Second Hour Exam **5.111**

Write your name and your TA's name below**. Do not open the exam until the start of the exam is announced.** The exam is closed notes and closed book.
1. Read each part of each problem carefully and thoroughly.
2. Show your work. Indicate units. Use correct significant figures.
3. Make your dots on Lewis structures clearly visible.
4. If you don't understand what the problem is requesting, raise your hand and a proctor will come to your desk.
5. Physical constants, formulas and a periodic table are given on the last page. You may detach this page **once the exam has started**.

1.	Periodic Table Trends	(14 points)
2.	Bonding	(12 points)
3.	Lewis Structures and VSEPR	(28 points)
4.	Molecular Orbital Theory	(25 points)
5.	Hybridization and VSEPR	(21 points)

Total (100 points) _____

Name Answer Key

TA _____

1. (14 points) **Periodic Table trends**

(**a**) (8 points) **<u>Ionization energy</u>**

(**i**) Which of the following (**Li, Be, B, Na, K**) has the highest **second** ionization energy (IE_2)? Briefly explain your answer.

Li

(**ii**) Which ionization energy is the **largest** of the following three: the fourth ionization energy for B, the third ionization energy for Be or the second ionization energy for Li? Briefly explain your answer.

B 4^{th} IE

(**b**) (3 points) Rank the following from smallest to largest **<u>radius</u>**: **Na, Na^+, Rb**

smallest… Na^+, Na, Rb ….largest

(**c**) (3 points) Rank the **<u>electron affinity</u>** from smallest to largest for **P, Cl, Ar**.

smallest… Ar, P, Cl ….largest

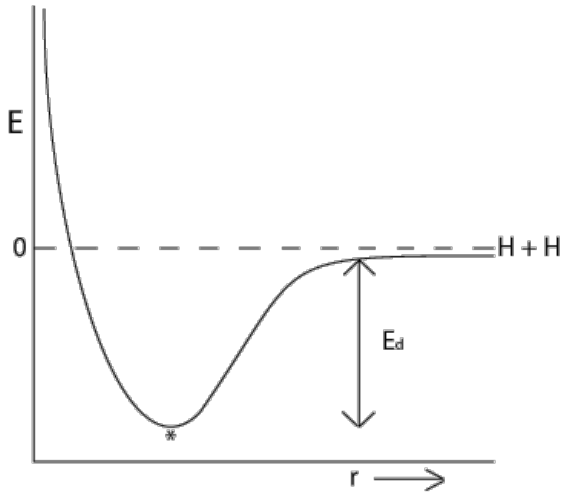
2. (12 points) **Bonding**

element	ionization energy	electron affinity
Rubridium (Rb)	403 kJ/mol	47 kJ/mol
Fluorine (F)	1680 kJ/mol	328 kJ/mol

(a) (8 points) For the ionic molecule RbF, calculate the maximum value of r for which the ionic bond is energetically allowed. For this problem, use the information above and assume Rb^+ and F^- are point charges.

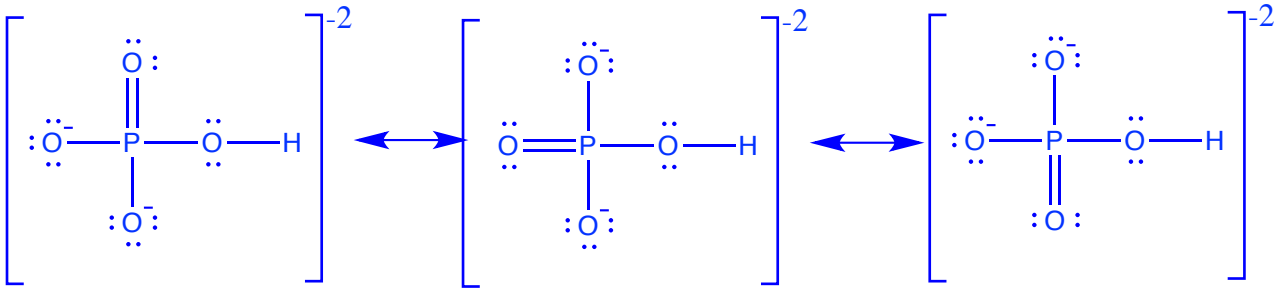
$r = 1.85 \times 10^{-9}$ m (accept both 1.8×10^{-9} m and 1.9×10^{-9} m, and 1.8 nm and 1.9 nm)

(b) (4 points) Draw an energy plot (with energy on the y-axis and internuclear distance, r, on the x-axis) for H_2. Label the (i) equilibrium bond distance with a *, and (ii) the dissociation energy with a double-headed arrow. Set the separated atom limit at zero energy.



