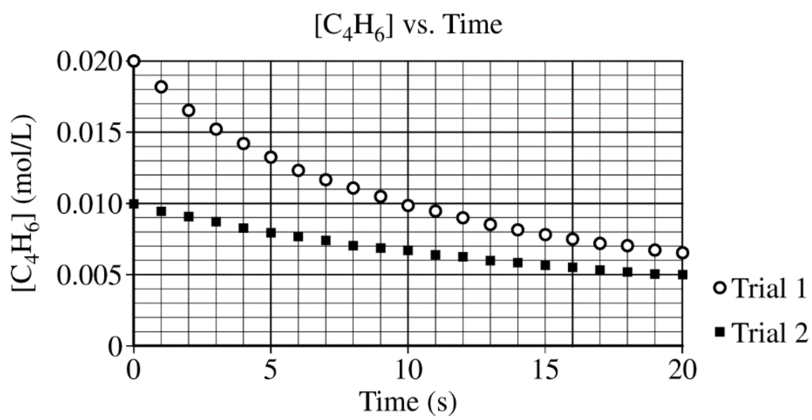
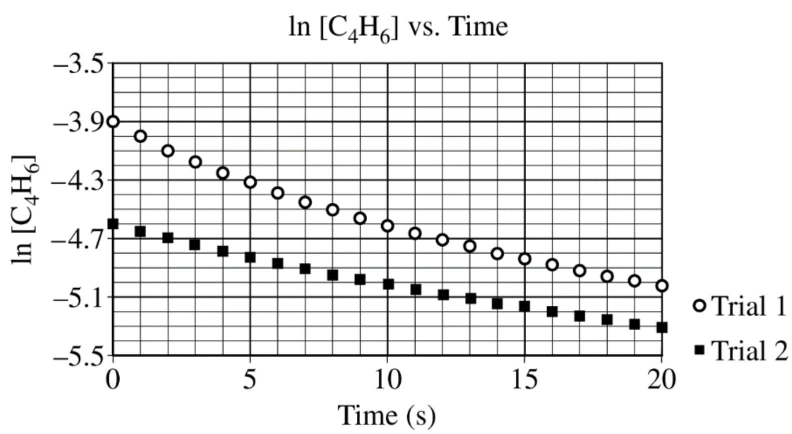
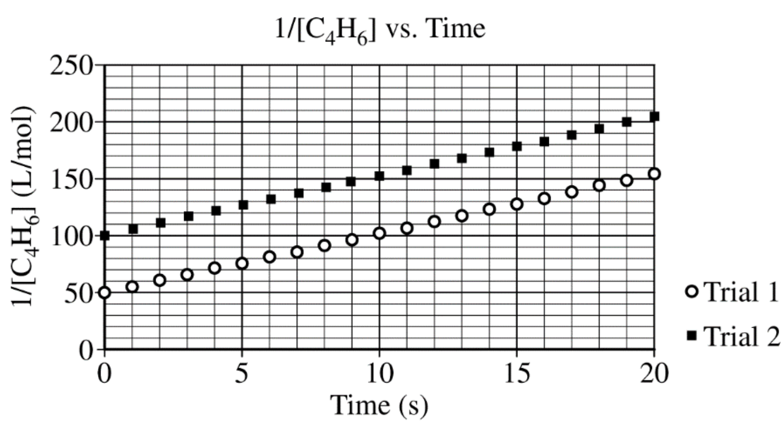
Question 5

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

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.