Course 343 Lecturer Hackenberger

Day Monday Date 09/09/13

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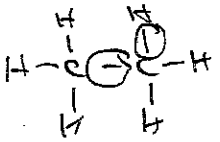
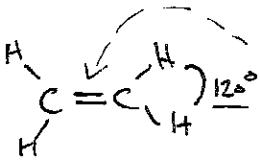
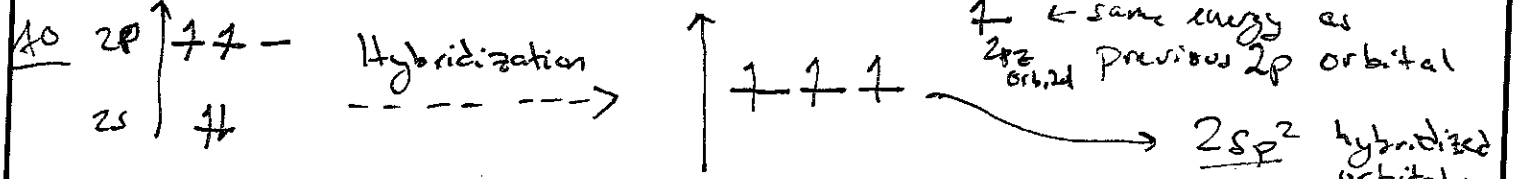
Last Lecture:

- atomic & molecular orbitals (AO) & (MO)
- σ bonds (MO)
- energy change and spatial discription of MOs
- alkanes contain different C-H and C-C σ bonds

Ethane C_2H_6  molecule is an alkane

Ethene (Ethylene) C_2H_4  double bond σ bond (C-C) π bond (C-C)

In order to use MO Theory, we hybridize 3 AO from our C, and leave one of them not hybridized



← same energy as previous 2p orbital

Spatial character of sp^2 AO

 sp^2 more s character, more electron density at nucleus (compared to sp^3)

the 3 sp^2 hybridized AO's, make 3 σ bonds

the 2p orbital makes a π bond

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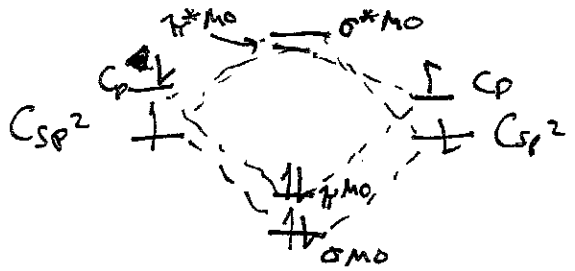
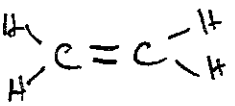
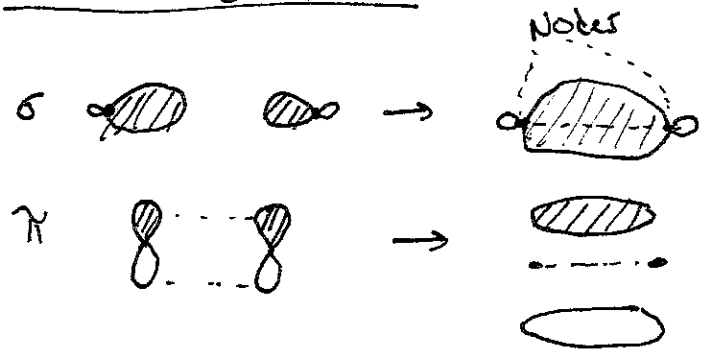
MO Diagrams: C–C σ bond + C–C π bond





π $e^{\ominus}$ are higher in energy than σ $e^{\ominus}$

Spatial Diagrams



Ethyne C_2H_2 type of alkyne – triple bond

2 π bonds

H–C≡C–H

1 σ bond

2 π bonds

σbond σbond

AO

2p ↑ ↑ —

2s ⇅

hybridize ---> Sp

50% s character

50% p character

hybridize 2 AO, leave 2 AO unchanged

Geometrical Consequences of hybridization

Sp^3 109.5° sp^2 120° Sp 180° } angle between σ bonds

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Bond length — more e⁻ shared, the shorter the bond

C–C	1.54 Å	nuclei are closer together
C=C	1.33 Å	
C≡C	1.20 Å	

Heteroatoms (atoms other than carbon) (O, N, Cl) in C-molecules

Polarity in bonds Table p.9

Electronegativity in different atoms – heteroatoms drastically d.ff in E/N

this difference results in different e⁻ distributions in bonds, thus they become polar and a dipole moment is generated.

μ (unit of dipole moment)

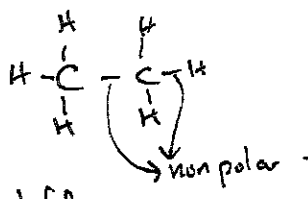
Different extremes: 1) identical atoms → H-H, Cl-Cl

nonpolar compounds

2) very different EN values $Na^{\oplus}\ Cl^{\ominus}$ → ionic bond (salt, polar)

In organic molecules we have both polar + non-polar bonds

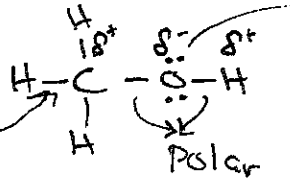
ethane



nonpolar

E/N diff. < 0.3

methanol CH_3OH



lone pairs → 2 filled orbitals on O

Polar

O has high E/N value 3.4, 2nd most E/N

δ & δ^+ → partial charges

both C–O & O-H bonds are polar

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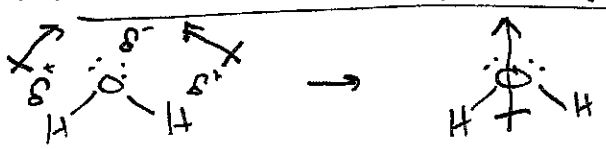
Differentiate bond and molecule dipole



Dipole of bond dipole moment of whole molecule

arrows are vectors so depend on direction