3. (28 points) **Lewis Structures and VSEPR**

(a) (i) (10 points) Draw the most stable Lewis structure for $(PO_4H)^{-2}$. Be sure to include any lone pairs and, if applicable, draw resonance forms. **I**ndicate the overall charge on the molecule as well as **any nonzero formal charges**. Note that there are **no** oxygen-oxygen bonds in this molecule.



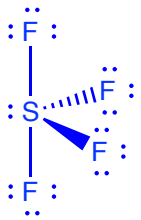
(ii) (3 points) Name the geometry around the phosphorus atom (example: square planar).

Tetrahedral

(iii) (3 points) What is (are) the O-P-O bond angle(s) in $(PO_4H)^{-2}$?

109.5˚ (109˚ is okay)

(b) (i) (6 points) Draw the most stable Lewis structure for (SF_4). Be sure to include any lone pairs and, if applicable, draw resonance forms.



(ii) (3 points) Name the geometry around the sulfur atom (example: square planar).

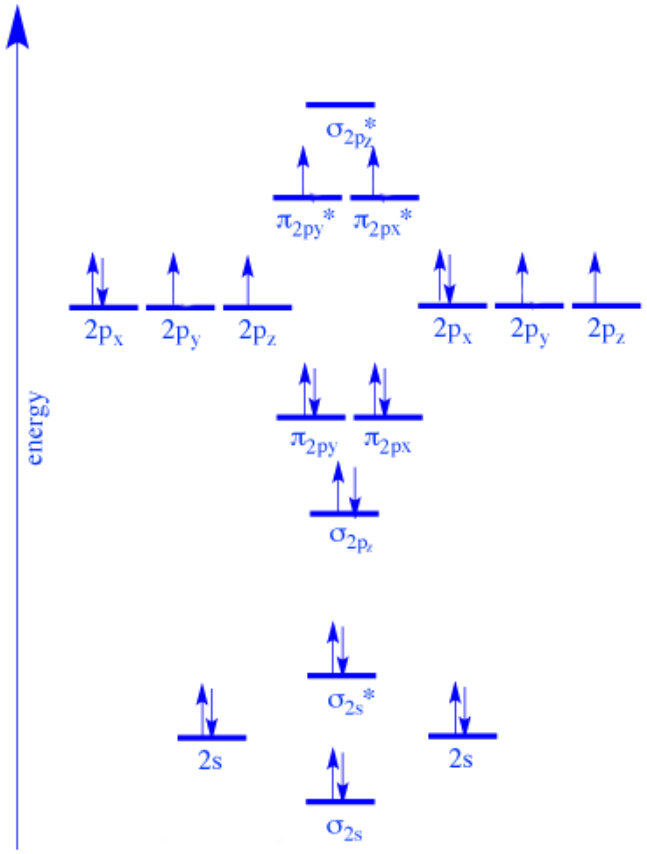
See-saw

(iii) (3 points) Name the formula type (example: AX).

AX_4E

4. (25 points) **Molecular Orbital Theory**

(a) (10 points) Draw the MO diagram for the **valence electrons** of **O_2**. Label the atomic and molecular orbitals, including the x, y and z designations where appropriate. Use the full space available to spread out your energy levels so that the labels for the orbitals fit easily.



(b) (3 points) Write the **valence electron configuration** for O_2 based on the diagram above.

$(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2pz})^2(\pi_{2px})^2(\pi_{2py})^2(\pi_{2px}^*)^1(\pi_{2py}^*)^1$

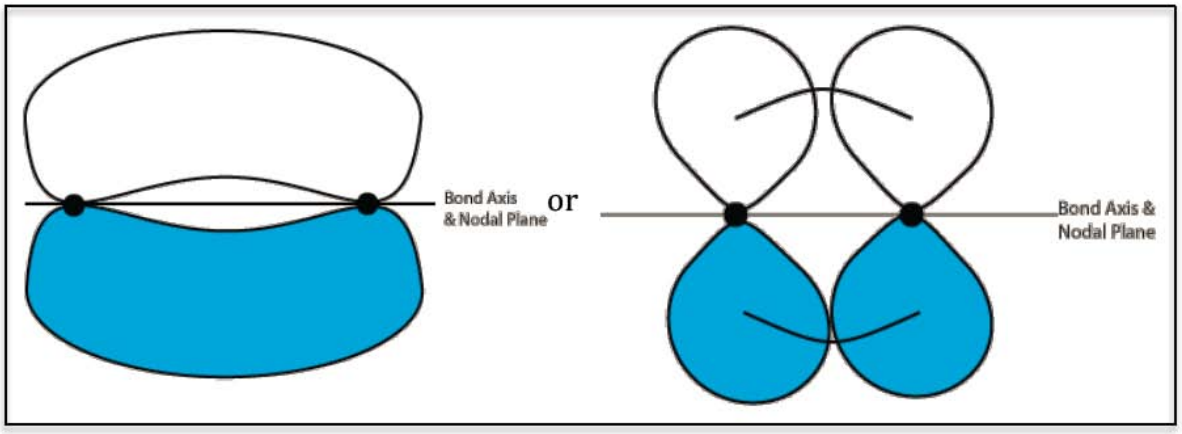
(c) (3 points) Calculate the **bond order** for O_2.

