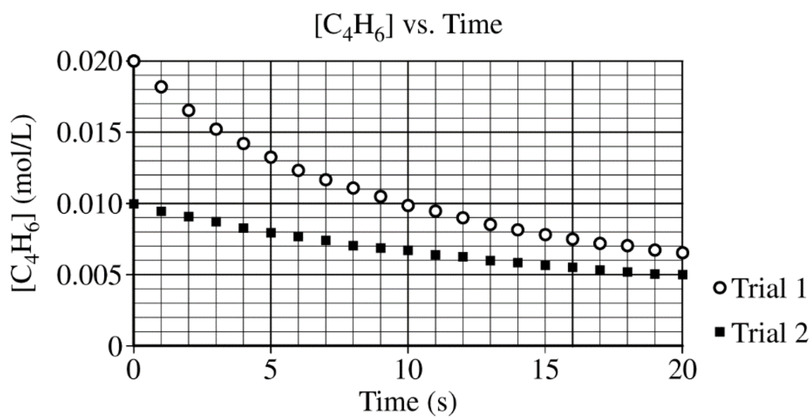
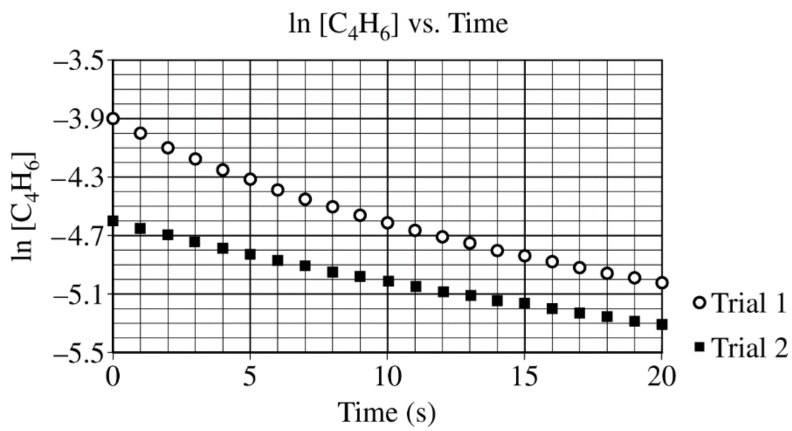
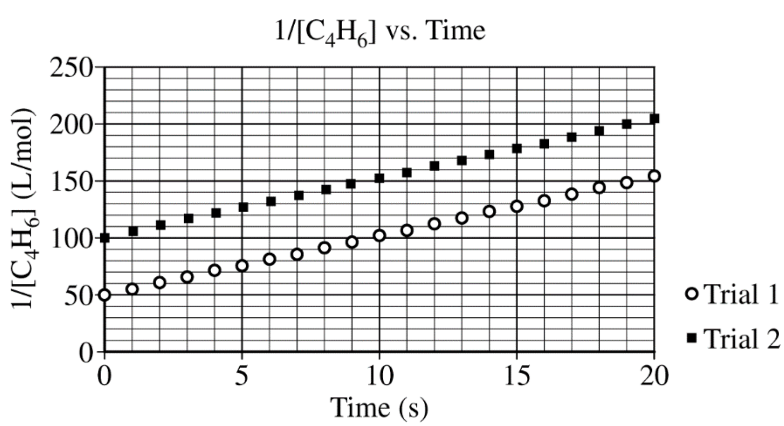
Question 5

$$2\ C_4H_6(g) \rightarrow C_8H_{12}(g)$$

At high temperatures the compound C_4H_6 (1,3-butadiene) reacts according to the equation above. The rate of the reaction was studied at 625 K in a rigid reaction vessel. Two different trials, each with a different starting concentration, were carried out. The data were plotted in three different ways, as shown below.







Question 5 (continued)

(a) For trial 1, calculate the initial pressure, in atm, in the vessel at 625 K. Assume that initially all the gas present in the vessel is C_4H_6.

For trial 1, $\frac{n}{V} = 0.020$ mol/L (or assume the volume of the vessel is 1.0 L; the number of moles of C_4H_6 in the vessel would then be 0.020 mol). $PV = nRT$ $P = \frac{nRT}{V} = \frac{(0.020 \text{ mol})(0.08206 \text{ L atm mol}^{-1} \text{ K}^{-1})(625 \text{ K})}{1.0 \text{ L}} = 1.0 \text{ atm}$	1 point is earned for a correct setup. 1 point is earned for the correct answer.

(b) Use the data plotted in the graphs to determine the order of the reaction with respect to C_4H_6.

Second order (because the plot of $1/[C_4H_6]$ is a straight line).	1 point is earned for the correct order.

(c) The initial rate of the reaction in trial 1 is 0.0010 mol/(L·s). Calculate the rate constant, k, for the reaction at 625 K.

From the second-order rate law (differential form): rate $= k[C_4H_6]^2$ $\Rightarrow k = \frac{\text{rate}}{([C_4H_6])^2} = \frac{0.0010 \text{ mol/(L}\cdot\text{s)}}{(0.020 \text{ mol/L})^2} = 2.5 \text{ L/(mol}\cdot\text{s)}$ OR From the second-order rate law (integrated form): $\frac{1}{[C_4H_6]_t} = 2kt + \frac{1}{[C_4H_6]_0}$ The coefficient of t is equal to $2k$ because of the reaction stoichiometry. The slope of the line in the plot of $\frac{1}{[C_4H_6]}$ versus time is $2k$. Thus slope = 5.0 L/(mol·s) = $2k$, therefore k = 2.5 L/(mol·s). Note: Students who choose the second method of determining k but omit the factor of 2, thereby getting an answer of 5.0 L/(mol·s), still earn the point.	1 point is earned for the correct value.

