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)***

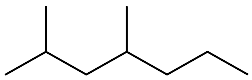
2) Procedure: During this period, you can check final score of the examination *on the website* again.
(No additional corrections. If no change in your score after reasoning, the claims were not accepted.)

***** For further information, please visit General Chemistry website at www.gencheminkaist.pe.kr***

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.

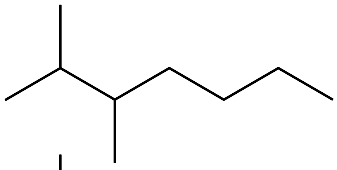
(for example: )

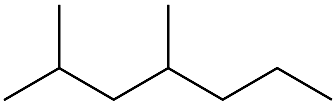
b) Identify the isomers with chiral center(s) among the 11 isomers and mark the chiral carbon(s).

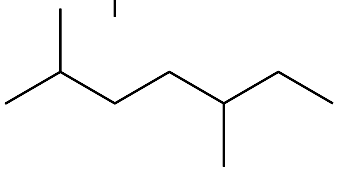
c) Identify the diastereomers.

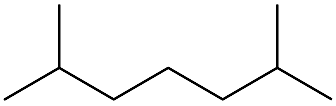
Answer

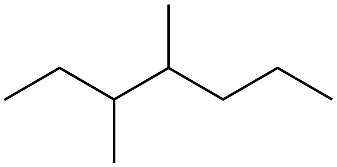
a) 10 pts (1 pt each, except 2))

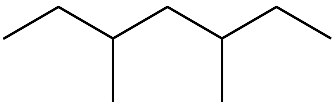
1) 

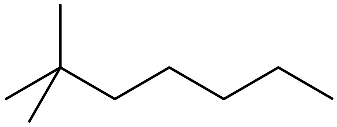
2) 

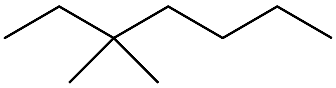
3) 

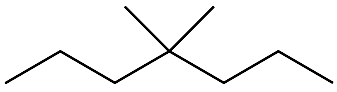
4) 

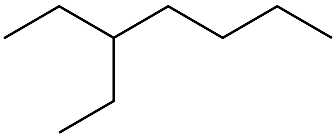
5) 

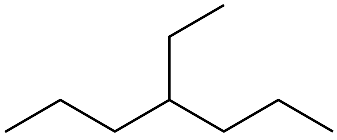
6) 

7) 

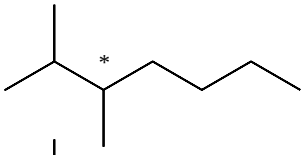
8) 

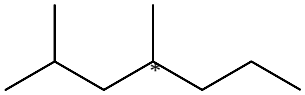
9) 

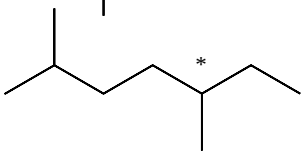
10) 

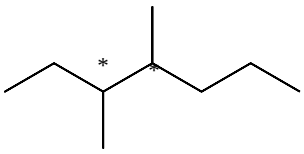
11) 

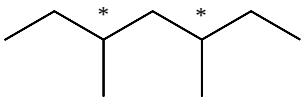
b) 5 pts (1 pt each)

1) 

2) 

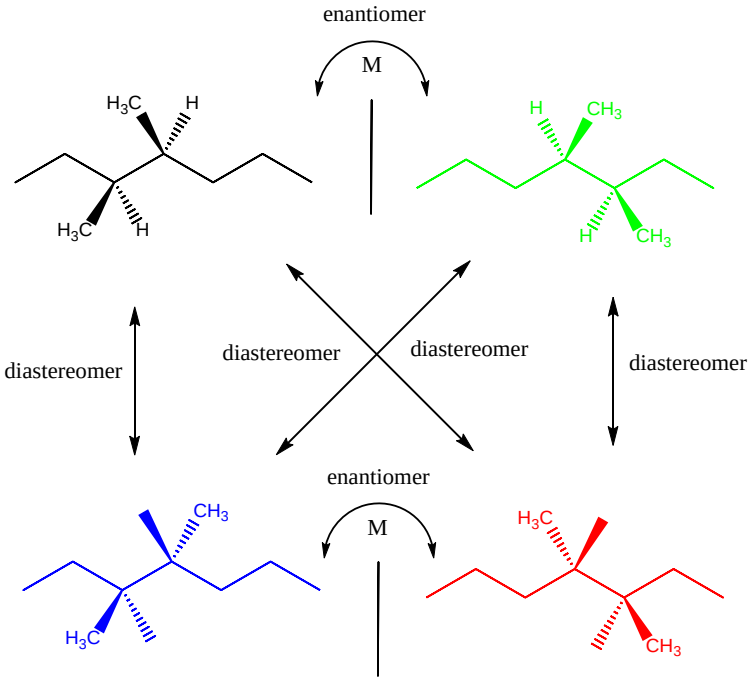
3) 

