# 2022 Fall Semester Midterm Examination For General Chemistry II

### Date: October 19 (Wed), Time Limit: 19:00 ~ 21:00

Write down your information neatly in the space provided below; print your Student ID in the upper right corner of every page.

Professor Name	Class	Student I.D. Number	Name

Problem	points	Problem	points	TOTAL pts
1	/17	6	/12	
2	/6	7	/10	
3	/10	8	/10	
4	/8	9	/9	/100
5	/8	10	/10	

\*\* This paper consists of 20 sheets with 10 problems (*page 18 - 19*: Equation, constants & periodic table, *page 20*: claim form). Please check all page numbers before taking the exam. Write down your work and answers in the Answer sheet. Please write down the unit of your answer when applicable. You will get 30% deduction for a missing unit.

### NOTICE: SCHEDULES on RETURN and CLAIM of the MARKED EXAM PAPER. (채점 답안지 분배 및 이의신청 일정)

## 1. Period, Location and Procedure

0 Return and Claim Period: October 24 (Mon, 20:00 ~ 21:00, 1 hr)

*The claim is permitted only on this period. Keep that in mind!* 0 Location: Each designated room of Creative Learning Bldg. (E11)

Class	Room(E11)	Class	Room(E11)
A/B	102	C/D	103

#### 0 Procedure

*Rule 1: Students cannot bring their writing tools into the rooms (Use a pen only provided by TA) Rule 2: With or without claim, you must submit the paper back to TA. (Do not go out of the room with it)*  If you have any claims on it, write them on the claim form and attach it to the top of the exam paper with a stapler. Give them to your TA.

#### WARNING!!

If you deliberately alter any original answers or insert something on your marked paper to achieve a better grade, you will get a F grade for this course. Or if you don't keep the rules above, we will regard it as a kind of cheating and give you 0 point. So please don't cheat.

## 2. Final Confirmation

1) Period: October 27(Thu) ~ 28(Fri)

2) Procedure: During this period, you can check final score of the examination on the website again.

(No additional corrections. If no change in your score after reasoning, the claims were not accepted.)

\*\* For further information, please visit General Chemistry website at <u>www.gencheminkaist.pe.kr</u>

### 1. (total 17 pts)

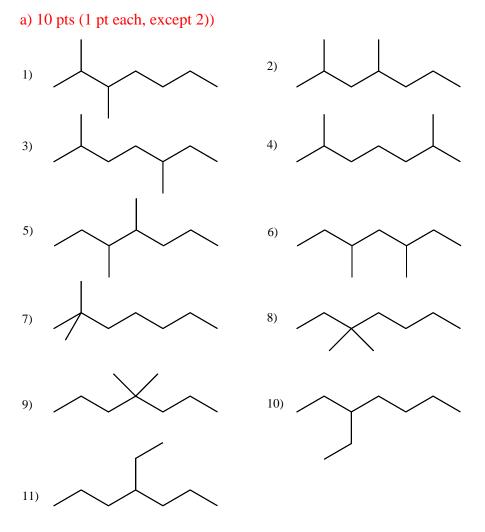
The alkane of molecular formula  $C_9H_{20}$  (nonane) has 35 structural (constitutional) isomers. a) Draw the 11 isomers with 7 carbon atoms in a chain.

(for example: )

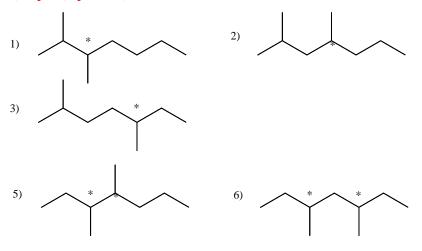
b) Identify the isomers with chiral center(s) among the 11 isomers and mark the chiral carbon(s).

c) Identify the diastereomers.

