Lecture 1: Introduction & Bonding Theories

Note Title 8/29/2016

Outline:

1) Syllabus

2) What is Physical Organic Chemistry?

3) Theories of Structure & Bonding

Announcements:

1) Problem Set 1 due Thurs, 9/8

2) Department Colloquium: Prof. Lars Gundlach, Fri, 9/2, 4pm, 101 BRL

What is Physical Organic Chemistry?

A & D : study of interrelationships between structure & reactivity of molecules

Mechanism : theory deduced from available experimental data.

↑ The facts.

↑ "conjecture based upon these facts"

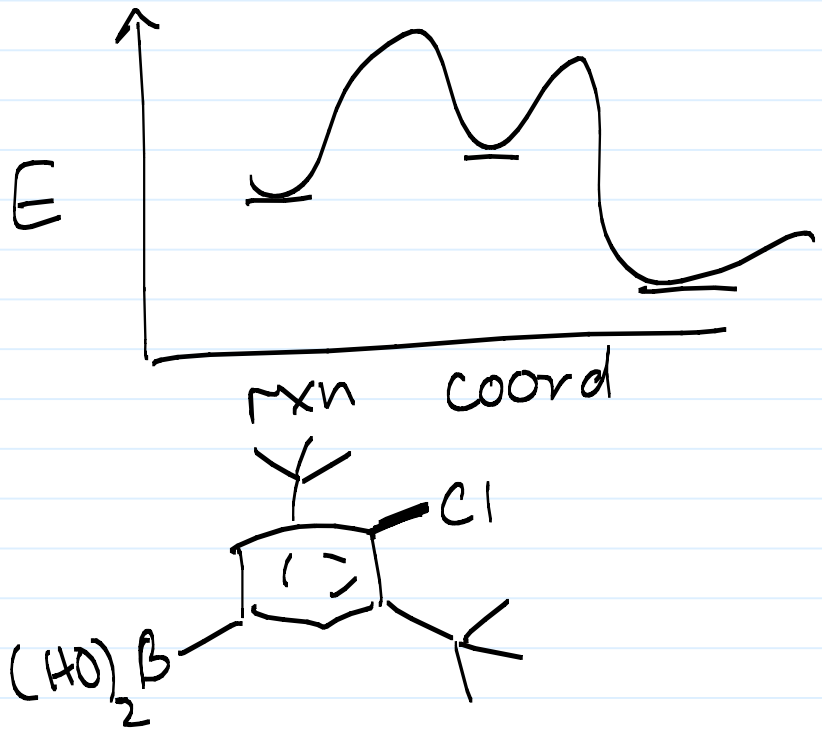
∴ Valid mech = simplest rationalization consistent w/ all data.

Corrolaries:

1) Should provide testable predictions.
2) can never be proven (can be disproven)
3) should obey Ockham's razor.

Simplest mech not always right, but priortized until disproven.