5) 

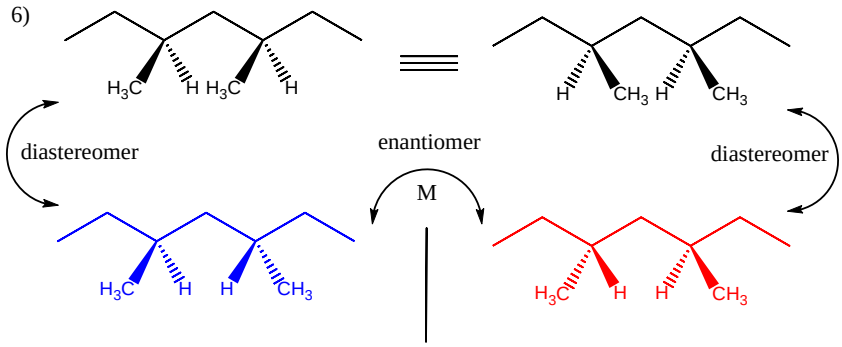
6) 

c) 1 pts each (total 2 pts)

5)



6)



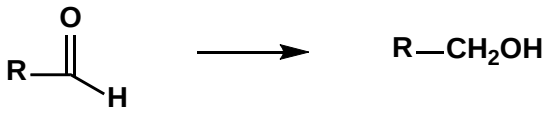
2. (total 6 pts)

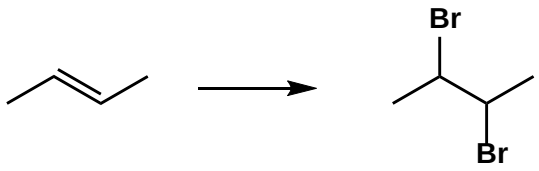
(a) List three important reactive intermediates in organic reactions.

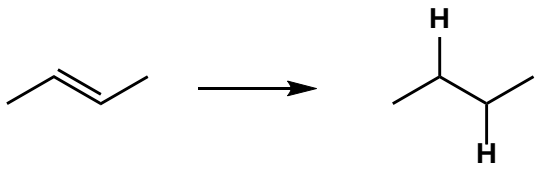
Answer 3 pts (1 pt each)

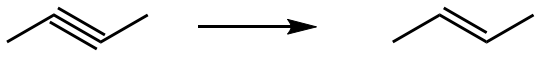
Radical, Carbanion Carbocation,

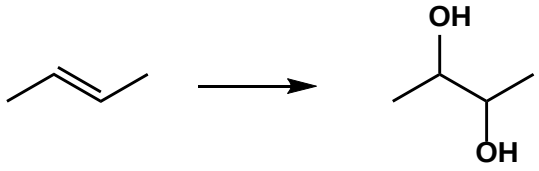
(b) Identify the oxidation reactions among the following reactions.

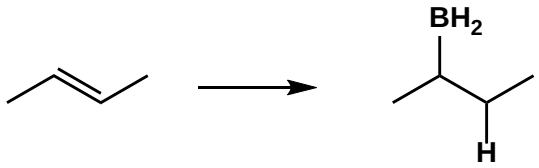
a) 

b) 

c) 

d) 

e) 

f) 

Answer 3 pts (1.5 pt each)

b), e)

3. (total 10 pts)

Polymerization of propylene (CH_2=CH-CH_3) produces so-called polypropylene with molecular weight of several hundred thousand.

