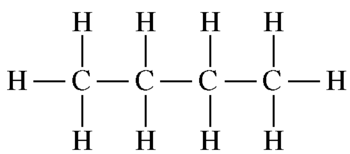
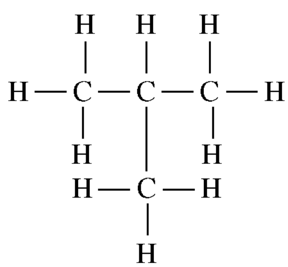
Question 1
(10 points)

The compound butane, C_4H_{10}, occurs in two isomeric forms, *n*-butane and isobutane (2-methyl propane). Both compounds exist as gases at 25°C and 1.0 atm.

(a) Draw the structural formula of each of the isomers (include all atoms). Clearly label each structure.

 *n*-butane  isobutane	Two points are earned for two correct structures with correct labels. (<u>Note:</u> 1 point can be earned for either two correct structures that are mislabeled or one correct structure with or without correct label.) *OR* 1 point can be earned for two skeletal structures (hydrogen atoms not shown) with proper labels.

(b) On the basis of molecular structure, identify the isomer that has the higher boiling point. Justify your answer.

The isomer *n*-butane has the higher boiling point. London (dispersion) forces are greater among molecules of *n*-butane than they are among molecules of isobutane because molecules of *n*-butane, with its linear structure, can approach one another more closely and can form a greater number of induced temporary dipoles than molecules of isobutane, with its more compact structure, can form.	One point is earned for the correct choice of isomer with justification.

The two isomers exist in equilibrium as represented by the equation below.

$$n\text{-butane}(g) \rightleftarrows \text{isobutane}(g) \qquad K_c = 2.5 \text{ at } 25°\text{C}$$

Suppose that a 0.010 mol sample of pure *n*-butane is placed in an evacuated 1.0 L rigid container at 25°C.

(c) Write the expression for the equilibrium constant, K_c, for the reaction.

$K_c = \dfrac{[\text{isobutane}]}{[n\text{-butane}]}$	One point is earned for the correct equation.

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Question 1 (continued)

(d) Calculate the initial pressure in the container when the *n*-butane is first introduced (before the reaction starts).

$P = \dfrac{nRT}{V} = \dfrac{(0.010\text{ mol})(0.0821\dfrac{\text{L}\times\text{atm}}{\text{mol}\times\text{K}})(298\text{ K})}{1.0\text{ L}}$ $= 0.24\text{ atm}$	One point is earned for the correct substitution and numerical answer.

(e) The *n*-butane reacts until equilibrium has been established at 25°C.

(i) Calculate the total pressure in the container at equilibrium. Justify your answer.

The total pressure in the container remains the same, 0.24 atm. As the reaction proceeds, the number of molecules in the container remains constant; one molecule of isobutane is produced for each molecule of *n*-butane consumed.	One point is earned for the correct answer with justification.

(ii) Calculate the molar concentration of each species at equilibrium.

$K_c = \dfrac{[\text{isobutane}]}{[n\text{-butane}]} = \dfrac{x}{(0.010 - x)} = 2.5$ $x = 2.5(0.010 - x) = 0.025 - 2.5x$ $3.5x = 0.025 \Rightarrow x = 0.0071\ M$ isobutane $(0.010\ M - 0.0071\ M) = 0.003\ M$ *n*-butane	One point is earned for the correct setup. One point is earned for both correct numerical answers.

(iii) If the volume of the system is reduced to half of its original volume, what will be the new concentration of *n*-butane after equilibrium has been reestablished at 25°C ? Justify your answer.

Halving the volume of the container at equilibrium doubles the pressure of both isobutane and *n*-butane, which has no effect on the equilibrium because the stoichiometry of the reaction is one mole of product produced for each mole of reactant consumed. Since the number of moles of each isomer is unchanged but the volume is reduced by half, concentrations of both isomers are doubled and the concentration of *n*-butane will be $2 \times 0.003\ M = 0.006\ M$.	One point is earned for the correct answer with justification.

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Question 1 (continued)

Suppose that in another experiment a 0.010 mol sample of pure isobutane is placed in an evacuated 1.0 L rigid container and allowed to come to equilibrium at 25°C.

(f) Calculate the molar concentration of each species after equilibrium has been established.

The concentrations of isobutane and *n*-butane would be the same as they were calculated in part (e)(ii), 0.0071 *M* and 0.003 *M*, respectively.	One point is earned for correct numerical answers or a correct statement regarding their equivalence to values obtained in part (e)(ii).

