

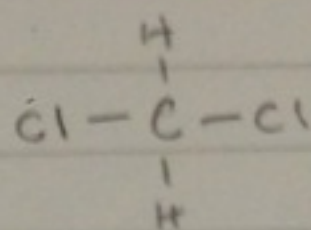
Unit 3 Day 4

- Why does a frog float in a magnetic field?
- IM 22/23 due Thurs. 9AM

Clicker question

Is the molecule CH_2Cl_2 ?

a) polar



Given a tetrahedral electronic geometry, which of the following hybridizations is possible?

a) sp^3

Molecular Orbital theory

- VB

- it's the bonds

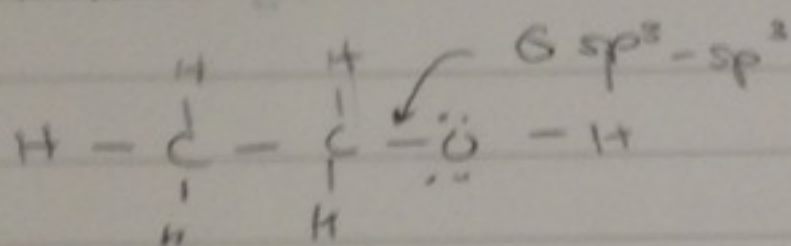
- "local"

- molecular thinks about the whole molecule

- mix atoms on all

- atom in molecule

- Ethanol $\text{C}_2\text{H}_5\text{OH}$



paramagnetic

• unpaired e⁻

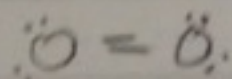
• attraction

diamagnetic

• paired

• repel

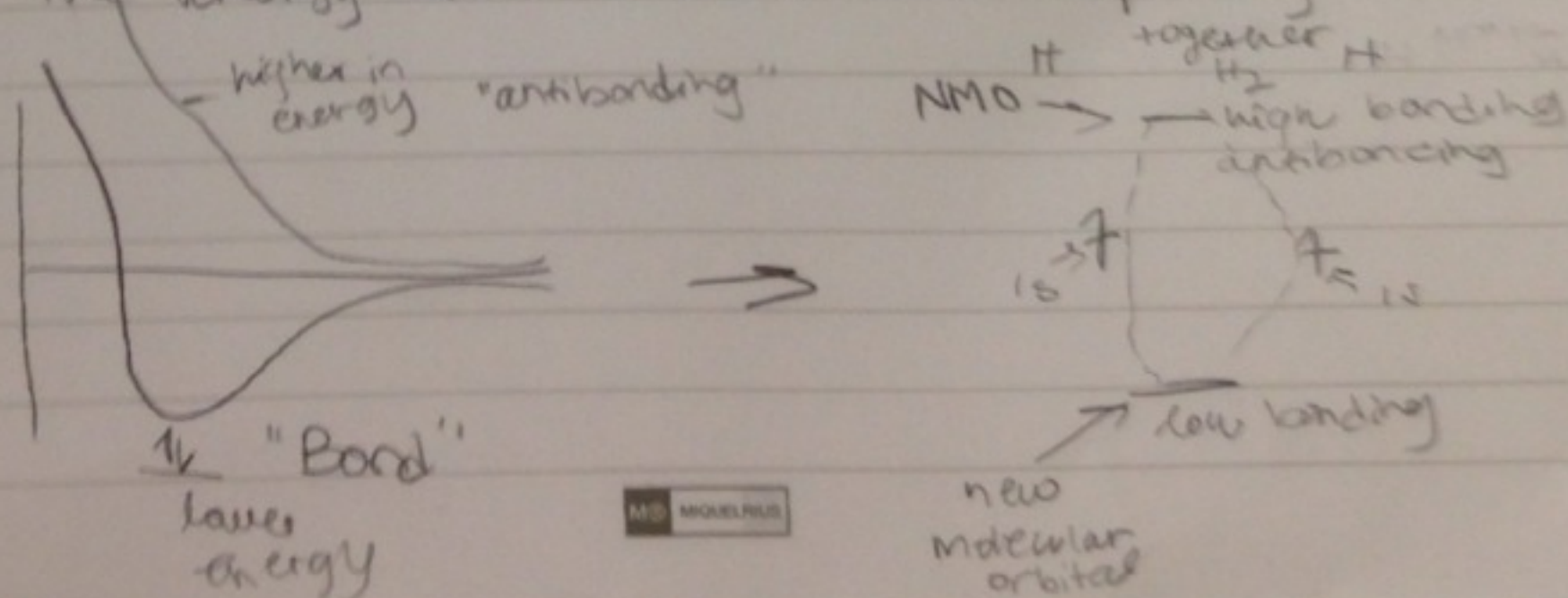
- Diatomic oxygen



paramagnetic

What is the bond strength/length of H_2 ?

