Question 3
(9 points)

$$H-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle \cdot\cdot}{}}{N}}-H \longrightarrow \overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}=\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{C} } \quad + \quad :\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle H}{|}}{N}}-H$$

A sample of $CH_3CH_2NH_2$ is placed in an insulated container, where it decomposes into ethene and ammonia according to the reaction represented above.

Substance	Absolute Entropy, $S°$, in J/(mol·K) at 298 K
$CH_3CH_2NH_2(g)$	284.9
$CH_2CH_2(g)$	219.3
$NH_3(g)$	192.8

(a) Using the data in the table above, calculate the value, in J/(mol$_{rxn}$·K), of the standard entropy change, $\Delta S°$, for the reaction at 298 K.

$\Delta S°_{rxn} = \Sigma S°_{products} - \Sigma S°_{reactants}$ $\Delta S°_{rxn} = [(219.3 + 192.8) - 284.9]$ J/(mol$_{rxn}$·K) $\quad = 127.2$ J/(mol$_{rxn}$·K)	1 point is earned for the correct $\Delta S°$.

(b) Using the data in the table below, calculate the value, in kJ/mol$_{rxn}$, of the standard enthalpy change, $\Delta H°$, for the reaction at 298 K.

Bond	C–C	C = C	C–H	C–N	N–H
Average Bond Enthalpy (kJ/mol)	348	614	413	293	391

$\Delta H°$ = enthalpy of bonds broken – enthalpy of bonds formed $\Delta H° = [5(\Delta H_{C-H}) + (\Delta H_{C-N}) + (\Delta H_{C-C}) + 2(\Delta H_{N-H})] -$ $\qquad [4(\Delta H_{C-H}) + (\Delta H_{C=C}) + 3(\Delta H_{N-H})]$ $\quad = [5(413) + 293 + 348 + 2(391)] - [4(413) + 614 + 3(391)] = 49$ kJ/mol$_{rxn}$ **OR** $\Delta H° = [(\Delta H_{C-H}) + (\Delta H_{C-N}) + (\Delta H_{C-C})] - [(\Delta H_{C=C}) + (\Delta H_{N-H})]$ $\quad = [413 + 293 + 348]$ kJ/mol $- [614 + 391]$ kJ/mol $= 49$ kJ/mol$_{rxn}$	1 point is earned for the correct bond count and use of values from table. 1 point is earned for the correct setup in terms of bonds broken minus bonds formed and calculated $\Delta H°$.

(c) Based on your answer to part (b), predict whether the temperature of the contents of the insulated container will increase, decrease, or remain the same as the reaction proceeds. Justify your prediction.

The temperature of the contents should decrease because the reaction is endothermic, as indicated by the positive $\Delta H°$.	1 point is earned for the correct choice with explanation.

An experiment is carried out to measure the rate of the reaction, which is first order. A 4.70×10^{-3} mol sample of $CH_3CH_2NH_2$ is placed in a previously evacuated 2.00 L container at 773 K. After 20.0 minutes, the concentration of the $CH_3CH_2NH_2$ is found to be 3.60×10^{-4} mol/L.

(d) Calculate the rate constant for the reaction at 773 K. Include units with your answer.

$\ln[A]_t - \ln[A]_o = -kt$ $\ln\left(3.60 \times 10^{-4}\,\text{mol/L}\right) - \ln\left(\dfrac{4.70 \times 10^{-3}\,\text{mol}}{2.00\,\text{L}}\right) = -k(20.0\,\text{min})$ $-7.929 - (-6.053) = -k(20.0\,\text{min})$ $k = 9.38 \times 10^{-2}\,\text{min}^{-1}$	1 point is earned for the initial concentration of $CH_3CH_2NH_2$. 1 point is earned for the correct setup of the first order integrated rate law equation. 1 point is earned for the calculated result with unit.

(e) Calculate the initial rate, in $M\,\text{min}^{-1}$, of the reaction at 773 K.

$initial\ rate = k[CH_3CH_2NH_2] = \left(9.38 \times 10^{-2}\,\text{min}^{-1}\right)\left(\dfrac{4.70 \times 10^{-3}\,\text{mol}}{2.00\,\text{L}}\right)$ $= 2.20 \times 10^{-4}\ M\,\text{min}^{-1}$	1 point is earned for the calculated result.

(f) If $\dfrac{1}{[CH_3CH_2NH_2]}$ is plotted versus time for this reaction, would the plot result in a straight line or would it result in a curve? Explain your reasoning.

The plot would produce a curve; had the reaction been second order the plot would have been a straight line. A plot of $\ln[CH_3CH_2NH_2]$ vs. t would have yielded a straight line.	1 point is earned for the correct choice with explanation.