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

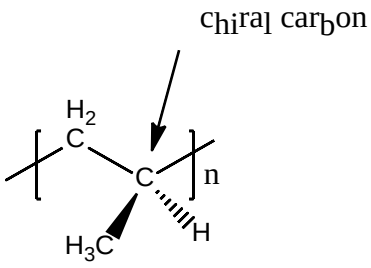
(b) Draw the repeating unit of polypropylene and identify the chiral carbon.

(c) Draw three isomeric structures of polypropylene including their name.

Answer

a) Addition (1 pt)

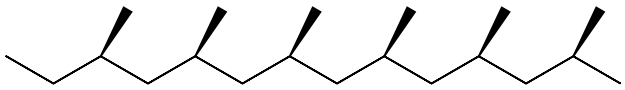
b) (3 pts)



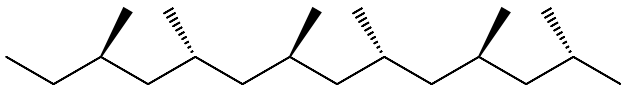
(no reduction for missing n)

c) 6 pts (2 pts each)

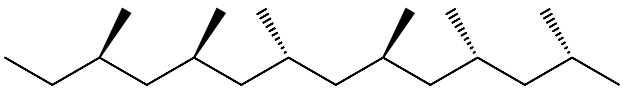
isotactic



syndiotactic



atactic



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_n) at 99% conversion. (molar mass of the repeating unit: M_0 = 113).

Answer (6 pts)

Number average of degree of polymerization: $X_n = M_n / M_o = 11{,}300 / 113 = 100$

Extent of reaction: p = 0.99

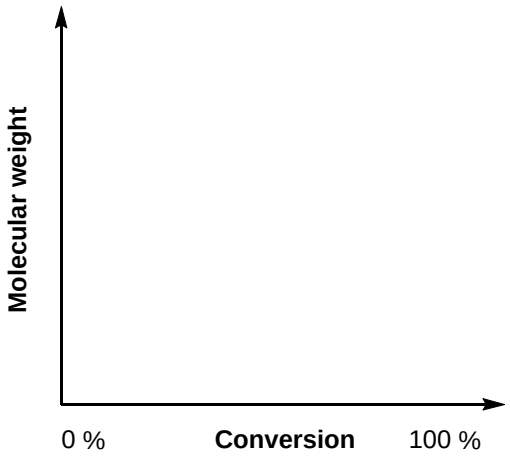
Feed ratio: r

$X_n = (1 + r) / (1 + r - 2rp) = (1 + r) / (1 + r - 2r \times 0.99) = 100$

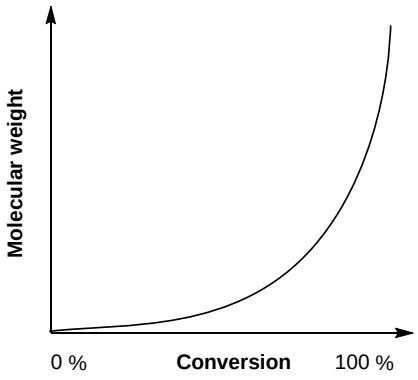
r = 1

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.



Answer (2 pts)



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)

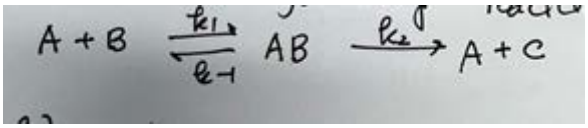
b) (X)

c) (O)

d) (X)

6. (total 12 pts)

Consider the following reaction



(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, $k_1([A]_0 - [AB])[B] - k_{-1}[AB] - k_2[\mathrm{AB}] = 0$

$$[\mathrm{AB}] = \frac{[A]_0[B]}{\frac{k_{-1} + k_2}{k_1} + [B]}$$

1-c) 3 pts

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

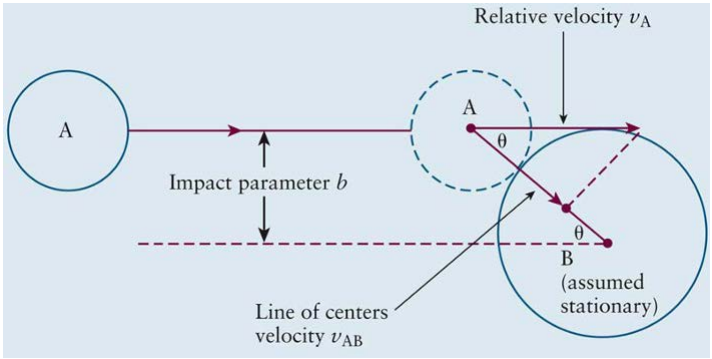
7. (total 10 pts)

