3.091 Fall Term 2004

Final Exam

Wednesday, December 15, 2004

9:00 a.m. — 12:00 noon

Name: MODEL SOLUTIONS

(please print in UPPER CASE)

Recitation Instructor: ____________________

A complete test consists of 13 questions.

Write your answers on these pages.

State your assumptions and show calculations that support your conclusions.

RESOURCES PERMITTED: PERIODIC TABLE OF THE ELEMENTS
TABLE OF CONSTANTS
AID SHEET (ONE PAGE 8½" × 11")
CALCULATOR.

NO BOOKS OR OTHER NOTES ALLOWED.

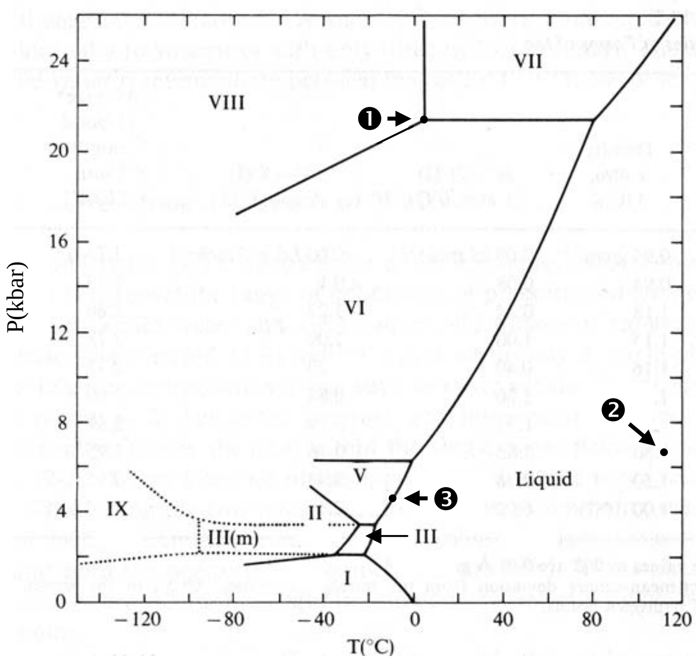
USE OF WIRELESS COMMUNICATIONS DEVICES STRICTLY FORBIDDEN.

#1	11 points	
#2	16 points	
#3	9 points	
#4	16 points	
#5	7 points	
#6	11 points	
#7	8 points	
#8	7 points	
#9	8 points	
#10	3 points	
#11	6 points	
#12	9 points	
#13	5 points	
Total	116 points	

% Score

Problem #1 (11 points)

Here is the phase diagram of water with attention given to phases present at high pressure.



(a) Name all phases present at ❶, ❷, and ❸.

6

❶ VI, VII, VIII

❷ liquid

❸ liquid, V

(b) Rank the following in order of increasing density: VI, VII, VIII, liquid. Justify your choice.

5

liquid < VI < VII = VIII

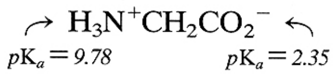
+ve slope of l + VI coexistence curve ⇒ $\rho_{VI} > \rho_{liq.}$

+ve slope of VI + VIII coexistence curve ⇒ $\rho_{VIII} > \rho_{VI}$

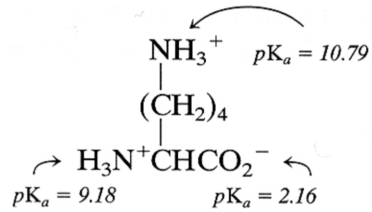
vertical pitch of VII + VIII coexistence curve ⇒ $\rho_{VII} = \rho_{VIII}$

Problem #2 (16 points)

The skeletal structures of the two amino acids, glycine and lysine, are given below along with the values of the relevant acid dissociation constants (pK_a).



glycine (Gly)

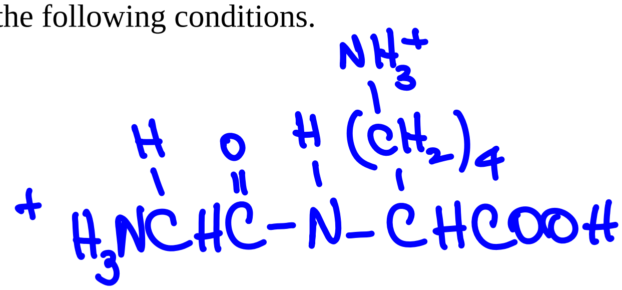


lysine (Lys)