BO = **2**

(d) (1 point) Based on the above diagram, state whether O_2 is **paramagnetic** or diamagnetic.

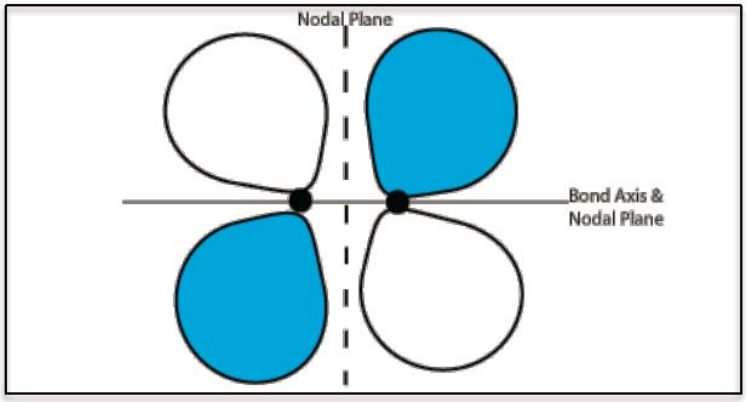
(e) (8 points) (i) Draw pictures of π_{2px} and π_{2px}^* **molecular orbitals** in the boxes below, (ii) draw **nuclei**, (iii) draw and label the **bond axis**, (iv) draw and label **nodal planes** (if any), and (v) indicate the number of nodal planes below the boxes.

π_{2px}



Total number of nodal planes in π_{2px}: **1**

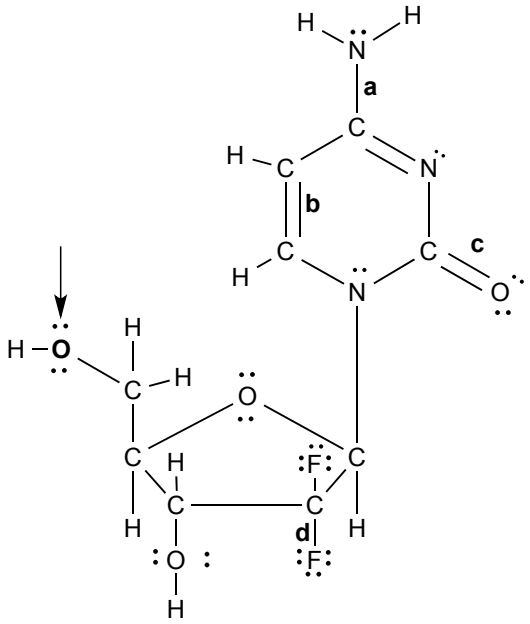
π_{2px}^*



Total number of nodal planes in π_{2px}^*: **2**

5. (21 points) **Hybridization and VSEPR**

(a) (12 points) The structure of chemotherapeutic agent gemcitabine is shown. For the indicated bonds, **a-d**, write the symmetry of each bond, and give the hybrid or atomic orbitals (with their principal quantum numbers) that overlap to form each of the bonds. Where appropriate, include the x, y, or z designations with the orbitals.



(i) The single C-N bond **a**:

σ(C2sp², N2sp³)

(ii) The double C=C bond **b**:

σ(C2sp², C2sp²)
π(C2p$_y$, C2p$_y$) or x

(iii) The double C=O bond **c**:

σ(C2sp², O2sp²)
π(C2p$_y$, O2p$_y$) or x

(iv) The single C-F bond **d**:

σ(C2sp³, F2p$_z$)

