

- INSTRUCTIONS:
- 1) Please read over the test carefully before beginning. You should have 6 pages of questions, a blank “overflow” page and a periodic table page.
 - 2) If your work is not legible, it will be given a mark of zero.
 - 3) Marks will be deducted for incorrect information added to an otherwise correct answer.
 - 4) Calculators are not permitted.
 - 5) You have 90 minutes to complete this test.
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Confidentiality Agreement:

I agree not to discuss (or in any other way divulge) the contents of this exam until after 8:00 pm Mountain Time on Thursday, February 9th, 2017. I understand that breaking this agreement would constitute academic misconduct, a serious offense with serious consequences. The minimum punishment would be a mark of 0/50 on this exam and removal of the “overwrite midterm mark with final exam mark” option for my grade in this course; the maximum punishment would include expulsion from this university.

Signature: _____

Date: _____

Course: CHEM 2000 (General Chemistry II)

Semester: Spring 2017

The University of Lethbridge

Question Breakdown

Q1	/ 18
Q2	/ 8
Q3	/ 3
Q4	/ 3
Q5	/ 18

Total	/ 50
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1. Consider the NO^+ cation according to molecular orbital (MO) theory. [18 marks]

(a) Provide a molecular formula for one neutral diatomic molecule that is isoelectronic with NO^+ . [1 mark]
 N_2 *or* CO

(b) Draw the Lewis structure for NO^+ . Include all non-zero formal charges. [1 mark]

