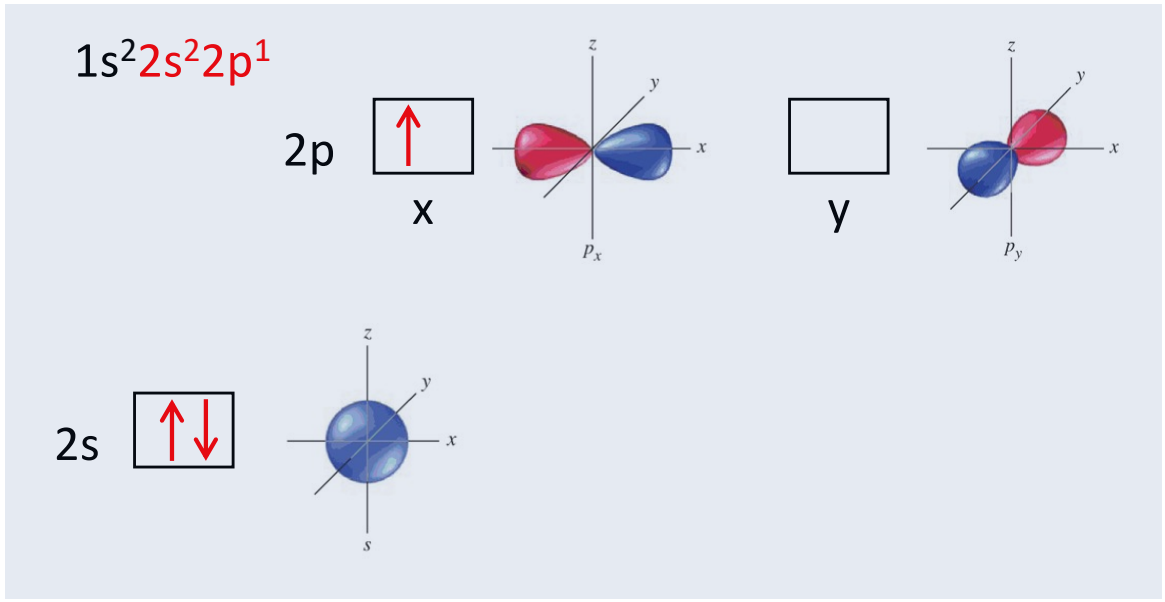
Hybridization for 3 electron groups

e.g. BF_3



Mix <u>three</u> valence orbitals to get <u>three</u> equivalent hybrid orbitals

Orbital Energy



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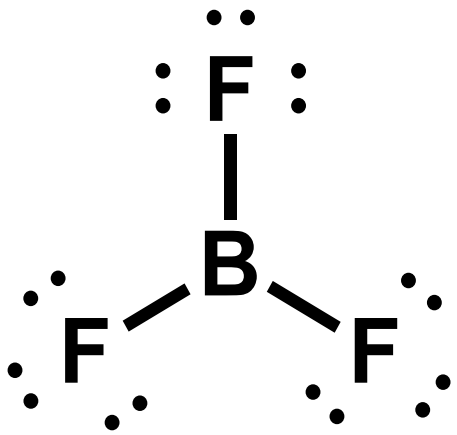
Hybridization for 3 electron groups

e.g. BF_3



Mix <u>three</u> valence orbitals to get <u>three</u> equivalent hybrid orbitals

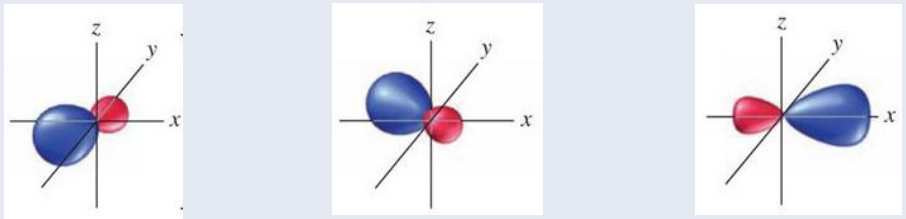
(s:p = 1:2 = "sp^2")