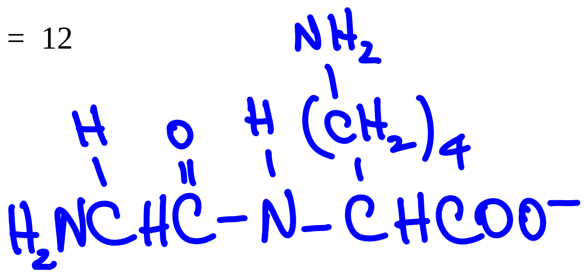
(a) Draw the skeletal structure of the dipeptide, Gly-Lys, when it is solvated in an aqueous solution under each of the following conditions.

9

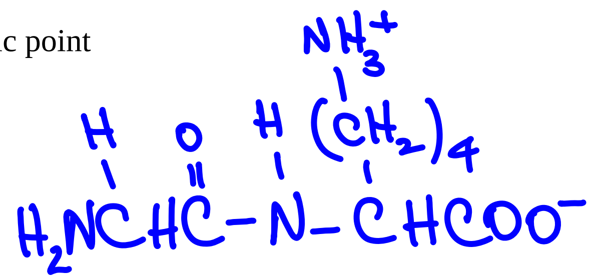
(i) $pH = 1$



(ii) $pH = 12$



(iii) $pH = pI$, the isoelectric point



(b) Calculate the value of pI of the dipeptide, Gly-Lys, assuming that there is negligible shift in the values of acid dissociation constants from the values of the constituent amino acids.

3

to counter the -ve charge of the COO^-, pH must be set at a value between pKas of the two amino groups ⇒

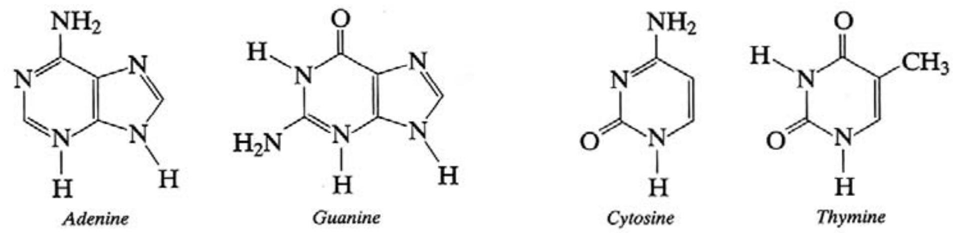
$$pI = \frac{9.78 + 10.79}{2} = 10.29$$

(continued on next page)

Problem #2 (continued)

(c) The structures of the four bases found in DNA are shown below.

4



(i) Erwin Chargaff observed that adenine (A) is always paired with thymine (T) and cytosine (C) always with guanine (G). With reference to molecular structure explain why there can be no exceptions to this.

① A & T have 2 H-bonding sites, while C & G have 3 H-bonding sites

② spacing between H-bonding sites will not allow linkage between A or T with C or G

(ii) Two strands of DNA are denatured by exposure to the same temperature and held there for the same length of time. Strand 1 is 75% AT - 25% CG. Strand 2 is 25% AT - 75% CG. Which strand is denatured to a greater extent? Explain.

CG linkages are stronger than AT linkages (3 bonds stronger than 2)

∴ strand 1 weaker & so more susceptible to denaturing under identical thermal stress

Problem #3 (9 points)

(a) Silicon is doped with boron in the amount of 3.091×10^{-4} g B / kg Si. Calculate the carrier concentration in units of carriers cm^{-3}. Neglect contributions from intrinsic carriers.

4

1 carrier / B atom

volume occupied by 1 kg Si $= \frac{m}{\rho} = \frac{1000\ g}{2.33\ g/cm^3} = 429\ cm^3$

$3.091 \times 10^{-4}\ g\ B \Rightarrow \frac{3.091 \times 10^{-4}}{10.811} = 2.86 \times 10^{-5}$ mol B $(\times N_{AV} = \text{atoms})$

$= 1.72 \times 10^{19}$ atoms B

$\therefore$ carrier conc. $= \frac{1.72 \times 10^{19}}{429\ cm^3} = 4.01 \times 10^{16}\ \frac{\text{carriers}}{cm^3}$

(b) The absorption edge, $\lambda_{abs\ edge}$, of the compound semiconductor, gallium arsenide (GaAs), has been measured to be 8.71×10^{-7} m. Calculate the maximum value of the de Broglie wavelength of an electron, λ_e, with enough energy to promote a valence electron in GaAs across the band gap.

