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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.

## Confidentiality Agreement:

I agree not to discuss (or in any other way divulge) the contents of this exam until after 8:00pm Mountain Time on Wednesday, February $13^{\text {th }}$, 2013. I understand that breaking this agreement would constitute academic misconduct, a serious offense with serious consequences. The minimum punishment would be a mark of $0 / 47$ 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: $\qquad$ Date: $\qquad$
Course: CHEM 2000 (General Chemistry II)
Semester: Spring 2013
The University of Lethbridge

Question Breakdown

|  | $/ 12$ |
| :--- | ---: |
| Q1 | $/ 5$ |
| Q2 | $/ 4$ |
| Q3 | $/ 15$ |
| Q4 | $/ 11$ |
| Q5 |  |

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1.
(a) Draw a valence molecular orbital diagram for $\mathrm{C}_{2}$. Your diagram must include labeled atomic and molecular orbitals and include electrons in the appropriate orbitals.
(b) Draw a valence molecular orbital diagram for $\mathrm{F}_{2}$. Your diagram must include labeled atomic and molecular orbitals and include electrons in the appropriate orbitals. You do not need to draw pictures of the orbitals.
(c) On each of your answers to part (a) and (b) of this question, clearly label the HOMO and LUMO. [2 marks]
(d) Calculate the bond order for $\mathrm{F}_{2}$.
(e) Does the bond order change when an electron is removed from $F_{2}$ ? If so, how?
(f) Does the bond order change when an electron is added to $\mathrm{F}_{2}$ ? If so, how?
[1 mark]
(g) Of the following species, which (if any) are paramagnetic: $\mathrm{F}_{2}, \mathrm{~F}_{2}{ }^{+}$and $\mathrm{F}_{2}{ }^{-}$?

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2. A photoelectron spectrum of $\mathrm{C}_{2}$ is obtained using an ultraviolet lamp producing a single wavelength of light. The electrons ejected with the highest kinetic energy have a kinetic energy of $9 \times 10^{-19} \mathrm{~J}$.
(a) From what orbital are the electrons with the highest kinetic energy being ionized? [2 marks] Hint: You drew a valence MO diagram for $C_{2}$ in question 1(a)
(b) What effect would the ionization process have on the vibrational spacing of the ion relative to the neutral molecule?
[3 marks]
3. The best Lewis structure for formamide is shown below.
[4 marks]

(a) Draw another Lewis structure for formamide that also obeys the octet rule. Your Lewis structure should have atoms with nonzero formal charges. Show those charges.
[2 marks]
(b) A typical $\mathrm{C}=\mathrm{O}$ bond has a stretching frequency (expressed as a wavenumber*) of $1700 \mathrm{~cm}^{-1}$ on an infrared spectrum. Would you expect the $\mathrm{C}=\mathrm{O}$ stretching frequency for formamide to be larger or smaller than $1700 \mathrm{~cm}^{-1}$ ? Explain briefly.
[2 marks]

[^0]$\qquad$
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4. The valence atomic orbital energies for Be and Cl are as follows:

|  | $\mathbf{B e}$ | $\mathbf{C l}$ |
| :---: | :---: | :---: |
| $2 s$ | -0.69 Ry |  |
| $2 p$ | +0.08 Ry |  |
| $3 s$ |  | -1.86 Ry |
| $3 p$ |  | -1.01 Ry |

While the $2 p$ orbital is unoccupied in a Be atom, we can still get molecular orbitals involving this atomic orbital since it is relatively low in energy.
(a) Draw the Lewis structure for $\mathrm{BeCl}_{2}$. Predict the geometry of this molecule as well as the $\mathrm{Be}-\mathrm{Cl}$ bond order.
[3 marks]
(b) Classify each of the atomic orbitals of Be and Cl as sigma or pi type.
(c) Indicate which (if any) of the atomic orbitals would not be expected to participate in bonding.
(d) Sketch the combination of atomic orbitals that produces the lowest-energy bonding sigma orbital of $\mathrm{BeCl}_{2}$ in LCAO-MO theory. Also, show the final shape of that molecular orbital. [2 marks]
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4. ...continued
(e) A sketch of the valence molecular orbital diagram of $\mathrm{BeCl}_{2}$ is shown below, along with pictures of all but the bottom three orbitals. The diagram is not entirely drawn to scale. In particular, the two orbitals at the bottom are closer in energy than suggested by this graphic. In the orbital pictures, approximate locations of nuclei are marked by heavy dots.