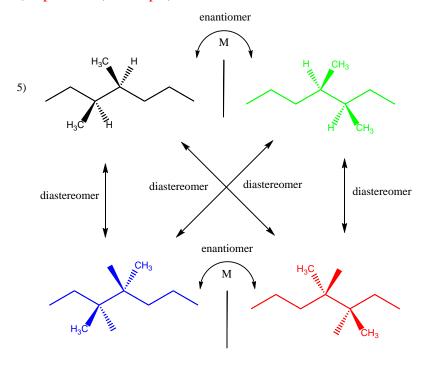
Answer

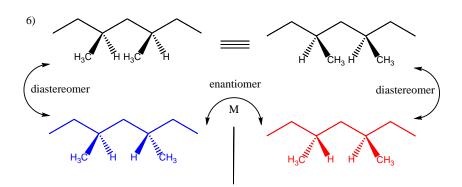


b) 5 pts (1 pt each)



c) 1 pts each (total 2 pts)





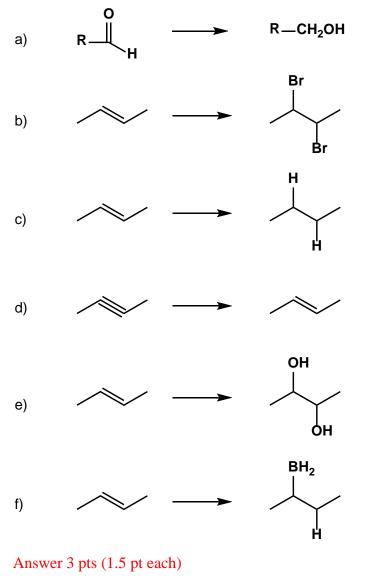
### 2. (total 6 pts)

(a) List three important reactive intermediates in organic reactions.

Answer 3 pts (1 pt each)

Radical,CarbanionCarbocation, $A^{\oplus}$  $A^{\odot}$  $A \bullet$ 

(b) Identify the oxidation reactions among the following reactions.



b), e)

### 3. (total 10 pts)

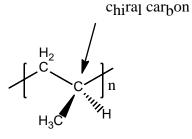
Polymerization of propylene (CH<sub>2</sub>=CH-CH<sub>3</sub>) produces so-called polypropylene with molecular weight of several hundred thousand.

(a) What kind of polymer it is, condensation or addition?

- (b) Draw the repeating unit of polypropylene and identify the chiral carbon.
- (c) Draw three isomeric structures of polypropylene including their name.

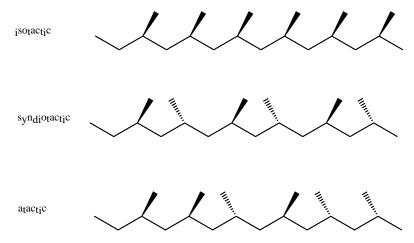
### Answer

- a) Addition (1 pt)
- b) (3 pts)



(no reduction for missing n)





### 4. (total 8 pts)

(a) Calculate the feed ratio of hexamethylene diamine  $[H_2N-(CH_2)_6-NH_2]$  and adipic acid  $[HOOC-(CH_2)_4-COOH]$  that should be employed to obtain polyamide (Nylon 66) of 11,300 number average molecular weight (M<sub>n</sub>) at 99% conversion. (molar mass of the repeating unit: M<sub>0</sub> = 113).

#### Answer (6 pts)

0 %

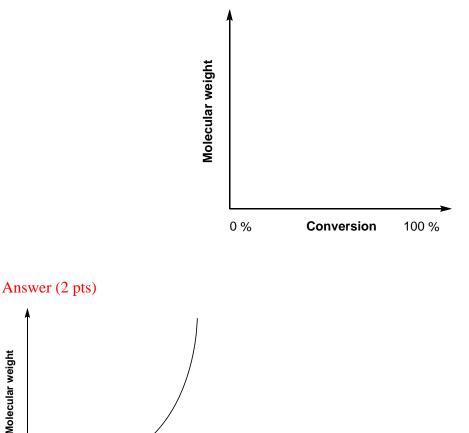
Conversion

100 %

Number average of degree of polymerization:  $X_n = M_n / M_o = 11,300 / 113 = 100$ Extent of reaction: p = 0.99Feed ratio: r $X_n = (1 + r) / (1 + r - 2rp) = (1 + r) / (1 + r - 2r \times 0.99) = 100$ r = 1

hexamethylene diamine : adipic acid = 1 : 1 (equal amount of the monomers should be used)

(b) Show the change in molecular weight as a function of conversion for Nylon 66.



