3.091 Introduction to Solid State Chemistry
Fall Term 2018
Exam 2
10/29/2018 (11:05 am – 11:55 am)

Name: _____

Recitation Section: _____ Recitation Instructor: _____

A complete exam consists of five (5) questions on a total of twelve (12) pages.
Write your answers on these pages (you can use the back for computation).
State your assumptions and show calculations that support your conclusions.

RESOURCES PERMITTED:
PERIODIC TABLE OF THE ELEMENTS
TABLE OF CONSTANTS
ONE AID SHEET (ONE PAGE 8.5" × 11", DOUBLE-SIDED O.K.)
A STAND-ALONE CALCULATOR – GRAPHING O.K.

NO BOOKS OR OTHER NOTES ALLOWED.

USE OF WIRELESS COMMUNICATIONS DEVICES STRICTLY FORBIDDEN.

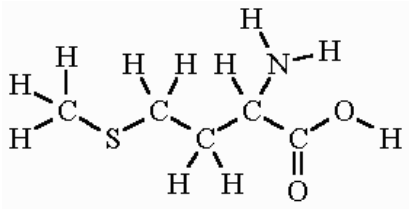
Problem 1	17 pts	
Problem 2	23 pts	
Problem 3	18 pts	
Problem 4	21 pts	
Problem 5	21 pts	
TOTAL	100 pts	

NAME _____

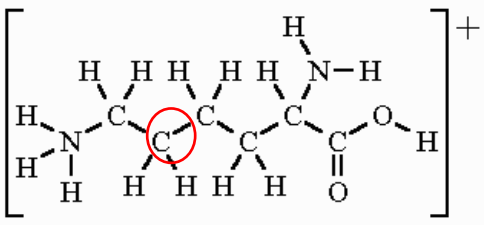
Problem 1 (17 POINTS)

a. Use the fact that $SeOF_2$ is trigonal pyramidal to write the Lewis Dot Structure, including lone pairs, for $SeOF_2$. (3 points)

b. Below is a drawing of two different amino acids, Methionine and Lysine, without any lone pairs drawn.



Methionine



Lysine

Name the VSEPR geometry around the following central atoms:

i. The sulfur in methionine (2 points)

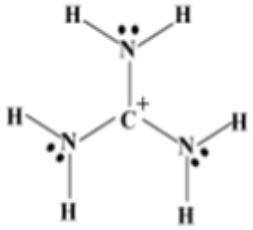
ii. The circled carbon in lysine. (2 points)

iii. Which of these angles is smaller? Explain why or why not in ONE sentence. (2 points)

CH_2-S-CH_2 OR CH_2-CH_2-CH_2

NAME _____

c. Below is one structure for the molecule $[CH_6N_3]^+$



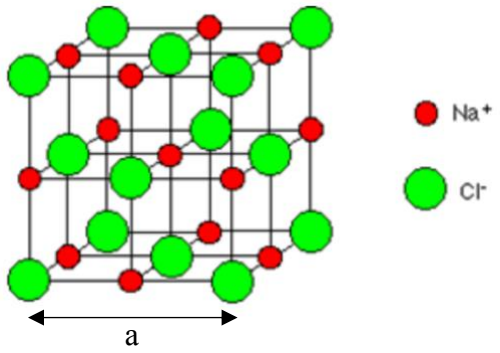
i. There are three other resonant structures for this molecule; what are they? (6 points)

ii. The structure that we gave you for $[CH_6N_3]^+$ contributes the least to the overall bonding of the molecule (it is the least stable). Why? (2 points)

NAME _____

Problem 2 (23 POINTS)

NaCl is a compound that forms a rock salt structure (unit cell below). The radius of the Na^+ atoms is 1.16 Å; the radius of the Cl^- atoms is 1.67 Å. (1Å = 10^{-10} m).