5

$E_e \geq E_g$ for promotion

$E_e = \frac{1}{2} m v^2 = \frac{p^2}{2m} = \frac{h^2}{2m\lambda_e^2} = \frac{hc}{\lambda_{abs\ edge}}$

$\therefore \lambda_e = \left(\frac{\lambda_{abs\ edge}\, h^{\cancel{2}}}{2m \cancel{h} c} \right)^{1/2}$

$= \left(\frac{8.71 \times 10^{-7} \times 6.6 \times 10^{-34}}{2 \times 9.11 \times 10^{-31} \times 3 \times 10^{8}} \right)^{1/2}$

$= 1.03 \times 10^{-9}$ m

Problem #4 (16 points)

(a) Is metallic glass opaque or transparent to visible light? Explain.

3

- opaque
- the atomic disorder does not change the energy levels so as to create a band gap

  ∴ visible light has enough energy to excite electrons in the material which in turn is not transparent

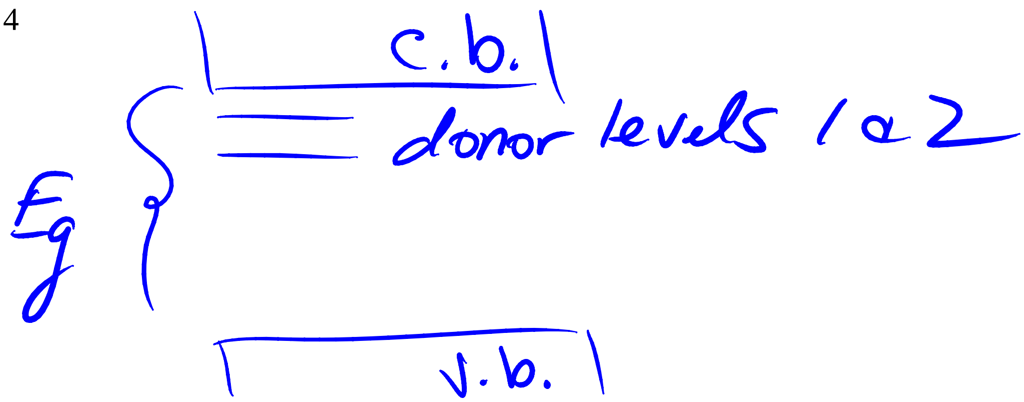
(b) Sodium chloride (NaCl) and magnesium oxide (MgO) both crystallize in the cubic rock salt structure. How does the value of the Madelung constant ($\mathscr{M}$) compare for the two compounds? Explain.

3

- identical
- the Madelung constant is a geometric quantity and unrelated to the specific charges on the ions in question

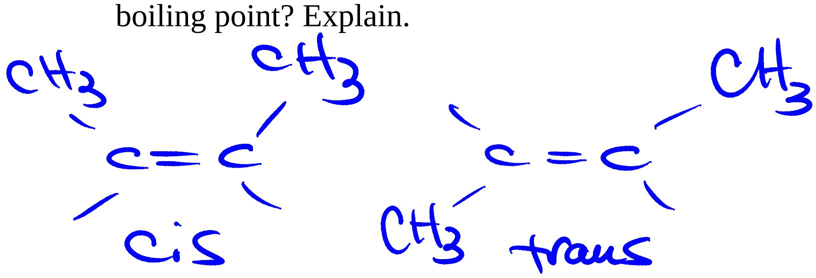
(c) Draw the energy level diagram of silicon (Si) doped with selenium (Se). Label the valence band, the conduction band, and any features associated with the impurity.

4



(d) There are two stereoisomers of butene (C_4H_8), *cis*-2-butene and *trans*-2-butene. Which has the higher boiling point? Explain.

3



cis is polar
Trans is nonpolar
→ cis has higher b.p.

(e) Two specimens of polyethylene {$(-CH_2-CH_2-)_n$}, one composed of linear chains, the other composed of branched chains, are solidified by identical cooling from the melt. The degree of polymerization, *n*, is the same in both specimens. Which is more likely to be suitable for use as plastic food wrap? Explain.