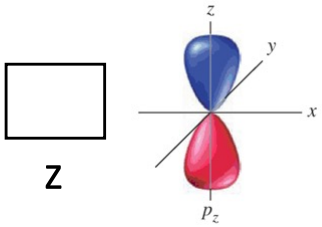
Orbital Energy

$1s^2 2(sp^2)^3$

sp^2 Hybrid Orbitals

sp^2 sp^2 sp^2





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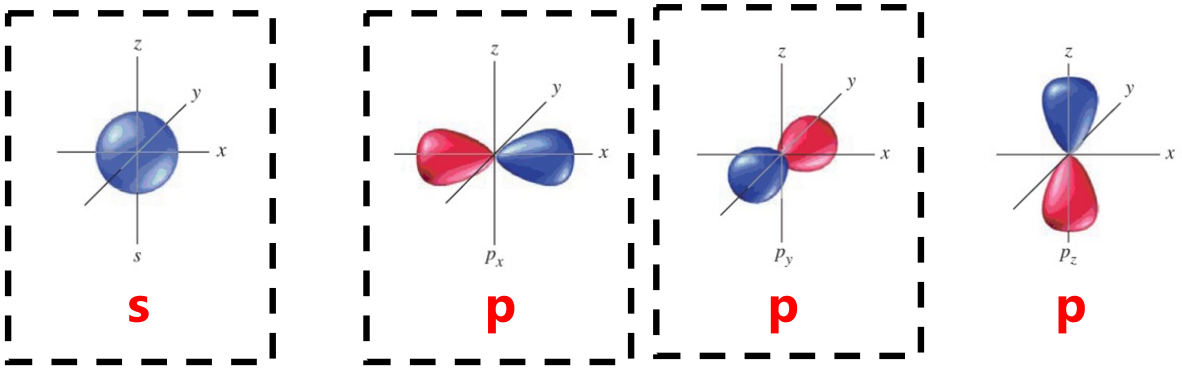
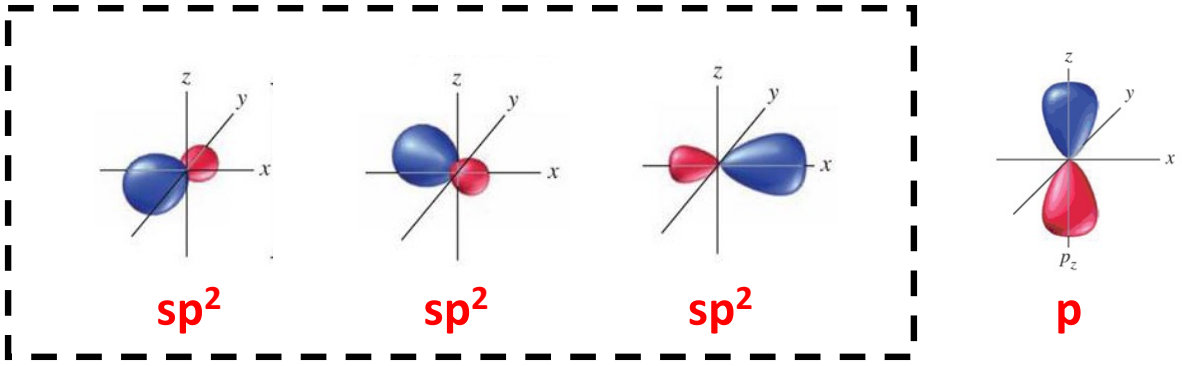
Hybridization

Mixing of valence orbitals in an element to obtain orbitals with appropriate geometry

Atomic B
Valence
Orbitals:



B atoms in BF_3
Valence
Orbitals:



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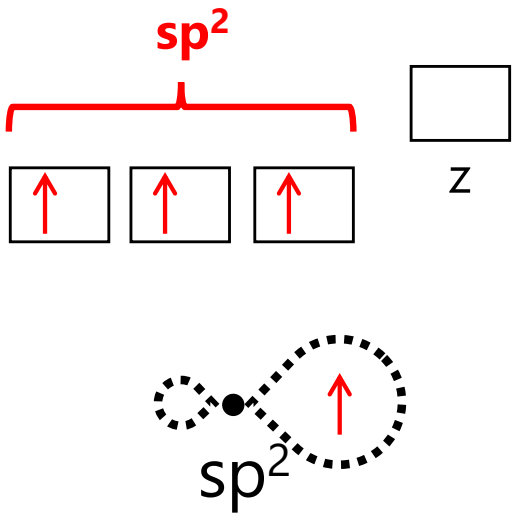
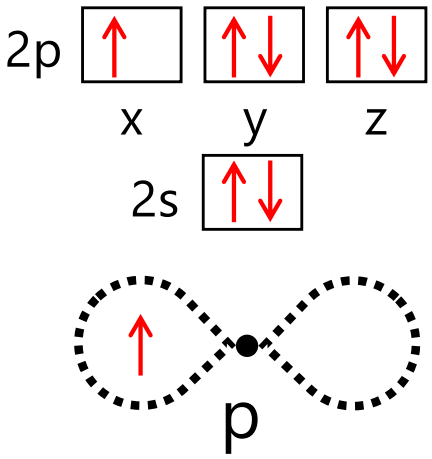
Depicting bond formation with hybrid orbitals