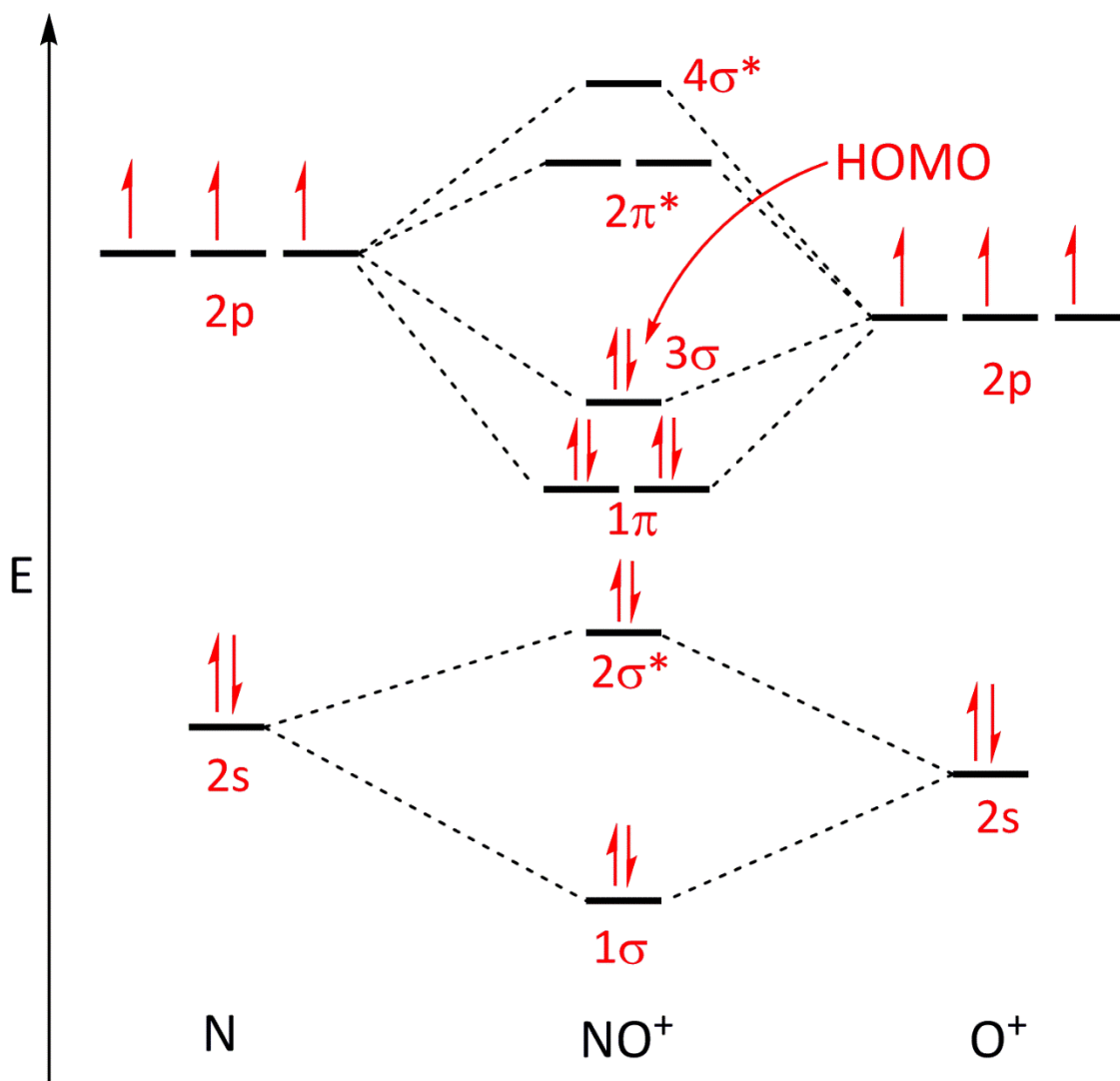


(c) What N–O bond order does your Lewis diagram predict for NO^+ ? [1 mark]

3

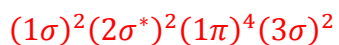
(d) The unlabeled valence MO energy level diagram for NO^+ is shown below. [7 marks]

- i. Label all atomic and molecular orbitals on this diagram.
- ii. Place the correct number of valence electrons into the atomic orbitals.
- iii. Place the correct number of valence electrons into the molecular orbitals.



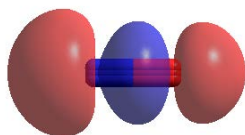
1. *continued...*

(e) Write the valence orbital occupancy (i.e. electron configuration) in line notation for NO^+ . [1 mark]



(f) On the MO energy level diagram on the previous page, clearly label the highest occupied molecular orbital(s) of NO^+ as the “HOMO”(s). [1 mark]

(g) In the space below, draw a picture of the orbital(s) you labeled as HOMO. Clearly indicate relative phase as well as the location of each nucleus. [1 mark]



(g) What bond order does your MO treatment predict for NO^+ ? Does it agree with the bond order from your Lewis diagram? [2 marks]

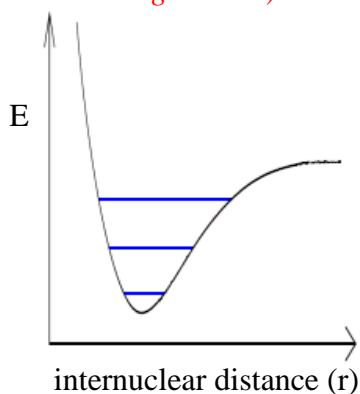
$$B.O. = \frac{1}{2}(8 - 2) = 3 \quad \text{Yes it agrees with the Lewis diagram}$$

(h) What is the bond order if an electron is added to NO^+ ? In other words, what is the bond order in NO ? [1 mark]

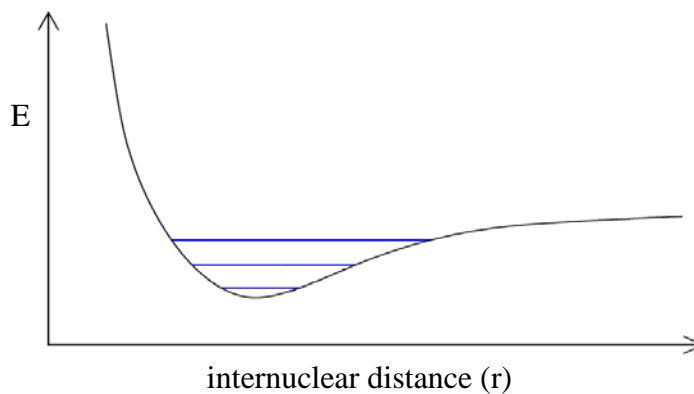
It will go into an antibonding orbital, so the bond order will decrease to 2.5.

