Course Chem 343-5 Lecturer Prof. Sam Gellman

Day Friday Date 9/9/16

Notes Taken By Sungho Park Total # of Pages 3

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Recall: bonding in organic molecules...

C atom valence shell = 2s + 3x2p

→ Hybridize AOs to be able to form 4 bonds → $4 \times sp^3$

CH_4 = "tetrahedral" geometry 109.5°

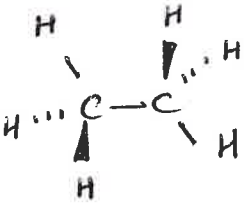
4 equivalent C–H bonds ("σ-bonds"; σ MO)

Ethane = C_2H_6

6x C–H σ bonds

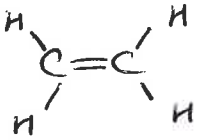
+

1 x C–C σ bonds



All angles ~109.5°

Example 3 : ethene (ethylene)

C_2H_4 

1 C–C σ-bond

1 C–C π-bond

4 x C–H σ bonds

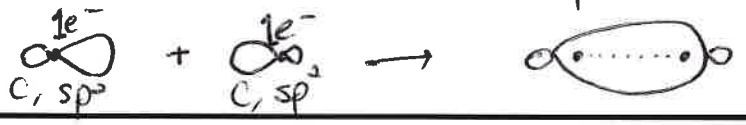
σ-bonds (# bonding partners) determines mode of hybridization.

Distribute s-character into only those AOs that engage in σ-bonds.

For C_2H_4, sp^2-hybridized C { sp^2 AO 33% s / 67% p ; $3 \times sp^2$ AOs + 1 p orbital for π bond }

C=C double bond : σ component + π component

Spatial characteristics: 1) σ-component



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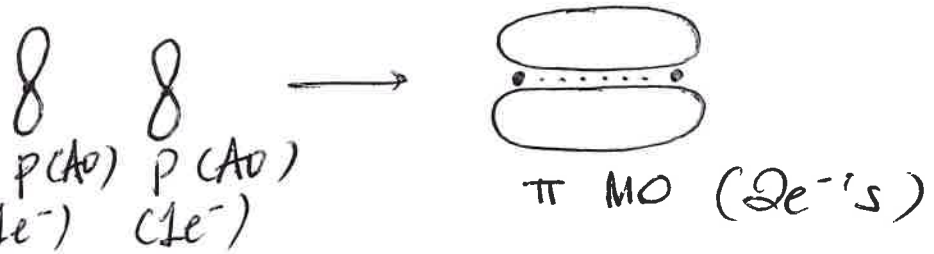
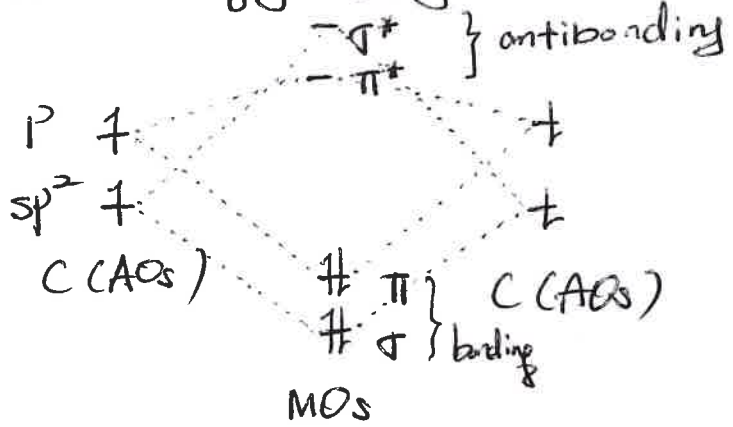
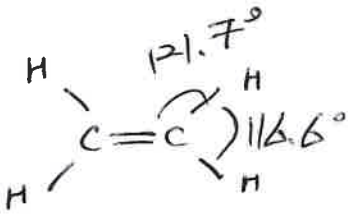
2) π Component