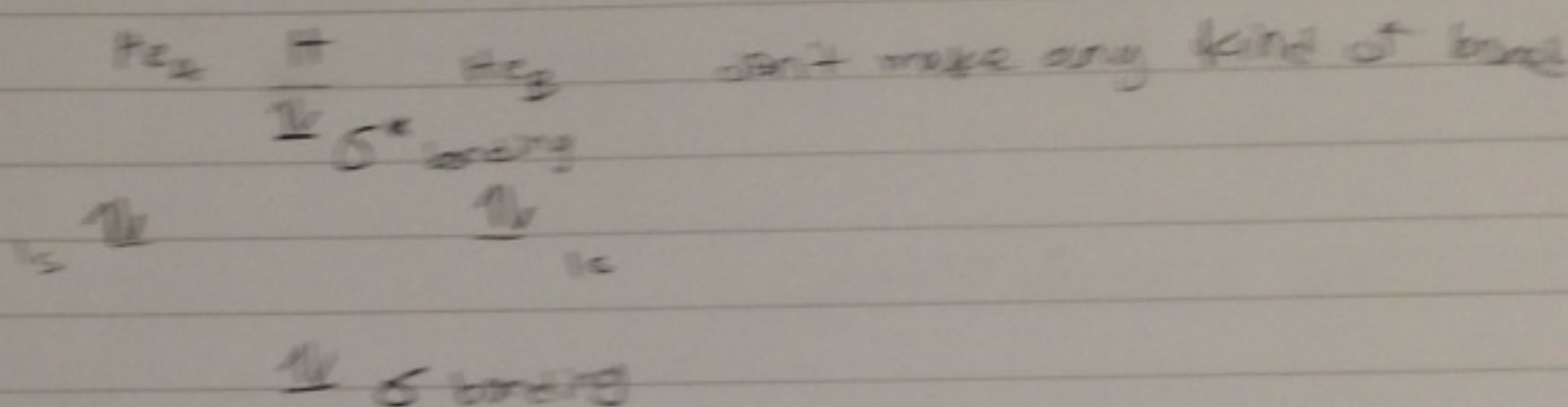
What is the energy of the molecule when pulling them apart?



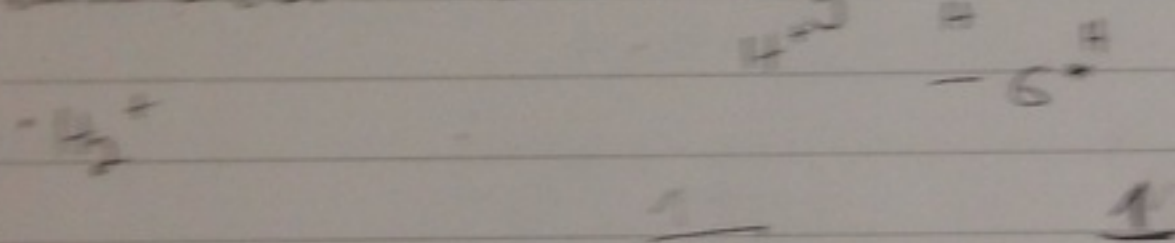
Things about MO

- combine atomic orbitals, $\frac{1}{2}$ time low energy / $\frac{1}{2}$ time high energy
- e⁻ have wave function
- constructive & destructive interference

What does the e⁻ config for H₂ look like?



bond order = $\frac{1}{2} (\# \text{ bonding} - \# \text{ antibonding})$



$$BO = \frac{1}{2}(1 - 0) = \frac{1}{2}$$

- bond order tells us bond strengths

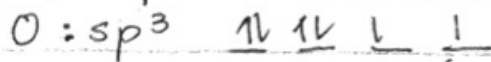
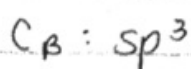
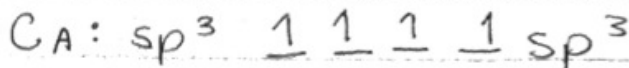
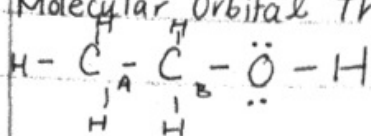
- high occupied MO } where all the chemistry occurs; lowest ant. of
- lowest unpaired MO } excitation

- Most molecules have have

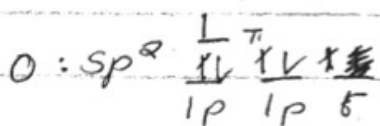
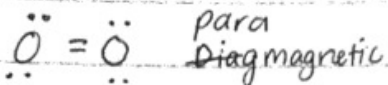
- an even # of e⁻
- diamagnetic

Molecular Orbital Theory

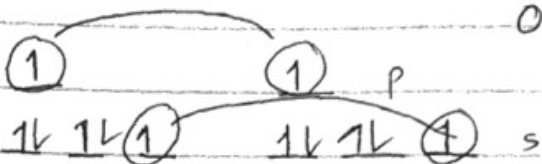
Ethanol



Diatom. O

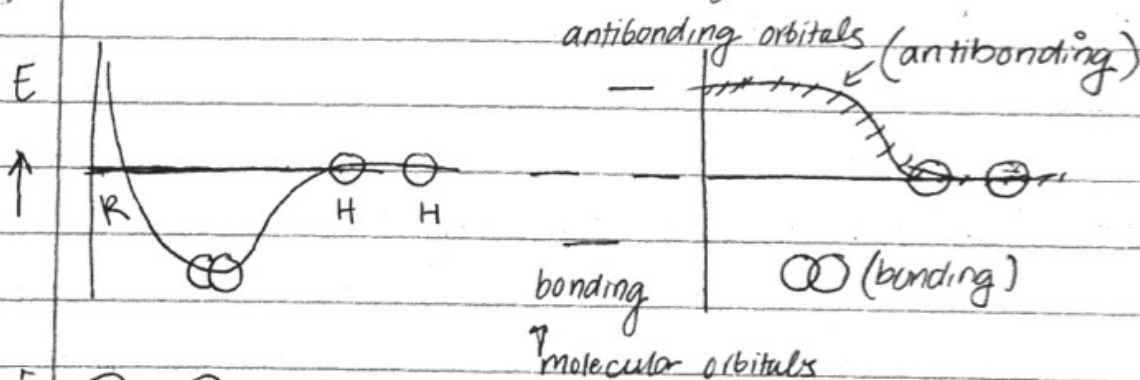


available for sigma bond



Molecular Orbital
de-localized

What is bond str + bond length in H₂?