(i) What will happen to the potential energy curve of the N-O bond if you remove an electron from NO^+ ? Be specific. You may find it helpful to sketch the potential energy curve before and after the electron is removed. [2 marks]

The electron that would be removed from NO^+ would come from the 3σ orbital – which is a bonding orbital. As such, the bond order would decrease from 3 to 2.5. This would make the bond longer and weaker. As such, the potential energy curve would get shallower (for the lower bond energy) and the minimum would be at a larger internuclear distance (for the longer bond):



NO^+



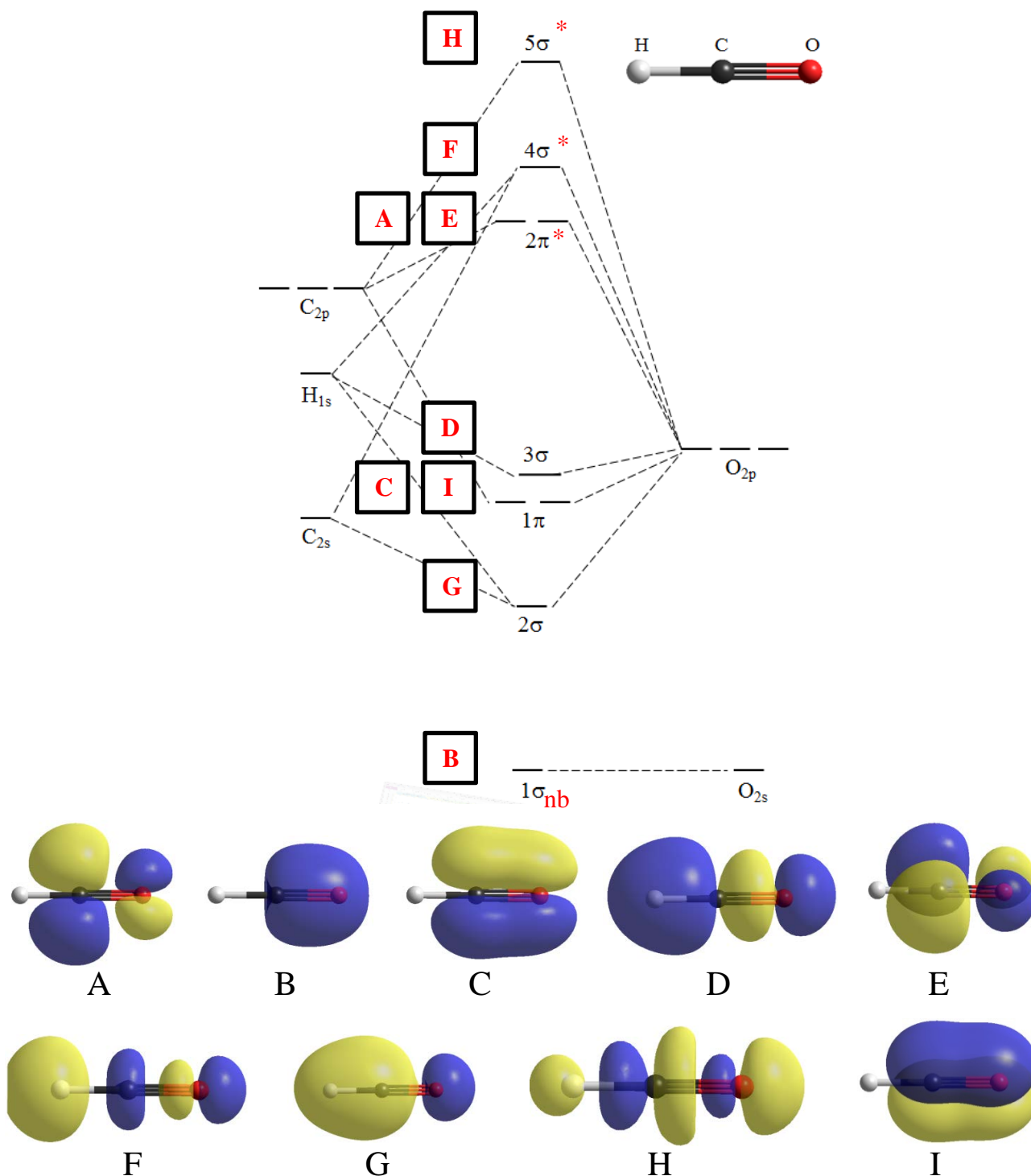
NO^{2+}

2.