### 5. (total 8 pts)

The following sentences describe the step polymerization reaction. Mark each argument as true (O) or false (X).

a) any two molecular species in the reaction mixture can react with each other. ( )

b) monomer concentration decreases steadily throughout the polymerization reaction. ( )

c) molecular weight of polymers rises steadily throughout the reaction. ( )

d) long reaction times give high yields but affect molecular weight little. ( )

### Answer 2 pts each

- a) (O)
- b) (X)
- c) (O)
- d) (X)

### 6. (total 12 pts)

Consider the following reaction

$$A + B \xrightarrow{k_1} AB \xrightarrow{k_2} A + C$$

(initial concentration of A is  $[A]_0$ )

(a) Fill in the right-hand side of the following rate expressions.

 $\frac{d[A]}{dt} = ?$   $\frac{d[B]}{dt} = ?$   $\frac{d[AB]}{dt} = ?$   $\frac{d[C]}{dt} = ?$ 

(b) If [AB] rapidly approaches to equilibrium, we can apply steady-state approximation. Express [AB] in terms of  $[A]_0$  and [B].

(c) Derive overall reaction rate. (Be sure to eliminate intermediates from the answer)

$$\frac{d[C]}{dt} = ?$$

Answer

1-a) 6 pts (1.5 each)

$$\frac{d[A]}{dt} = -k_1[A][B] + k_{-1}[AB] + k_2[AB]$$
$$\frac{d[B]}{dt} = -k_1[A][B] + k_{-1}[AB]$$
$$\frac{d[AB]}{dt} = k_1[A][B] - k_{-1}[AB] - k_2[AB]$$
$$\frac{d[C]}{dt} = k_2[AB]$$

1-b) 3 pts

$$[A]_{0} = [A] + [AB]$$
  
SSA:  $k_{1}[A][B] - k_{-1}[AB] - k_{2}[AB] = 0$   
so,  $k_{1}([A]_{0} - [AB])[B] - k_{-1}[AB] - k_{2}[AB] = 0$   

$$[AB] = \frac{[A]_{0}[B]}{\frac{k_{-1} + k_{2}}{k_{1}} + [B]}$$

1-c) 3 pts

$$\frac{d[C]}{dt} = v = \frac{k_2[A]_0[B]}{\frac{k_{-1} + k_2}{k_1} + [B]}$$

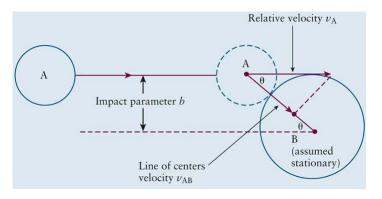
### 7. (total 10 pts)

Total rate of collision between A molecule with B molecule in a gas/unit volume is expressed as follows.

$$Z_{AB} = \sigma_c \sqrt{\frac{8k_BT}{\pi\mu}} (\frac{N_A}{V}) (\frac{N_B}{V})$$

(a) Derive  $\sigma_c$  and  $\mu$ .

(b) Let  $v_A$  be the relative velocity of A with respect to B and the component of the velocity directed along the line of the center be  $v_{AB}$ . Using impact parameter b, derive  $v_{AB}$  and corresponding energy  $\varepsilon_{AB}$ .



