

## CH 1101, Mid Semester Exam

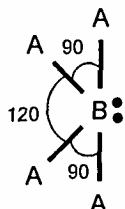
Total Points = 20; Time = 60 min

~~You need to answer all the questions in both Section A and Section B. Section A must be answered in the OMR sheets while Section B in the answer sheet provided to you.~~

### Section A

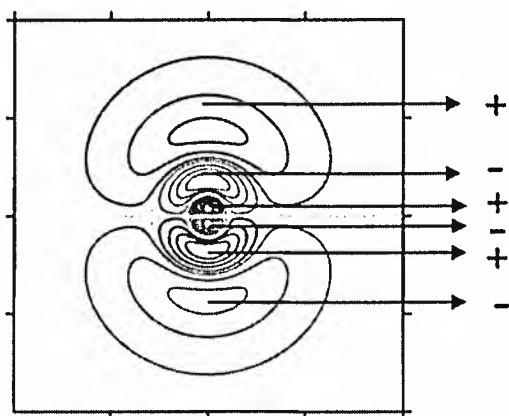
Consider all the statements in the following groups and select the single statement that most correctly answers the question posed. There is one correct answer for each problem. (8 X 1 = 8 points)

1. An electron is excited from the ground state to the  $n = 3$  state in a hydrogen atom. Which of the following statements is true?  
A) It takes more energy to ionize (remove) the electron from  $n = 3$  than from the ground state.  
B) The electron is farther from the nucleus on average in the  $n = 3$  state than in the ground state.  
C) The wavelength of light emitted if the electron drops from  $n = 3$  to  $n = 2$  is shorter than the wavelength of light emitted if the electron falls from  $n = 3$  to  $n = 1$ .  
D) The first excited state corresponds to  $n = 3$
2. The Radial Probability Distribution (RPD) Function of Hydrogen 1d orbital will have how many radial nodes: (NOTE: DONOT consider  $RPD=0$  at  $r=0$  as a node)  
A) 7  
B) 8  
C) 9  
D) 10
3. The following statements highlight the difference between H-atom orbitals and their corresponding Na-atom orbitals. Which of the following statements is **NOT** correct?  
(A) The Na-atom orbitals are lower in energy than H-atom orbitals  
(B) The radial probability distribution function of Na-atom is similar to that of H-atom (consider just the shape of the curve)  
(C) In Na-atom the maxima of the radial distribution function from the nucleus increases in the order:  $3d > 3p > 3s$   
(D) The energy of an electron in the 2s orbital of H-atom is lower than that in the 2p orbital
4. Which of the following molecules will have a see-saw structure as shown below:



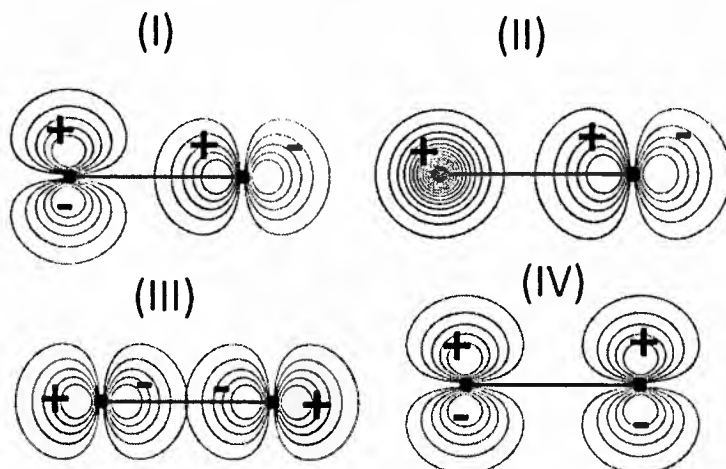
- (A)  $CF_4$
- (B)  $XeF_4$
- (C)  $TeCl_4$
- (D)  $PCl_4^+$

