

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.**
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|----|----------------------------|-------------|
| 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) **Ionization energy**

(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 4th IE

(b) (3 points) Rank the following from smallest to largest **radius**: **Na, Na⁺, Rb**

smallest... **Na⁺, Na, Rb**largest

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

smallest... **Ar, P, Cl**largest

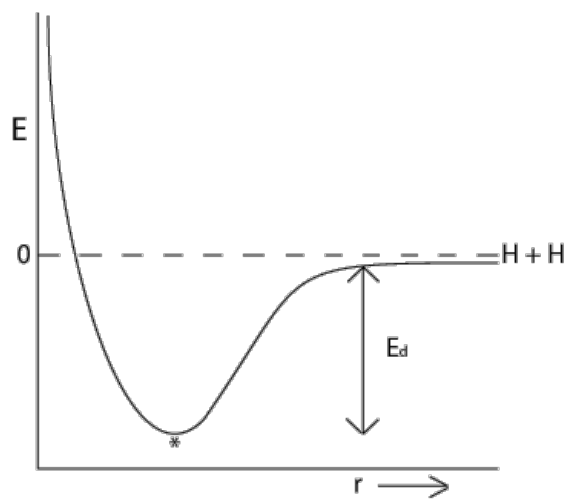
2. (12 points) **Bonding**

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.

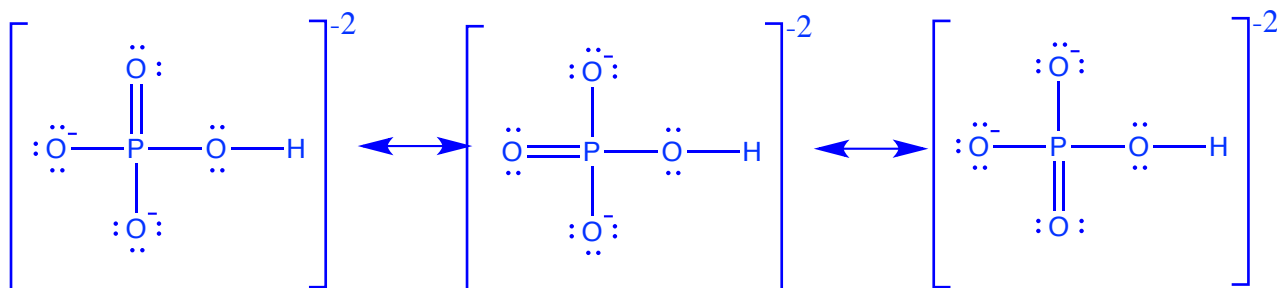
$r = 1.85 \times 10^{-9} \text{ m}$ (accept both $1.8 \times 10^{-9} \text{ m}$ and $1.9 \times 10^{-9} \text{ m}$, and 1.8 nm and 1.9 nm)

(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 $(\text{PO}_4\text{H})^{-2}$. Be sure to include any lone pairs and, if applicable, draw resonance forms. Indicate the overall charge on the molecule as well as **any nonzero formal charges**. Note that there are **no** oxygen-oxygen bonds in this molecule.



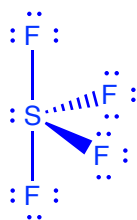
- (ii) (3 points) Name the geometry around the phosphorus atom (example: square planar).

Tetrahedral

- (iii) (3 points) What is (are) the O-P-O bond angle(s) in $(\text{PO}_4\text{H})^{-2}$?

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).

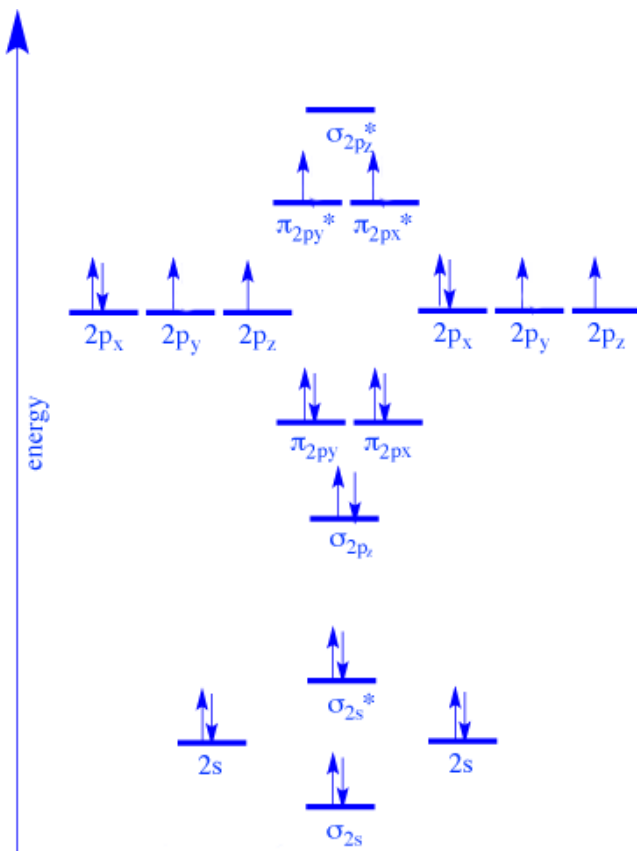
See-saw

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

AX₄E

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.