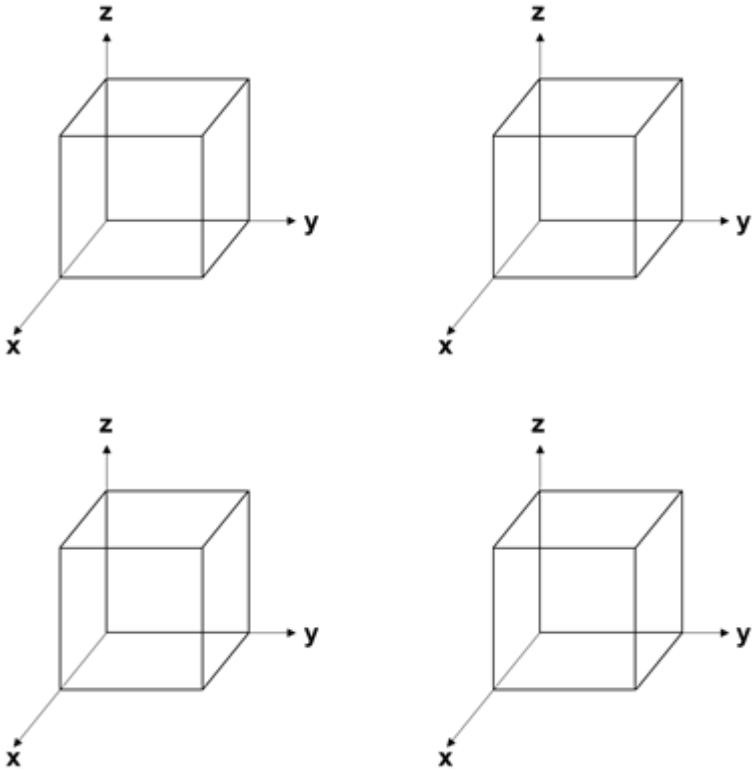
a. Name the Bravais lattice (lattice type) of NaCl. What is the basis? (2 points)

b. How many Na^+ ions are in the unit cell? How many Cl^- ions? (4 points)

c. Determine the close-packed direction of this structure and use it to calculate the lattice parameter, a. (3 points)

NAME _____

d. Draw (211), [$0\bar{2}1$], [301], and ($1\bar{1}0$) in the boxes below. Make sure to label which is which. (8 points)



e. Which of the planes in part d is closer in distance to its equivalent plane in a neighboring cell? Show how you arrived at this answer. (4 points)

f. Using atomic packing factor, explain why calcium is denser than potassium. (2 points)

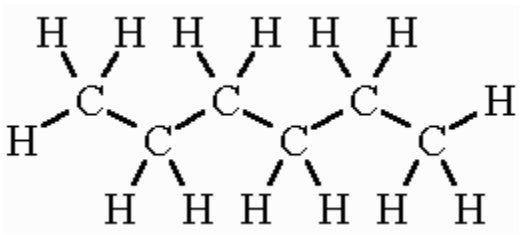
NAME _____

Problem 3 (18 POINTS)

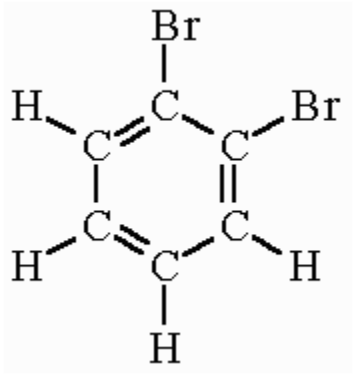
a. Rank the following intermolecular forces in terms of their average relative strength: London dispersion, hydrogen bonding, dipole-dipole, and dipole-induced-dipole. (4 points)

1. _____ (strongest)
2. _____
3. _____
4. _____ (weakest)

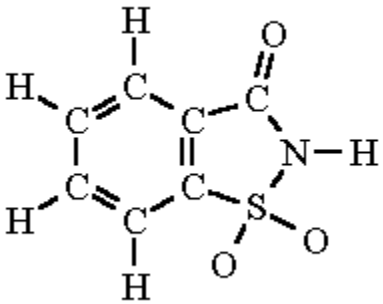
You have the four following molecules in liquid form in your lab cabinet.



