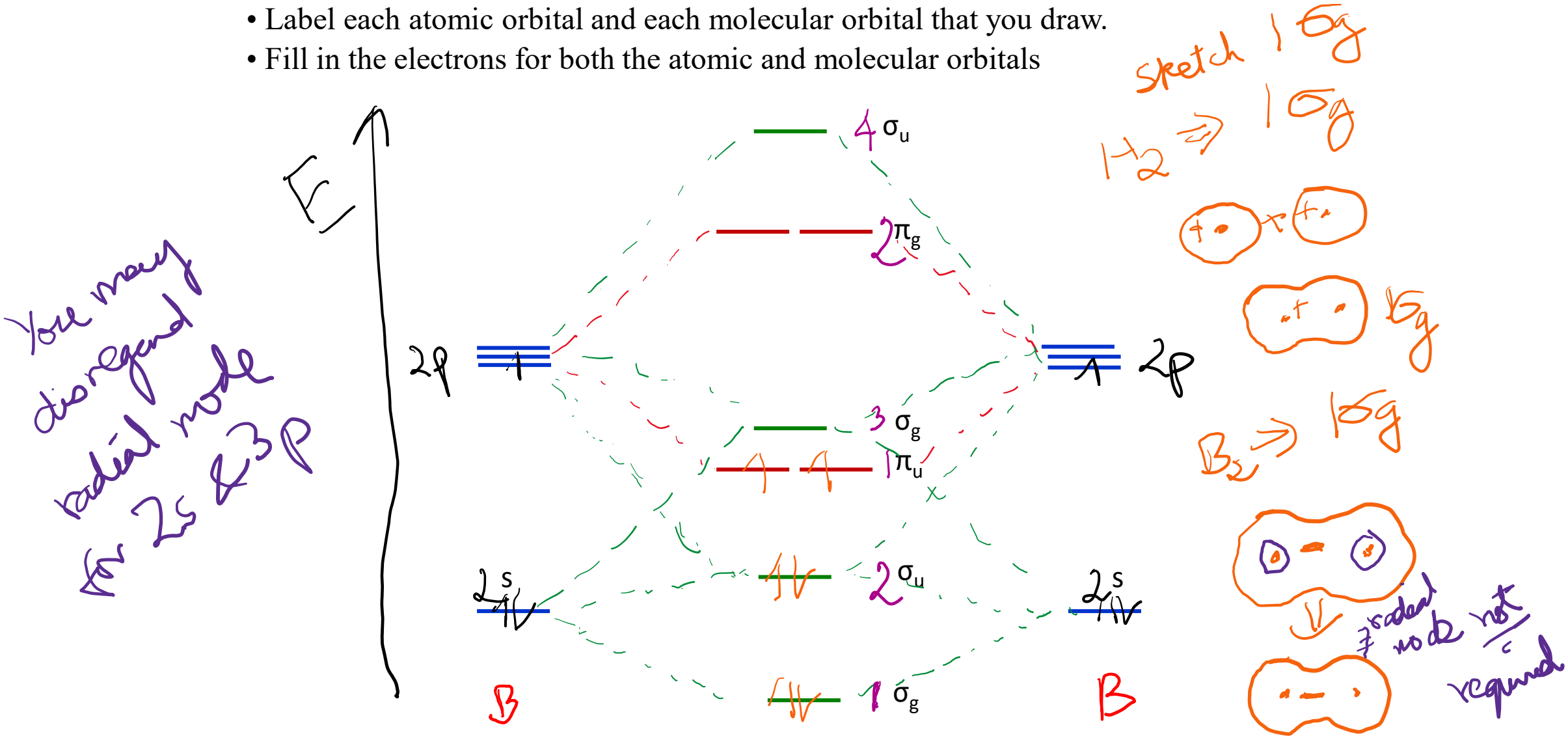
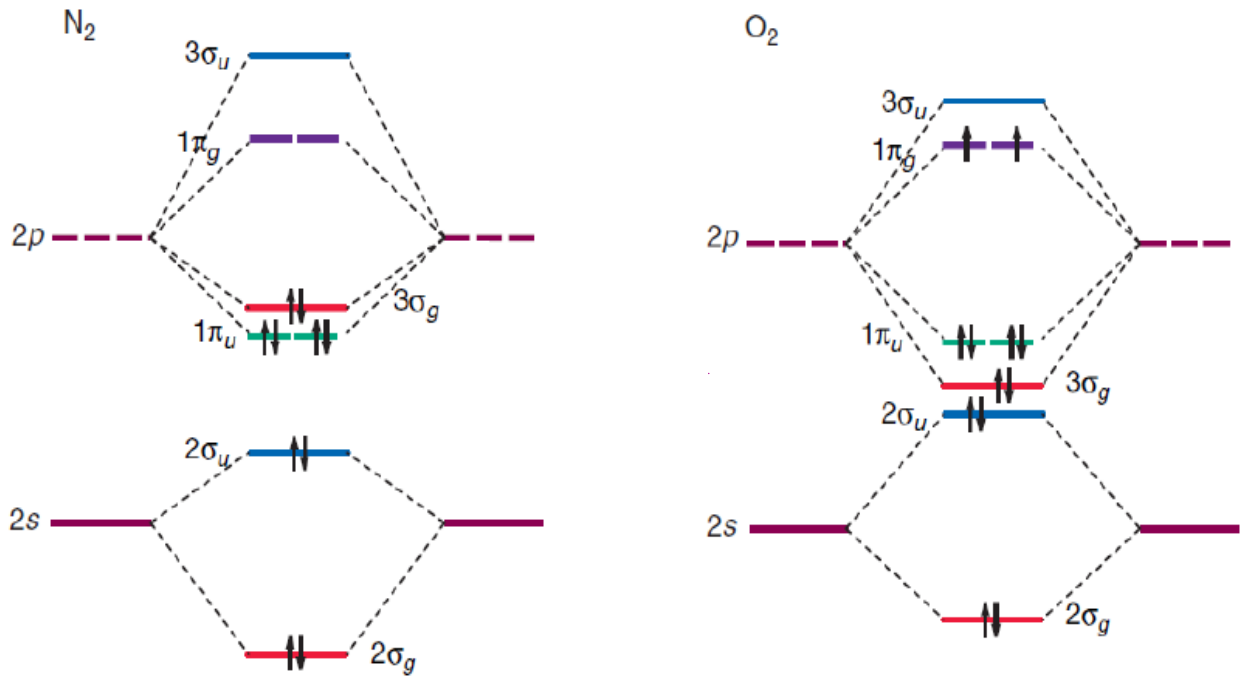
1. Draw a molecular orbital diagram and determine the bond order expected for the molecule B_2. For full credit on MO diagrams,