H	H ₂	H	
1s	σ _{1s} *	1s	
1	1↓ σ _{1s}	1	

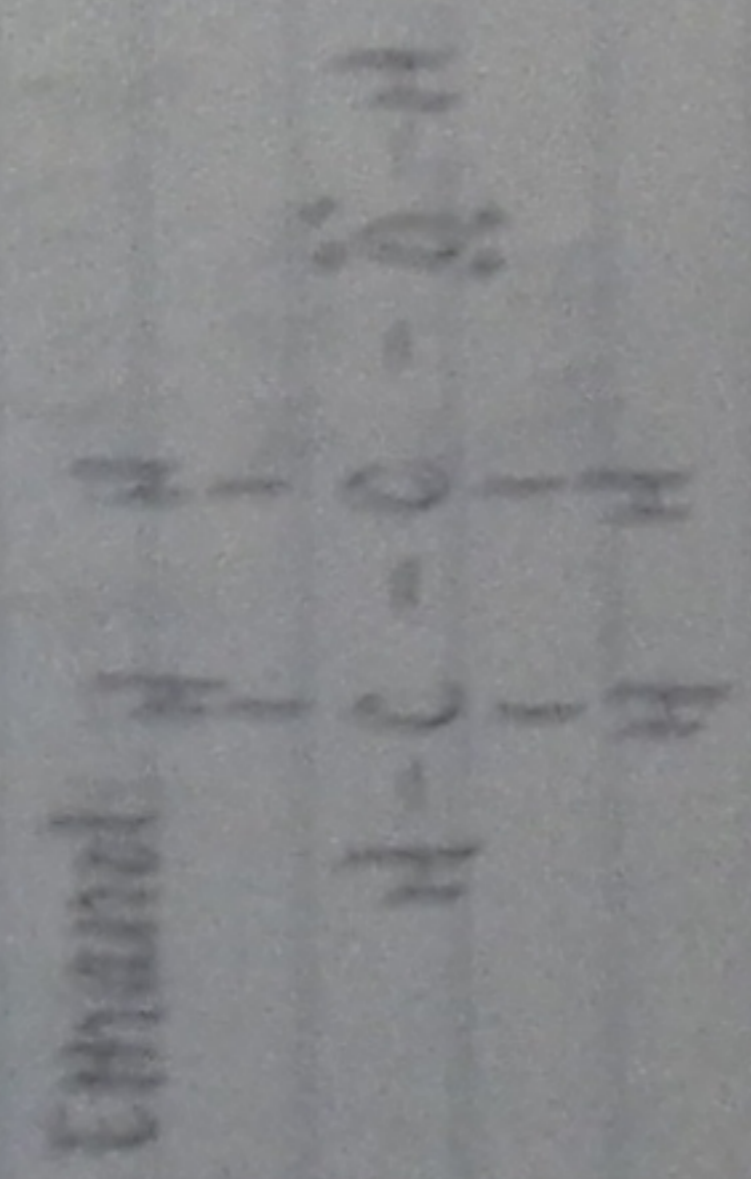
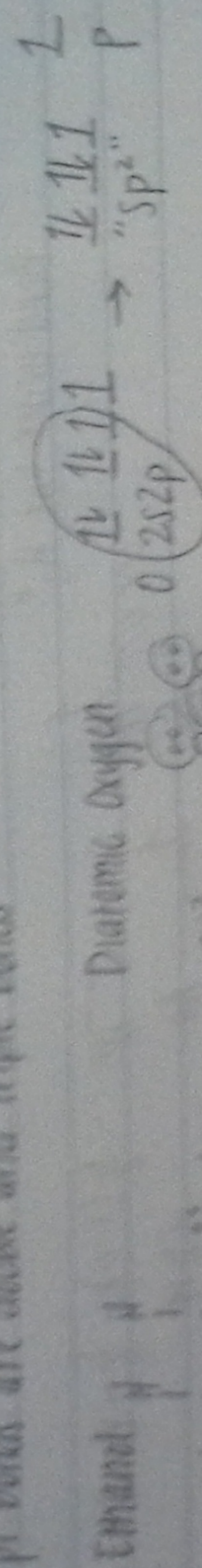
combine atomic orbitals, 50% higher E
50% lower E

constructive interfer σ
destructive interfer σ*

2/12/22

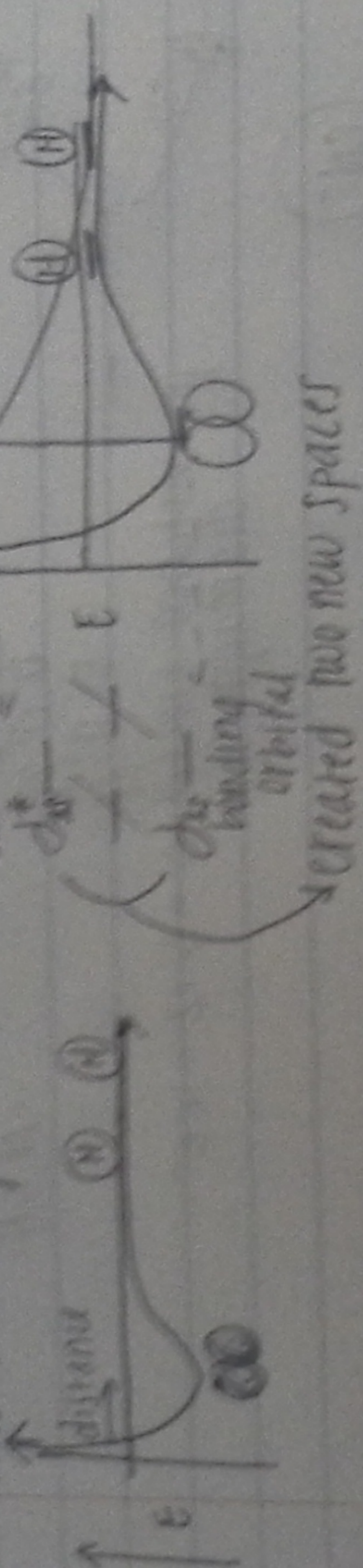
CH₂Cl₂ $\begin{matrix} \text{:Cl:} \\ | \\ \text{H}-\text{C}-\text{H} \\ | \\ \text{:Cl:} \end{matrix}$ tetrahedral given a tetrahedral electronic geometry, which hybridization is possible? sp^3