3

- food wrap ideally should be transparent to visible light and plastically deformable
- crystallization will result in opacity due to variation in index of refraction and will stiffen the material reducing its plasticity
- since branched chains entangle, pack less well, and raise melt viscosity, branched PE will be more successful in averting crystallization and thus more suitable as the material from which to make food wrap

Problem #5 (7 points)

Allene or propadiene has the chemical formula CH_2=C=CH_2.

(a) Identify the hybridization of each of the three carbon atoms.

3

CH_2=C=CH_2

sp^2

CH_2=**C**=CH_2

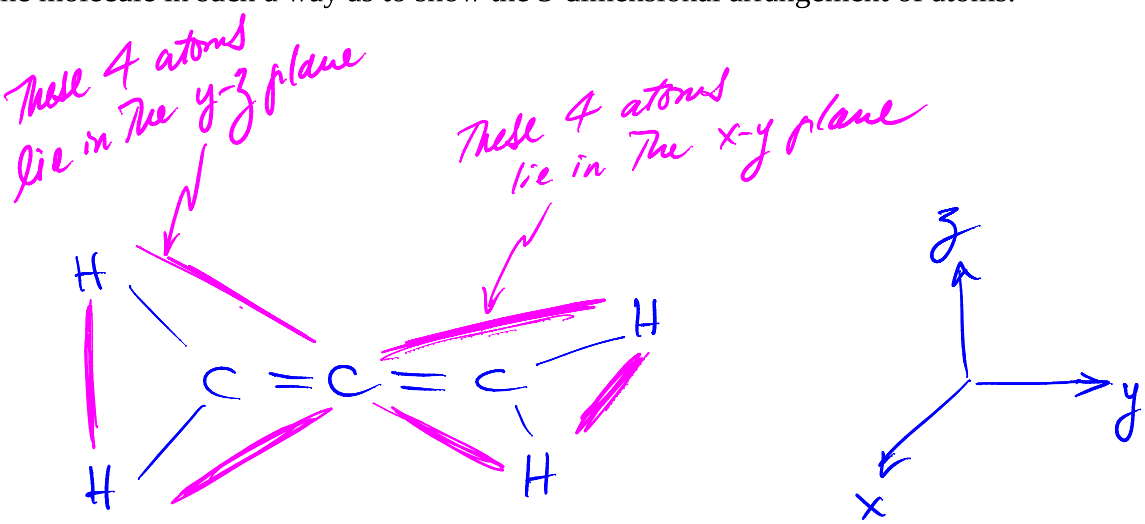
sp

CH_2=C=**C**H_2

sp^2

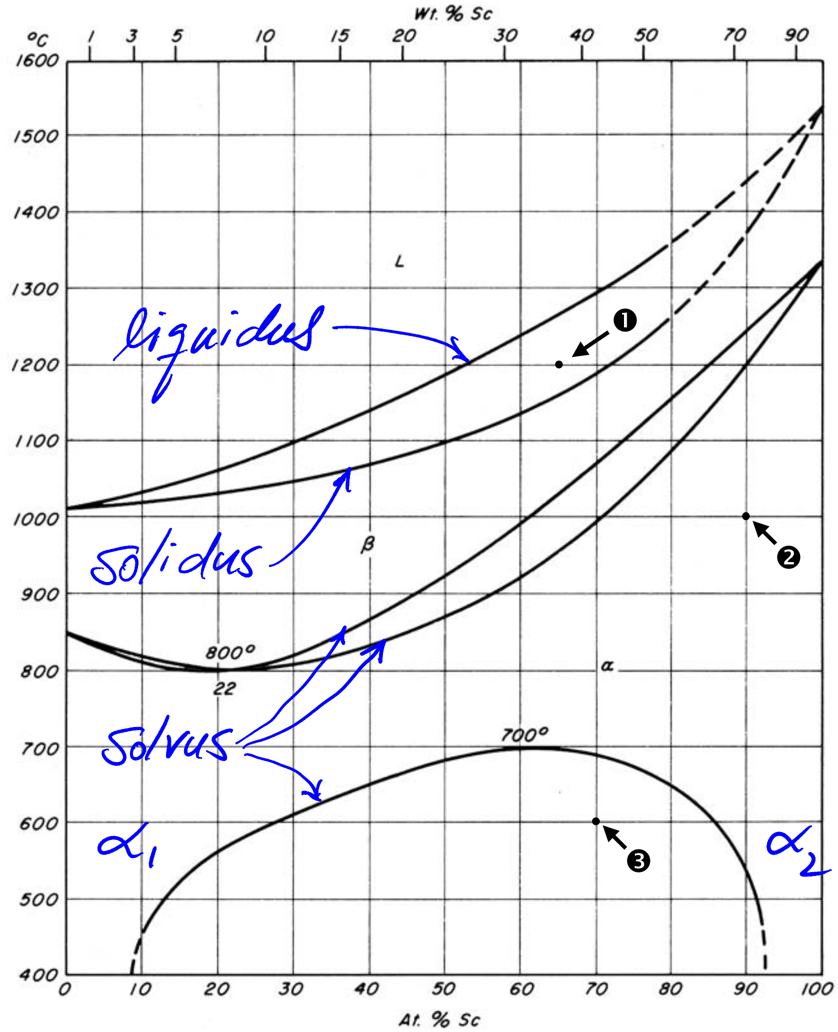
(b) Draw a cartoon of the molecule in such a way as to show the 3-dimensional arrangement of atoms.