i. One of the orbitals for which a picture isn't shown is the bonding orbital you sketched in part (d). Which of the bottom three lines in the molecular orbital diagram corresponds to your bonding orbital?
[1 mark]
ii. What are the other two orbitals for which a picture isn't shown?
[1 mark]
iii. Label all orbitals in the diagram using our usual numbering scheme ( $1 \sigma, 2 \sigma, 1 \pi$, etc.). Clearly label any nonbonding orbitals with a subscript nb.
iv. Show the ground state orbital occupancy on the diagram using up/down arrows to symbolize electrons.
[1 mark]
v. Use the completed valence molecular orbital diagram to estimate the $\mathrm{Be}-\mathrm{Cl}$ bond order. Does it agree with the bond order from your Lewis structure in part (a)?
[2 marks]
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5.
[11 marks]
Table 1: Atomic Orbital Energy Values for Hydrogen, Fluorine and Bromine

|  | Hydrogen | Fluorine | Bromine |
| :---: | :---: | :---: | :---: |
| $1 s$ | -1.0 Ry | -51.2 Ry | -993.0 Ry |
| $2 s$ |  | -3.0 Ry | -131.7 Ry |
| $2 p$ |  | -1.4 Ry | -115.6 Ry |
| $3 s$ |  |  | -19.9 Ry |
| $3 p$ |  |  | -13.8 Ry |
| $3 d$ |  |  | -4.5 Ry |
| $4 s$ |  |  | -1.8 Ry |
| $4 p$ |  |  | -0.93 Ry |

(a) Why is the difference in energy between the $1 s$ orbital of hydrogen and the $1 s$ orbital of bromine much larger than that between hydrogen and fluorine?
(b) Complete the valence molecular orbital energy level diagram for HBr by adding electrons to the appropriate orbitals and labeling the orbitals as bonding, nonbonding or antibonding. [2 marks]
 4s
(c) Sketch a picture of each molecular orbital and clearly indicate which atomic orbitals were used to generate it.
[4 marks]
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$\qquad$ Student Number: $\qquad$
5. ...continued
(d) The valence molecular orbital energy level diagram for HBr has been redrawn below. To its left is the valence molecular orbital energy level diagram for HF. You will need to add the electrons again.


Use these two diagrams to explain why HBr is a stronger Lewis acid than HF.

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## Overflow Page

If you use this page for any answers, please clearly indicate which question is being answered and make sure you note on the page for the question itself that the answer continues here.

| 1 | Chem 2000 Standard Periodic Table |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 18 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1.0079 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 4.0026 |
| ${ }_{1} \mathbf{H}$ | 2 |  |  |  |  |  |  |  |  |  |  | 13 | 14 | 15 | 16 | 17 | ${ }_{2} \mathrm{He}$ |
| 6.941 | 9.0122 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 10.811 | 12.011 | 14.0067 | 15.9994 | 18.9984 | 20.1797 |
| Li | Be |  |  |  |  |  |  |  |  |  |  | B | C | N | 0 | F | Ne |
| 3 | 4 |  |  |  |  |  |  |  |  |  |  | 5 | 6 | 7 | 8 | 9 | 10 |
| 22.9898 | 24.3050 |  |  |  |  |  |  |  |  |  |  | 26.9815 | 28.0855 | 30.9738 | 32.066 | 35.4527 | 39.948 |
| Na | Mg |  |  |  |  |  |  |  |  |  |  | Al | Si | P | S | Cl | Ar |
| 11 | ${ }_{12} \mathrm{Mg}$ |  |  |  |  |  |  |  |  |  |  | ${ }_{13}{ }^{\text {Al }}$ | 14 | 15 | 16 | 17 | 18 |
| 39.0983 | 40.078 | 44.9559 | 47.88 | 50.9415 | 51.9961 | 54.9380 | 55.847 | 58.9332 | 58.693 | 63.546 | 65.39 | 69.723 | 72.61 | 74.9216 | 78.96 | 79.904 | 83.80 |
| K | Ca | Sc | Ti | V | Cr | Mn | Fe | Co | Ni | Cu | Zn | Ga | Ge | As | Se | Br | Kr |
| 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 |
| 85.4678 | 87.62 | 88.9059 | 91.224 | 92.9064 | 95.94 | (98) | 101.07 | 102.906 | 106.42 | 107.868 | 112.411 | 114.82 | 118.710 | 121.757 | 127.60 | 126.905 | 131.29 |
| Rb | Sr | Y | Zr | Nb | Mo | Tc | Ru | Rh | Pd | Ag | Cd | In | Sn | Sb | Te | I | Xe |
| 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 |
| 132.905 | 137.327 |  | 178.49 | 180.948 | 183.85 | 186.207 | 190.2 | 192.22 | 195.08 | 196.967 | 200.59 | 204.383 | 207.19 | 208.980 | (210) | (210) | (222) |
| Cs | Ba | La-Lu | Hf | Ta | W | Re | Os | Ir | Pt | Au | Hg | Tl | Pb | Bi | Po | At | Rn |
| 55 | 56 |  | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 |
| (223) | 226.025 |  | (261) | (262) | (263) | (262) | (265) | (266) | (281) | (283) |  |  |  |  |  |  |  |
| Fr | Ra | Ac-Lr | Rf | Db | Sg | Bh | Hs | Mt | Dt | Rg |  |  |  |  |  |  |  |
| 87 | 88 |  | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 |  |  |  |  |  |  |  |