Structure & Bonding Theories



energies, structure } ground states

↓

SM, Pdts, intermediates

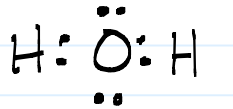
&

transition states

Valence Bond Theory

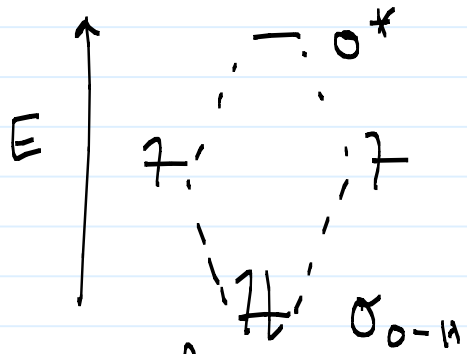
H_2O

Lewis dot structure

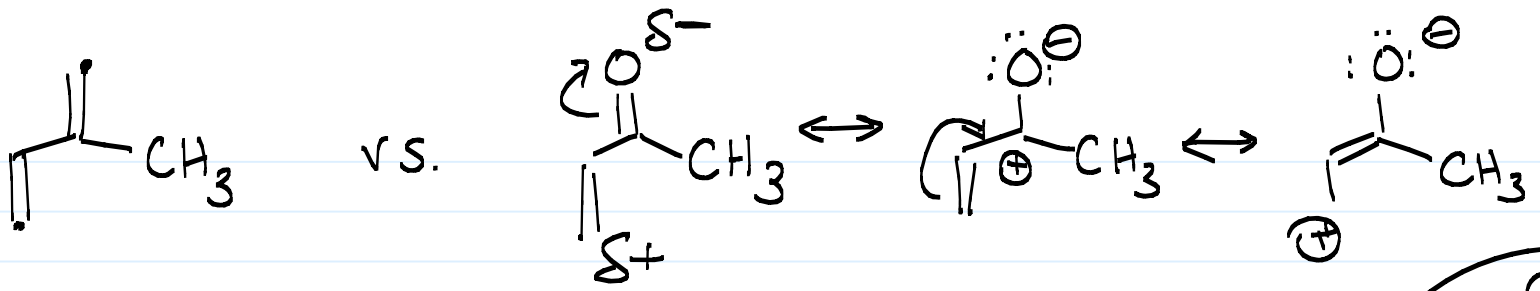


↳ localized bond (covalent)

↳ equal sharing = 2 e⁻s between atoms = bond



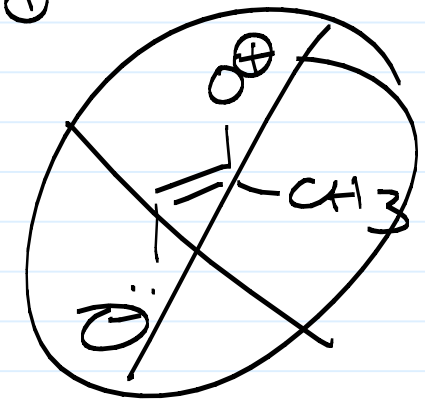
↳ octet rule



e-s are not shared evenly

ELECTRONEGATIVITY

Pauling EN Scale: 0.7 — 4.0 ← F

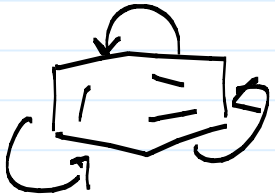


Covalent vs. Ionic Bonds

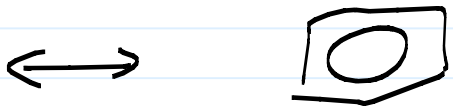
$\Delta < 1.5$ $\Delta > 1.5$

C = 2.5 ⇒ All bonds to C have <u>covalent character</u>.