sigma bond is lone pairs and single bonds
pi bonds are double and triple bonds

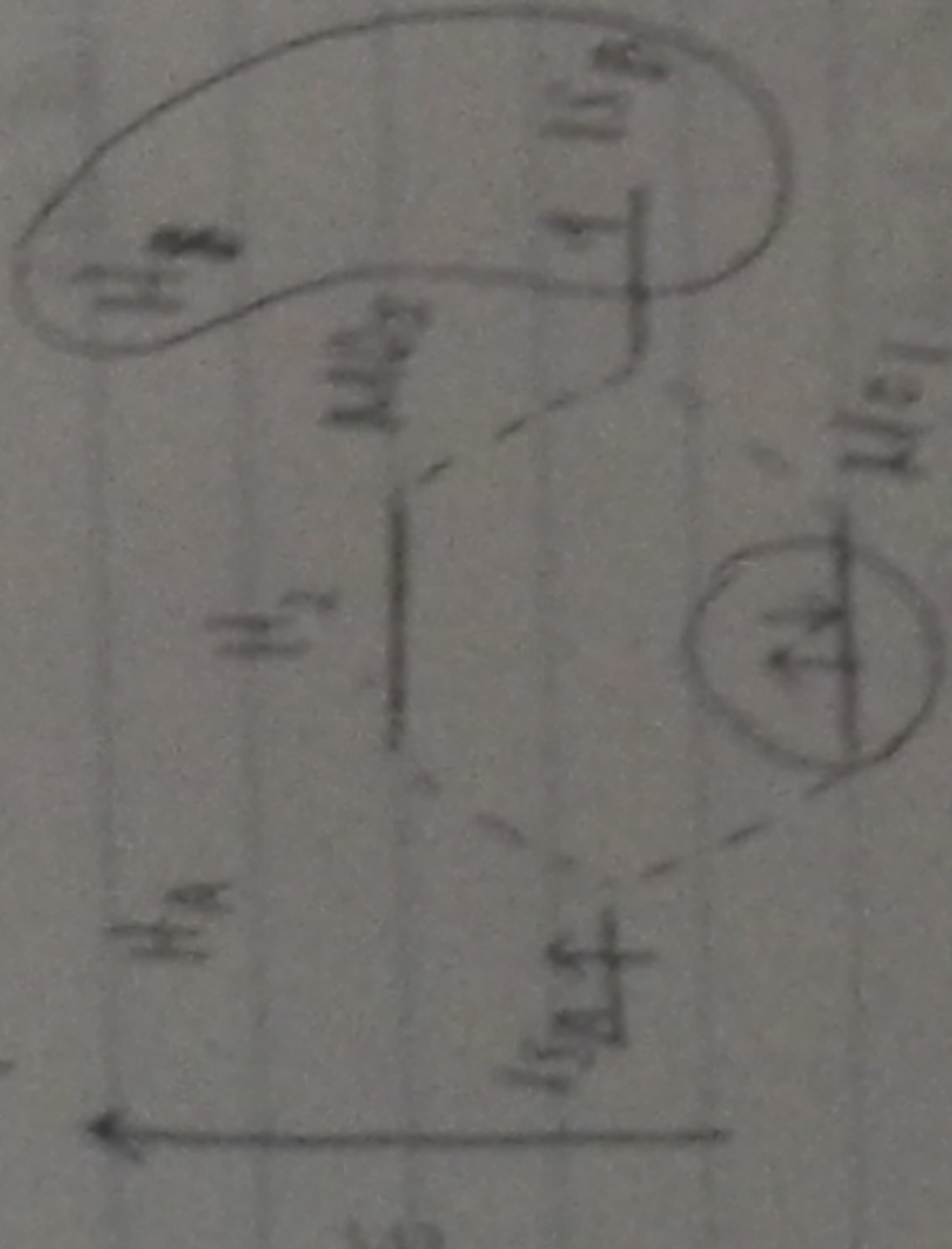


VB: Valence Bond theory is a localized theory, looking at each individual atom
MB: Molecular orbital Bond theory is de-localized, mixing all regions

What is the bond strength and bond length in H₂?
How can we get that?