- label increasing energy with an arrow next to the diagram.
- for any bonding orbital drawn, include the corresponding anti-bonding orbital, even if it is not filled with any electrons.
- Label each atomic orbital and each molecular orbital that you draw.
- Fill in the electrons for both the atomic and molecular orbitals



2. The dissociation energy of N_2 is 942 kJ/mol, where as that for N_2^+ is 842 kJ/mol. The dissociation energy of O_2 is 494 kJ/mol, whereas that for O_2^+ is 642 kJ/mol. Rationalize these data.

The electron is removed from a bonding MO in N_2. This leads to a reduction in bond order and also a decrease in the BDE. In contrast, for O_2, electron is removed from the anti-bonding MO and this leads to an increase in the BO and an increase in BDE.



3. Sketch an MO diagram for BeH. On the basis of your diagram, would you expect this molecule to be stable with respect to dissociation into atoms.? Use your MO diagram to predict any other properties you can.

Be $\Rightarrow 1s^2 2s^2$

Be
- 8 eV (2s)
- 130 eV (1s)

H
- 14 eV (1s)

$1s^1 \Leftarrow H$

-140 eV
$\downarrow$
$Be(1s) + H(1s) \Rightarrow$ (-14 eV) $\Rightarrow S \neq 0 \Rightarrow$ Huge energy mismatch

$Be(2s) + H(1s) \Rightarrow S \neq 0 \Rightarrow$ Energy match
-8 eV -14 eV

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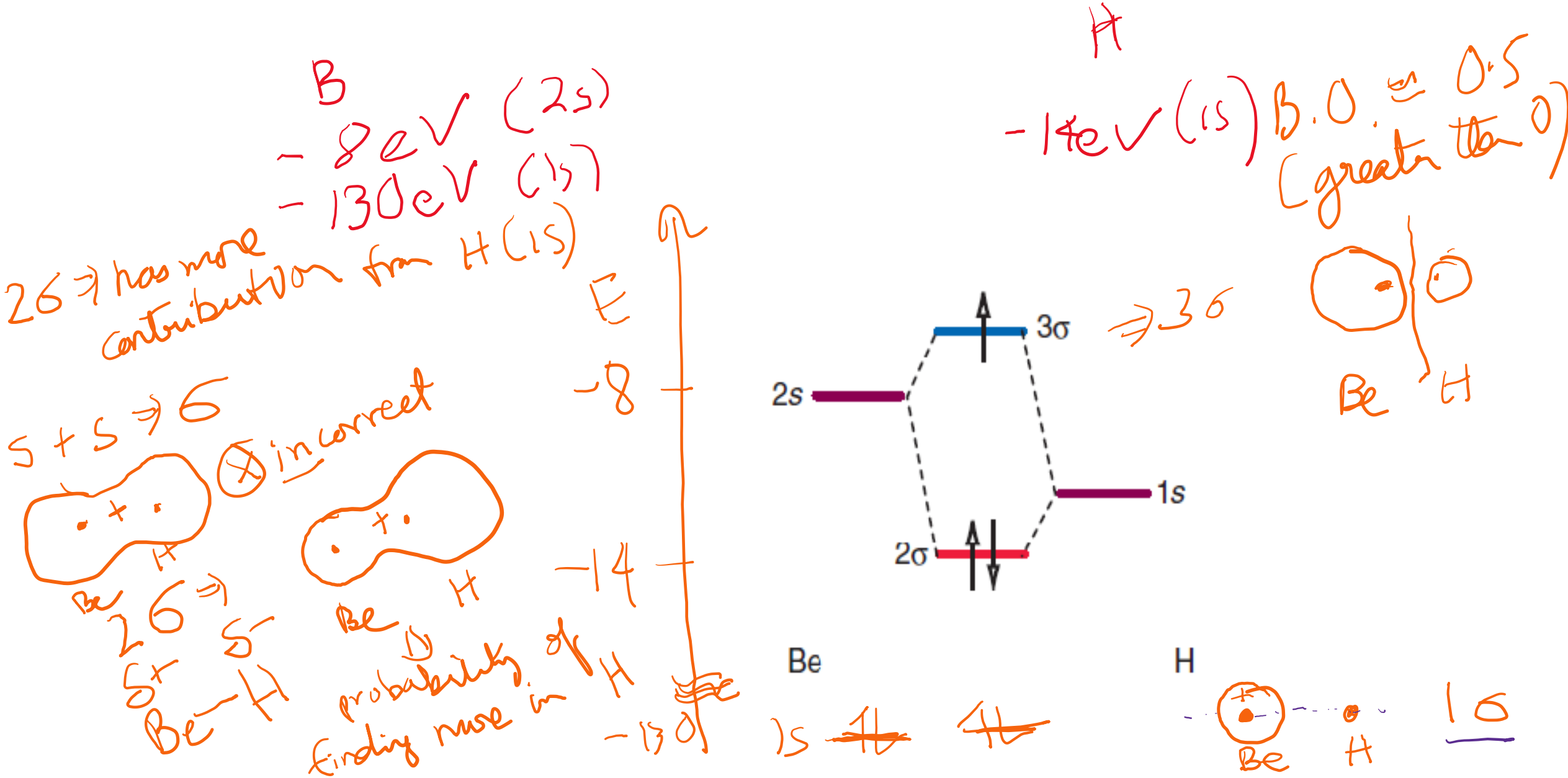
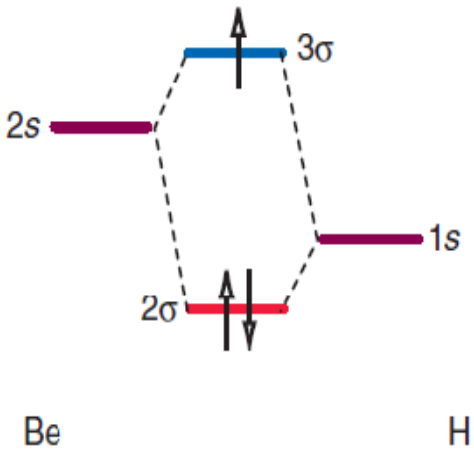
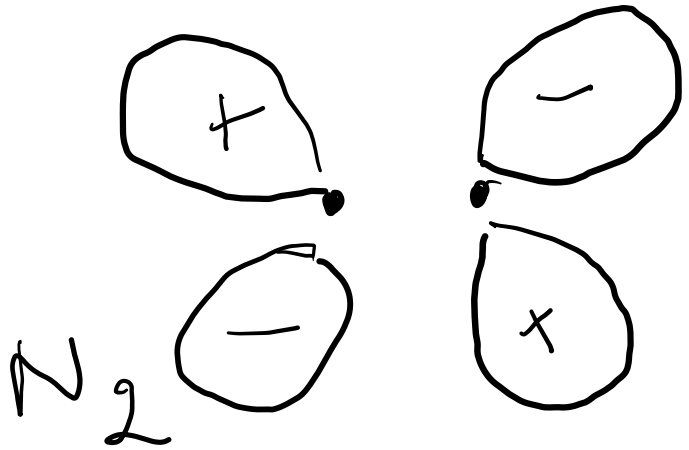