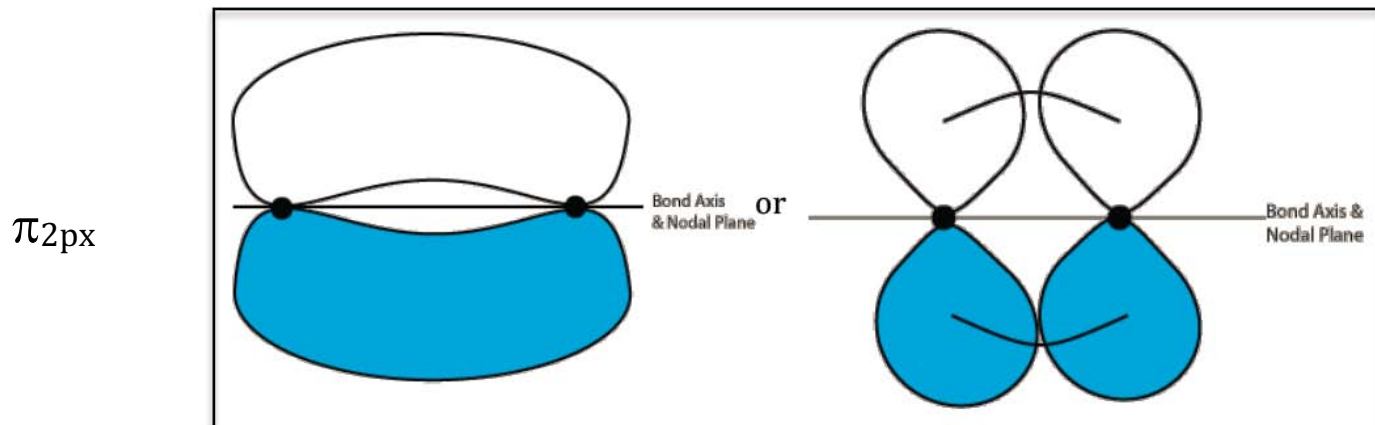
$$(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p_x})^2(\pi_{2p_y})^2(\pi_{2p_x}^*)^1(\pi_{2p_y}^*)^1$$

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

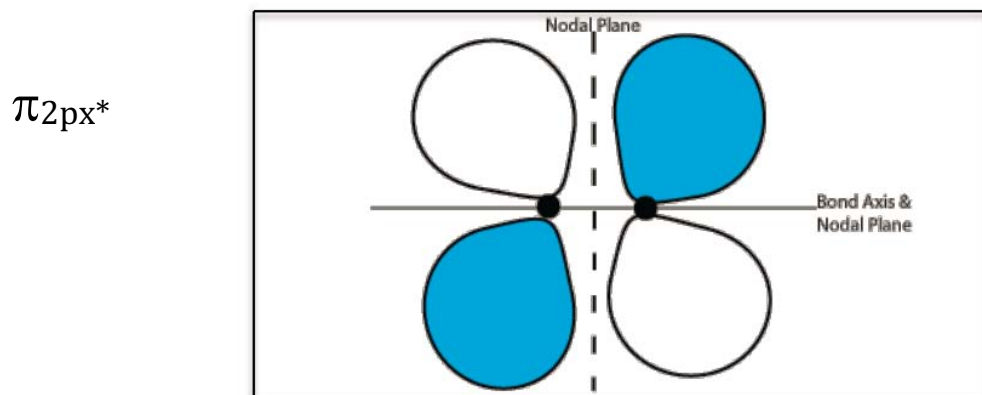
$$BO = 2$$

(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.