C=C bond energy diagram

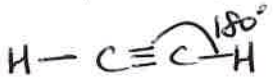




sp² C bond angles

~120°

Example #4 Ethyne (acetylene) C_2H_2



2x C–H σ-bonds
1 x C–C σ-bond
2 x C–C π-bonds

Polarity in bonds & molecules → electronegativity

- Non-polar: e⁻'s are perfectly shared

nonpolar bond

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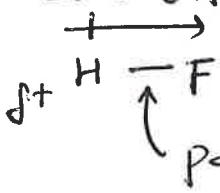
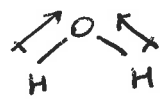
Bond dipole



polar bond!

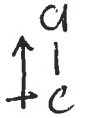
Molecular dipole - sum of bond dipoles

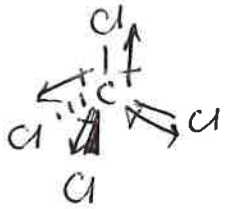


bond dipoles

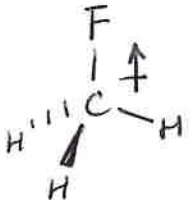
molecular dipole

Bond dipoles can cancel out!



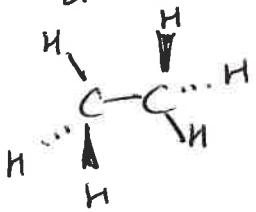


bond dipoles cancel out; NON POLAR



net dipole

C & H not very electronegative



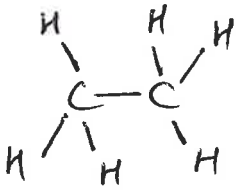
Each bond is non-polar

∴ Molecule is nonpolar

O, N, Cl, F, Br : more electronegative than C

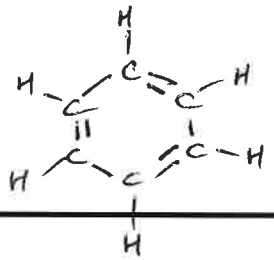
→ polar bonds

localized vs. delocalized bonding



each line = 1 bond = $2e^-$

Benzene C_6H_6



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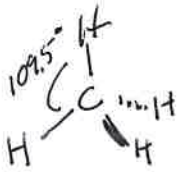
Recall: Bonding in organic molecules...

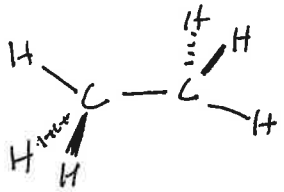
C atom valence shell: S + 3p → Hybridize AOs to be able to form 4 bonds... ⇒ 4 x sp^3

CH_4 = 

"tetrahedral geometry"

4 equivalent C–H bonds ("σ-bonds"; σ MO)

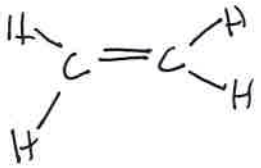
Ethane = C_2H_6



6x C–H σ-bonds
+
1x C–C σ-bond

} All angles ~ 109.5°

Example #3 = Ethene (Ethylene)

C_2H_4 

1 x C–C σ-bond
1 x C–C π-bond
4 x C–H σ-bond

σ-bonds (# bonding partners) determines mode of hybridization

Distribute s-character into only those AOs that engage in σ-bonds.

For C_2H_4, sp^2 hybridized C

sp^2 AO = 33% s / 67% p

3 x sp^2 AOs + 1 p-orbital for π bond

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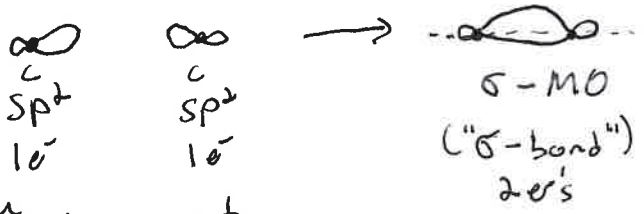
Bare down on the C=C double bond.

