More Questions for Exam 3

[✓ T] F The orbital picture in molecules is an approximation of the true electronic wavefunction for the molecule. Orbitals as a whole are approximations

[✓ T] F In molecular orbital theory for diatomics, bonding orbitals arise from constructive interference between the atomic orbitals.

[✓ T] F π bonds in diatomics always have a node parallel to the bond axis (along the bond)

The Born-Openheimer approximation assumes that in a molecule the nuclei are essentially fixed on the timescale of the motion of the electrons because

A. The electron-electron repulsion is so large
B. It's a subtle affect based on the effective nuclear charge
C. There is no justification for this assumption it simply makes the calculation easier
D. Because the mass of the nuclei are so large compared to the mass of the electron
E. Because the electron and nuclei are "self-consistent"

D

Draw a correlation diagram for F_2 $(\sigma_{2s})^2(\sigma^*_{2s})^2(\sigma_{2p})^2(\pi_{2p})^4(\pi^*_{2p})^4$

What is the electronic configuration?

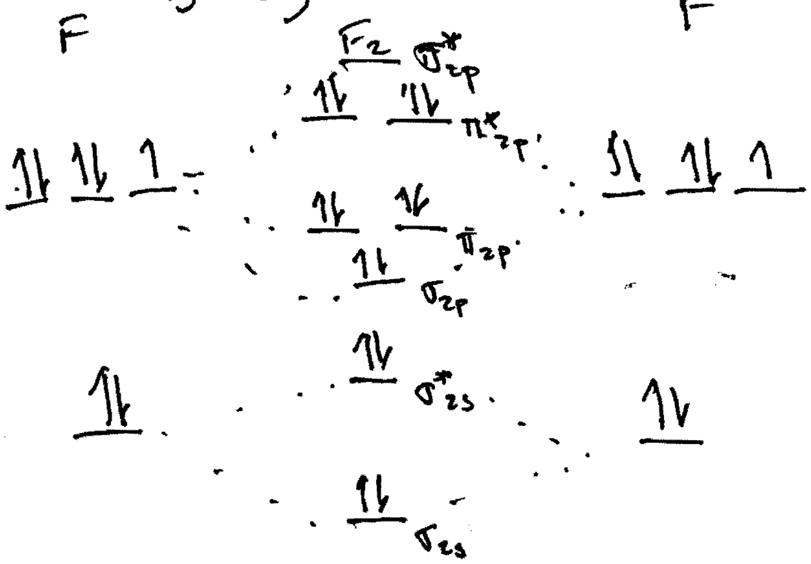
What is the bond order? B.O. $= \frac{1}{2}(6-4) = 1$

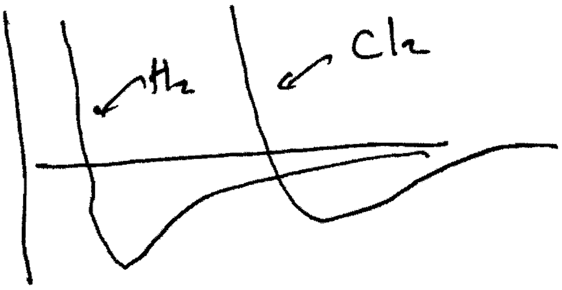
Which would you expect F_2 to be most stable than F_2, F_2^-, or F_2^+?

F_2^+ 1 less antibonding
↳ stronger bond BO = 1½

F_2^- 1 more antibonding
~~tes~~ weaker bond BO = ½

ignoring the 1s core





similar shape
Cl_2 longer bond length
weaker bond

Sketch a diagram of the energy of a H_2 molecule as a function of the internuclear distance. On the same sketch what do you think a plot of Cl_2 would look like? What are the key differences and similarities?

What is the bond order and molecular electronic configuration for N_2^+?