5. The following diagram represents the equal probability iso-surface of which orbital:



- A) 3p
- B) 4p
- C) 2p
- D) 5p

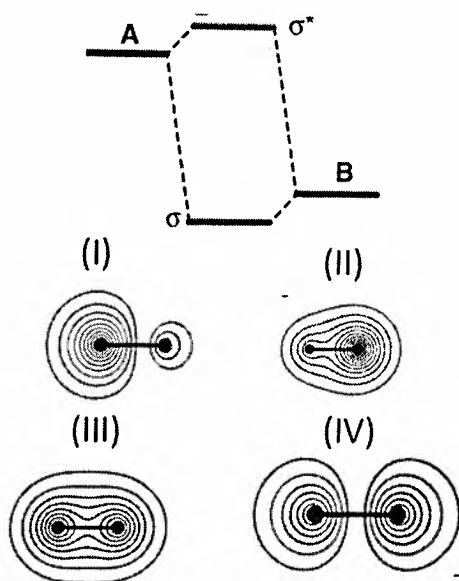
6. The illustration below represents four possible combinations of 1s and 2p orbitals than can lead to the formation of MO's. In which combination the overlap integral  $S$  will be zero.



- (A) I
- (B) II
- (C) III
- (D) IV

7. The illustration below represents the formation of MO's  $\sigma$  and  $\sigma^*$  from the AO of A and AO of B having different energy. Which of the following contour plots best represent the MO  $\sigma$ .

*Handwritten scribble*



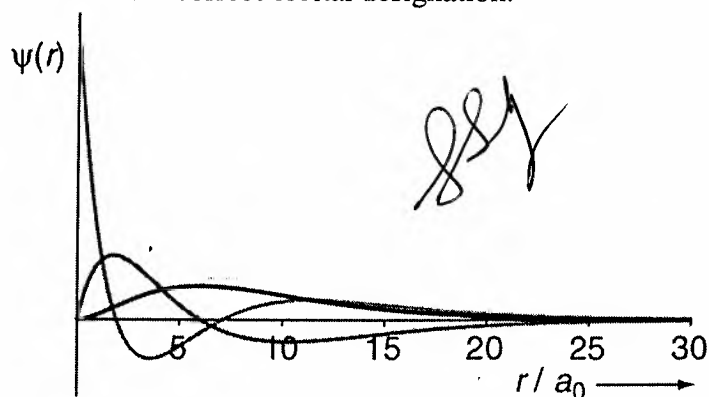
- (A) I  
(B) II  
(C) III  
(D) IV

8. Consider the group I elements Li to Cs. Which of the following statements is NOT correct?

- (A) The effective nuclear charge  $Z_{\text{eff}}$  increases as we go down the group  
(B) The valance s-orbital energy decreases (more negative values in eV) as we go down the group  
(C) The bond strengths of the dimers in gas phase (such as  $\text{Li}_2$ ) decreases as we go down the group  
(D) The valance s-orbital energy depends on both  $Z_{\text{eff}}$  and  $n$  (principal quantum no).

## SECTION B

9. In the illustration below, the radial parts of 3s, 3p and 3d AOs of H-atom are shown. Sketch the Radial Probability Distribution Function of the corresponding AO's in one graph. Label them with the correct orbital designation.

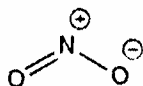


(2 marks)

10. Suppose that some all powerful being suddenly decided to change the Schrödinger wave equation. After this change, the energies in *ALL* atoms depends on the principal quantum number *n only*. Everything else would remain the same. (a) Write the electronic configuration of Ni (Atomic no 28) under the new rules (b) What ions, if any, would Nickel tend to form.

(2 marks)

11.  $\text{NO}_2$  is known to be a free radical (i.e. it has an unpaired electron) and adopt a bent geometry. One possible representation of the bonding in  $\text{NO}_2$  is shown below: indicate in the usual way the location of the electrons in the molecule by drawing the Lewis structure and verify that the formal charges shown are correct.



(2 marks)

12. Methylidyne is an organic molecule with the formula  $\text{CH}$  and is abundant in the interstellar medium. Construct an MO diagram for this diatomic molecule  $\text{CH}$ , label the MOs, indicate which orbitals are occupied, and sketch the form of the occupied orbitals. The relevant orbital energies are:  $\text{H } 1s -14 \text{ eV}$ ;  $\text{C } 2s -19 \text{ eV}$ ;  $\text{C } 2p -12 \text{ eV}$ . To a first approximation, you can ignore the interaction between the  $\text{H } 1s$  and the  $\text{C } 2s$ . Why? What does your MO diagram predict about the magnetic properties (diamagnetic or paramagnetic) of  $\text{CH}$  and its ion  $\text{CH}^+$ ?

(6 marks)