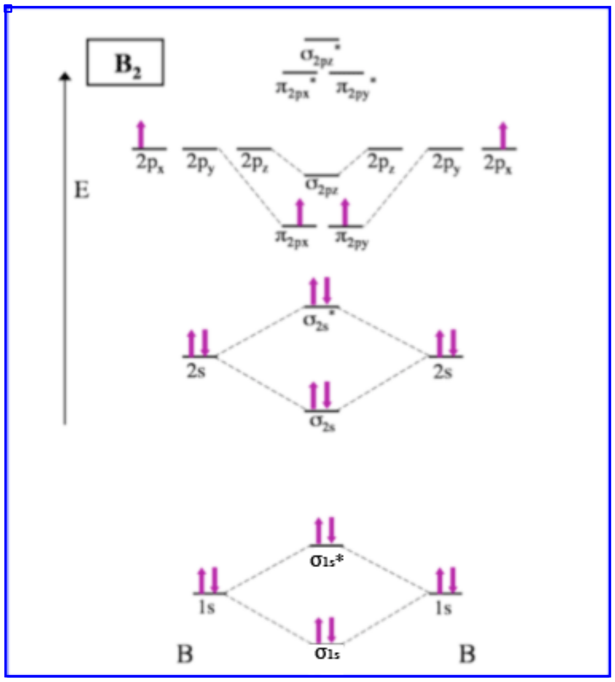
LECTURE 13

1. Draw a molecular orbital diagram and determine the bond order expected for the molecule B_2. For full credit on MO diagrams,
   - label increasing energy with an arrow next to the diagram.
   - pay attention to whether the question asks for valence electrons or all electrons.
   - for any bonding orbital drawn, include the corresponding anti-bonding orbital, even if it is not filled with any electrons.
   - Label each atomic orbital (1s, 2s, $2p_x$, $2p_y$, $2p_z$ etc.) and each molecular orbital ($\sigma 2s$, $\pi 2p_x$, $\pi 2p_y$, etc.) that you draw.
   - Fill in the electrons for both the atomic and molecular orbitals.

Bond order = ½(6-4) = **1**



2. (a) Write the valence electron configuration (from lowest to highest orbital energies) for the ion N_2^{-1}. Your answer should be in a form similar to $(\sigma 2s)^2$, which is the valence configuration for Li_2.
   (b) What is the bond order of N_2^{-1}?
   (c) Which has a **longer** bond, N_2^{-1} or N_2? Justify your answer using bond order.

(a) $(\sigma 2s)^2(\sigma 2s^*)^2(\pi 2p_x)^2(\pi 2p_y)^2(\sigma 2p_z)^2(\pi 2p_x^*)^1$

(b) 2.5

(c) The N-N bond is stronger in N_2 since an electron is removed from an anti-bonding orbital, increasing the bond order from 2.5 to 3.

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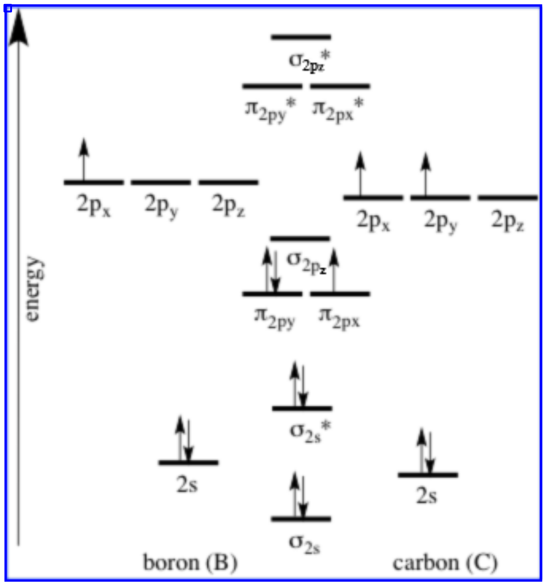
3. (a) Draw a MO diagram for the valence electrons of BC. Label all atomic and molecular orbitals.
(b) Write the molecular orbital configuration for the valence electrons in BC and in BC^{1-}.
(c) Which of the molecular orbitals in BC do <u>not</u> have a planar node along the internuclear axis?
(d) Which has the stronger B–C bond, BC or BC^{1-}? Justify your answer using bond order.

(a)



(b)

BC: 7 valence electrons
$(\sigma 2s)^2(\sigma 2s^*)^2(\pi 2px)^2(\pi 2py)^1$

BC^{1-}: 8 valence electrons
$(\sigma 2s)^2(\sigma 2s^*)^2(\pi 2px)^2(\pi 2py)^2$

(c) Only π orbitals have planar nodes at the internuclear (bonding) axis. The following orbitals do not have nodal planes along the bonding axis: σ2*s*, σ2*s, σ2*pz*, and σ2*pz*****

(d) The B-C bond is stronger in BC^{1-} since an electron is added to a bonding orbital, increasing the bond order from 1.5 to 2.

4. For each of the following molecules, (i) write the valence electron configuration (Your answer should be in a form similar to $(\sigma_{2s})^2$, which is the valence configuration for Li_2) and (ii) determine if the molecule is paramagnetic (has unpaired electrons) or diamagnetic (does not have unpaired electrons). If the species is paramagnetic, identify the number of unpaired electrons. (a) Cl_2^{1+}; (b) O_2^{1+}

(a) Cl_2^+: **13** valence electrons
$(\sigma 3s)^2(\sigma 3s^*)^2(\sigma 3pz)^2(\pi 3px)^2(\pi 3py)^2(\pi 3px^*)^2(\pi 3py^*)^1$
paramagnetic: **1** unpaired electron

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(b) O_2^+: **11** valence electrons

$(\sigma 2s)^2(\sigma 2s^*)^2(\sigma 2pz)^2(\pi 2px)^2(\pi 2py)^2(\pi 2px^*)^1$

paramagnetic: **1** unpaired electron