$(\sigma_{g2s})^2(\sigma^*_{u2s})^2(\sigma_{g2p})^2(\pi_{u2p})^3$ B.O = 2.5

Each of the following is characteristic of either a bonding anti-bonding or non-bonding molecular orbitals in diatomic molecules. For each fill in the blank as BB (bonding), AB (antibonding) or NB (nonbonding) (10 points)

AB Energy is always higher than corresponding atomic orbitals

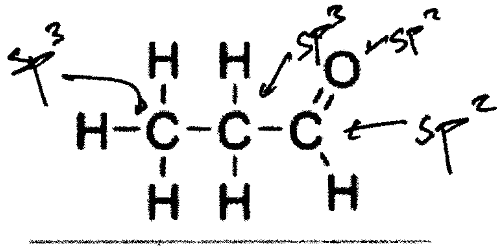
BB Energy has a minimum at a particular distance between the two nuclei

NB Energy is not a strong function of the distance between the two nuclei

AB Electron density is greater on the atom with the smallest electronegativity

AB The wavefunction has a node between the two nuclei

For each of the following carbons what is the hybridization?



How many total sigma bonds does the molecules have?

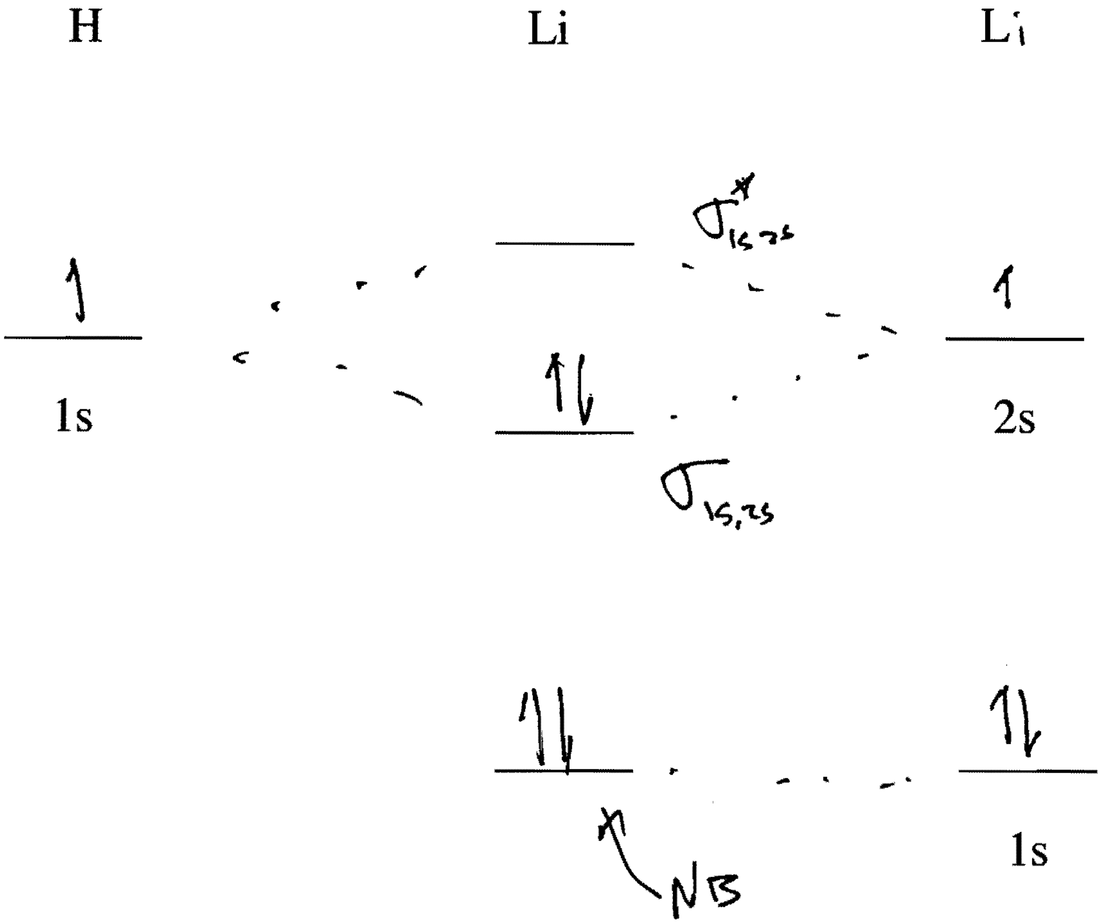
2 C-C σ
6 C-H σ → 9 σ
1 C-O σ

How many pi bonds? 1 C-O π

Using the VB picture describe the double bond between the carbon and the oxygen?

