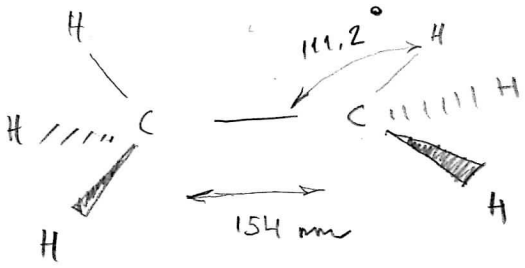
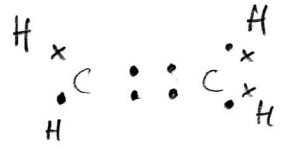
20160916

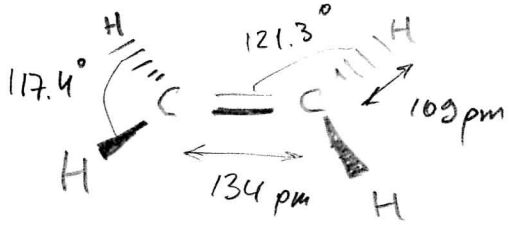
CHM 151: VB Theory II & MO



sp^2 Hybrid Orbitals:



ALKENE



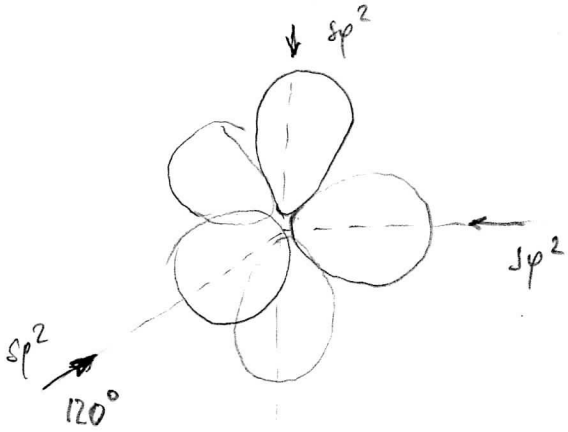
THE DOUBLE BOUND IN ETHYLENE IS MADE UP OF A σ BOND

