Name Jorge F

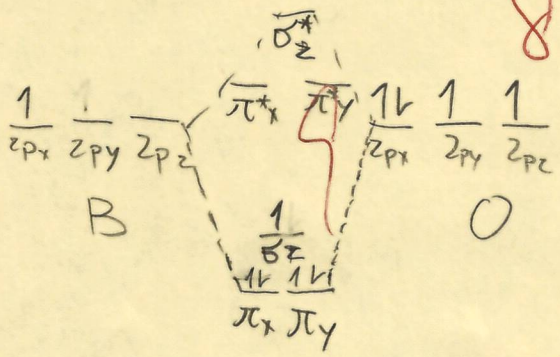
Midterm (Continued) **Chem 20A, Winter 2016**

1. (30 points total) The boron oxide molecule (BO) is known to be a stable although highly reactive diatomic, and its structure has been deduced in various spectroscopy experiments.

   (a) (20 points) Write down a molecular orbital energy (correlation) diagram for the BO molecule; you do *not* need to include the filled MO's formed by LCAOs of the 1s or 2s orbitals, only those formed from the LCAO's of the 2p valence electrons. Be sure to fill the molecular energy levels with the appropriate number of electrons for BO. Label each of the AO's and MO's in your diagram, and be sure to *briefly* justify how you picked the ordering of the MO energy levels.

BO

$2s^2 2p^2$ $2s^2 2p^4$



8

The switch in E between π bonding & sigma bonding takes place between N & O. Since, O is on the low side & B_2's π are definitely lower in E, I choose to predict the π were lower in energy.

Antibonding are always higher in energy than bonding b/c of the unstabilization.

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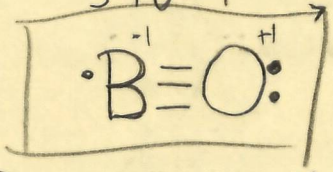
Name Jorge F

1. (Continued)

(b) (10 points) Write down a Lewis structure for BO, and make sure to indicate formal charges on each atom. Based on your MO diagram in part (a), what is the bond order of BO? Does this agree with the Lewis structure (yes or no)? Would you expect BO to be paramagnetic or diamagnetic?

3+6=9 — 9/2 are recessive bond



* triple bond are 1 sigma bond & 2 pi bonds

B F.C 3-4 = -1 B

O F.C 6-5 = +1 O

2

Based on MO diagram in a, the B.O would be 2.5

2

Based on the Lewis dot, it would be 3 ← ≠ different, Lewis Dot & MO disagree slightly

The molecule has one unpaired e^-, so its paramagnetic

2

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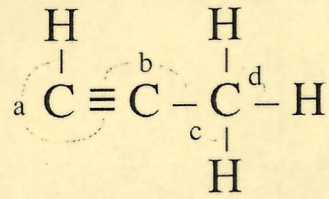
Name Jorge F

Midterm (Continued) **Chem 20A, Winter 2016**

2. (20 pts total) The Lewis structure (but not necessarily the chemical structure!) for the hydrocarbon molecule propyne (C_3H_4) is shown at right. Keep in mind that although the structure is drawn co-planar with bonds at right angles, the actual chemical structure and bond angles are likely to be different. Note: No MO diagram is needed for this problem!



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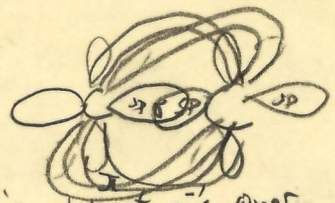
(a) (16 points) Use the ideas of the VSEPR theory to estimate the four bond angles (*a*, *b*, *c* and *d*) shown in the picture. For each of the 4 bond angles, do you expect the actual bond angle to be slightly larger, slightly smaller, or equal to your estimate? Briefly explain why for each angle.

There are no lone pairs on any of the atoms.

a) 180° (2) because S.N = 2 & L.P. = 0 so linear (2)



– triple bonds are 2 π bonds & a sigma bond, so there is a lot of e⁻'s over on that side pretty symetrical along nuclear axis so I would say equal (1)

b) 180° (2) b/c SN = 2 & L.P = 0 so linear (2)

– the σ is between the sp & sp^3 C MO's, & the sp^3 tetrahedral shape & π bonds are symetrical along nuclear axis so again equal (1)

c) 109.5° (2) b/c SN = 4 & L.P = 0 so tetrahedral

The sp & sp^3 MO combination has more charge than the H so I would say the H's would be compresed & be ~~smaller~~ (0) angle

d) 109.5° (2) b/c SN = 4 & LP = 0 so tetrahedral

Since sp & sp^3 MO & entire left of molecule contains lot of charge, I would say H's would be compressed & so < bac would be ~~larger~~ (0)

4

(b) (4 points) List the hybridization of each of the three C atoms (left, center, and right) in the molecule; no justification is needed.

Left	Center	Right
C	C	C
sp	sp	sp^3
(1)	4 (1)	(1)

needs 2 left over for π bonds (triple bond)

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Name Jorge Fuentes

Midterm (Continued) **Chem 20A, Winter 2016**

3. (50 points) A microwave spectroscopy experiment on the $^{12}C-^{32}S$ molecule shows a series of evenly spaced absorption lines, with the lowest frequency line having a wavelength of 6.10 mm (= 6.10×10^{-3} m). An infrared absorption experiment on this same molecule shows a single line at 1277 cm^{-1}. The bond dissociation energy of CS is 573 kJ/mole. The dipole moment of CS is 1.95 D units. Calculate the fraction ionicity (that is, the degree of charge separation) of the C–S bond.

Rotational Spec (Microwaves)

$2B = 6.10$ mm

- B will tell you I which can tell you R since we know m's

4 6 = 10

C S — not paramagnetic, 150 microwaves, not for ESR

573 kJ Bond dissociation

fi... forgot this step

Infrared (Vibrational Spec)

$E = h\nu$ unit of E → $1277\,cm^{-1} = h\nu_{osc}$

wave # $\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$ - can tell me force constant & reduced mass

$= h\frac{c}{\lambda}$

$= 3.26 \cdot 10^{-23}$

$B = \frac{\hbar^2}{2I}$ $2B = 3.26 \cdot 10^{-23}$

$B = \frac{h^2}{8\pi^2 I}$ $2\frac{h^2}{8\pi^2 I} = 3.26 \cdot 10^{-23}$

$I = \frac{h^2}{4\pi^2 \cdot 3.26 \cdot 10^{-23}}$

$I = \frac{m_1 m_2}{m_1 + m_2}R^2$ that small → $I = 3.414 \cdot 10^{-46}$

$R = \sqrt{I\frac{m_1+m_2}{m_1 m_2}}$ $R = \sqrt{3.414 \cdot 10^{-46} \cdot \frac{(12+32)1.6605 \cdot 10^{-27}}{12 \cdot 32 \cdot (1.6605 \cdot 10^{-27})^2}}$

$C_m = 12$ amu

$S_m = 32$ amu

1 amu $= 1.6605 \cdot 10^{-27}$ kg

~~R = 7.0096 · 10^{-22}~~

$R = 1.535 \cdot 10^{-10}$

Dipole Moment

$-\mu = R\delta / 0.2082$ D

- can tell you charge separation if you know R

$\mu = R\delta / 0.2082$

$\delta = \frac{0.2082\,\mu}{R}$

$\delta = \frac{0.2082 \cdot 1.95}{1.535 \cdot 10^{-10}}$

R must be in Å

$\delta = 264462331$

sig fig

$\delta = 2.65 \cdot 10^{9}$

+45