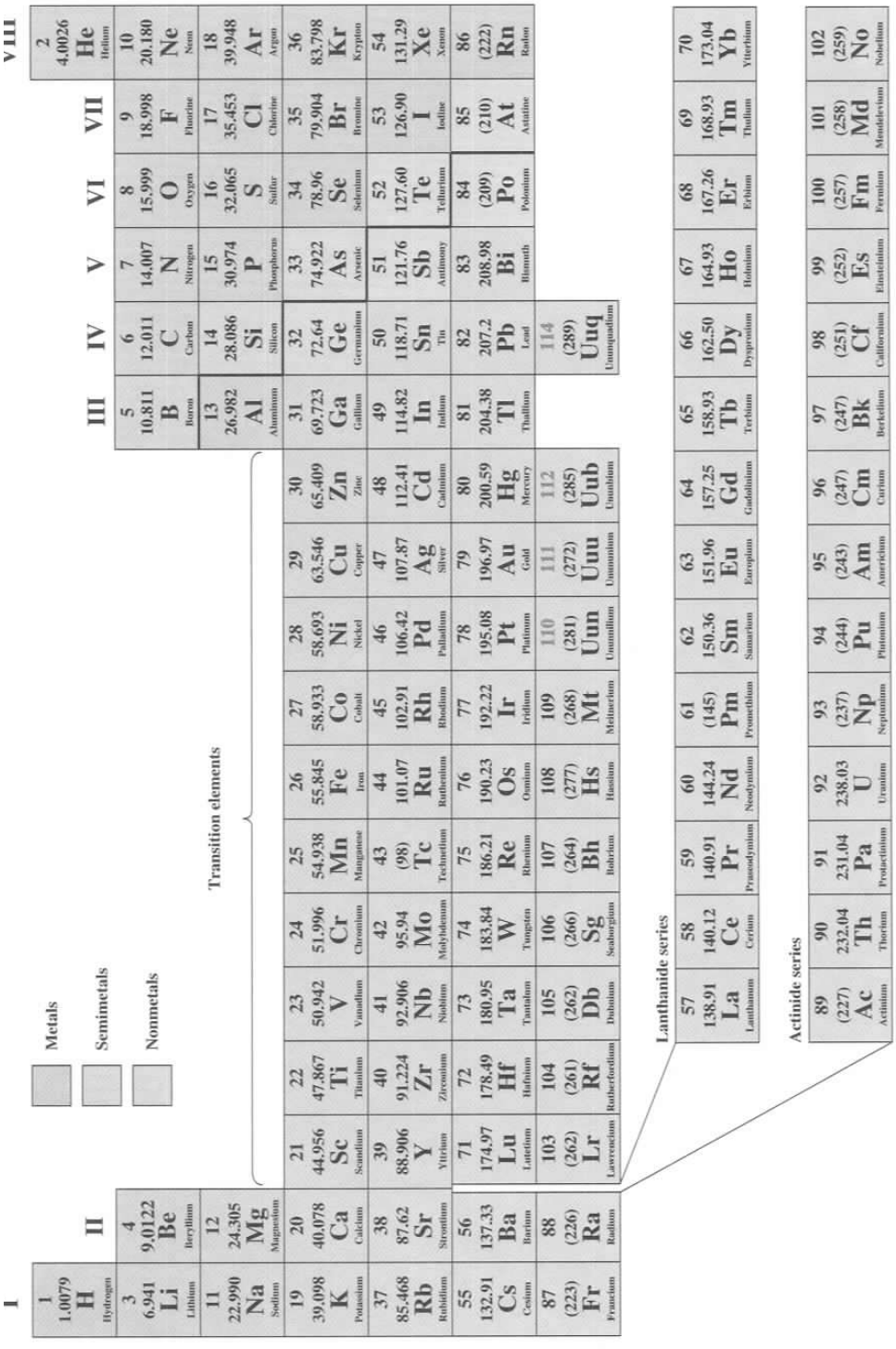
(b) (9 points) For oxygen indicated <u>with an arrow</u> in the above molecule

(i) (3 points) Write the SN number.
4

(ii) (3 points) Name the geometry around this oxygen (example: square planar).
Bent

(iii) (3 points) Circle the one value that best describes the H-O-C bond angle.

< 90°; 90°; > 90°; **< 109.5°**; 109.5°; > 109.5°; < 120°; 120°; > 120°



$c = 2.99792 \times 10^{8}$ m/s

$h = 6.62608 \times 10^{-34}$ J s

$N_a = 6.02214 \times 10^{23}$ mol^{-1}

1 eV = 1.60218×10^{-19} J

$m_e = 9.10939 \times 10^{-31}$ kg

$e = 1.60218 \times 10^{-19}$ C

$U(r) = (z_1 z_2 e^2)/(4\pi\varepsilon_0 r)$

$\varepsilon_0 = 8.8542 \times 10^{-12}$ C^2/(Jm)

Electronegativity = (IE + EA)/2

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