### Answer

2-a) 4 pts (2 pts each)  $\sigma_c = \pi d^2$   $\mu = \frac{m_A m_B}{m_A + m_B}.$ 2-b) 6 pts (3 pts each)

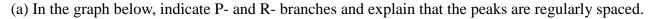
$$v_{AB} = v_A \cos\theta, \qquad \sin\theta = \frac{D}{d}$$
  

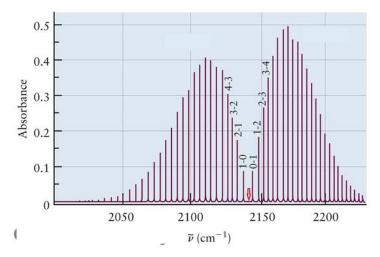
$$\cos\theta = [1 - \sin^2\theta]^{\frac{1}{2}}$$
  

$$v_{AB} = v_A \left[\frac{d^2 - b^2}{d^2}\right]^{\frac{1}{2}}$$
  

$$\varepsilon_A = \frac{1}{2}\mu v_A^2 \rightarrow \varepsilon_{AB} = \varepsilon_A (d^2 - b^2)/d^2$$

#### 8. (10 pts)





Above graph is the vibration-rotation spectrum of CO in the gas phase, measured using IR absorption spectroscopy

(b) Explain the Born-Oppenheimer approximation.

#### Answer

#### 8-a) 6 pts

Vibrational excitation과 더불어 rotational excitation 및 de-excitation이 수반됨을 언급하고 selection rule  $\Delta v = \pm 1, \Delta J = \pm 1$  이며 P-branch는  $\Delta J = -1$  R-branch는  $\Delta J = +1, \Delta E_j \propto (J + 1)$  임을 언급하고  $\Delta E_v$  는 Quantum number v와 independent 함을 언급하면 만점

#### 8-b) 4 pts

Molecular wave function  $\Psi_{ne}(\{r_e\}, \{\mathbb{R}_n\})$ 이  $\varphi((\{r_e\}, \{R_n\}) X_n(\{R_n\}) \supseteq z$  decoupling 하는 근사라고 언급하면 만점. 여기서  $\varphi((\{r_e\}, \{R_n\}))$ 의  $\{R_n\}$ 은 variable이 아니고 parameter라는 것을 언급하여야 함. (+핵은 전자보다 훨씬 무겁기 때문에 운동 속도가 전자에 비해 훨씬 낮으므로 전자의 파동함수를 도출할

때 핵은 고정되어 있다고 가정하는 것이라고 이야기해도 답으로 인정해 줘야 한다고 생각합니다.)

### 9. (total 9 pts)

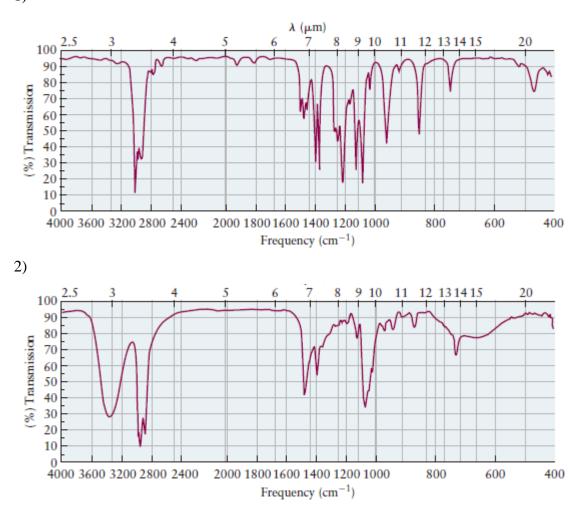
The three IR spectra are from 1-hexanol( $C_6H_{13}OH$ ), nonane( $C_9H_{20}$ ), and tert-butyl methyl ether(( $CH_3$ )<sub>3</sub>OCH<sub>3</sub>). Identify which is which, and explain the characteristic bonds with each answer.