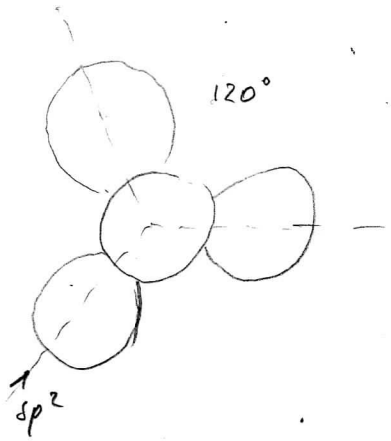
$\therefore$ sp^2-sp^2 HEAD-ON OVERLAP

AND

A π BOND

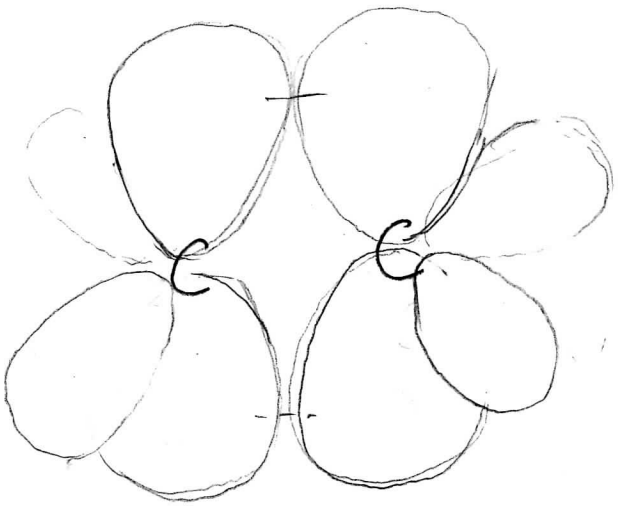
$\therefore$ p-p SIDE-ON OVERLAP



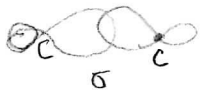


BONDING IN ETHYLENE

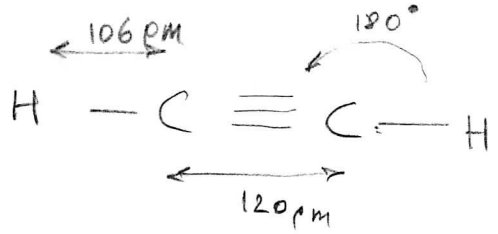
π BONDING



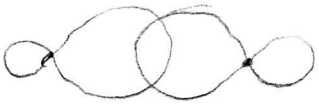
σ BONDING



sp HYBRID BONDING

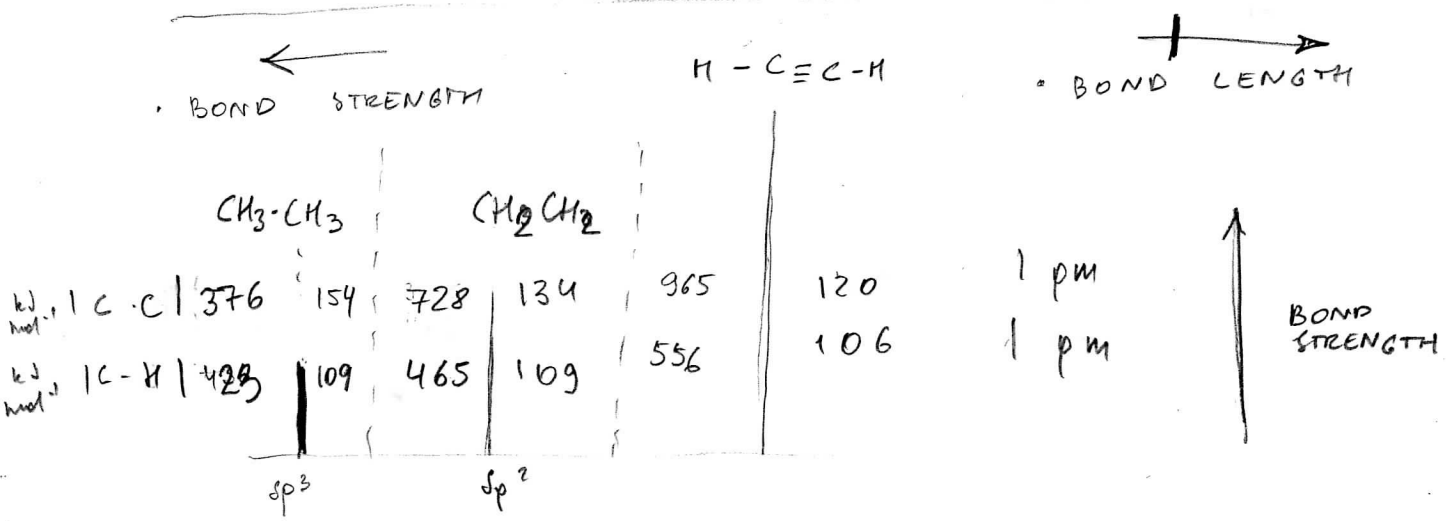


2 × π BONDING



σ BONDING

TRENDS IN C-C BOND STRENGTH & LENGTH



C = C > C-C ;; NOT 2x

C ≡ C > C-C ;; NOT 3x

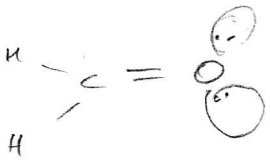
HYBRIDIZATION OF HETEROATOMS

! KEEP TRACK OF LONE PAIRS

EXAMPLE

METHYLAMINE

FORMALDEHYDE



METHANOL

vs

109.5° CH_4

HOW MANY GROUPS ARE BOUND TO THE ELEMENT INVOLVED?

# OF GROUPS AROUND ATOM	# ORBITALS USED	TYPE OF HYBRID ORB
4	4	sp^3
3	3	sp^2
2	2	sp

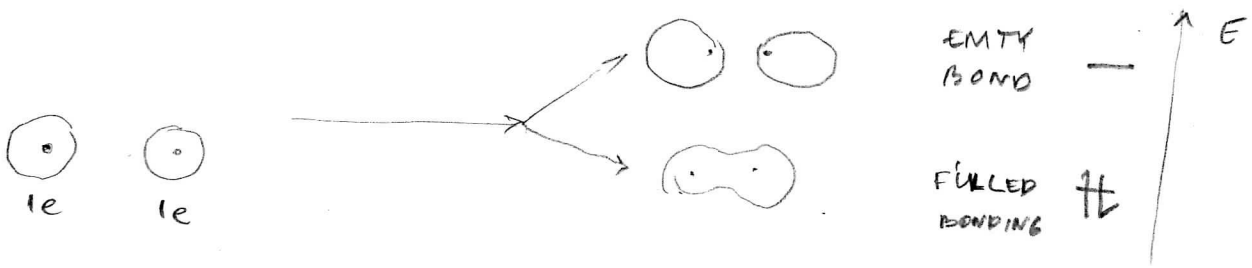
MOLECULAR ORBITAL THEORY

MATHEMATICAL COMBINATION OF ATOMIC ORBITALS ON DIFFERENT ATOMS GIVES RISE TO MOLECULAR ORBITALS

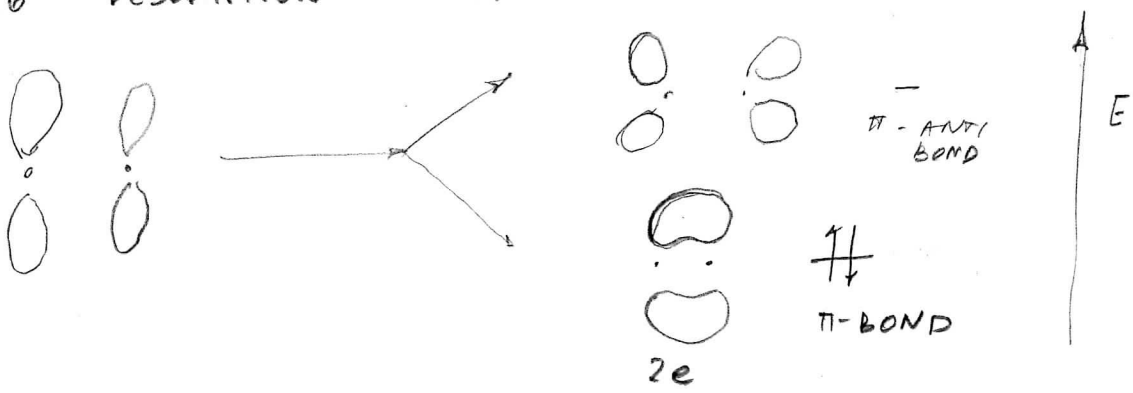
! NOT THE SAME AS VB THEORY

4. CONCEPT OF ANTIBONDING ORBITALS ORIGINATES FROM MO THEORY
2. MO THEORY IS ABLE TO DESCRIBE BONDING THAT IS NOT WELL DEPICTED BY A SINGLE LINE STRUCTURE.

EXAMPLE



MO DESCRIPTION OF DOUBLE BOND



→ MORE ON BONDING AFTER DISCUSSING ALKANES AND CYCLOALKANES

DRAWING CHEMICAL STRUCTURES

n-butane:

$CH_3CH_2CH_2CH_3$