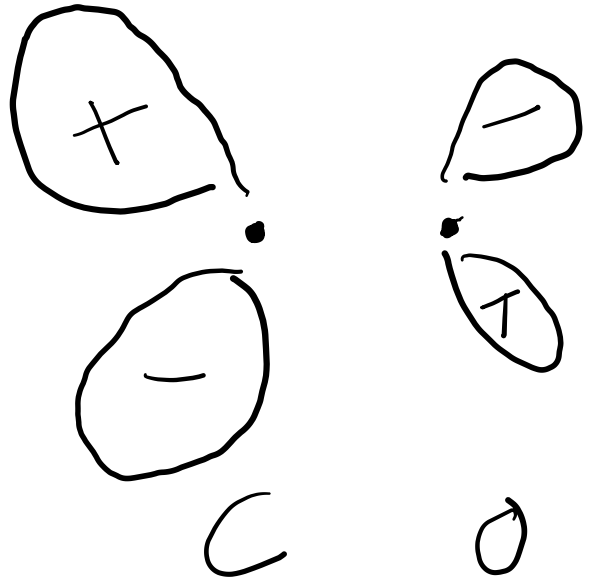
3. Sketch an MO diagram for BeH. On the basis of your diagram, would you expect this molecule to be stable with respect to dissociation into atoms.? Use your MO diagram to predict any other properties you can.



4. Draw the π and π* MO's for N_2 and CO. Qualitatively show the difference. Comment on the contribution from individual AO's in the resulting MO's.