#### TABLE 20.4

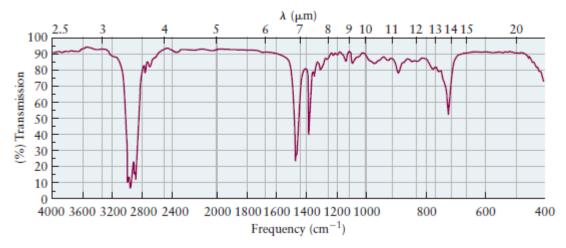
Characteristic Vibrational Frequencies and Infrared Absorption Intensities of Selected Vibrations and Functional Groups

Frequency (cm <sup>-1</sup> )	Bond or Group	Vibration	<b>Relative Intensity</b>
3650-3200	0-н	Stretching	Weak to strong
3550-3100	N-H	Stretching	Medium
3300-2700	C—H	Stretching	Weak to medium
2250-2100	C≡C	Stretching	Weak
1820–1630	C=0	Stretching	Strong
1680–1600	C=C	Stretching	Weak to medium
1430–1390	C-N	Stretching	Strong
1250–1000	C-O	Stretching	Strong

1)



3)



### Answer 3 pts each

- 1) tert-butyl methyl ether((CH<sub>3</sub>)<sub>3</sub>OCH<sub>3</sub>) / C–O peaks are observed around 1200 cm<sup>-1</sup>.
- 2) 1-hexanol(C<sub>6</sub>H<sub>13</sub>OH) / O–H peak observed around 3300 cm<sup>-1</sup>.
- 3) nonane(C<sub>9</sub>H<sub>20</sub>) / Only C–H peaks observed.

### 10. (total 10 pts)

Consider trans-1,3-butadiene.

(a) What is the total number of valence electrons?

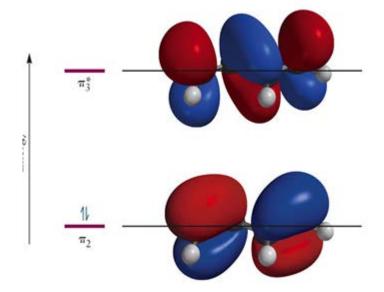
How many valence electrons are involved in  $\sigma$  – and  $\pi$  – bond?

(b) Draw a schematic diagram of HOMO and LUMO.

#### Answer

10-a) 4 pts 22 valence electrons

10-b) 6 pts (3 each)



Node 표시 확실하게 해야 만점.

