 Student name: _____ Student ID#: _____

Multiple Choice Questions **Circle one answer**, unless noted. (5 points each, 30 total)

1) Which of the following molecular species are paramagnetic?

A) N_2^{2+} **B)** F_2^{2-} **C)** O_2^{2+} **D)** Cl_2 **(E)** Ne_2^{3+}

2) How many radial nodes are in a 4d orbital?

(A) 1 **B)** 2 **C)** 3 **D)** 4 **E)** 5

3) Which of the following molecules contain sp^2 hybridization?

A) Acetylene, C_2H_2 **B)** Water, H_2O **C)** Ethane, C_2H_6

(D) Benzene, C_6H_6 **E)** Ammonia, NH_3

4) Ψ^2 for the 2*s* orbital of Na is $\frac{27}{32\pi a_0^3}\left(2-\frac{11r}{a_0}\right)^2 e^{\frac{-11r}{a_0}}$

The position of the node is:

A) $r=\frac{a_0}{11}$ **B)** $r=\frac{2}{3}a_0$ **C)** $r=a_0$ **D)** $r=\frac{32}{27}a_0$ **(E)** $r=\frac{2}{11}a_0$

5) Which element does not have a ground state electron configuration with a half-filled *d* orbital (d^5)?

A) Mn **B)** Tc **C)** Cr **(D)** Ru **E)** Mo

6) Which of the following explains why silicon-silicon multiple bonds are less common than carbon-carbon multiple bonds? **Circle all that apply.**

(A) Si is less electronegative than C

(B) Si atoms are larger than C atoms

C) Si atoms are smaller than C atoms False

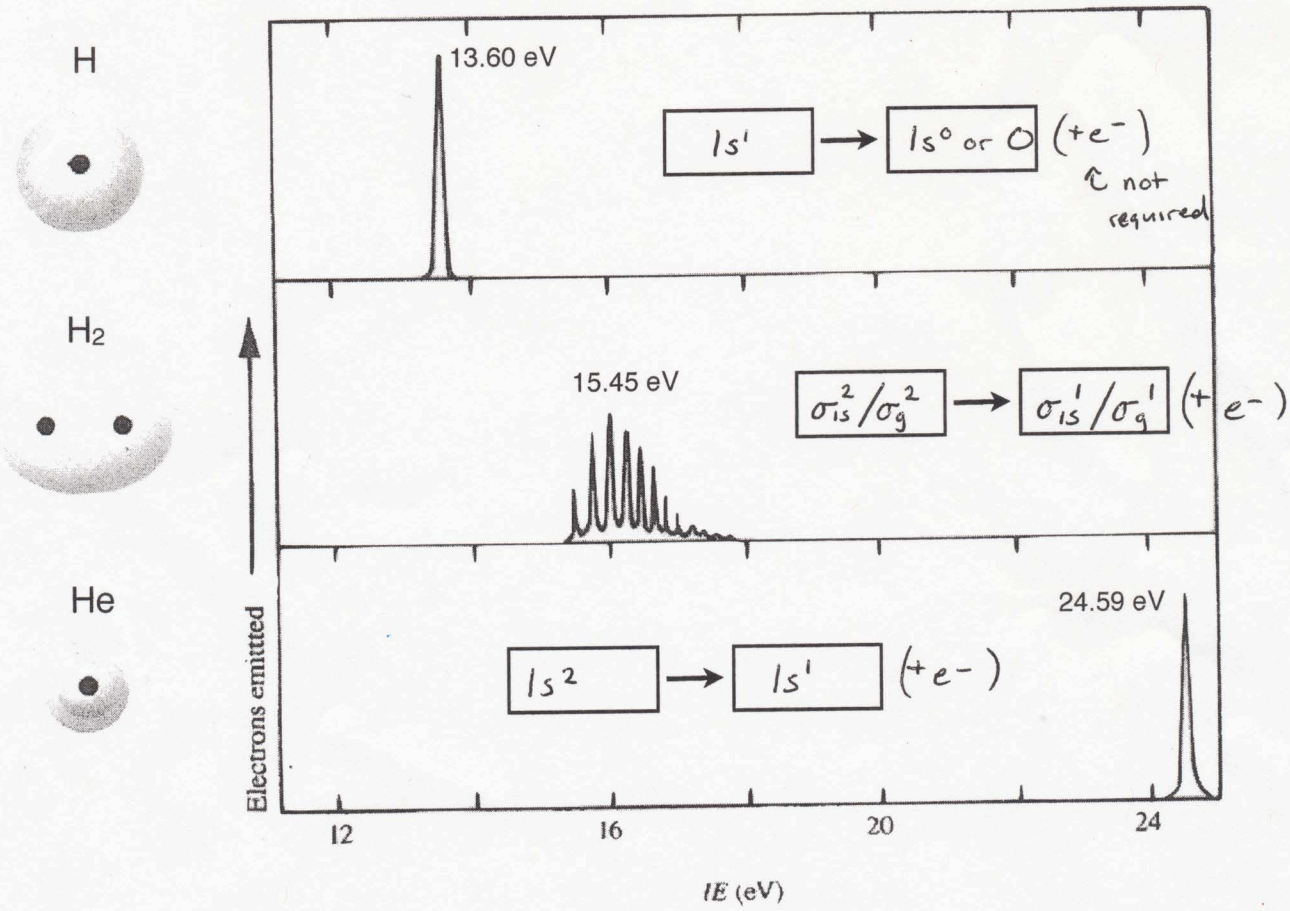
(D) Si can use more than 8 valence electrons