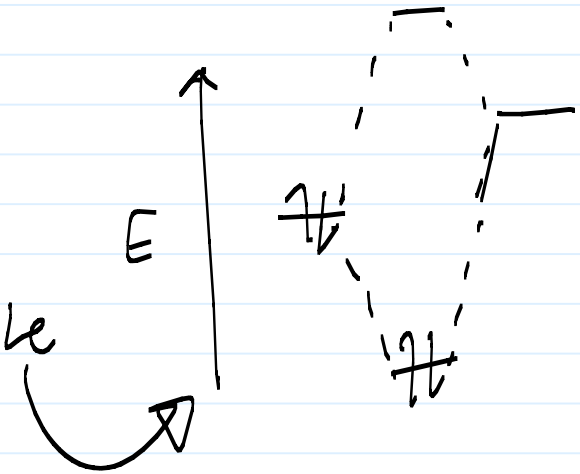
Resonance



≠ 3 single bonds + 3 double bonds

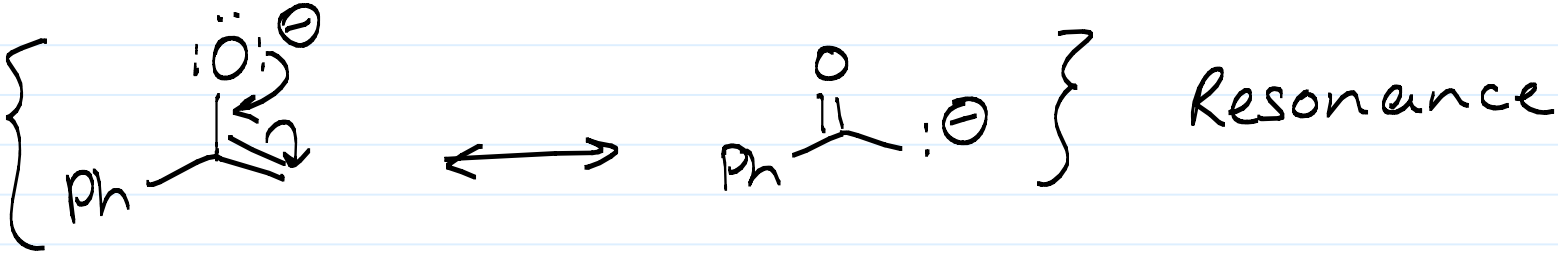


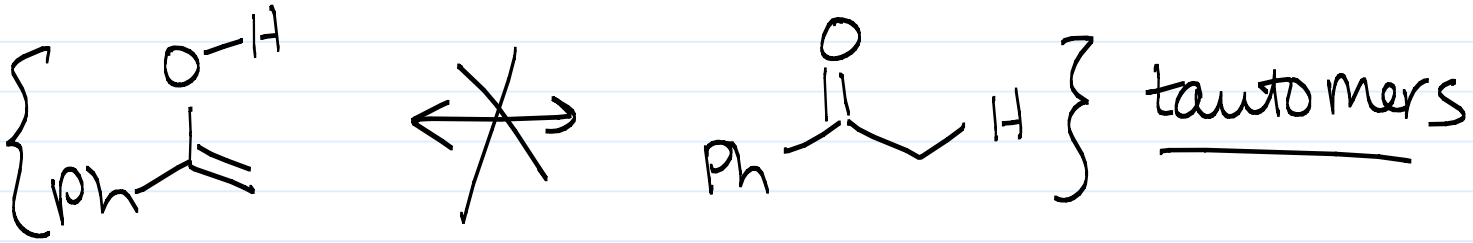
Delocalize e^- density => more stable



Rules of Resonance

1) No nuclear movement

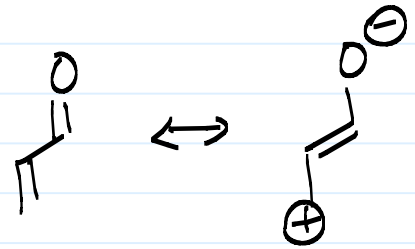