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

$$Z_{AB} = \sigma_c \sqrt{\frac{8k_B T}{\pi\mu}} \left(\frac{N_A}{V}\right)\left(\frac{N_B}{V}\right)$$

(a) Derive σ_c and μ.

(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 ε_{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)

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

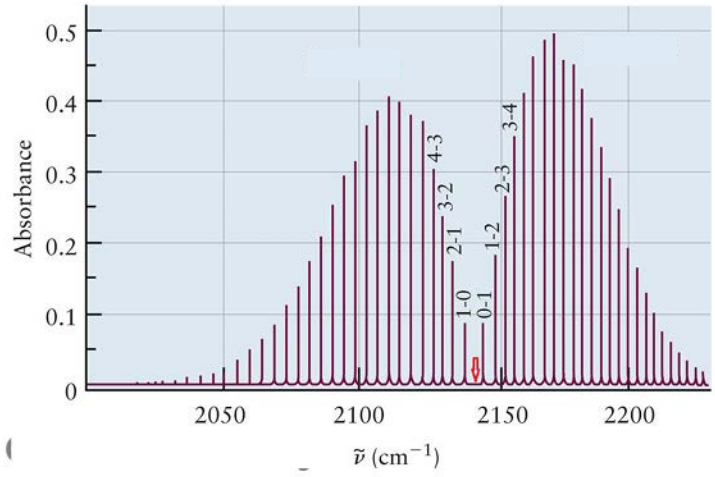
$$\cos\theta = [1 - \sin^2\theta]^{\frac{1}{2}}$$

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

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

8. (10 pts)

(a) In the graph below, indicate P- and R- branches and explain that the peaks are regularly spaced.



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 ΔE_v 는 Quantum number v와 independent 함을 언급하면 만점

8-b) 4 pts

Molecular wave function $\Psi_{ne}(\{r_e\},\{\mathbb{R}_n\})$이 $\varphi((\{r_e\};\{R_n\})\, X_n(\{R_n\})$으로 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)

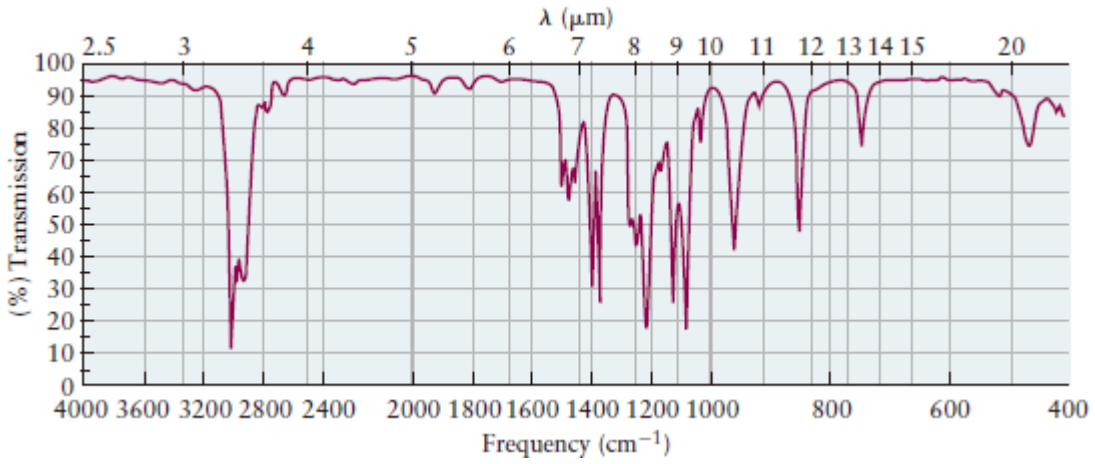
The three IR spectra are from 1-hexanol($C_6H_{13}OH$), nonane(C_9H_{20}), and tert-butyl methyl ether($(CH_3)_3OCH_3$). Identify which is which, and explain the characteristic bonds with each answer.