(a) For trial 1, calculate the initial pressure, in atm, in the vessel at 625 K. Assume that initially all the gas present in the vessel is C_4H_6.

(b) Use the data plotted in the graphs to determine the order of the reaction with respect to C_4H_6.

(c) The initial rate of the reaction in trial 1 is 0.0010 mol/(L·s). Calculate the rate constant, k, for the reaction at 625 K.

a. $PV = nRT$

$P = \frac{nRT}{V} = \left(\frac{n}{V}\right)RT = (0.020\ mol\,L^{-1})(0.08206\ L\,atm\,mol^{-1}K^{-1})(625\,K)$

$\approx 1.03\ atm \approx 1.0\ atm$

b. Second order with respect to C_4H_6

The plot of $\frac{1}{[C_4H_6]}$ versus time shows a linear relationship indicating secondorder.

c. $Rate = k[C_4H_6]^2$

$k = \frac{Rate}{[C_4H_6]^2} = \frac{0.0010\ mol/(L\cdot s)}{(0.020\ mol/L)^2} = \frac{0.0010\ Ms^{-1}}{(0.020\ M)^2} = \frac{2.5\,s^{-1}}{M}$

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5B

(a) For trial 1, calculate the initial pressure, in atm, in the vessel at 625 K. Assume that initially all the gas present in the vessel is C_4H_6.

(b) Use the data plotted in the graphs to determine the order of the reaction with respect to C_4H_6.

(c) The initial rate of the reaction in trial 1 is 0.0010 mol/(L·s). Calculate the rate constant, k, for the reaction at 625 K.

a) $P = \frac{nRT}{V} = \frac{0.020 \text{ mol}(0.08206 \text{ atm mol}^{-1}\text{K}^{-1})(625\text{ K})}{1 \text{ L}} = 1.0 \text{ atm}$

b) Because $\frac{1}{[C_4H_6]}$ vs Time is linear, it is second order.

c) $\frac{\ln[A_t] - \ln[A_0]}{-t} = k$

$= \frac{\ln[0.010] - \ln[0.020]}{-10 s}$

$= 0.069$

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5C

(a) For trial 1, calculate the initial pressure, in atm, in the vessel at 625 K. Assume that initially all the gas present in the vessel is C_4H_6.

(b) Use the data plotted in the graphs to determine the order of the reaction with respect to C_4H_6.

(c) The initial rate of the reaction in trial 1 is 0.0010 mol/(L·s). Calculate the rate constant, k, for the reaction at 625 K.

(a) PV=nRT

$\frac{P(1L)}{1L} = \frac{(2mol)(0.0821 L\cdot atm\cdot mol^{-1}\cdot K^{-1})(625K)}{1L}$

P = 102.625 atm

(b) The order of reaction is first order.

(c) rate = k[C4H6]

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Question 5

Overview

Question 5 assessed students' understanding of the ideal gas law, kinetics and reaction-order, and the ability to interpret real experimental data and patterns from graphs. In part (a) students were asked to determine the initial concentration of the gas C_4H_6 for trial 1 from a graph of kinetic data for concentration versus time, and then use this value to determine the initial pressure of C_4H_6 for trial 1. In part (b) the students had to examine three different graphical representations of the same data – $[C_4H_6]$ vs time, ln $[C_4H_6]$ vs time, and $1/[C_4H_6]$ – and determine the order of the reaction with respect to C_4H_6. In part (c) students were asked to calculate the rate constant k from the given initial rate of the reaction for trial 1.

Sample: 5A
Score: 4

In part (a) 1 point was earned for the correct setup of the numerical values of n/V, R, and T in the equation $P = nRT/V$ and 1 point was earned for correctly using the values of n/V, R, and T to calculate the initial pressure. Students who displayed units with their numerical values benefited by being able to see the units of mole, L, and Kelvin cancel, leaving units of atm. In part (b) 1 point was earned for stating that the reaction is second order. In part (c) 1 point was earned for using rate = $k[C_4H_6]^2$ and calculating the correct value of k, the rate constant.

Sample: 5B
Score: 3

In part (a) 1 point was earned for the correct setup of the numerical values of n, V, R, and T in the equation $P = nRT/V$ and 1 point was earned for correctly using the values of n, V, R, and T to calculate the initial pressure. In part (b) 1 point was earned for stating that the reaction is second order. In part (c) the student incorrectly uses the first-order integrated rate equation and did not earn the point.

Sample: 5C
Score: 1

In part (a) 1 point was earned for a correct setup of $P = (n/V)RT$ with two of the three values correct. The student does not use the correct value for the initial concentration of butadiene, so did not earn the second point. In part (b) the point was not earned because the student states that the reaction is first order. In part (c) the student gives a rate-law equation consistent with the answer in part (b), but the point was not earned because the student does not calculate a value of k, the rate constant.