Boron atom

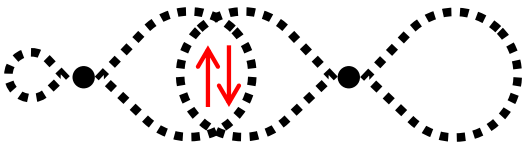


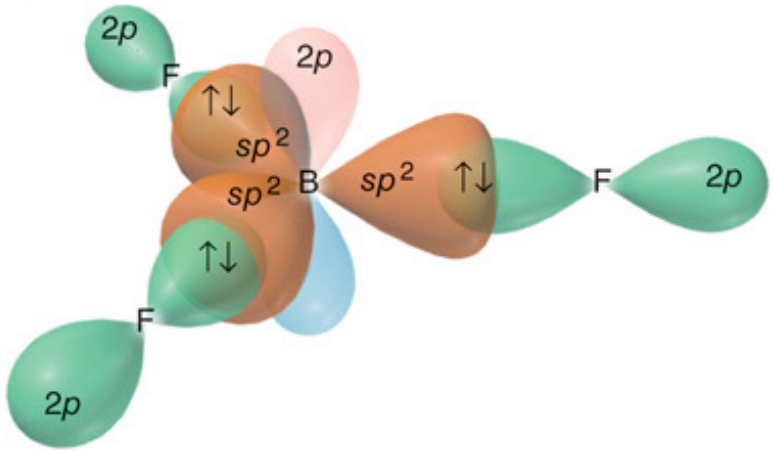
Fluorine atom



THREE IDENTICAL "sp^2-p" σ-bonds

<u>ONE</u> B-F sp^2-p σ-bond:





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What about sp^2 hybridization when there are multiple bonds?

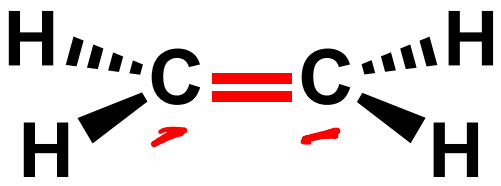
Trigonal Planar Geometry

3 electron groups : 3 bonding groups (no lone pairs)

Bond Angle (XAX): 120˚

e.g. C_2H_4 (ethene)

Number of electron groups = number of hybrid orbitals



3 hybrid orbitals: sp^2 hybridization

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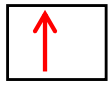
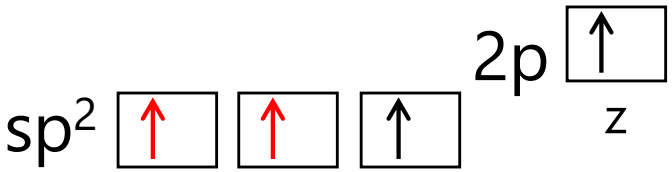
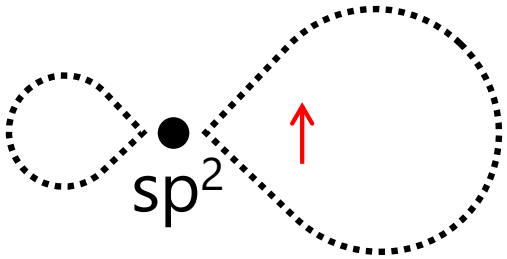
C-H bonds in C_2H_4 (ethene): Sigma bond