TABLE 20.4

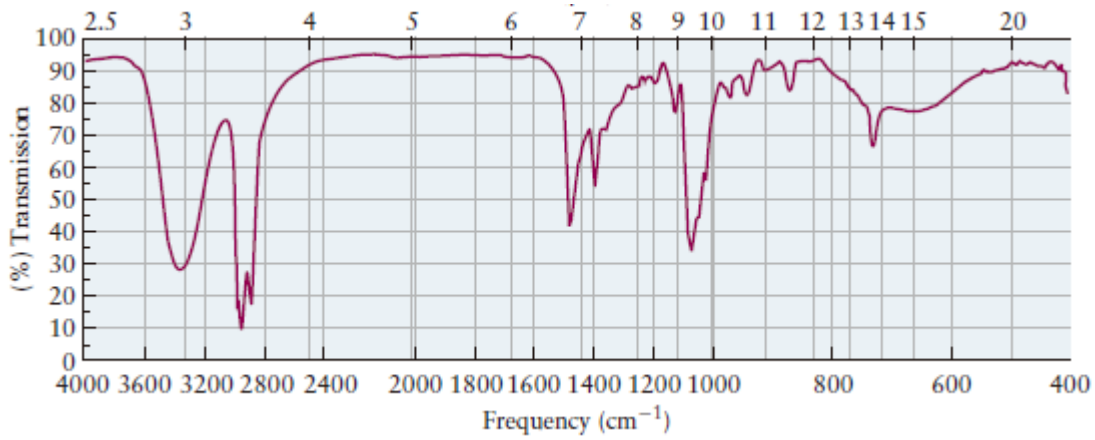
Characteristic Vibrational Frequencies and Infrared Absorption Intensities of Selected Vibrations and Functional Groups

Frequency (cm^{-1})	Bond or Group	Vibration	Relative Intensity
3650–3200	O—H	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=O	Stretching	Strong
1680–1600	C=C	Stretching	Weak to medium
1430–1390	C—N	Stretching	Strong
1250–1000	C—O	Stretching	Strong

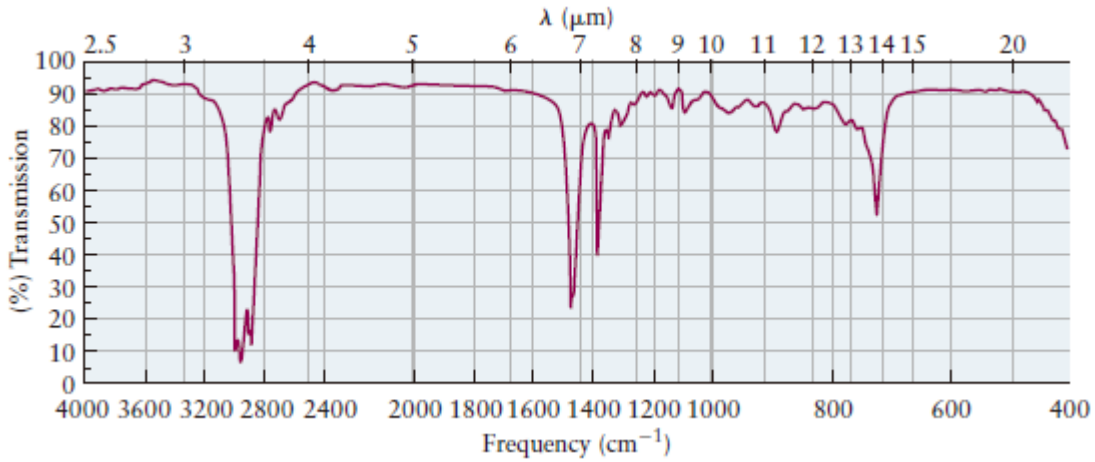
1)



2)



3)



Answer 3 pts each

1) tert-butyl methyl ether($(CH_3)_3OCH_3$) / C–O peaks are observed around 1200 cm^{-1}.

2) 1-hexanol($C_6H_{13}OH$) / O–H peak observed around 3300 cm^{-1}.

3) nonane(C_9H_{20}) / 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?