[8 marks]

Shown below is the valence MO energy level diagram for the *linear* HCO^+ cation, also known as the acylium cation. Below that, pictures of the nine valence molecular orbitals are given, each labeled with a letter (A-I). All the pictures have HCO^+ in the same orientation (H at the left; O at the right).

- (a) None of the MOs on this diagram have been labeled as bonding, nonbonding or antibonding. Mark the antibonding MOs with a * and mark the nonbonding MOs with the subscript 'nb'.
- (b) In the box next to each energy level on the MO diagram, use the letters provided to identify the picture(s) corresponding to each energy level. *There should be one letter per box.*

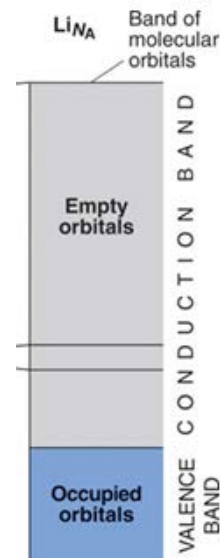


3.

[3 marks]

In band theory, compounds with a band gap smaller than or close to $k_B T$, (which is very small) can be considered metallic conductors. Briefly explain the band structure of metals and why metals are considered electric conductors. *You may find it helpful to include a diagram in your answer.*

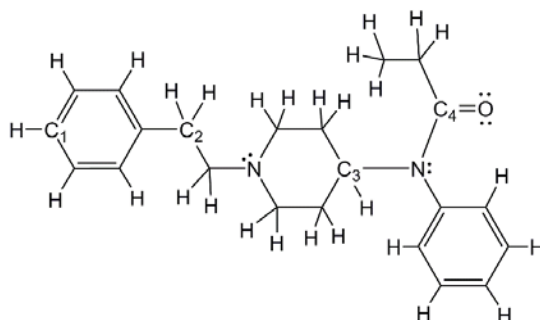
- Electrons in a metal are in states (analogous to MOs in small molecules). States of similar energy form bands.
- The highest energy electrons in a metal are in the valence band (analogous to HOMO in small molecules).
- The lowest energy empty states are in the conduction band (analogous to LUMO in small molecules)
- In a metal, the energy gap between the highest energy electrons and lowest energy empty states is very small. Often, there is no gap at all! (This can either be because the valence band is only half full so also functions as the conduction band, or it can be because the valence band and conduction band overlap in energy.)
- For a substance to conduct electricity, it must be easy to excite an electron from the valence band into the conduction band. The smaller the energy gap between the valence and conduction bands, the easier this excitation will be.



4.

[3 marks]

Fentanyl (a synthetic opioid pain medication) was originally developed in 1960s, but more recently the combination of its extreme potency and use/distribution as a recreational drug has resulted in a significant increase in deaths by overdose to the general public. Consider the fentanyl molecule in accordance with valence bond theory:



Parts of the structure above are drawn using the “line-bond” method meaning that not all carbon atoms are explicitly represented by a C.

- (a) What is the hybridization for each of the four labeled carbon atoms in this molecule? [2 marks]