| $\begin{gathered} 138.906 \\ \mathbf{L a} \\ 57 \end{gathered}$ | $\begin{gathered} 140.115 \\ \mathbf{C e} \\ 58 \end{gathered}$ | $\begin{gathered} 140.908 \\ \mathbf{P r} \\ 59 \end{gathered}$ | $\begin{aligned} & \hline 144.24 \\ & \mathbf{N d} \\ & 60 \end{aligned}$ | $\begin{gathered} \hline(145) \\ \mathbf{P m} \\ 61 \\ \hline \end{gathered}$ | $\begin{gathered} 150.36 \\ \text { Sm } \end{gathered}$ <br> 62 | $\begin{aligned} & 151.965 \\ & \mathbf{E u} \\ & 63 \end{aligned}$ | $\begin{gathered} 157.25 \\ \text { Gd } \\ 64 \end{gathered}$ | $\begin{gathered} 158.925 \\ \mathbf{T b} \\ 65 \end{gathered}$ | $\begin{gathered} 162.50 \\ \mathbf{D y} \\ 66 \end{gathered}$ | $\begin{gathered} 164.930 \\ \text { Ho } \end{gathered}$ $67$ |  | $\begin{gathered} 168.934 \\ \mathbf{T m} \\ 69 \end{gathered}$ | $\begin{gathered} 173.04 \\ \mathbf{Y b} \\ 70 \end{gathered}$ | $\begin{gathered} 174.967 \\ \mathbf{L u} \\ 71 \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 227.028 | 232.038 | 231.036 | 238.029 | 237.048 | (240) | (243) | (247) | (247) | (251) | (252) | (257) | (258) | (259) | (260) |
| Ac | Th | Pa | U | Np | Pu | Am | Cm | Bk | Cf | Es | Fm | Md | No | Lr |
| 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 | 101 | 102 | 103 |

Developed by Prof. R. T. Boeré

| Region | Frequency range, $\left(\mathrm{cm}^{-1}\right)$ | Bond types | Functional groups |
| :---: | :---: | :---: | :--- |
| 1 | $3500-3200$ | $\mathrm{O}-\mathrm{H}$ | Alcohol, phenol <br> Amine, amide |
| 2 | $2300-2100$ | $\mathrm{~N}-\mathrm{H}$ | Am <br>  <br> 3 |
|  | $1800-1650$ | $\mathrm{C} \equiv \mathrm{C}$ | Alkyne <br> Nitrile |
|  | $\mathrm{C}=\mathrm{N}$ | Aldehyde <br> Amide |  |
|  |  | Anhydride (2 bands) <br> Carboxylic acid |  |
|  |  |  | Acid chloride <br> Ester |
|  |  | $\mathrm{C}=\mathrm{C}$ | Alkene |
| 4 | $\mathrm{C}=\mathrm{C}$ | Arene |  |
|  |  | $\mathrm{C}=\mathrm{N}$ | Imine |
|  | $\mathrm{N}=\mathrm{O}$ | Nitro compound |  |
|  |  |  |  |


[^0]:    ${ }^{*}$ wavenumber: $1 \mathrm{~cm}^{-1}=2.997925 \times 10^{10} \mathrm{~Hz}$