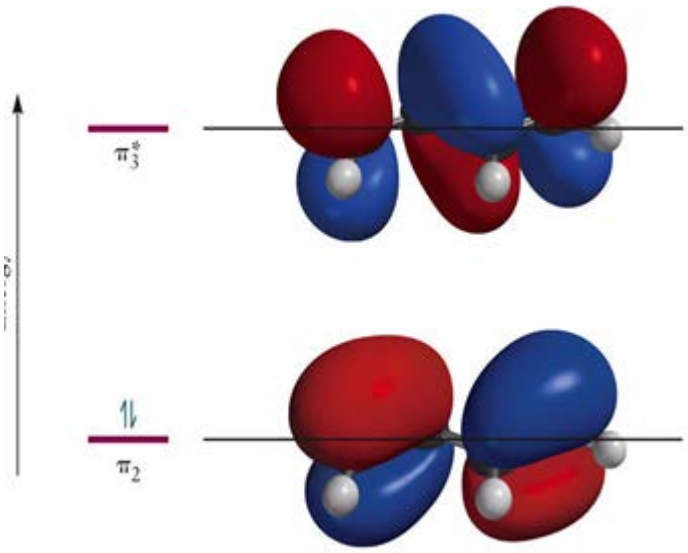
(b) Draw a schematic diagram of HOMO and LUMO.

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 x 10^{23} mol^{-1}
Bohr radius	a_0 = 0.52917720859 Å = 5.2917720859 x 10^{-11} m
Boltzmann's constant	K_B = 1.3806504 x 10^{-23} J K^{-1}
Electronic charge	e = 1.602176487 x 10^{-19} C
Faraday constant	F = 96485.3399 C mol^{-1}
Masses of fundamental particles:	
Electron	m_e = 9.10938215 x 10^{-31} kg
Proton	m_P = 1.672621637 x 10^{-27} kg
Neutron	m_n= 1.674927211 x 10^{-27} kg
Permittivity of vacuum	ε_o = 8.854187817 x 10^{-12} C^{-2} J^{-1} m^{-1}
Planck's constant	h = 6.62606896 x 10^{-34} J s
Ratio of proton mass to electron mass	m_P / m_e = 1836.15267247
Speed of light in a vacuum	c = 2.99792458 x 10^{8} m s^{-1} (exactly)
Standard acceleration of terrestrial gravity	g = 9.80665 m s^{-2} (exactly)
Universal gas constant	R = 8.314472 J mol^{-1} K^{-1} = 0.0820574 L atm mol^{-1} 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^{-10} m
Atomic mass unit	1 u = 1.660538782 x 10^{-27} 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 x 10^{-19} J = 96.485335 kJ mol^{-1}
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^{-18}J = 1312.7136 kJ mol^{-1} = 13.60569193 eV
Standard atmosphere	1 atm = 1.01325 x 10^{5} Pa = 1.01325 x 10^{5} kg m^{-1} s^{-2} (exactly)
Torr	1 torr = 133.3224 Pa

PERIODIC TABLE OF THE ELEMENTS

http://www.ktf-split.hr/periodni/en/

GROUP NUMBERS IUPAC RECOMMENDATION (1985) — GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986)