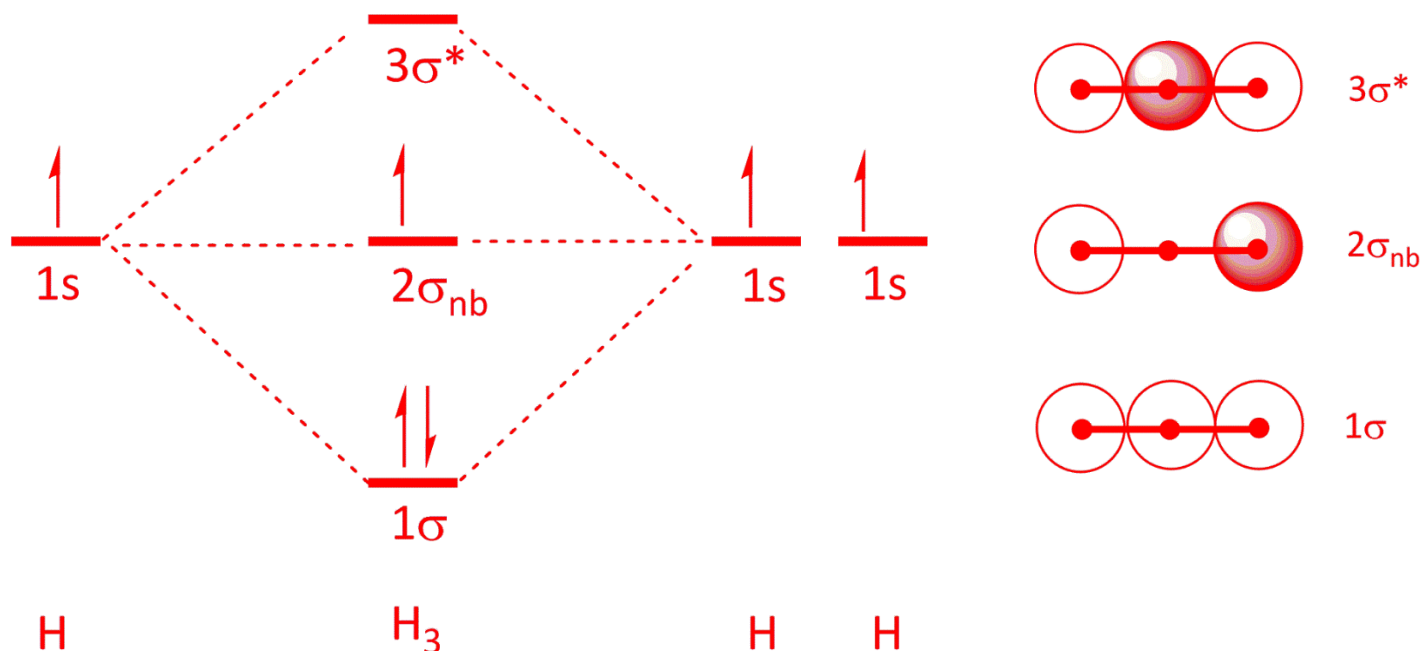
Carbon #	Hybridization
C ₁	sp^2
C ₂	sp^3
C ₃	sp^3
C ₄	sp^2

- (b) How many π bonds are there in this molecule?

[1 mark]

[18 marks]

5. (a) Consider the **linear** neutral H_3 molecule. It has one central hydrogen atom and two terminal hydrogen atoms. [9 marks]
- Draw a molecular orbital energy level diagram for H_3 .
 - Label all atomic and molecular orbitals on your diagram, clearly indicating if each MO is bonding, nonbonding or antibonding.
 - Populate the atomic orbitals with the correct number of electrons.
 - Populate the molecular orbitals with the correct number of electrons.



- (b) Draw a picture of each molecular orbital next to your MO energy level diagram. Clearly indicate relative phase as well as the location of each nucleus. [3 marks]
see above

- (c) Calculate the H–H bond order for the H_3 molecule. [1 mark]

$$B.O. = \frac{\frac{1}{2}(2-0)}{2} = \frac{1}{2}$$

*Remember that the two bonding electrons are shared by two H–H links/bonds/regions!
 The nonbonding electron has no effect on bond order.*

- (d) What are the H–H bond orders for H_3^+ and for H_3^- ? [2 marks]

$$H_3^+ \text{ bond order} = \frac{1}{2}$$

$$H_3^- \text{ bond order} = \frac{1}{2}$$

The nonbonding electron has no effect on bond order.

5. *continued...*

(e) What are the magnetic properties of H_3 , H_3^+ , and H_3^- ? (paramagnetic or diamagnetic) [1 mark]

H_3 is paramagnetic

H_3^+ is diamagnetic

H_3^- is diamagnetic

(f) Sketch a UV-photoelectron spectrum for the H_3 molecule. Label the bands with the labels of the appropriate MOs. You do not need to provide numerical values for the energies. [2 marks]