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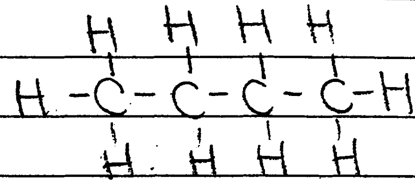
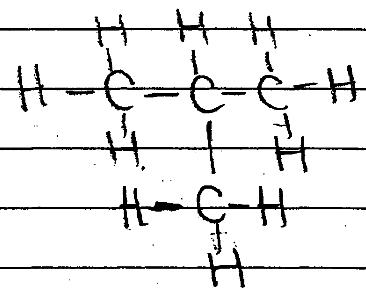
1)

a. n-Butane → 

isobutane → 

b. For butane, the main intermolecular force is the London dispersion force, which is weaker when the molecule is more symmetrically arranged. Since n-butane's structure is more symmetric than isobutane's, its London dispersion forces are weaker. The boiling pt. increases as the strength of intermolecular forces increases – thus, isobutane has a higher boiling point.

c. $K_C = \frac{[\text{isobutane}]}{[\text{n-butane}]}$

d. $PV = nRT$

$P(1.0L) = (0.010 mol)(0.0821\ L\,atm\,mol^{-1}K^{-1})(25+273K)$

$P = 0.24 atm$

*0.24 atm.

e. i. Since n-butane & isobutane are in a 1:1 ratio, the # of moles of gas remains the same. Therefore, the total pressure is 0.24 atm.

GO ON TO THE NEXT PAGE.

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1A2

ii) $K_c = 2.5 = \frac{[\text{isobutane}]}{[\text{n-butane}]}$ → *volume = 1L.

	n-butane ⟷	isobutane
I	0.010	0
C	$-x$	$+x$
E	$0.010-x$	x

$K_c = 2.5 = \frac{x}{0.010-x}$

$x = 0.0071$

[isobutane] = 0.0071 M

[n-butane] = 0.010 − 0.0071

= 0.0029M.

GO ON TO THE NEXT PAGE.

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1A3

iii) The equilibrium position doesn't change b/c there are equal moles of gas on each side of the equation.

[N-butane] = 0.0029mol / 0.5L
= 0.0058 M

f) isobutane ⟷ N-butane $K_c = \frac{1}{2.5}$

	isobutane	N-butane
I	0.010mol	0
C	$-x$	$+x$
E	$0.010-x$	x

$K_c = \frac{1}{2.5} = \frac{[N\text{-butane}]}{[\text{isobutane}]}$.

$\frac{1}{2.5} = \frac{x}{0.010-x}$

$x = 0.0029$

[N-butane] = 0.0029 M
[isobutane] = 0.010 − 0.0029
= 0.0071 M.

GO ON TO THE NEXT PAGE.

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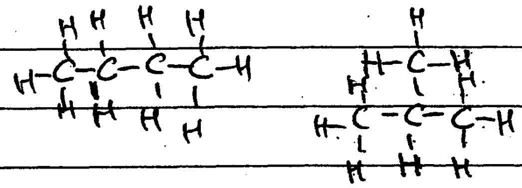
1a) 

b) isobutane has higher boiling point because it has more complex structure than ~~n-butane~~ isobutane, so ~~it~~ requires more energy.

$Kc = \frac{\text{Product}}{\text{Reactant}}$

c) $K_c = \frac{[\text{isobutane}]}{[\text{n-butane}]}$

d) $PV = nRT$

$P = \frac{nRT}{V}$

$= \frac{(0.01\text{ mol})(0.0821)(25°C + 273)}{1L}$

$= 0.24$ atm.

e) i) ~~KA = isobutane / n-butane~~

$K_p = K_c (RT)^{\Delta n}$

$K_p = 2.5((0.0821)(25°C + 273))^0$

$=$ 2.5 atm

ii) n-butane ⇄ isobutane

	n-butane	isobutane
i	$\frac{0.01\text{mol}}{1.0\text{ L}} = 0.01M$	0
c	$-x$	$+x$
e	$0.01M - x$	x M.

$Kc = \frac{[\text{isobutane}]}{[\text{n-butane}]} = \frac{x}{0.01 - x} = 2.5$

$x = 2.5(0.01 - x)$

$x = 0.025 - 2.5x$

$3.5x = 0.025$

$x = 0.0071$ M.

n-butane ⇒ 0.01M − 0.0071 M = 0.0029 M

isobutane ⇒ 0.0071M

GO ON TO THE NEXT PAGE.

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iii) $\frac{1.0L \text{ (original)}}{2} = 0.5L$

	n-butane ⇌	isobutane
i	$\frac{0.01 mol}{0.5L} = 0.02M$	0
c	$-x$	$+x$
e	$0.02M - x$	$+x$

$Kc = \frac{[isobutane]}{[n\text{-}butane]} = \frac{[+x]}{[0.02M - x]} = 2.5$

$2.5(0.02 - x) = x$

$0.05 - 2.5x = x$

$0.05 = 3.5x$

$x = 0.014M$

concentration of n-butane after equilibrium $= 0.02 - 0.014 = 0.006M$.

f)

	isobutane ⇌	n-butane
i	$\frac{0.01 mol}{1.0L} = 0.01M$	0
c	$-x$	$+x$
e	$0.01M - x$.	$+x$

reverse reaction = $\frac{1}{Kc} = \frac{1}{2.5} = 0.4$

$Kc = \frac{[n\text{-}butane]}{[isobutane]} = 0.4$.

