

Bonding in Organic Molecules and Reactivity

- ✓ Valence Bond Theory (VBT): Resonance, Hybridization
 - ✓ Molecular Orbital Theory (MOT): Molecular orbitals
-
- Organic chemists like to use the concept of hybridization and resonance whenever possible
 - Molecular Orbital Theory is more sophisticated and more precise
 - However, *in many instances a better picture of bonding is described by combining the hybrid approach with delocalized MO approach*

Course Content for my part

- ✓ Hybrid Atomic Orbitals (VBT)
- ✓ Conjugation and Delocalization (VBT / MOT)
- ✓ Molecular Orbitals and Organic Reactions

S_N1 and **S_N2**

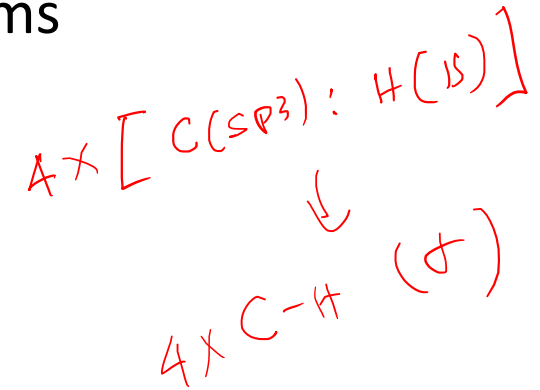
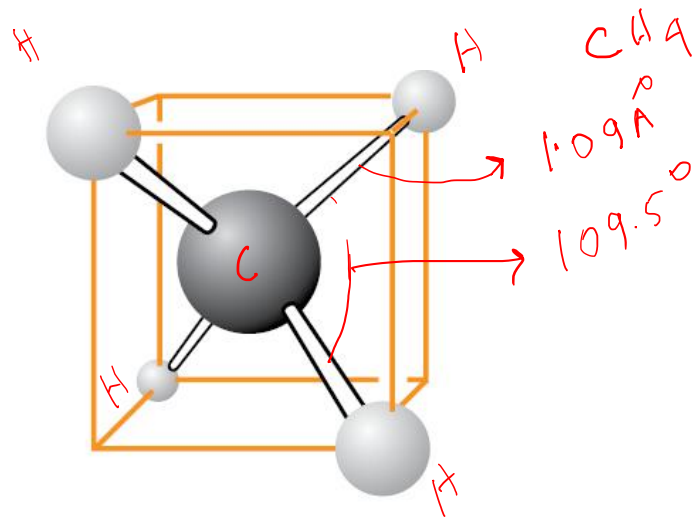
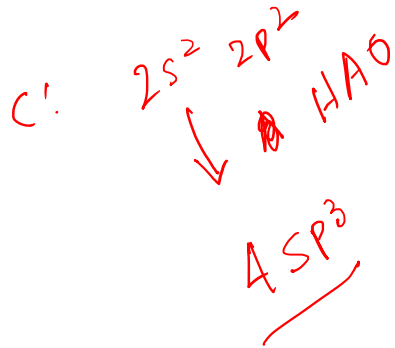
Study Material

First 3 classes: Mostly from Keeler-Wothers, 2nd Edition (Chapter 5)

❖ **Page 164 to 176**

Hybrid Atomic Orbitals

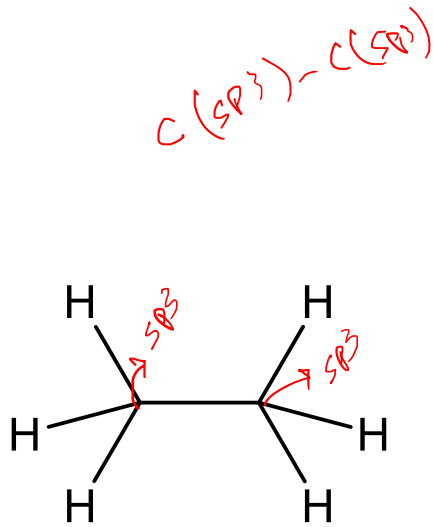
- ✓ As CH_4 is tetrahedral, we should construct some new orbitals on the carbon that point towards the corners of a tetrahedron
- ✓ The important thing is that we're combining the AOs from the same atom, in contrast to when MOs are formed where we combine AOs from different atoms



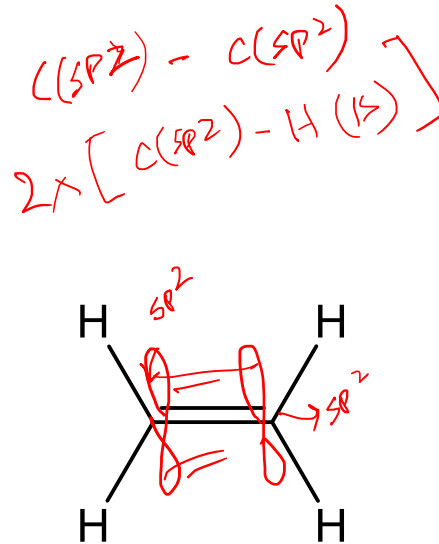
a molecule of methane
enclosed in a cube

Bonding In Organic Molecules

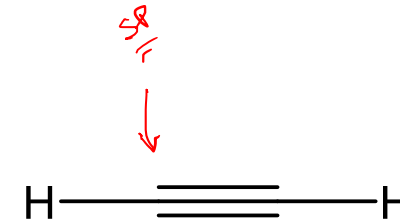
- ✓ Hybrid orbitals to describe the bonding in organic molecules
- ✓ In reactions, the form of HOMO and LUMO are quite important (we will see later)