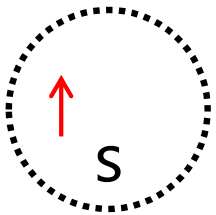
Hydrogen atom

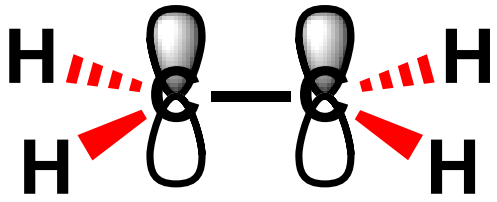
1s 

Carbon atom



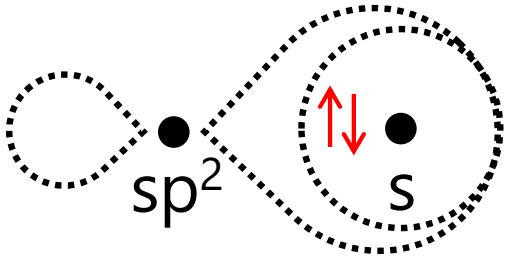






<u>ONE</u> C-H Single Bond:

sp^2-s σ-bond



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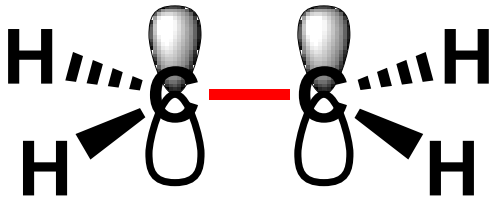
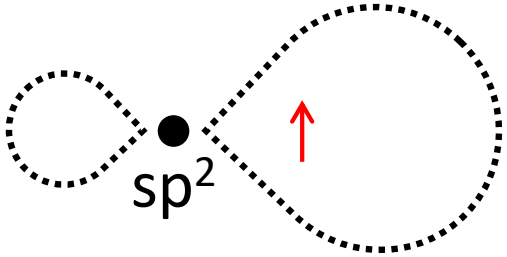
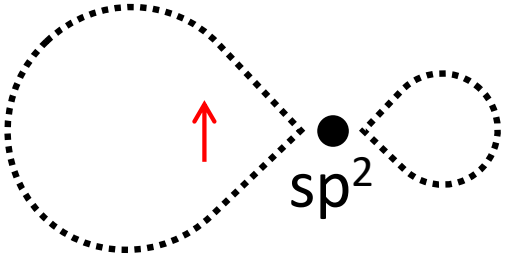
C-C bonds in C_2H_4 (ethene): Sigma bond



Carbon atom

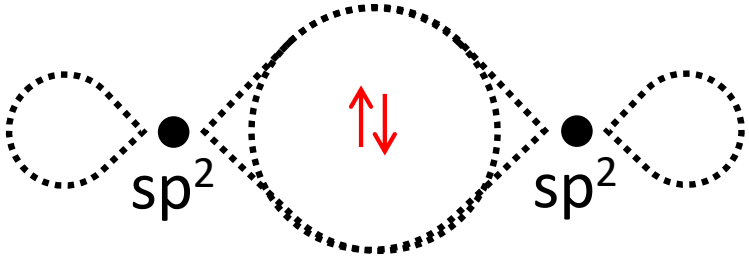


Carbon atom



<u>ONE</u> C-C σ Bond:

sp^2-sp^2 σ-bond



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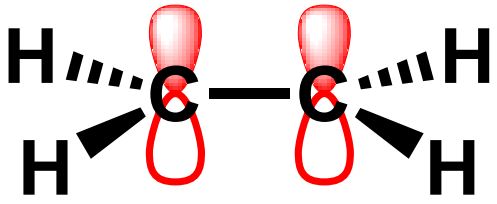
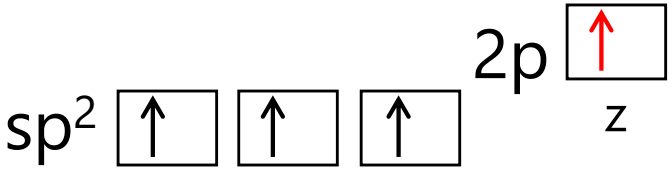
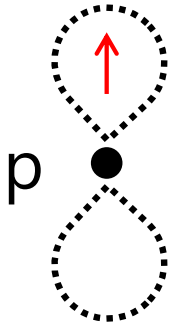
C-C bonds in C_2H_4 (ethene): Pi bond