σ C_{sp} - O_{sp} π C_{2p} - O_{2p}

Below is a correlation diagram for LiH.



How many bonding, anti-bonding, and non-bonding electrons are in the molecule?

2 bonding, 2 non-bonding

What is the bond order?

B.O = 1

If you excited the highest energy electron to the next highest orbital would the molecule fall apart? Explain.

Yes. then B.O = 0

Would LiH^+ have a stronger or a weaker bond

LiH^+ would have 1 less bonding e^-

∴ B.O = ½ weaker.

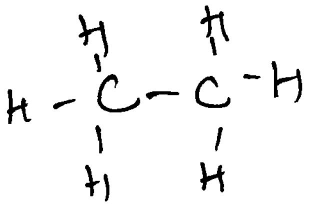
Acetylene (ethyne) gas C_2H_2 reacts with hydrogen H_2 in the presence of a catalyst to form ethane C_2H_6..

Write a balanced equation for this reaction.

How many isomers of ethane are formed

$$C_2H_2 + 2H_2 \rightarrow C_2H_6$$

there is only on farm of ethane



$$\begin{array}{ccccccc} & & H & & H & & \\ & & | & & | & & \\ H & - & C & - & C & - & H \\ & & | & & | & & \\ & & H & & H & & \end{array}$$

Can you draw and name two isomers of C_2H_6O that have different functional groups?