$Kc = \frac{[x]}{[0.01M - x]} = 0.4$

$0.4(0.01 - x) = x$

$0.004 - 0.4x = x$

$0.004 = 1.4x$

$x = 0.0029M$.

After equilibrium:

isobutane: $0.01M - 0.0029M = 0.0071M$

n-butane: $0.0029M$.

GO ON TO THE NEXT PAGE.

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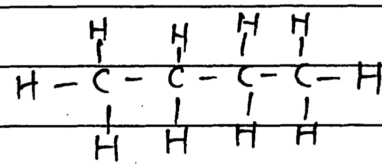
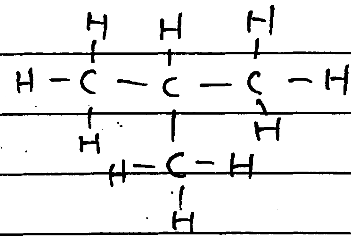
1C₁

1. a) n-butane :



isobutane :



b). Both n-butane and isobutane have london Dispersion force as their inter-molecular forces. However, this type of induced diple force is stronger for larger size molecules like n-butane as compared to isobutane which is more compact. Hence, more heat energy is needed to overcome the inter molecular forces between n-butane molecules than for isobutane. Therefore, n-butane has a higher boiling point than isobutane.

c) $K_c = \dfrac{\text{molar concentration of isobutane}}{\text{molar concentration of n-butane}} = \dfrac{n_{\text{isobutane}}}{n_{\text{n-butane}}} = 2.5$

d) $VP = nRT$

$1L \cdot P_i = 0.010\,mol \cdot (25+273)K \cdot 0.0821\,L\,atm\,mol^{-1} \cdot K^{-1}$

$P_i = 0.245\,atm.$

e) i) Each mol of n-butane become 1 mol of isobutane after reaction, so there is no change in pressure, hence, pressure in the container is still 0.245 atm

ii) Next page.

GO ON TO THE NEXT PAGE.

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1C2

ii) $K_c = 2.5$

$\frac{n_{isobutane}}{n_{n\text{-}butane}} = 2.5$

⇒ Molar concentration of isobutane = $\frac{n_{isobutane}}{n_{total}} = \frac{1}{3.5} = 0.286$

~~$= \frac{0.01}{3.5}$ mol L^{-1} = 0.286 × 10^{-3} mol L^{-1}~~

$1 - 0.286 = 0.714$

⇒ Molar concentration of n-butane = ~~$\frac{2.5}{3.5} \times 0.01$ mol L^{-1}~~

iii) Number of moles of n-butane does not change with pressure, because 1 mole of n-butane form 1 mol of isobutane.

So Molar concentration is still 0.714

f) Same as part (e), ii). Molar concentration of isobutane = 0.286

" " " of n-butane = 0.714

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Question 1

Sample: 1A
Score: 9

This response earned 9 of the possible 10 points: 2 points for part (a), 1 point for part (c), 1 point for part (d), 1 point for part (e)(i), 2 points for part (e)(ii), 1 point for part (e)(iii), and 1point for part (f). In part (b) the point was not earned because the student incorrectly identifies isobutane as the isomer with the higher boiling point.

Sample: 1B
Score: 7

This response earned 7 of the possible 10 points. In part (a) only 1 of the possible 2 points was earned because the student does not label the two correctly drawn structures. In part (b) the point was not earned because the student incorrectly identifies isobutane as the isomer with the higher boiling point. In part (e)(i) the point was not earned because the student calculates the value of K_P rather than the total pressure at equilibrium.

Sample: 1C
Score: 6

This response earned 6 of the possible 10 points. In part (a) 2 points were earned for the two correctly labeled structures. In part (b) 1 point was earned because the student correctly identifies *n*-butane as the isomer with the higher boiling point and gives a reasonable explanation related to the stronger London forces between less compact molecules. In part (c) 1 point was earned for the correct equilibrium expression even though it is stated in words. In part (d) 1 point was earned for the correct calculation of the initial pressure using the ideal gas law. In part (e)(i) 1 point was earned for indicating that the total pressure in the container is the same as the initial pressure, with a reasonable justification. In part (e)(ii) the points were not earned because the student does not correctly calculate the concentrations of isobutane and *n*-butane. In part (e)(iii) the point was not earned because the student says the concentration does not change. In part (f) the point was not earned because the student does not calculate the correct concentrations of both species under equilibrium conditions.

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