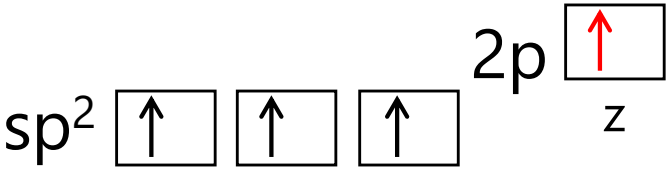


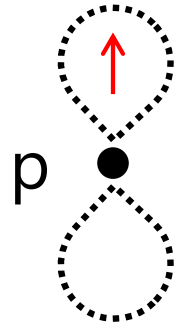
Carbon atom





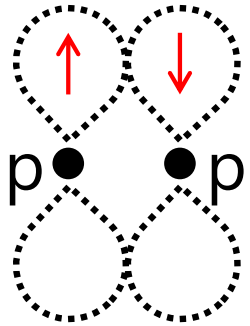
Carbon atom





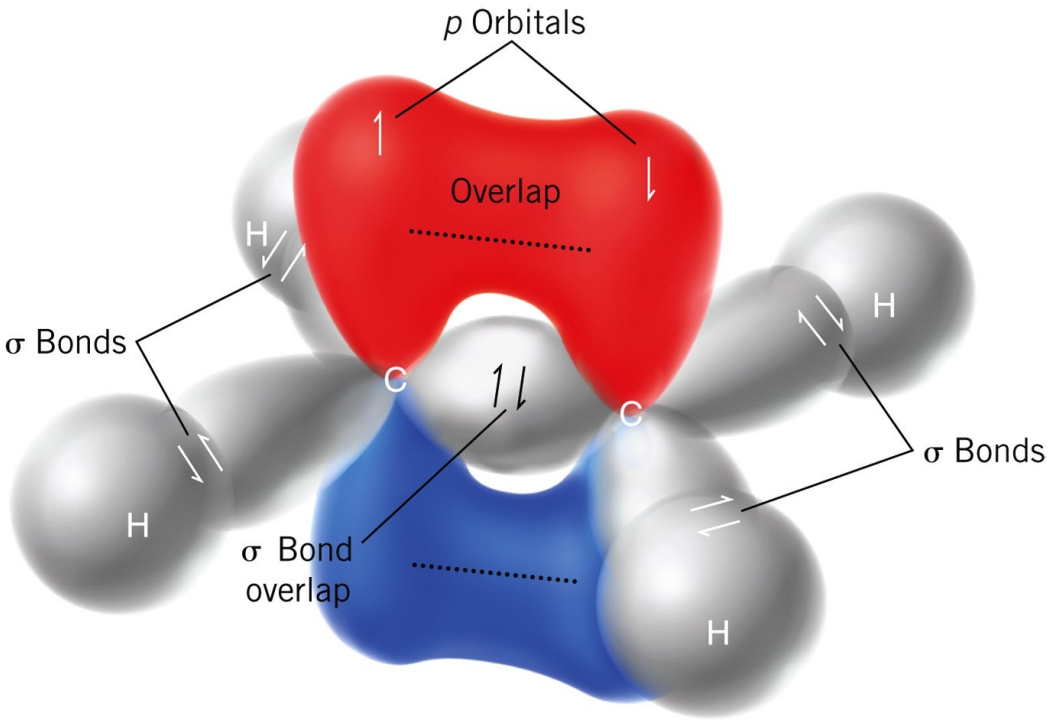
<u>ONE</u> C-C π Bond:

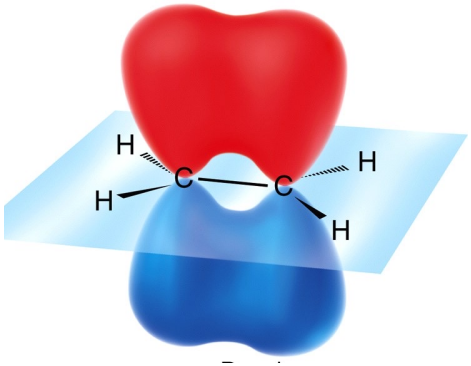
p-p π-bond

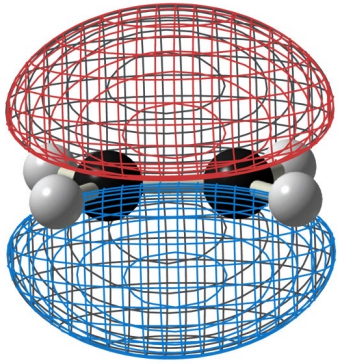


McGill

Structure of Ethene







THREE σ-bonds per C
sp^2-s (x2), sp^2-sp^2