CH 1101, Mid Semester Exam

Total Marks = 30; Time = 90 min

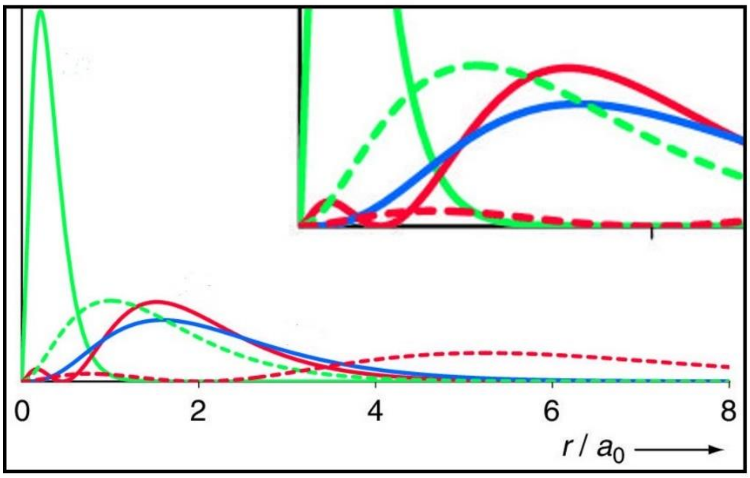
There are **Six** questions and you will have to answer all the questions. There is an optional **Question 7**. You can get **extra credit** for answering this question.

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

1. For the **$3p_z$** hydrogen-like atomic orbitals, sketch the following:
(i) The radial function R(r).
(ii) The radial distribution function (RDF). Label the axes, but do not include numbers or units. Label the r_{max} (the value of r where RDF becomes maximum) and indicate any nodes with an arrow.
(iii) Sketch the contour maps (plots) of the orbital. Indicate the signs of the wavefunction, radial node, and nodal planes in the diagram.
(5 marks)

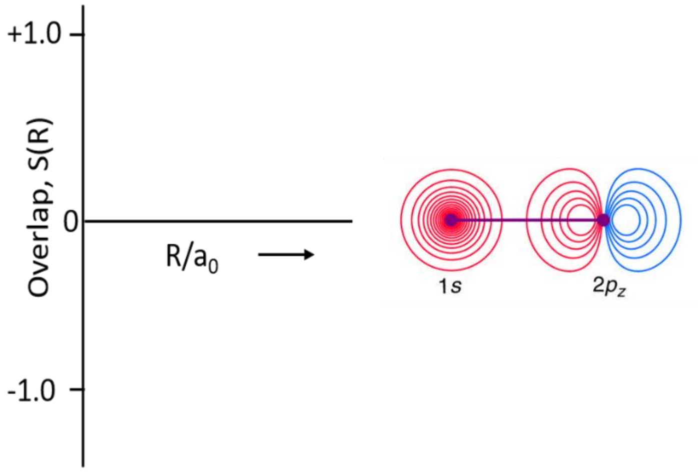
2. Shown below is the plot of the radial distribution function (RDF) of **B** (1s, 2s and 2p) and **H** (1s and 2s) AOs (the inset shows a blow-up of the graph between 0 and 2 r/a_0). The solid lines and dashed lines represent different elements. Match the following:

Orbital	Color of Line
H(2s)	Green solid
B(1s)	Red solid
H(1s)	Blue solid
B(2s)	Green dashed
B(2p)	Red dashed



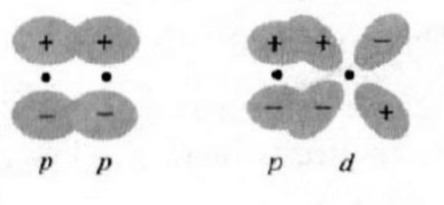
(5 marks)

3. Plot of the overlap integral as a function of internuclear distance between one **1s** orbital and one **$2p_z$** to give σ MO as shown below.



(3 marks)

4. Draw qualitative MO pictures with proper signs (**+ or -**) and assign the symmetries (**g/u**) of MO's formed from the AO's as shown below.



(3 marks)

5. The diatomic molecule **OH** exists in the gas phase. **OH** plays an important role in combustion reactions and is a reactive oxidizing agent in polluted air. Assume that the **OH** molecule is analogous to the HF molecule discussed in class and the **O-H** bond lies along the z axis.

A) Knowing that only the 2p orbitals of oxygen interact significantly with the 1s orbital of hydrogen, complete the **MO energy-level diagram for OH**. Place the correct number of electrons in the energy levels.

B) Which of the two MO's has the greater hydrogen 1s character?

C) Draw pictures of the sigma bonding and antibonding molecular orbitals in OH?

(7 marks)

6. (a) **NF** is a known molecule. **Draw** the MO interaction diagram for the **valence electrons** of **NF** (assume s-p mixing similar to what you have been taught for N_2 or CO). Label the atomic and molecular orbitals. Use the full space available to spread out your energy levels so that the labels for the orbitals fit easily.

(b) Calculate the **bond order** for **NF**.

(c) Based on the above diagram, state whether **NF** is paramagnetic or diamagnetic.

(d) Draw picture of the π^* molecular orbitals of NF. Make sure that you (i) draw nuclei, (ii) draw and label the bond axis, (iii) draw and label nodal planes (if any), and (iv) indicate the number of nodal planes.
(7 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:

α = 1,2,3,5,8,13,21….

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

γ takes on all odd integer values from - β to + β and zero

δ = -1/2, ½

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 α = 13, β = 5?

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

TABLE 5.2 Orbital Potential Energies

		Orbital Potential Energy (eV)						
Atomic Number	Element	1*s*	2*s*	2*p*	3*s*	3*p*	4*s*	4*p*
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.