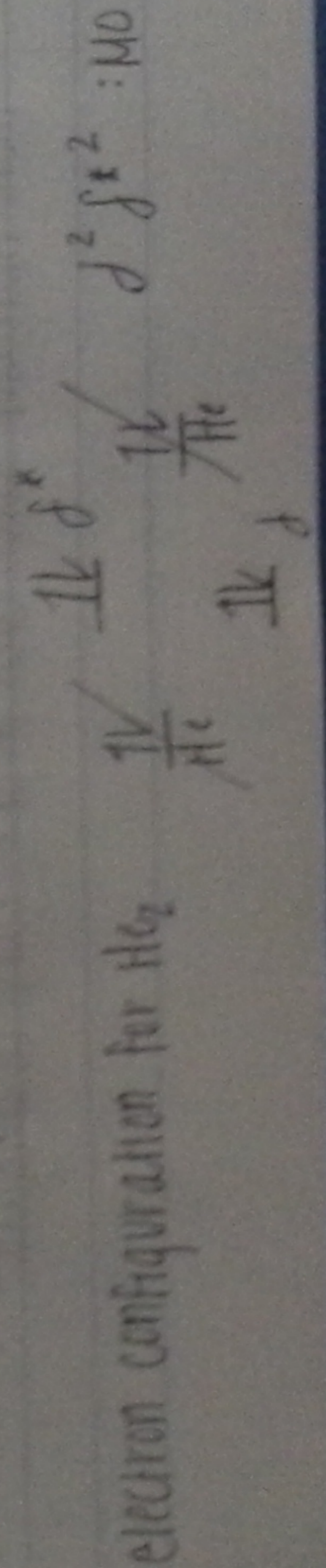


Compare MO to VB for H₂



- combine atomic orbitals, 1/2 the time
you get higher and 1/2 the time
you get lower energy

get smaller as they move closer



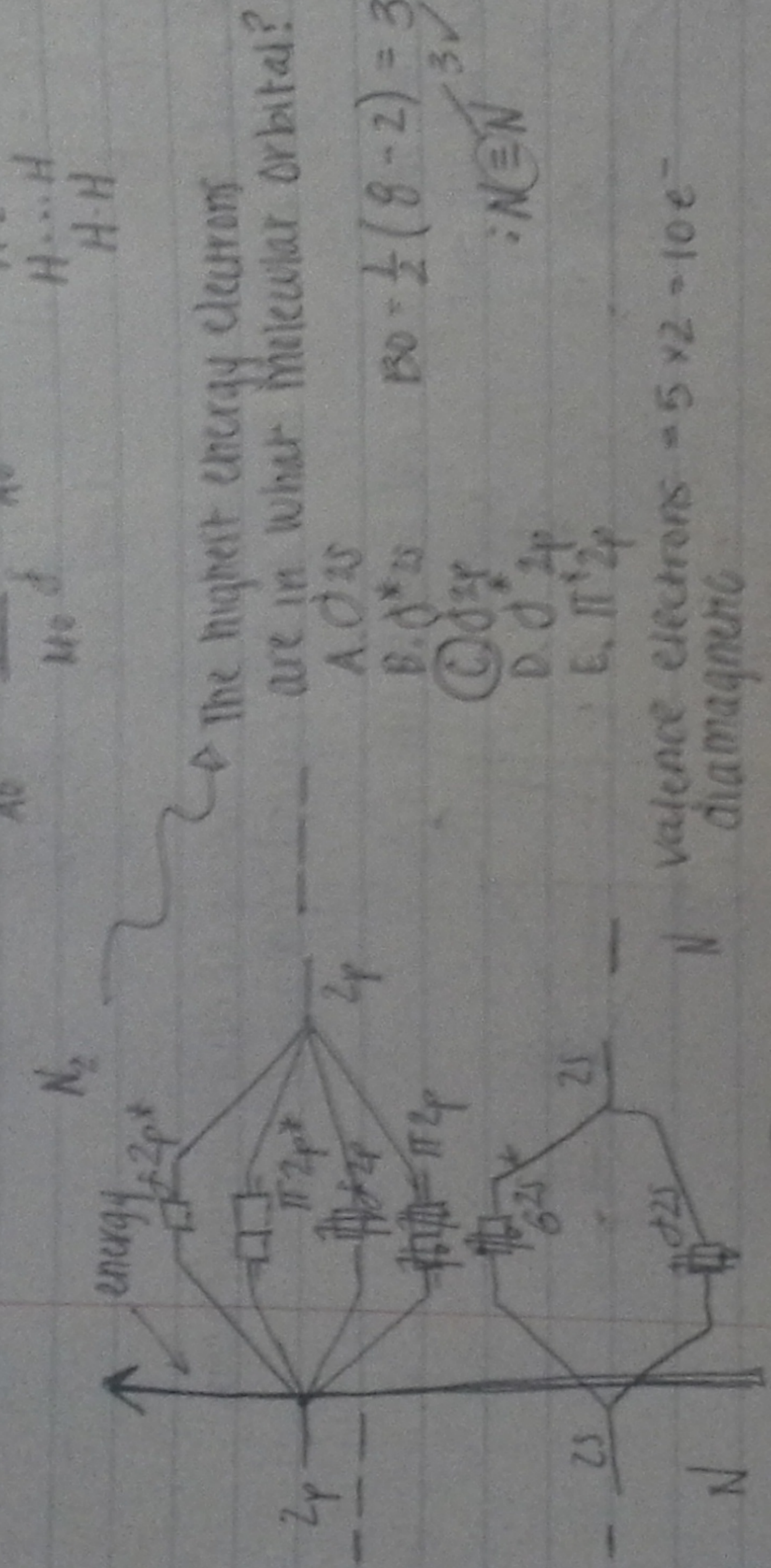
electron configuration for H₂

$\sigma^2 \sigma^{*2} : MO$

Bond order = $\frac{1}{2} (\# \text{ Bonding} - \# \text{ Antibonding})$
 ↑ bond order, ↑ bond strength
 He_2 Bond Order = $\frac{1}{2} (2 - 2) = 0$ not possible