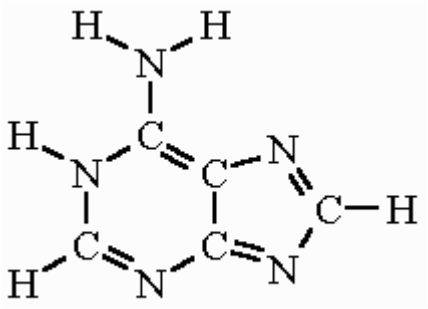
Molecule 1



Molecule 2



Molecule 3



Molecule 4

b. Which has the highest boiling point? (2 points)

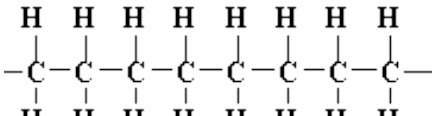
NAME _____

c. You make a mixture of two of the liquids.

i. If you wanted your mixture to have the LOWEST possible boiling point, which **two** of the four molecules would you choose? (4 points)

ii. If you want your mixture to have the HIGHEST possible boiling point, which **two** of the four molecules would you choose? (4 points)

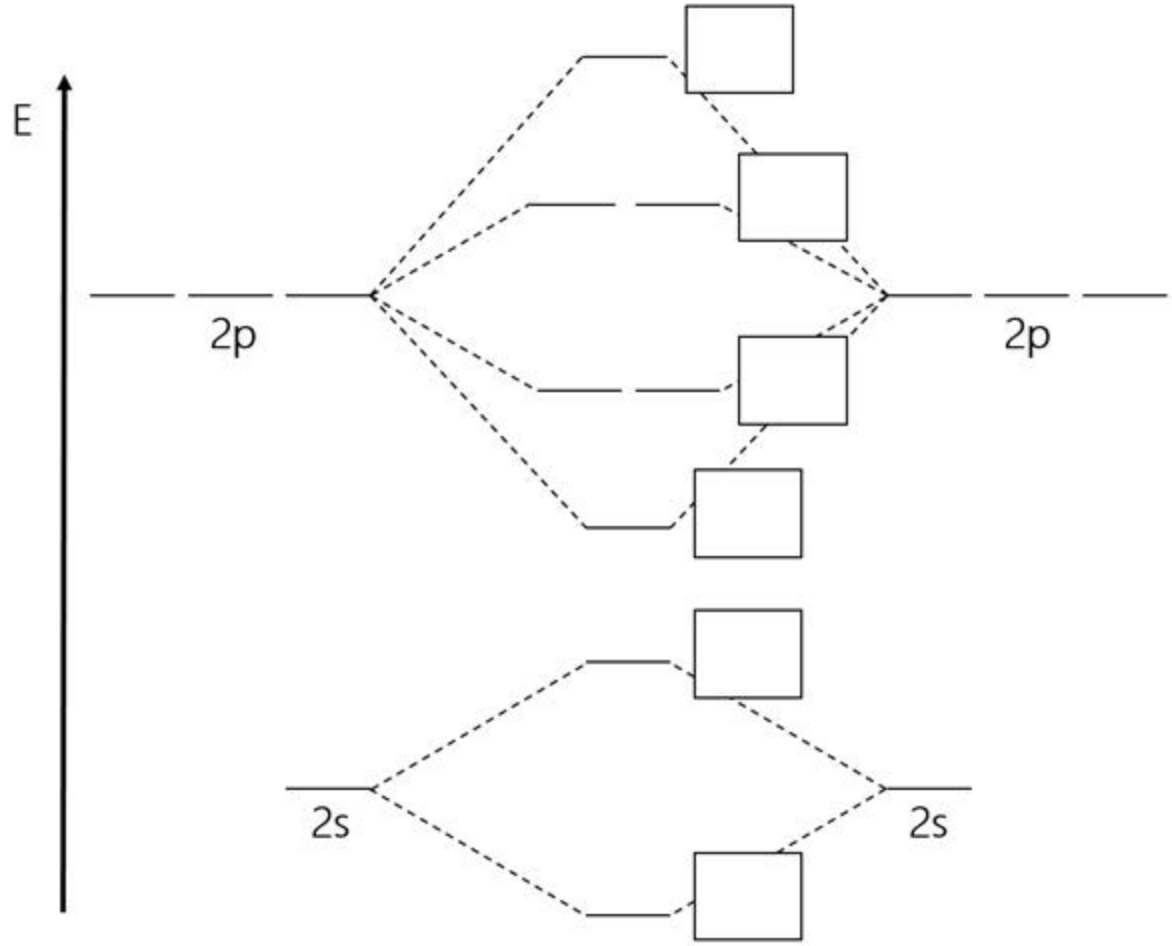
d. You have two samples of polyethylene, a polymer made of chains of carbon and hydrogen, as shown below. For one sample, each molecule chain is 50 units long and in the next sample, each chain is 500 units long. Which sample of plastic will be stronger? Why? (4 points)