2) e⁻ density on more EN atom

3) maximize # of bonds

4) minimize charge separation



5) Complete octets

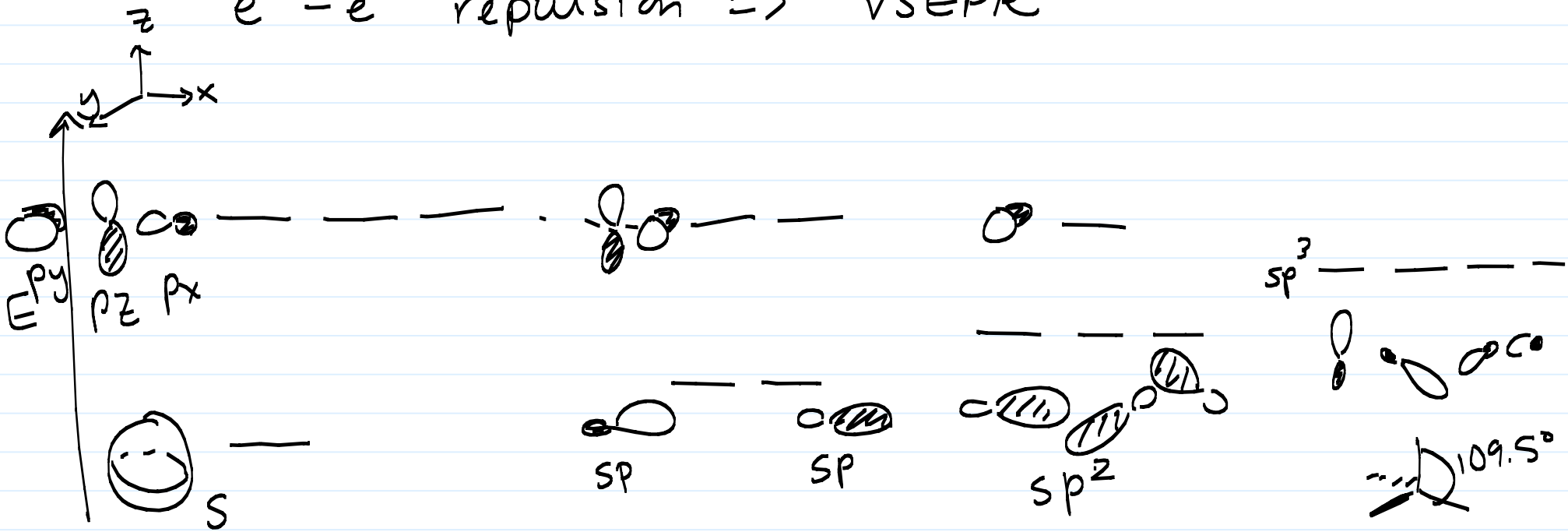
6) Structural requirements

Hybridization

↳ way to fit the data

↳ predict molecular shape by orienting lp's & bonds away from each other.