4



Problem #6 (11 points)

The phase diagram of the binary system, neodymium-scandium (Nd-Sc), is given below. There are two polymorphs in the solid state: α which is hexagonal close packed (HCP) and β which is body centered cubic (BCC).



3 (a) On the phase diagram at right, label one example of each: liquidus, solidus, and solvus.

6 (b) At each point, ❶, ❷, and ❸, identify all phases present at equilibrium.

❶ liquid + β

❷ α

❸ two compositions of α
one is Nd-rich, α_1
one is Sc-rich, α_2

2 (c) At point ❸ calculate the relative amounts of all phases present.

$$\% \alpha_1 = \frac{85-70}{85-28} \times 100\% = 26\%$$

$$\% \alpha_2 = \frac{70-28}{85-28} \times 100\% = 74\%$$

Problem #7 (8 points)

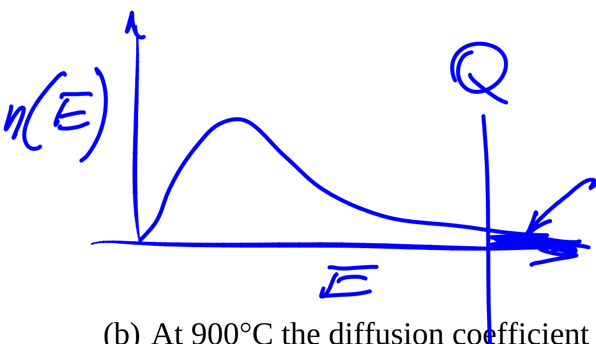
Carbon diffuses interstitially through iron. The values of the diffusion coefficient, D, are given below.

	$D_o(m^2s^{-1})$	$Q(kJ\ mol^{-1})$
C in BCC-Fe	6.2×10^{-7}	81
C in FCC-Fe	2.3×10^{-5}	148

where $D = D_o \exp\left(-\frac{Q}{RT}\right)$.

(a) At 900°C diffusion of carbon through iron is relatively fast. How is it that this can be the case when, even at this elevated temperature, $RT=N_{Av}k_BT<<Q$? In other words, what accounts for the observed high degree of thermal activation?

2 – not all atoms possess the same thermal energy



$e^{-Q/RT}$ is fraction of distribution possessing $E > Q$

(b) At 900°C the diffusion coefficient of carbon through BCC Fe is ~100 times greater than that in FCC iron at the same temperature. Explain with reference to the relevant atomistics.

3 - FCC is more tightly packed than BCC
∴ interstitial volume is smaller in FCC
∴ activation energy for motion is greater in FCC
note values of $Q_{FCC} > Q_{BCC}$

(c) A piece of BCC-iron is carburized (infused with carbon) so as to attain a carbon concentration of c_{spec} at a depth of 100 μm in 1 hour. Make a crude estimate of the depth at which the carbon concentration would reach the value of c_{spec} in a physically identical piece of ***FCC-iron*** subjected to the identical carburization conditions?

3 use $x \approx \sqrt{Dt}$

∴ $x_{FCC} \approx \sqrt{D_{FCC} \cdot 1hr}$ & $x_{BCC} \approx \sqrt{D_{BCC} \cdot 1hr}$

So $x_{FCC} = x_{BCC}\sqrt{\frac{D_{FCC}}{D_{BCC}}} = 100\,\mu m\sqrt{\frac{1}{100}} = 10\,\mu m$