E) The Si-Si bond is weaker than the C-C bond True, but not relevant

1 pt for each statement.

Short Answer Question #1 [15 points]

In the boxes provided, label the initial and final electron configurations for each of the following atomic and molecular photoelectron spectra. Assume only one electron is emitted.



5 points each, 3 for initial e⁻ configuration.
2 for final e⁻ configuration showing 1 less e⁻

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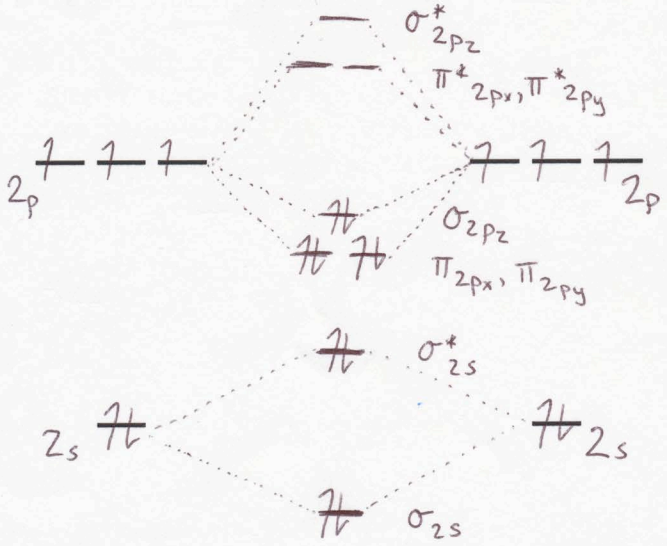
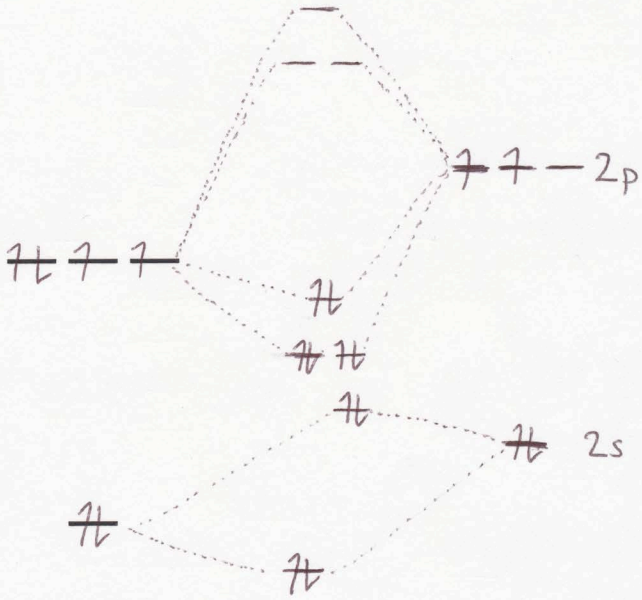
Short Answer Question #2 [24 points total]

a) The valence atomic orbitals (AOs) for nitrogen are shown below on a molecular orbital energy-level diagram. Complete the diagram for N_2 with MO energy levels and label i) the type of orbital from which they are made, ii) whether they are σ- or π-orbitals, and iii) whether they are bonding or antibonding. [8 points]



N +2 energy level order N
+2 electrons
+2 σ/π, bonding/antibonding
+2 orbital contribution/orientation

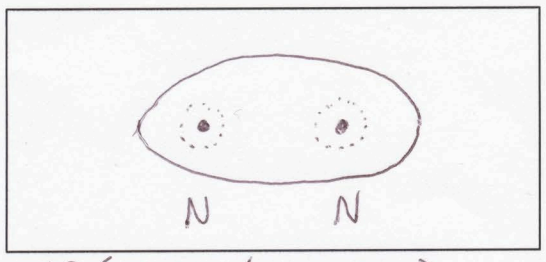
b) The orbital structure and order of CN^-, a heteronuclear diatomic ion, is similar to that of N_2. Using the preplaced nitrogen AOs and your knowledge of electronegativity, predict the position on the carbon AOs and the MO energy-level diagram for CN^-. [8 points]