Bond order for H_2^+
 $\frac{1}{2} (1 - 0) = \frac{1}{2}$ = Bond order

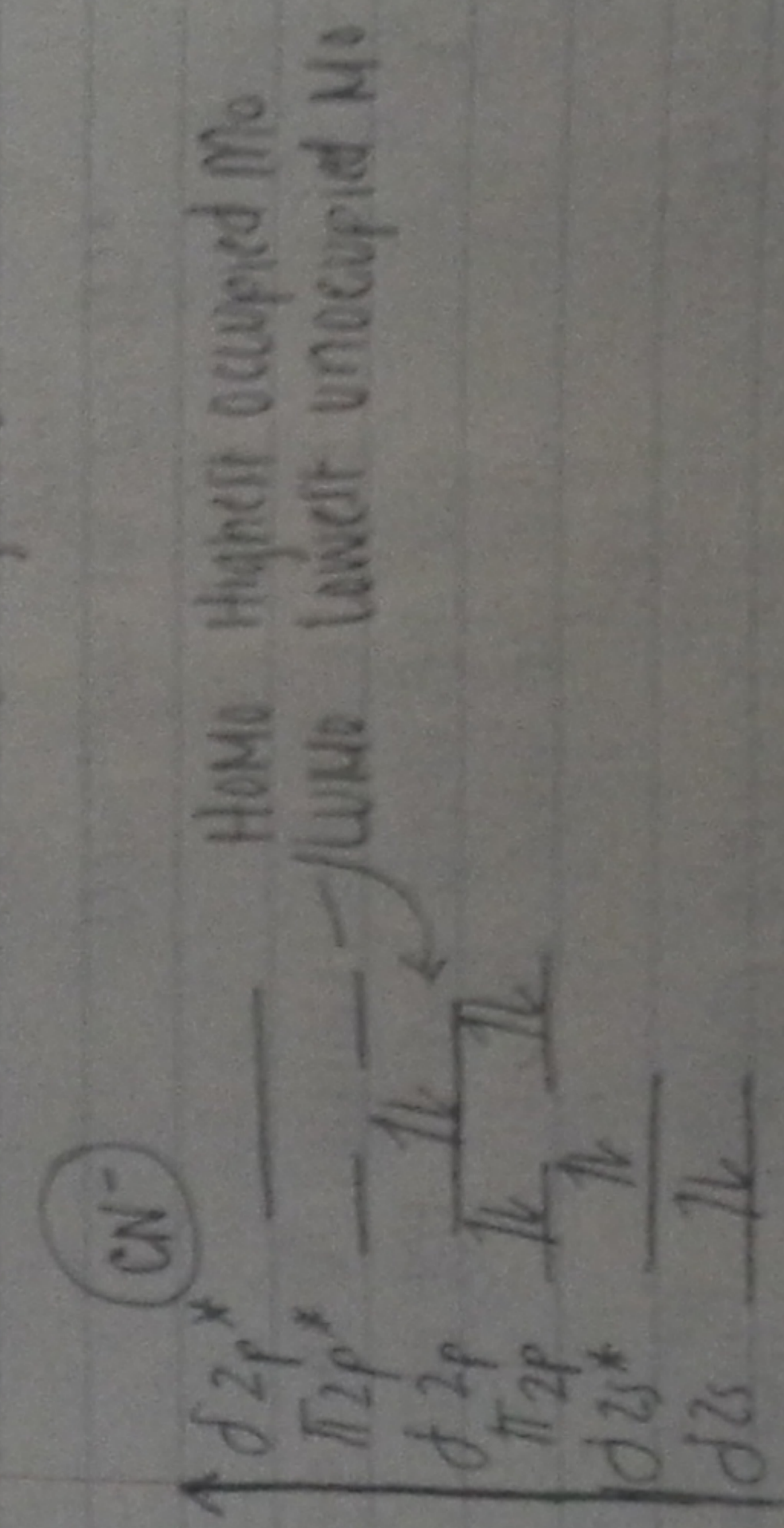
$\text{H} \quad \text{H}^+$
 $\text{A}_0 \quad \text{A}_0$
 $\frac{1}{2} \quad \frac{1}{2}$
 $\text{H} \frac{1}{2} \text{H}$
 $\text{H} \cdots \text{H}$
 $\text{H} \cdot \text{H}$



The highest energy electrons are in what molecular orbital?
 A. σ_{2s}
 B. σ_{2s}^*
 C. π_{2p}
 D. σ_{2p}
 E. π_{2p}^*

Answer: C. π_{2p}

valence electrons = $5 \times 2 = 10 e^-$
 diamagnetic



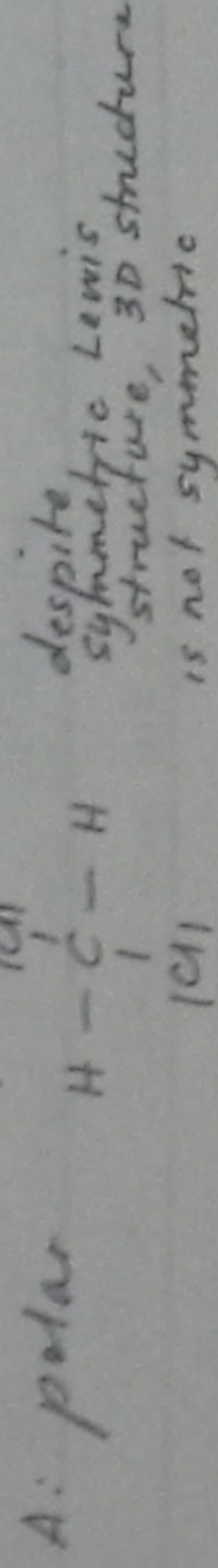
Most molecules have even # of e^- ; are diamagnetic

MOLECULAR ORBITAL THEORY

10/22/2013
10/21/2013

- note: typically, diff. in electroneg. < 0.3 is considered nonpolar by chemists. However, 0.4 is the Δ electroneg. btw C & H, and that is considered nonpolar.