$H_3C-O-CH_3$ dimethyl ether

or

CH_3CH_2OH ethanol

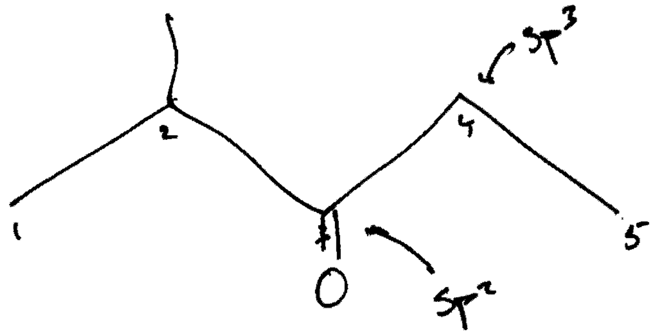
2 methyl petan-3-one

side Chan 1 at position 2

5 C chain

position of =O

ketone



$C_6H_{12}O$

C-O bond

$\sigma_{Csp^2-Osp^2}$

$\pi_{C_{2p}-O_{2p}}$

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3 ethyl heptane

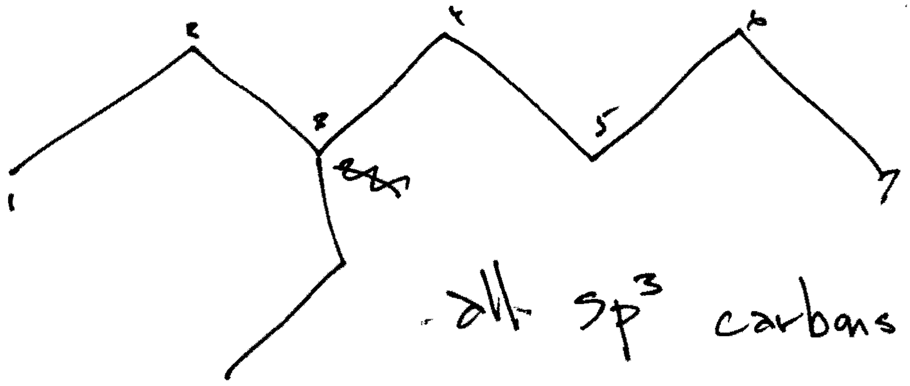
position 3

2 C side chain

7 C chain

alkane

C_9H_{20}



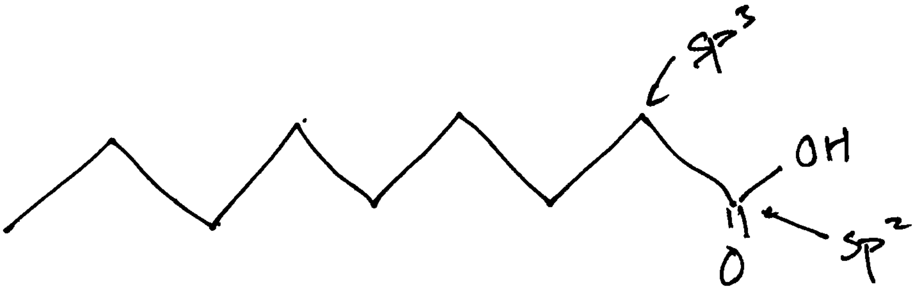
all sp³ carbons

C-H σ bond $\sigma_{Csp^3-H_{1s}}$

nonanoic acid

↑ 9 C chain

carboxylic acid



$C_8H_{17}COOH$

or $C_9H_{18}O_2$

C-O bond

$\sigma_{C_{sp^2}-O_{sp^2}}$

$\pi_{C_{2p}-O_{2p}}$

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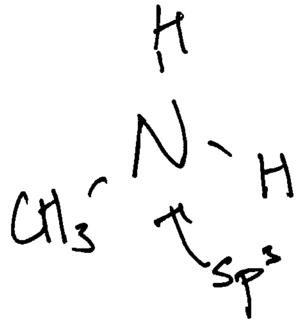
methyl amine



CH_3NH_2 ← better

or

CNH_5

N-H

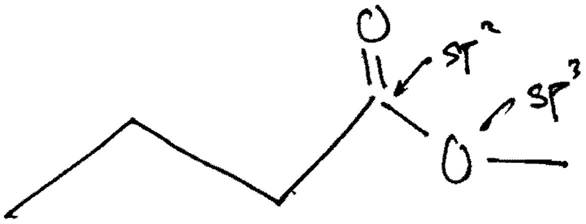
$\sigma_{N_{sp^3}-H_{1s}}$

methyl butanoate

side chain 1 C

main chain 4 C

ester



$C_3H_7COOCH_3 \rightarrow C_4H_{10}O_2$

C-O bond (single)

$\sigma\, C_{sp^3} - O_{sp^3}$

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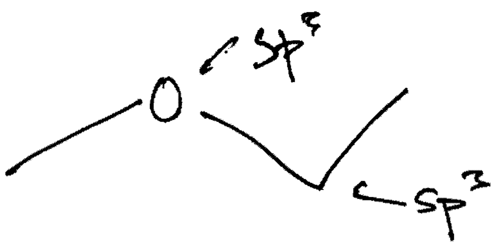
methyl ethyl ether