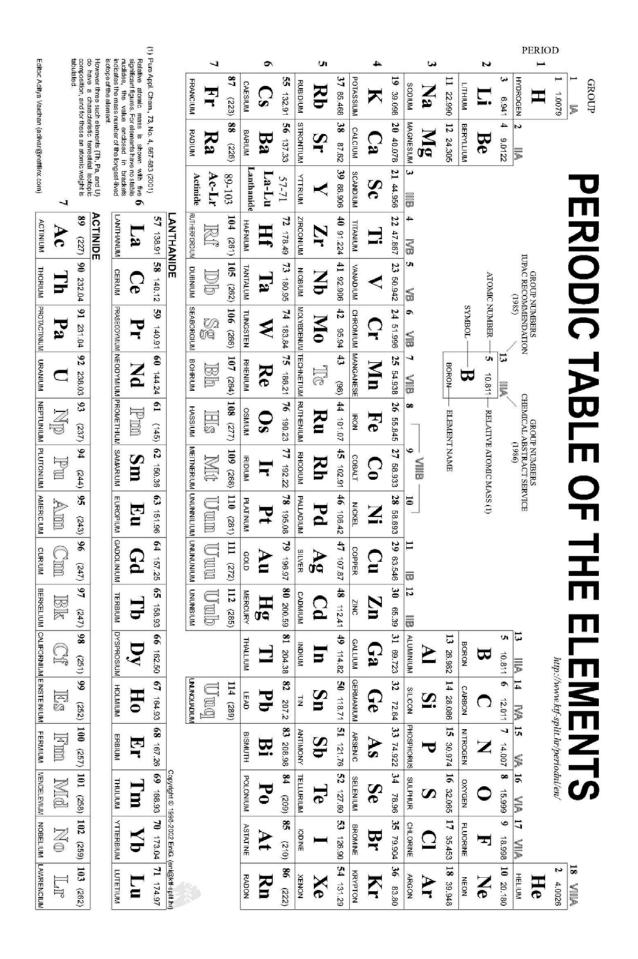
## **Physical Constants**

Avogadro's number	$N_A = 6.02214179 \times 10^{23} \text{ mol}^{-1}$		
Bohr radius	<i>a</i> <sub>0</sub> = 0.52917720859 Å = 5.2917720859 × 10 <sup>-11</sup> m		
Boltzmann's constant	$K_B = 1.3806504 \times 10^{-23} \text{ J K}^{-1}$		
Electronic charge	<i>e</i> = 1.602176487 × 10 <sup>-19</sup> C		
Faraday constant	<i>F</i> = 96485.3399 C mol <sup>-1</sup>		
Masses of fundamental particles:			
Electron	$m_e = 9.10938215 \times 10^{-31} \text{ kg}$		
Proton	$m_P = 1.672621637 \times 10^{-27} \text{ kg}$		
Neutron	$m_n = 1.674927211 \times 10^{-27} \text{ kg}$		
Permittivity of vacuum	$\epsilon_o = 8.854187817 \text{ x } 10^{-12} \text{ C}^{-2} \text{ J}^{-1} \text{ m}^{-1}$		
Planck's constant	$h = 6.62606896 \times 10^{-34} \text{ J s}$		
Ratio of proton mass to electron mass	$m_P / m_e = 1836.15267247$		
Speed of light in a vacuum	$c = 2.99792458 \times 10^8 \text{ m s}^{-1}$ (exactly)		
Standard acceleration of terrestrial gravity	$g = 9.80665 \text{ m s}^{-2}$ (exactly)		
Universal gas constant	$R = 8.314472 \text{ J mol}^{-1} \text{ K}^{-1}$ = 0.0820574 L atm mol}{-1} \text{ K}^{-1}		

Values are taken from the 2006 CODATA recommended values, as listed by the National Institute of Standards and Technology.

## **Conversion factors**

Ångström	1 Å= 10 <sup>-10</sup> m		
Atomic mass unit	$1 \text{ u} = 1.660538782 \times 10^{-27} \text{ kg}$		
	1 u = 1.492417830 x $10^{-10}$ J = 931.494028 MeV (energy equivalent form $E = mc^2$ )		
Calorie	1 cal = 4.184 J (exactly)		
Electron volt	1 eV = 1.602177 $\times$ 10 <sup>-19</sup> J = 96.485335 kJ mol <sup>-1</sup>		
Foot	1 ft = 12 in = 0.3048 m (exactly)		
Gallon (U. S.)	1 gallon = 4 quarts = 3.785412 L (exactly)		
Liter	$1 L = 10^{-3} m^{-3} = 10^3 cm^3$ (exactly)		
Liter-atmosphere	1 L atm = 101.325 J (exactly)		
Metric ton	1 t = 1000  kg (exactly)		
Pound	1 lb = 16 oz = 0.4539237 kg (exactly)		
Rydberg	1 Ry = 2.17987197 x 10 <sup>-18</sup> J = 1312.7136 kJ mol <sup>-1</sup> = 13.60569193 eV		
Standard atmosphere	1 atm = 1.01325 x 10 <sup>5</sup> Pa = 1.01325 x 10 <sup>5</sup> kg m <sup>-1</sup> s <sup>-2</sup> (exactly)		
Torr	1 torr = 133.3224 Pa		



### Claim Form for General Chemistry Examination

Class:

\_, Professor Name:\_\_\_\_\_, I.D.# :\_\_\_\_\_, Name:\_\_\_\_

If you have any claims on the marked paper, please write down them on this form and *submit this with your paper in the assigned place*. (And this form should be attached **on the top of the marked paper with a stapler**.) Please, **copy this sheet if you need more bef** 

By Student		By TA		
		Accepted? Yes( $\checkmark$ ) or No( $\checkmark$ )		
Question #	Claims	Yes: 🗆	No: 🗆	
		Pts (+/-)	Reasons	