CQ1 Is CH₂Cl₂ polar/nonpolar?



- MOLECULAR ORBITAL THEORY (MO)

(explains bonding in orbitals w/ electrons)

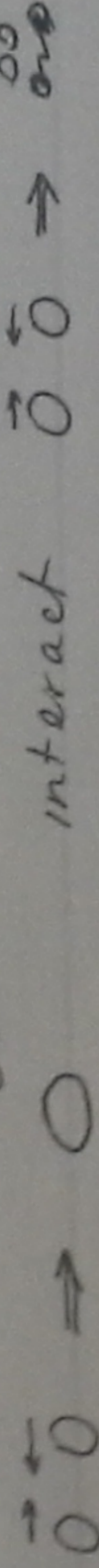
- better than valence bond (localized, meaning looking at individual atoms and their electrons)

- MO is delocalized; taking all atomic orbitals and mixing

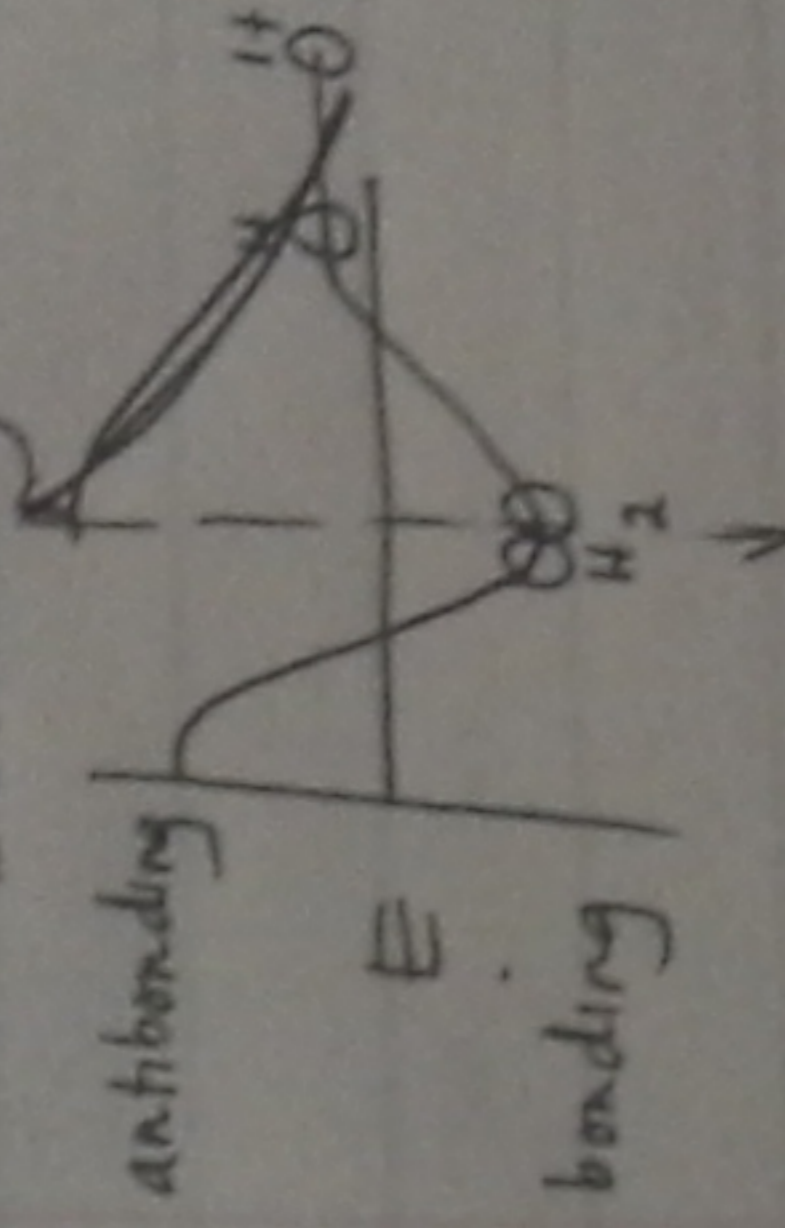
- predicts bond strength & length

- e.g. bond length/strength for H₂

- distance and energy → how individual H atoms in H₂



- bonding orbital (σ_{1s}) vs. antibonding orbital (σ*_{1s})
↳ higher energy

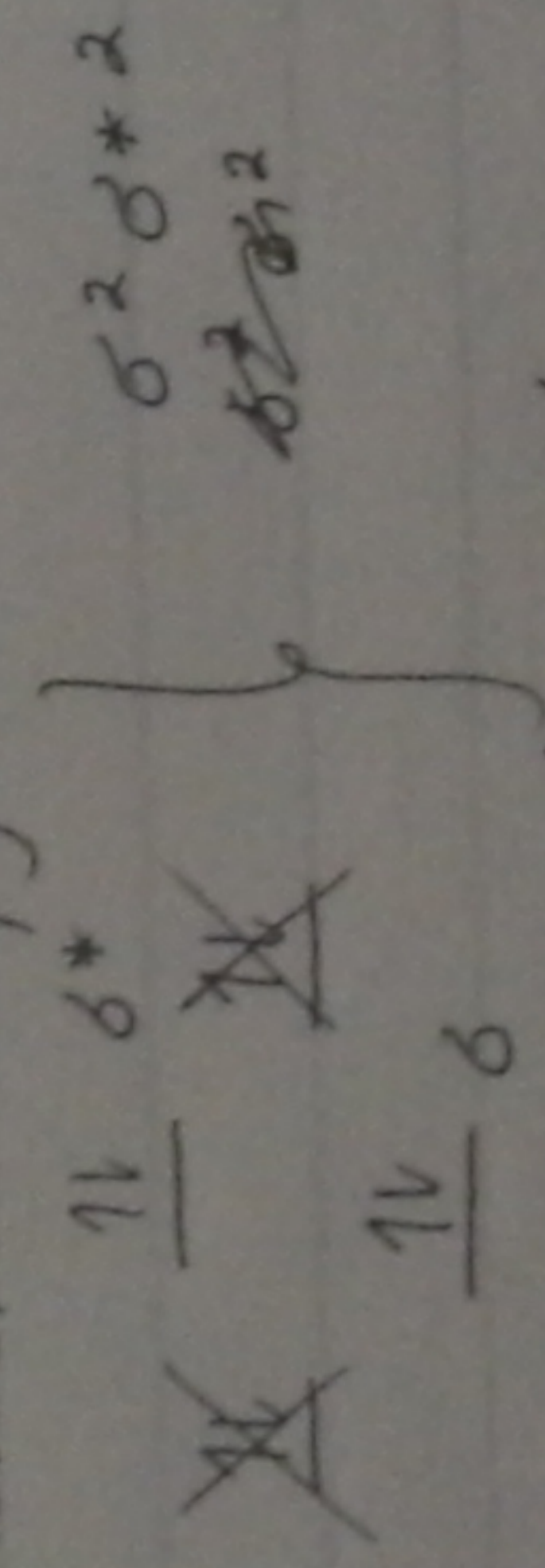


- number of MO in orbital = total AO in atom

- combine atomic orbitals: 1/2 you get higher energy, 1/2 you get lower energy

- e.g. H₂

- electron configuration: 1s² 2s²



bond order =