Ethane

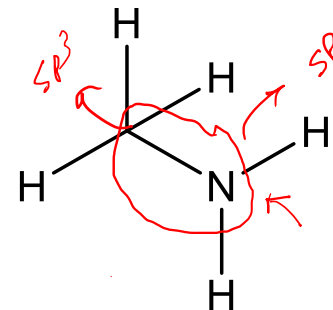
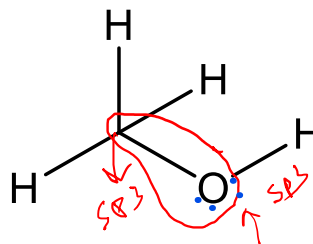
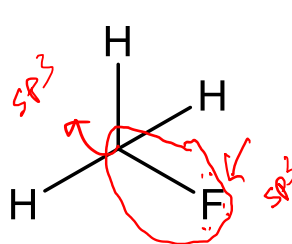


Ethylene

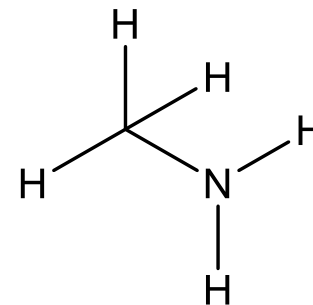
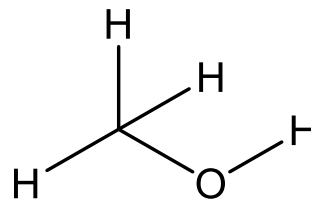
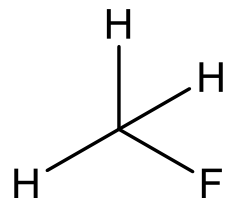
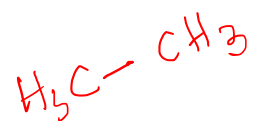


Acetylene

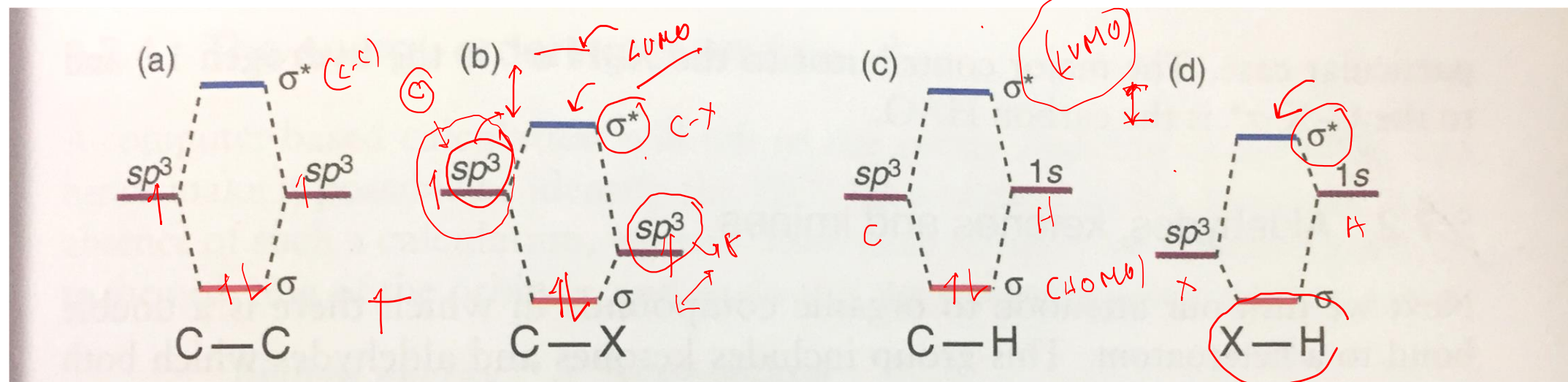
Halides, Alcohols and Amines



- ✓ CH_3F , CH_3OH and CH_3NH_2 : 3 very common organic molecules
- ✓ The arrangement of atoms around the carbon is close to tetrahedral: sp^3 hybridized
- ✓ We will also assume the heteroatom (F, O and N) are also sp^3 hybridized
- ✓ In all the molecules, the HOMO is essentially one of the heteroatom hybrid atomic orbitals not involved in bonding
- ✓ LUMO are σ^* antibonding MOs associated with C-H, X-H and C-X bonds.

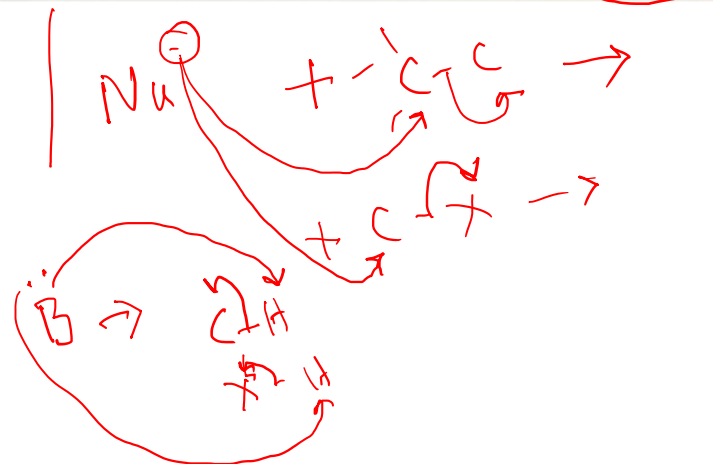


EN
C: 2.5
N: 3.0
O: 3.5
F: 4.0



✓ σ^* (C-X) is lower in energy than the σ^* (C-C)

✓ σ^* (X-H) is lower in energy than the σ^* (C-H)



Handwritten red annotations: "SOMO" with arrows pointing to the σ^* orbitals in diagrams (b) and (d). Below are circled numbers: 4, 4, 4.

4e