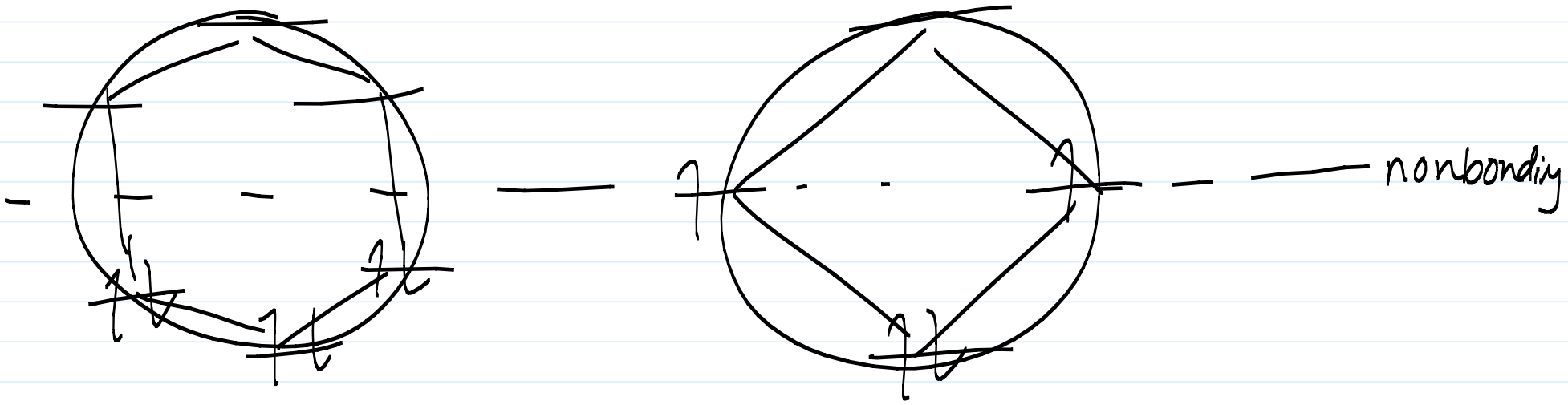
$e^- - e^-$ repulsion ⇒ VSEPR



stable

unstable

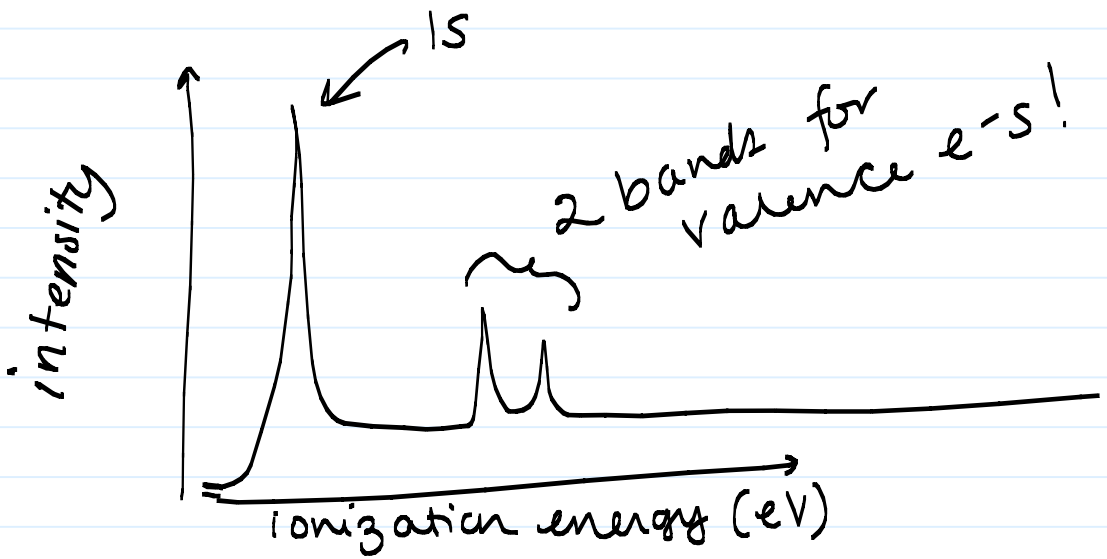
Molecular Orbital Theory



CH_4 : Valence Bond Theory

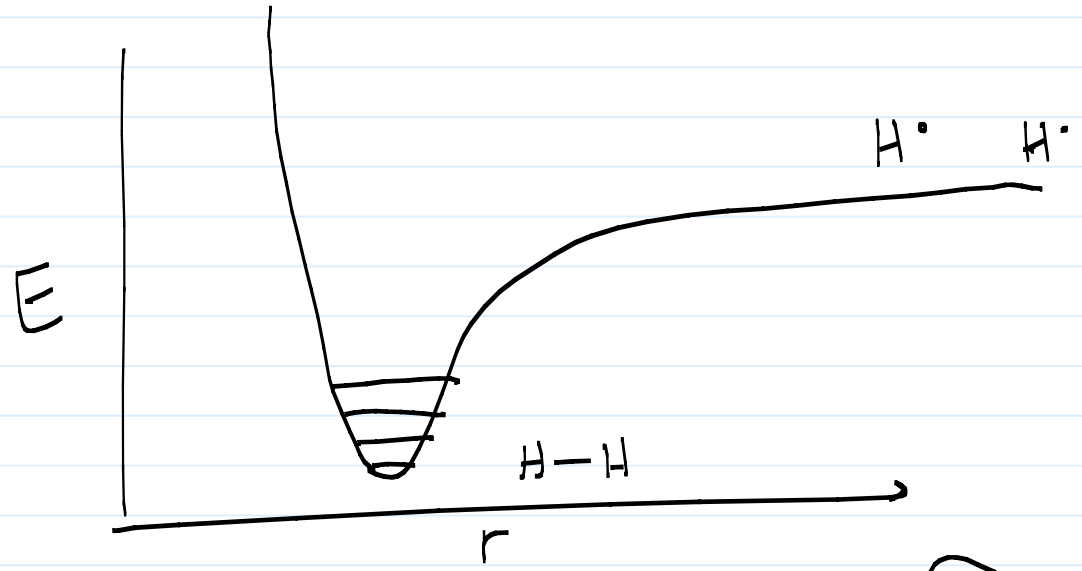
Valence $4\ sp^3$ (C) + $4\ s$ (H) $\longrightarrow$ 4 C–H

core: $1s^2$ $\longrightarrow$ 2 energy levels



H_2 :

Perturbation Theory



Atomic Orbitals

$H_{1s} + H_{1s}$

$\Downarrow$

$\psi_1 + \psi_2$

$\psi_1 = c_1 H_{1s} + c_2 H_{1s}$ in phase bonding

$\psi_2 = c_1 H_{1s} - c_2 H_{1s}$ out of phase antibonding