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



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**:

$\sigma(\text{C}2\text{sp}^2, \text{N}2\text{sp}^3)$

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

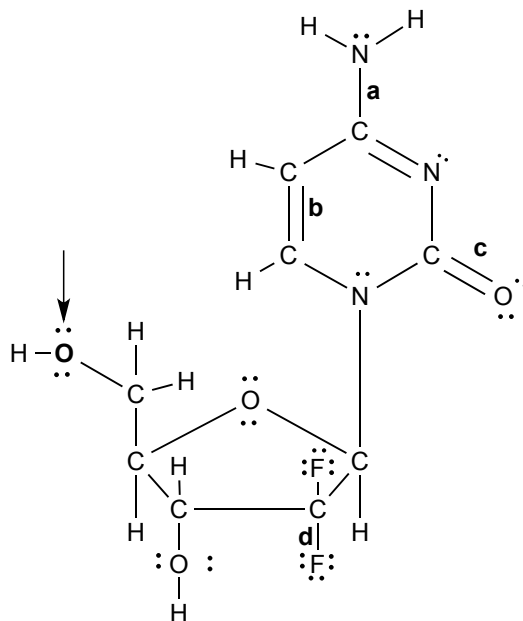
$\sigma(\text{C}2\text{sp}^2, \text{C}2\text{sp}^2)$
 $\pi(\text{C}2\text{p}_y, \text{C}2\text{p}_y)$ or x

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

$\sigma(\text{C}2\text{sp}^2, \text{O}2\text{sp}^2)$
 $\pi(\text{C}2\text{p}_y, \text{O}2\text{p}_y)$ or x

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

$\sigma(\text{C}2\text{sp}^3, \text{F}2\text{p}_z)$



(b) (9 points) For oxygen indicated with an arrow 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°

VIII

		I								II										III		IV		V		VI		VII		VIII					
		Metals				Semimetals						Nonmetals																							
		1 1.0079 H Hydrogen				3 6.941 Li Lithium				11 22.990 Na Sodium		19 39.098 K Potassium		27 72.64 Rb Rubidium		35 85.468 Cs Cesium		55 132.91 Fr Francium																	
		4 9.0122 Be Beryllium				12 24.305 Mg Magnesium				20 40.078 Ca Calcium		28 78.972 Strontium		36 87.62 Ba Barium		54 137.33 Ra Radium																			
		21 44.956 Sc Scandium		22 47.867 Ti Titanium		23 50.942 V Vanadium		24 51.996 Cr Chromium		25 54.938 Mn Manganese		26 55.845 Fe Iron		27 58.933 Co Cobalt		28 58.933 Ni Nickel		29 63.546 Cu Copper		30 65.409 Zn Zinc		31 69.723 Ga Gallium		32 72.64 Ge Germanium		33 74.922 As Arsenic		34 78.96 Se Selenium		35 79.904 Br Bromine		36 83.798 Kr Krypton			
		37 88.906 Y Yttrium		38 88.906 Zr Zirconium		39 91.224 Nb Niobium		40 92.906 Mo Molybdenum		41 95.94 Tc Technetium		42 95.94 Ru Rhodium		43 101.07 Rh Rhenium		44 106.42 Pd Palladium		45 107.87 Ag Silver		46 112.41 Cd Cadmium		47 114.82 In Indium		48 121.76 Sn Tin		49 127.60 Sb Antimony		50 127.60 Te Tellurium		51 126.90 I Iodine		52 131.29 Xe Xenon			
		56 174.97 Lu Lutetium		57 174.97 Hf Hafnium		58 180.95 Ta Tantalum		59 183.84 W Tungsten		60 186.21 Re Rhenium		61 190.23 Os Osmium		62 192.22 Ir Iridium		63 196.97 Pt Platinum		64 200.59 Hg Mercury		65 204.38 Tl Thallium		66 207.2 Pb Lead		67 208.98 Bi Bismuth		68 209 Po Polonium		69 210 At Astatine		70 222 Rn Radon					
		71 174.97 La Lanthanum		72 174.97 Ce Cerium		73 174.97 Pr Praseodymium		74 174.97 Nd Neodymium		75 174.97 Pm Promethium		76 174.97 Sm Samarium		77 174.97 Eu Europium		78 174.97 Gd Gadolinium		79 174.97 Tb Terbium		80 174.97 Dy Dysprosium		81 174.97 Ho Holmium		82 174.97 Er Erbium		83 174.97 Tm Thulium		84 174.97 Yb Ytterbium		85 174.97 Lu Lutetium					
		86 174.97 Ac Actinium		87 174.97 Th Thorium		88 174.97 Pa Protactinium		89 174.97 U Uranium		90 174.97 Np Neptunium		91 174.97 Pu Plutonium		92 174.97 Am Americium		93 174.97 Cm Curium		94 174.97 Bk Berkelium		95 174.97 Cf Californium		96 174.97 Es Einsteinium		97 174.97 Fm Fermium		98 174.97 Md Mendelevium		99 174.97 No Nobelium							

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

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

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

$$1 \text{ eV} = 1.60218 \times 10^{-19} \text{ J}$$

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

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

$$U(r) = (z_1 z_2 e^2) / (4\pi\epsilon_0 r)$$

$$\epsilon_0 = 8.8542 \times 10^{-12} \text{ C}^2 / (\text{Jm})$$

$$\text{Electronegativity} = (\text{IE} + \text{EA}) / 2$$

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5.111 Principles of Chemical Science
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