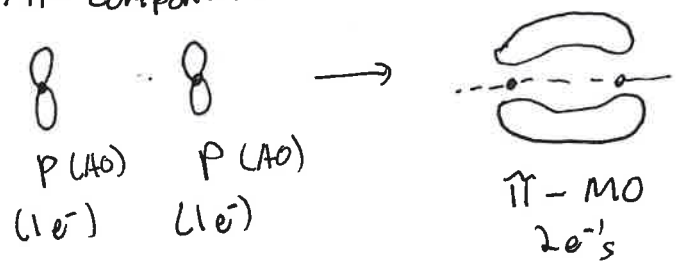
σ-component and π-component

Spatial characteristics:

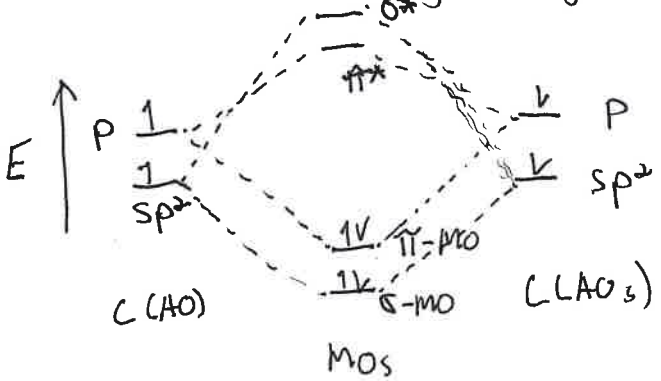
1) σ-component

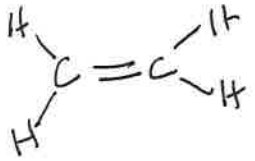


2) π-component



C=C bond energy diagram:





sp^2 C-bond angles ~120°

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Example #4 : Ethyne (Acetylene) C_2H_2

$H-C\equiv C-H$

2x σ C-H bonds

1x σ C-C bond

2x π C-C bonds

$H-C\equiv C-H$

180°

Polarity in bonds and molecules

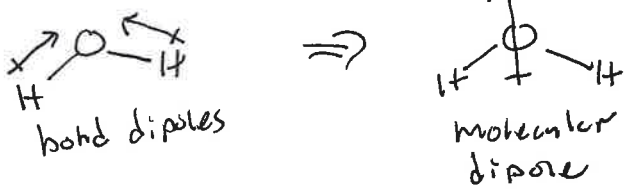
→ Electronegativity

"Non-polar" = e⁻'s are perfectly shared ex; H–H, F–F (non polar bond)

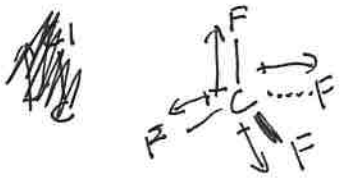
but → $\overset{\delta+}{H}-\overset{\delta-}{F}$ (δ⁻ partial negative; polar bond; δ⁺ partial positive)

H–F contains a bond dipole

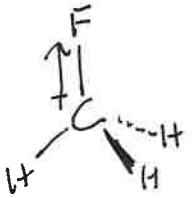
Molecular dipole – Sum of bond dipoles



Bond dipoles can cancel out.



The bond dipoles cancel out. Non-polar molecule



net dipole

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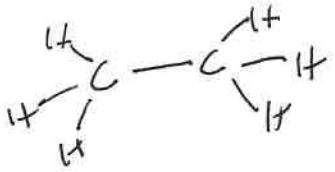
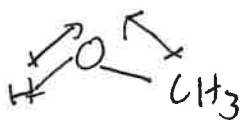
C and H are not very electro negative

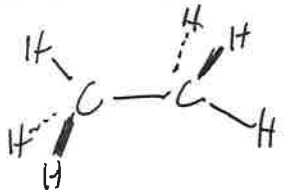


C-H bond is non-polar, molecule is nonpolar.

O, N, Cl, F, Br ⇒ more electronegative than C ⇒ polar bonds.



Localized vs. Delocalized bonding



each line stands for 1 bond = 2 e⁻'s. Localized bonds.

Benzene C_6H_6