(continued to the left)  (continued to the right)

NAME _____

Problem 4 (21 POINTS)

a. The molecular orbitals of a second-row diatomic molecule are shown in this figure. Label them each as σ, σ*, π, or π* by filling in the boxes provided. (The 2p and 2s atomic orbitals are labelled for reference). (6 points)



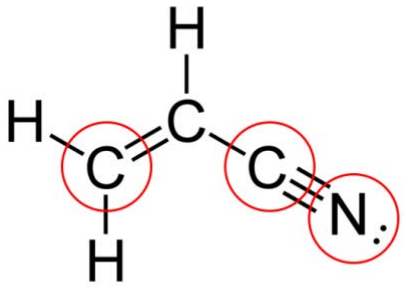
b. Circle which of the following this skeleton MO diagram could correspond to. (2 points)

C-C N-O H-F

NAME _____

c. Rank the following molecules in terms of stability: Li_2, Be_2 B_2, C_2.
Be sure to show your work (no need to show MO diagrams). (8 points)

c. Acrylonitrile is a feedstock chemical used for the manufacture of "nitrile" polymers. Pictured below is its chemical structure. What is the hybridization of the circled atoms? (3 points)



Carbon on the right	Nitrogen	Carbon on the left

d. Give the total number of σ bonds and total number of π bonds in acrylonitrile. (2 points)

NAME _____

Problem 5 (21 POINTS)

a. UV light corresponds to wavelengths from 10-400nm. What is the range of band gaps corresponding to UV light? (3 points)

b. You only have two materials in the lab to build an LED: GaAs (band gap 1.42 eV at 300K) and GaN (band gap 3.2 eV at 300 K). Which would you choose as a UV emitter? (3 points)

c. UV light can damage eyes, so you decide that for safety, your LED should emit in the visible range too. You recall that you can tune the band gap by alloying your material. Determine the fraction x of GaAs in your alloy such that $GaAs_xN_{1-x}$ will emit red light (wavelength 700nm). Remember that the band gap of an alloy is the weighted average of the band gaps of its components. (3 points)

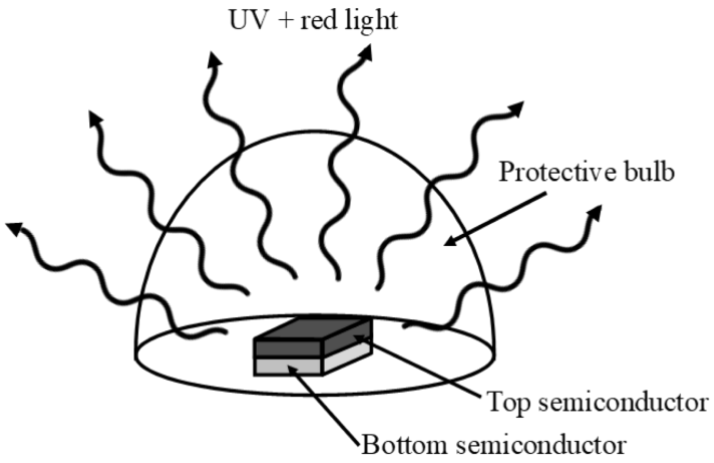
NAME _____

d. If you place the $GaAs_xN_{1-x}$ adjacent to *your answer from (B)* your LED will emit both UV light and red light. However, you observe that it is really dim: you decide to dope it with Mg.

   i. Is Mg an n- or p-type dopant in $GaAs_xN_{1-x}$? (2 points)

   ii. If you dope 1g GaN with Mg such that 1 Mg atom replaces 1 in every 10^6 Ga atoms, how many extra carriers are produced? What kind of carriers are these? (4 points)

NAME _____



e. In order to get enough current to $GaAs_xN_{1-x}$ and *your answer from (B)* processing requires that the two are stacked. Which should be on top to ensure no light is blocked? (3 points)

f. Do you expect a larger temperature-dependence of conductivity in the doped or the undoped GaAsN, at moderate temperatures? (3 points)

END OF 3.091 EXAM 2

3.091 Introduction to Solid-State Chemistry
Fall 2018