

More Questions for Exam 3

- T F The orbital picture in molecules is an approximation of the true electronic wavefunction for the molecule.
- 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"
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Draw a correlation diagram for F_2

What is the electronic configuration?

What is the bond order?

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

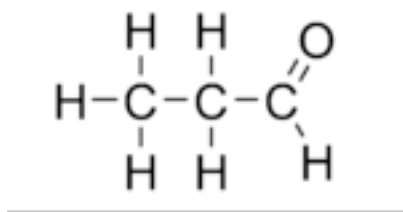
Sketch a diagram of the energy of a H_2 molecule as a function of the internuclear distance. On the same sketch what do you think a plot of Cl_2 would look like? What are the key differences and similarities?

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

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)

- _____ Energy is always higher than corresponding atomic orbitals
- _____ Energy has a minimum at a particular distance between the two nuclei
- _____ Energy is not a strong function of the distance between the two nuclei
- _____ Electron density is greater on the atom with the smallest electronegativity
- _____ The wavefunction has a node between the two nuclei

For each of the following carbons what is the hybridization?

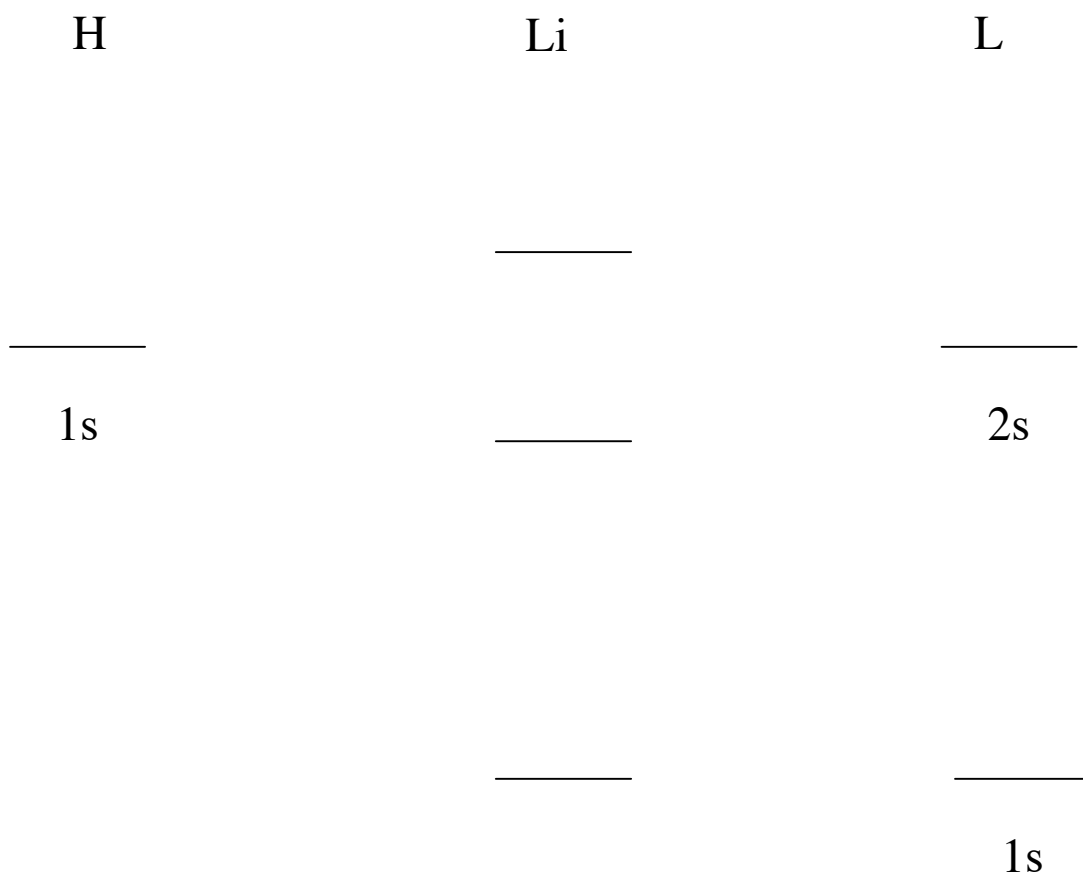


How many total sigma bonds does the molecules have?

How many pi bonds?

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

Below is a correlation diagram for LiH.



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

What is the bond order?

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

Would LiH^+ have a stronger or a weaker bond

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

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

Draw the following molecules

2 methyl pentan-3-one

3 ethyl heptane

nonanoic acid

methyl amine

methyl butanoate

methyl ethyl ether

octan-2-ol

4 methyl hex-2-yne

For any of the above, pick an atom and look at its hybridization.

For any of the above, write down the molecular formula

For any of the above, describe a sigma bond using the VB picture

For any of the above that have a double bond, describe the pi bond with the VB picture

What ether would you expect to form from a reaction of methanol with itself?

What would you expect to form from a condensation reaction involving butanoic acid and dimethyl amine?

If you reacted 2 methyl propane with Cl_2 gas to form a new alkyl halide with one chlorine atom (substituting a hydrogen with a chlorine). How many different isomers would you expect to form?

Draw a Lewis Dot structure (and resonance structures for CO_3^{2-})

Describe the sigma bond frame work in the VB picture.

Describe the pi bond in terms of MO (what orbitals make up the MO's, how many bonding orbitals are there, how many antibonding, how many electrons are in them,...)

Do you think it is best to describe the O's as sp^3 or sp^2 hybridized?

Do you think there are any electrons in anti-bonding MO's?

If you had to guess, how many NB orbitals do you think there are?