$CH_3OC_2H_5 \rightarrow C_3H_8O$

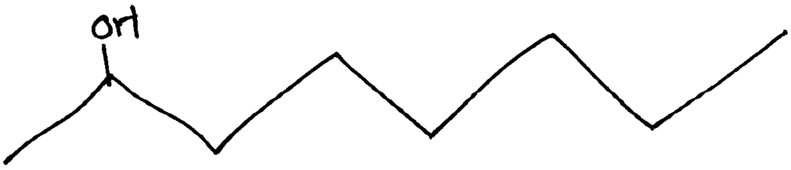
C-O $\sigma_{C_{sp^3}-O_{sp^3}}$

octan-2-ol

8 C chain

position 2 -OH

alcohol



all sp^3 $C_8H_{19}OH$ $C_8H_{20}O$

O-H $\sigma_{O_{sp^3}-H_{1s}}$

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4 methyl hex-2-yne

sidechain position 4

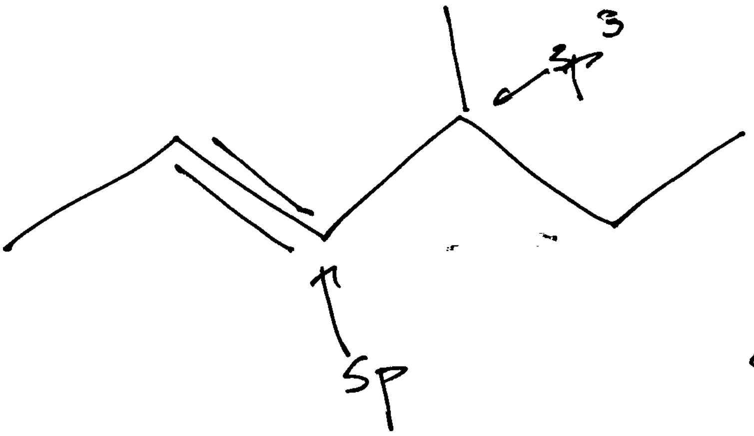
1 C sidechain

6 C chain

triple bond @ carbon #2

alkyne

C_7H_{12}



C–C triple bond

$\sigma_{C_{sp}-C_{sp}}$

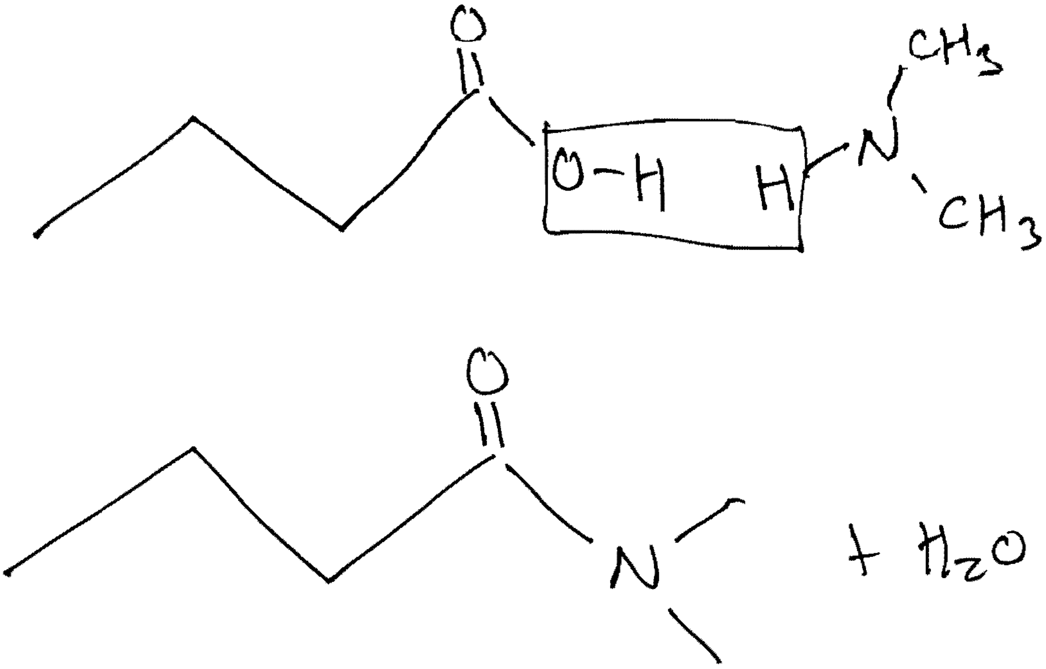
$2\times \pi_{C_{2p}-C_{2p}}$

$$CH_3-\boxed{OH + H}-O-CH_3$$

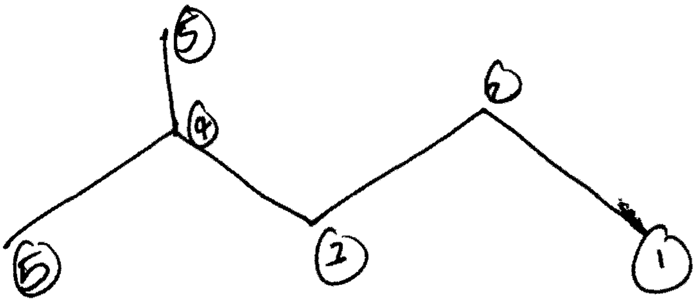
$$\downarrow$$

$$CH_3-O-CH_3 + H_2O$$

dimethyl ether



N,N dimethyl butanamide.



+ Cl_2

unique places to add a Cl.

