CH 1101, Mid Semester Exam

Total Marks = 30; Time = 90 min

There are **Six** questions, and you will have to answer all the questions. There is an optional **Question 7**. You can get **extra credit** for answering this question.

All the orbital energy values have been provided in a table in the last page.

1a) The binding energy of a calcium 2p electron is -349.7 eV. What would be the effective nuclear charge experienced by a calcium 2p electron? (R_H = 13.6 eV)

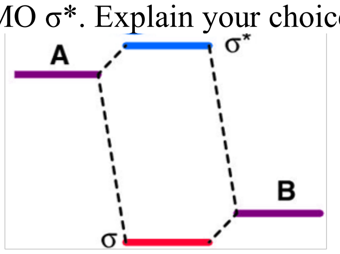
b) The radial part of the 2s AO wave function is:

$$\left(\frac{1}{2a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right)e^{-\frac{r}{2a_0}}$$

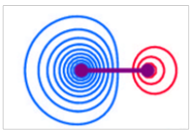
Determine the position of the radial node(s) in the 2s orbital?

c) For the Li atom, compare the 2s and 2p electrons in terms of shielding ability? Explain in brief.

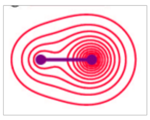
d) The illustration below represents the formation of MO's σ and σ* from the AO of **A** and AO of **B** having different energy. Which of the following contour plots (I – IV) best represent the MO σ*. Explain your choice briefly.



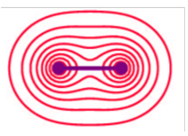
(I)



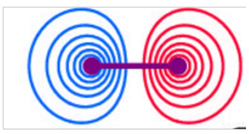
(II)



(III)



(IV)

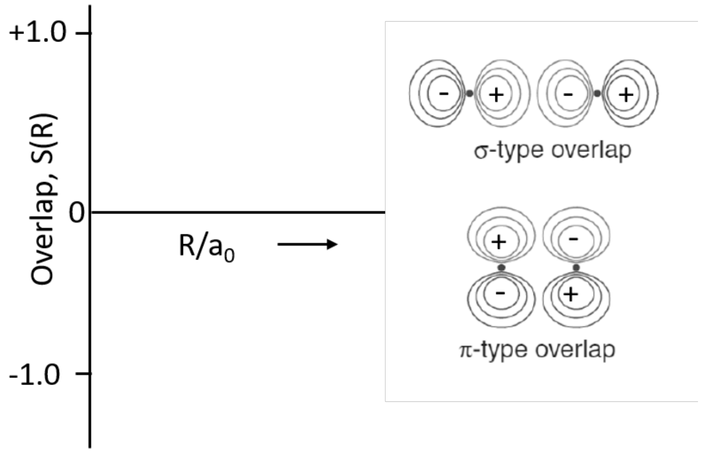


(2 X 4 marks)

2. The angular part of the p_x orbital, dependent on both θ and φ, is given by $\sqrt{\left(\frac{3}{4\pi}\right)}\sin\theta\cos\varphi$. Show that the plot of this function would generate yz plane as the nodal plane.

(4 marks)

3. Plot the overlap integral between two 2p orbitals. Depict the sideways –on overlap to give π MO's **(as a solid line)**, and the head-on overlap to give σ MO's **(as a dashed line)** on the same plot.



4. The organic molecule NH is found in the interstellar clouds interstellar. Construct an MO diagram for this diatomic molecule NH, label the MOs, indicate which orbitals are occupied, and sketch the form of the occupied orbitals. The relevant orbital energies are: H 1s -13.6 eV; N 2s -25.6 eV; N 2p -13.2 eV.

A) Complete the **MO energy-level diagram for NH**. Place the correct number of electrons in the energy levels.
B) What would be the possible spin state(s) of NH? Which would be the ground state electronic configuration of NH?
C) Sketch the molecular orbital of NH which can be designated as π MO?
(6 marks)

5. (a) Draw a MO diagram for the **valence electrons** of **BC**. Label all atomic and molecular orbitals.
(b) Write the molecular orbital configuration for the valence electrons in **BC** and in **BC^{1-}**.
(c) Which has the stronger **B–C bond**, **BC** or **BC^{1-}**? You may justify your answer using bond order.
(4 marks)

6. Draw the MO diagram of LiF and LiBr based on the relevant orbital energies given in the table in the next page. Based on the MO diagram, the charge on the Li atom will be higher in LiF or LiBr? Explain.
(4 marks)

Extra Credit (5 marks)

7. Assume yourself to be Dedalus. As a celebrated Greek philosopher, the Gods have invited you to classify the celestial elements found at Mount Olympus.

Electrons at Mount Olympus are described by four quantum numbers with meanings similar to those used by mortals on earth. We will call these quantum numbers α, β, γ, and δ. The rules for these quantum numbers are as follows:

$\alpha = 1,2,3,5,8,13,21\ldots.$

β takes on all integer values from 0 to $(\alpha-1)/2$ (for α = odd) and 0 to $\alpha/2$ (for α = even).

γ takes on all odd integer values from $-\beta$ to $+\beta$ and zero

$\delta = -1/2,\ \frac{1}{2}$

Consider that the 'basic ideas' of Hund's rule, Aufbau principle, and Pauli's Exclusion principle are applicable here also and the notion of stability remains the same.

A) Sketch the first five periods of the periodic table formulated for Olympian elements.

B) Stygian Iron (Sy) reacts with Cretan Sulfur (Ct) to form an ionic compound with the formula Sy_3Ct_2. What are the possible atomic numbers of Sy and Ct? Consider only the first five rows. Both Sy and Ct have a single oxidation state.

C) How many electrons can have $\alpha = 13$, $\beta = 5$?

D) What will be the electronic configuration of the element bearing atomic number 38 ? (Note: $\beta = 0 =$ s, $\beta = 1 =$ p….)

TABLE 5.2 Orbital Potential Energies

		Orbital Potential Energy (eV)						
Atomic Number	Element	1s	2s	2p	3s	3p	4s	4p
1	H	−13.61						
2	He	−24.59						
3	Li		−5.39					
4	Be		−9.32					
5	B		−14.05	−8.30				
6	C		−19.43	−10.66				
7	N		−25.56	−13.18				
8	O		−32.38	−15.85				
9	F		−40.17	−18.65				
10	Ne		−48.47	−21.59				
11	Na				−5.14			
12	Mg				−7.65			
13	Al				−11.32	−5.98		
14	Si				−15.89	−7.78		
15	P				−18.84	−9.65		
16	S				−22.71	−11.62		
17	Cl				−25.23	−13.67		
18	Ar				−29.24	−15.82		
19	K						−4.34	
20	Ca						−6.11	
30	Zn						−9.39	
31	Ga						−12.61	−5.93
32	Ge						−16.05	−7.54
33	As						−18.94	−9.17
34	Se						−21.37	−10.82
35	Br						−24.37	−12.49
36	Kr						−27.51	−14.22

J. B. Mann, T. L. Meek, L. C. Allen, *J. Am. Chem. Soc.*, 2000, *122*, 2780.

All energies are negative, representing average attractive potentials between the electrons and the nucleus for all terms of the specified orbitals.

Additional orbital potential energy values are available in the online Appendix B-9.