 $\frac{1}{2} (\# \text{ bonding electrons} - \# \text{ antibonding electrons})$

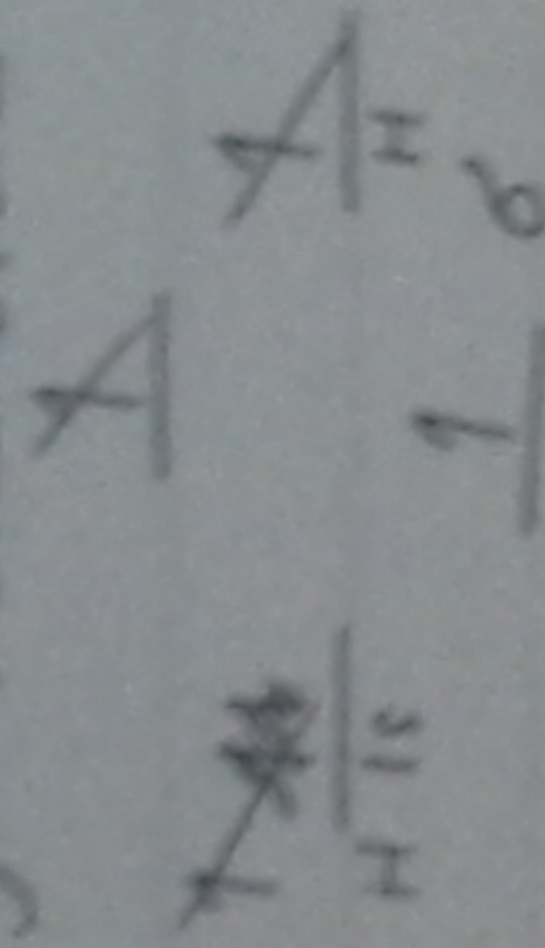
- higher bond order, stronger the bond

- bond order = 1/2 (2 - 2) = 0 ← impossible molecule

MOLECULAR ORBITAL THEORY

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- e.g: bond order H_2^+



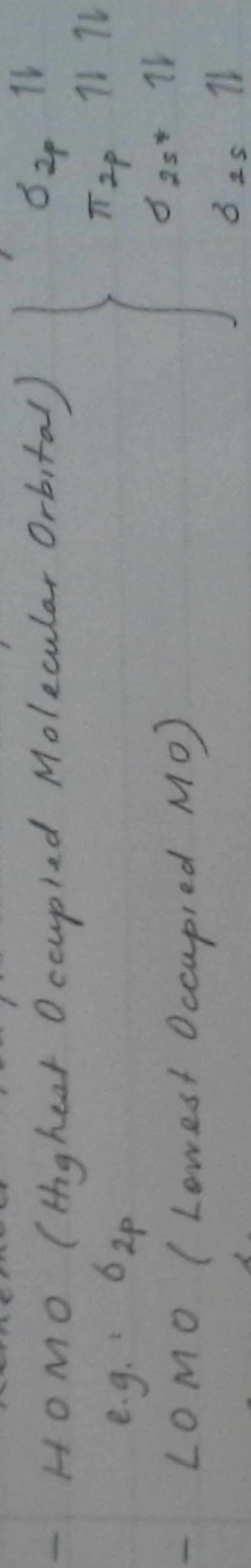
bonding order: $\frac{1}{2}(1 - 0) = \frac{1}{2}$

very weak, unstable bond

Q23 The highest energy electrons are in what molecular orbital?

AKA, These are where the electrons could be, but where are they actually.

Remember: You fill the orbitals from bottom to top (low to high)



- HOMO (Highest Occupied Molecular Orbital)
e.g: σ_{2p}

- LOMO (Lowest Occupied MO)

e.g: σ_{2s}

Q24 Most molecules have

A. An even number of electrons, thus diamagnetic.