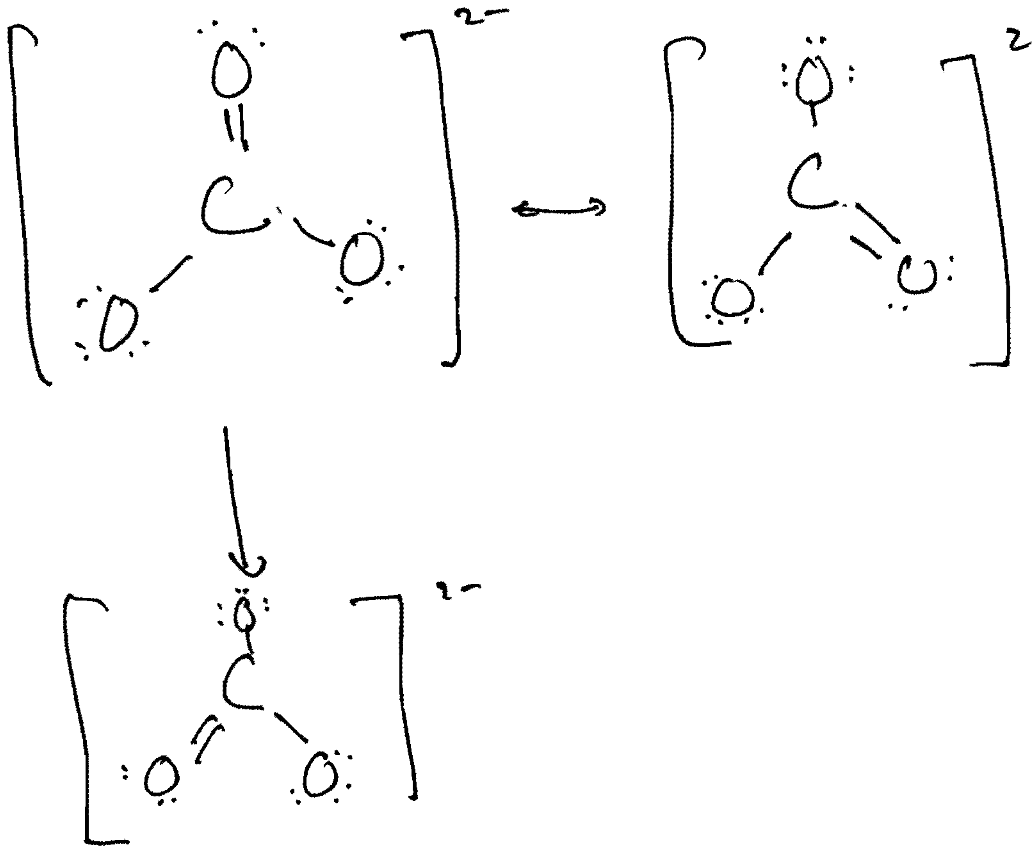
① end away from branch
② next to end away from branch
③ C next to branch
④ at the branch
⑤ at the end close to branch 2x

5 potential isomers.

1 chloro 4 methyl pentane
2 chloro 4 methyl pentane
3 chloro ~~4~~ 2 methyl pentane
2 chloro 2 methyl pentane
1 chloro 2 methyl pentane

I'm not certain of this name.

switch # scheme for lower option.



VB σ frame work.

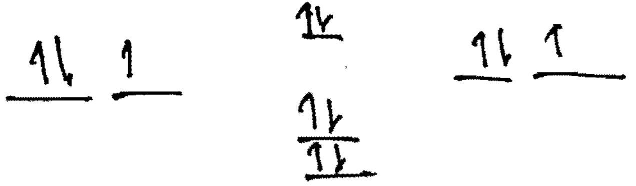
C sp^2 hybrid.

all oxygens the same ∴ O sp^2 as wel

C-O bond $\sigma_{C_{sp^2}-O_{sp^2}}$.

MO "left over" 2p on C & 3×O.

4 × 2p orbitals → 4 MO → 2 bonding
2 antibonding



6 e^- in MO's

B.O = 1. 1 double bond

ØN

Here the MO only deals with the delocalized π e^-'s.

4 e^- 1 each from C, 3×O

+ 2 e^- as it is a ~~the~~ 2^- ion!

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all other e^- in core
or σ framework