ATOMIC NUMBER — SYMBOL — RELATIVE ATOMIC MASS (1) — ELEMENT NAME

PERIOD	1 IA												13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 1.0079 **H** HYDROGEN	2 IIA																2 4.0026 **He** HELIUM
2	3 6.941 **Li** LITHIUM	4 9.0122 **Be** BERYLLIUM											5 10.811 **B** BORON	6 12.011 **C** CARBON	7 14.007 **N** NITROGEN	8 15.999 **O** OXYGEN	9 18.998 **F** FLUORINE	10 20.180 **Ne** NEON
3	11 22.990 **Na** SODIUM	12 24.305 **Mg** MAGNESIUM	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIIIB	10	11 IB	12 IIB	13 26.982 **Al** ALUMINIUM	14 28.086 **Si** SILICON	15 30.974 **P** PHOSPHORUS	16 32.065 **S** SULPHUR	17 35.453 **Cl** CHLORINE	18 39.948 **Ar** ARGON
4	19 39.098 **K** POTASSIUM	20 40.078 **Ca** CALCIUM	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 58.693 **Ni** NICKEL	29 63.546 **Cu** COPPER	30 65.39 **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 83.80 **Kr** KRYPTON
5	37 85.468 **Rb** RUBIDIUM	38 87.62 **Sr** STRONTIUM	39 88.906 **Y** YTTRIUM	40 91.224 **Zr** ZIRCONIUM	41 92.906 **Nb** NIOBIUM	42 95.94 **Mo** MOLYBDENUM	43 (98) **Tc** TECHNETIUM	44 101.07 **Ru** RUTHENIUM	45 102.91 **Rh** RHODIUM	46 106.42 **Pd** PALLADIUM	47 107.87 **Ag** SILVER	48 112.41 **Cd** CADMIUM	49 114.82 **In** INDIUM	50 118.71 **Sn** TIN	51 121.76 **Sb** ANTIMONY	52 127.60 **Te** TELLURIUM	53 126.90 **I** IODINE	54 131.29 **Xe** XENON
6	55 132.91 **Cs** CAESIUM	56 137.33 **Ba** BARIUM	57-71 **La-Lu** Lanthanide	72 178.49 **Hf** HAFNIUM	73 180.95 **Ta** TANTALUM	74 183.84 **W** TUNGSTEN	75 186.21 **Re** RHENIUM	76 190.23 **Os** OSMIUM	77 192.22 **Ir** IRIDIUM	78 195.08 **Pt** PLATINUM	79 196.97 **Au** GOLD	80 200.59 **Hg** MERCURY	81 204.38 **Tl** THALLIUM	82 207.2 **Pb** LEAD	83 208.98 **Bi** BISMUTH	84 (209) **Po** POLONIUM	85 (210) **At** ASTATINE	86 (222) **Rn** RADON
7	87 (223) **Fr** FRANCIUM	88 (226) **Ra** RADIUM	89-103 **Ac-Lr** Actinide	104 (261) **Rf** RUTHERFORDIUM	105 (262) **Db** DUBNIUM	106 (266) **Sg** SEABORGIUM	107 (264) **Bh** BOHRIUM	108 (277) **Hs** HASSIUM	109 (268) **Mt** MEITNERIUM	110 (281) **Uun** UNUNNILIUM	111 (272) **Uuu** UNUNUNIUM	112 (285) **Uub** UNUNBIUM		114 (289) **Uuq** UNUNQUADIUM				

LANTHANIDE 6	57 138.91 **La** LANTHANUM	58 140.12 **Ce** CERIUM	59 140.91 **Pr** PRASEODYMIUM	60 144.24 **Nd** NEODYMIUM	61 (145) **Pm** PROMETHIUM	62 150.36 **Sm** SAMARIUM	63 151.96 **Eu** EUROPIUM	64 157.25 **Gd** GADOLINIUM	65 158.93 **Tb** TERBIUM	66 162.50 **Dy** DYSPROSIUM	67 164.93 **Ho** HOLMIUM	68 167.26 **Er** ERBIUM	69 168.93 **Tm** THULIUM	70 173.04 **Yb** YTTERBIUM	71 174.97 **Lu** LUTETIUM
ACTINIDE 7	89 (227) **Ac** ACTINIUM	90 232.04 **Th** THORIUM	91 231.04 **Pa** PROTACTINIUM	92 238.03 **U** URANIUM	93 (237) **Np** NEPTUNIUM	94 (244) **Pu** PLUTONIUM	95 (243) **Am** AMERICIUM	96 (247) **Cm** CURIUM	97 (247) **Bk** BERKELIUM	98 (251) **Cf** CALIFORNIUM	99 (252) **Es** EINSTEINIUM	100 (257) **Fm** FERMIUM	101 (258) **Md** MENDELEVIUM	102 (259) **No** NOBELIUM	103 (262) **Lr** LAWRENCIUM

(1) Pure Appl. Chem., 73, No. 4, 667-683 (2001)

Relative atomic mass is shown with five significant figures. For elements have no stable nuclides, the value enclosed in brackets indicates the mass number of the longest-lived isotope of the element.

However three such elements (Th, Pa, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.

Editor: Aditya Vardhan (adivar@nettlinx.com)

Claim Form for General Chemistry Examination

Page (/)

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By Student		By TA	
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		Pts (+/-)	Reasons