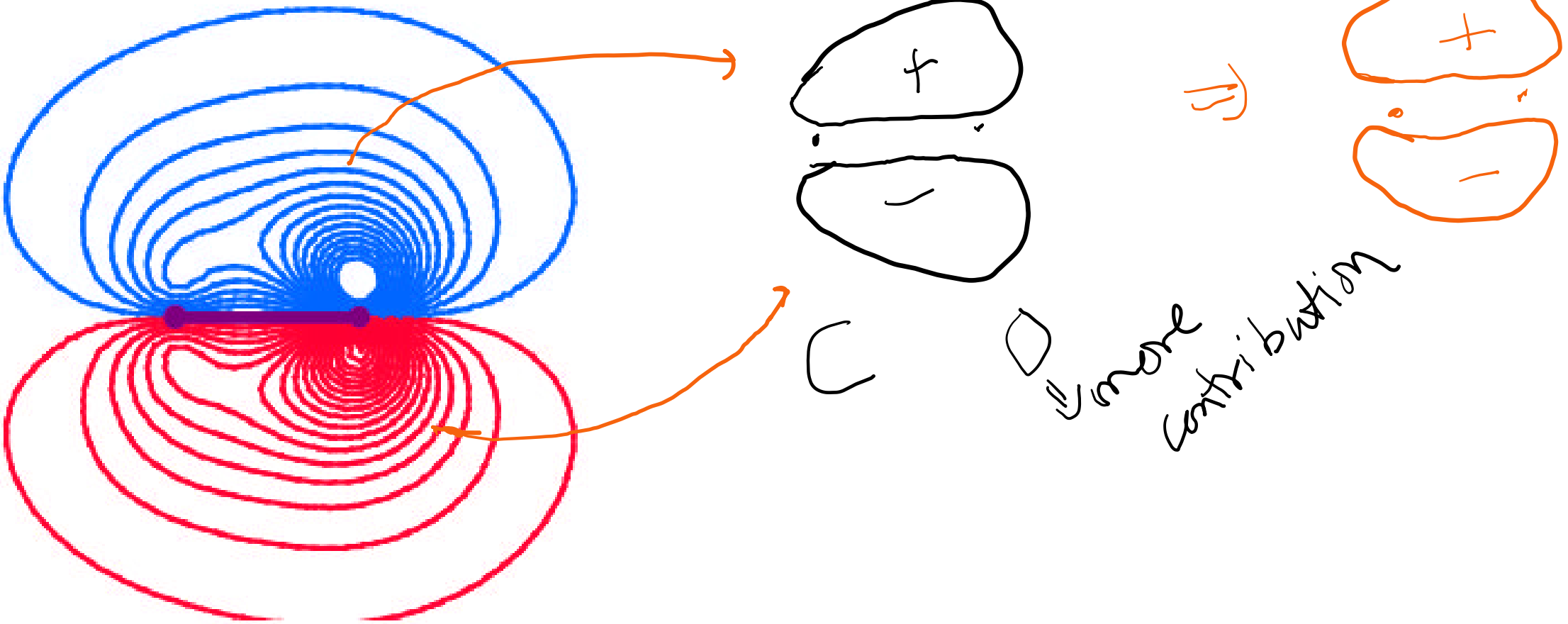


π* MO for N_2

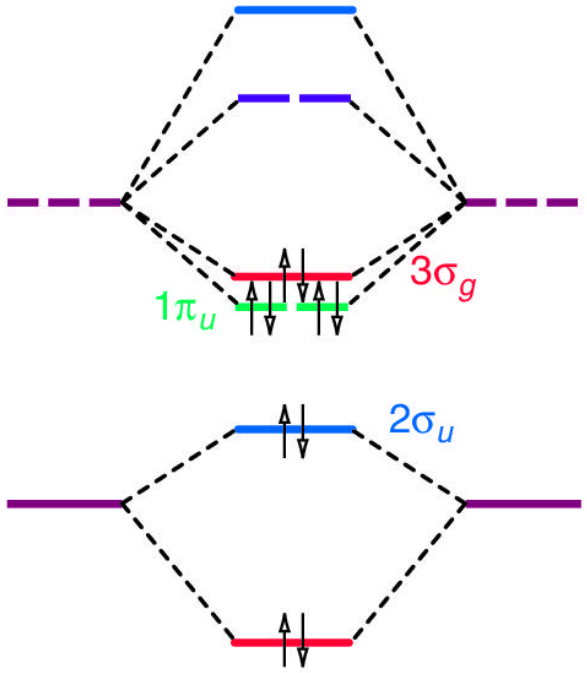


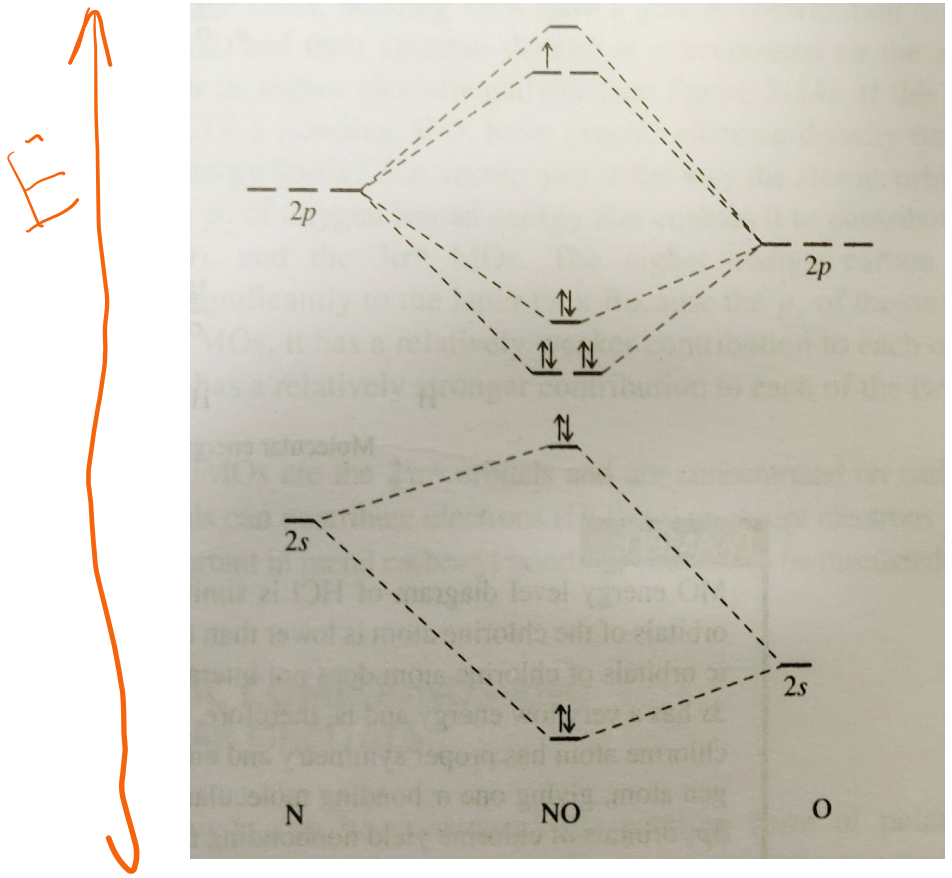
π* MO for CO

π^* has more contribution from C


+
−
C
O
more
contribution
N2
+
−

5. Consider that the orbital structure of the heteronuclear diatomic ion NO^+ is similar to that of N_2. Use this information to draw the energy level diagram for NO^+. In the molecular orbital, will the electrons have a higher probability of being at N or at O? Why?





→ NO
NO^+ → remove $\bar{e}$ from π^* → 10e system

6. Photoelectron spectrum of a second row homonuclear diatomic molecule was recorded using 21.21ev photons. It is observed that $K.E_{max}$ of the ejected electrons from the top three HOMO's were 10.01, 8.23, and 5.22 eV, having intensity ratios of 1:2:1. Sketch the molecular orbital energy level diagram and identify the molecule.