N +2 energy level order (same) C
+2 electrons
+4 C AO placement

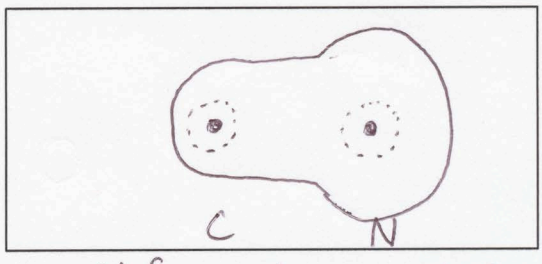
c) Draw the lowest energy bonding orbital (excluding 1*s*) for N_2 in the box provided. Draw the corresponding orbital for CN^-, showing the effect of electronegativity on the electron probability density. [4 points each]

N_2



+3 for σ_{2s} (symmetric)
+1 for radial nodes from 2s

CN^-



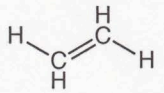
+1 for σ_{2s} (or same orbital as N_2)
+2 asymmetric e⁻ density
+1 asymmetric towards N
(or consistant w/ above diagram)

1pt - show E axis
i, ii, iii) (each)
1 point # of E levels
1 point E level arrangement
1 point # of electrons

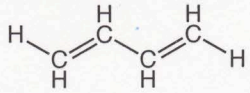
iv)
2 points for band formation
1 point for x filled,
1 point for x unfilled energy levels

Short Answer Question #3 [31 points total]

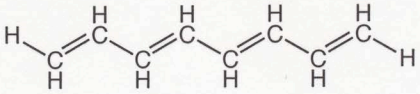
a) Consider the series of organic compounds:



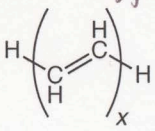
i) ethylene



ii) butadiene

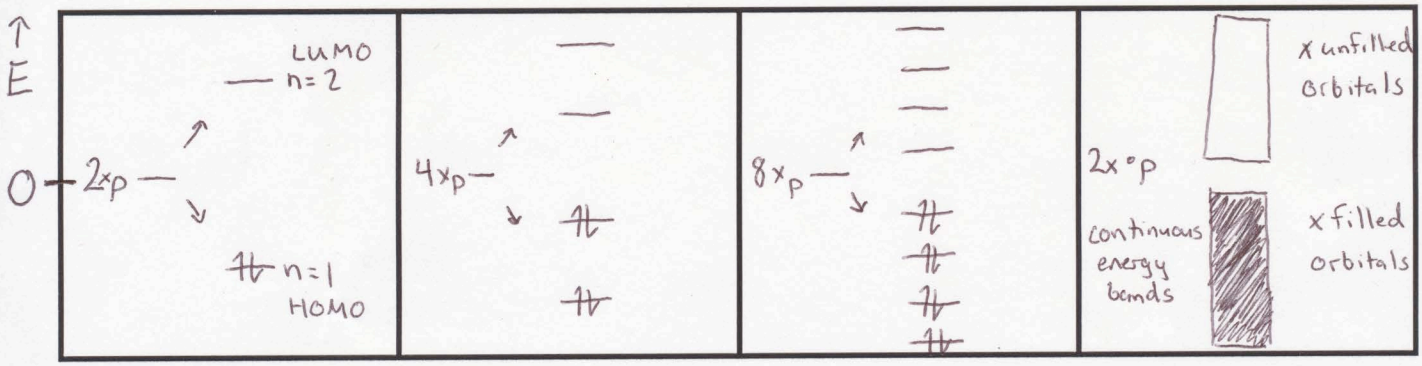


iii) octatetraene



iv) poly(acetylene)

Using the boxes provided, sketch the energy diagram for the conjugated π electrons in each system. Label the number of filled and unfilled energy levels in each case. [14 points]



b) Use the FEMO method to determine the wavelength of the HOMO-LUMO transition in octatetraene. Assume that the C bonds form a linear (180°) chain and the average C–C bond length is 0.140 Å. [14 points]

4 points: $L = 7(0.140\text{ Å}) = 0.980\text{ Å}$
Using "½ bonds at end" from lecture also acceptible

HOMO n=4
LUMO n=5
2 points

Incorrect reference data. Should be 1.40 Å.
λ = 353 nm is also acceptable.

4 points: $\Delta E = \dfrac{h^2(n^2_{LUMO} - n^2_{HOMO})}{8 m_e L^2}$

4 points: $\lambda = \dfrac{hc}{\Delta E} = 3.53\text{ nm}$

c) Which molecule has the lowest (most stable) energy level for $n = 1$? **Circle one response.** [3 points]

A) ethylene **B)** butadiene **(C)** octatetraene