9.4   a.   Endothermic. The reactor will have to be heated to keep the temperature constant. The temperature would decrease under adiabatic conditions. The energy required to break the reactant bonds is more than the energy released when the product bonds are formed.

     b. $\Delta \hat{U}_r^\circ = \Delta \hat{H}_r^\circ - RT \left[\sum_{\substack{\text{gaseous} \\ \text{products}}} v_i - \sum_{\substack{\text{gaseous} \\ \text{reactants}}} v_i \right] = 69.36 \dfrac{kJ}{mol} - \dfrac{8.314\ J}{mol \cdot K} \left| \dfrac{1\ kJ}{10^3\ J} \right| \dfrac{298\ K}{} \left| (7-0) \right.$

         $= 52.0\ kJ/mol$

$\Delta \hat{U}_r^\circ$ is the change in internal energy when 1 g-mole of CaC_2(s) and 5 g-moles of H_2O(l) at 25°C and 1 atm react to form 1 g-mole of CaO(s), 2 g-moles of CO_2(g) and 5 g-moles of H_2(g) at 25°C and 1 atm.

c. $Q = \Delta U = \dfrac{n_{CaC_2} \Delta \hat{U}_r^\circ}{v_{CaC_2}} = \dfrac{150\ g\ CaC_2}{} \left| \dfrac{1\ mol}{64.10\ g} \right| \dfrac{52.0\ kJ}{1\ mol\ CaC_2} = \underline{121.7\ kJ}$

Heat must be transferred to the reactor.

9.5   a. $\underline{\text{Given reaction} = (1) - (2)} \overset{\text{Hess's law}}{\Rightarrow} \Delta \hat{H}_r^\circ = \Delta \hat{H}_{r1}^\circ - \Delta \hat{H}_{r2}^\circ = (1226 - 18,935)\ \text{Btu/lb-mole}$

                                               $= \underline{-17,709\ \text{Btu/lb-mole}}$

     b. $\underline{\text{Given reaction} = (1) - (2)} \overset{\text{Hess's law}}{\Rightarrow} \Delta \hat{H}_r^\circ = \Delta \hat{H}_{r1}^\circ - \Delta \hat{H}_{r2}^\circ = (-121,740 + 104,040)\ \text{Btu/lb-mole}$

                                               $= \underline{-17,700\ \text{Btu/lb-mole}}$

9.8   a.

         $\Delta \hat{H}_{r1}^\circ = \left(\Delta \hat{H}_f^\circ \right)_{C_2H_3Cl_3(l)} - \left(\Delta \hat{H}_f^\circ \right)_{C_2H_4(g)} \Rightarrow \left(\Delta \hat{H}_f^\circ \right)_{C_2H_3Cl_3(l)} = -385.76 + 52.28 = \underline{-333.48\ kJ/mol}$

         $\Delta \hat{H}_{r2}^\circ = \left(\Delta \hat{H}_f^\circ \right)_{C_2HCl_3(l)} + \left(\Delta \hat{H}_f^\circ \right)_{HCl(g)} - \left(\Delta \hat{H}_f^\circ \right)_{C_2H_2Cl_4(l)} = -276.2 - 92.31 + 333.48 = \underline{-35.03\ kJ/mol}$

     b.

         Given reaction $= (1) + (2) \Rightarrow -385.76 - 35.03 = \underline{-420.79\ kJ/mol}$

     c. $Q = \Delta H = \dfrac{300\ mol\ C_2HCl_3}{h} \left| \dfrac{-420.79\ kJ}{mol} \right. = \underline{-1.26 \times 10^5\ kJ/h}\ (= -35\ kW)$

       Heat is evolved.

9.14 a. $C_7H_{16}(g) \rightarrow C_6H_5CH_3(g) + 4H_2(g)$

Basis: 1 mol C_7H_{16}

1 mol C_7H_{16}
400°C

1 mol $C_6H_5CH_3$
4 mol H_2
400° C
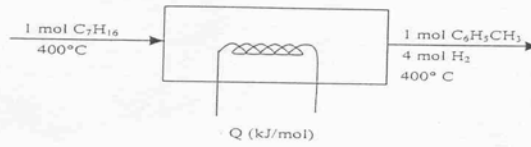
Q (kJ/mol)

b.

References: $C(s)$, $H_2(g)$ at 25°C

substance	n_{in} (mol)	$\hat{H}_{in}$ (kJ/mol)	n_{out} (mol)	$\hat{H}_{out}$ (kJ/mol)
C_7H_{16}	1	$\hat{H}_1$	—	—
C_7H_8	—	—	1	$\hat{H}_2$
H_2	—	—	4	$\hat{H}_3$

$C_7H_{16}(g,400°C)$: $\hat{H}_1 = (\Delta\hat{H}_f^{\circ})_{C_7H_{16}(g)} + \left[\int_{25}^{400} \overset{Table B.2}{\downarrow} \hat{C}_p\, dT\right]$

$= (-187.8 + 104.1)\ kJ/mol = \underline{-83.7\ kJ/mol}$

$C_6H_5CH_3(g,400°C)$: $\hat{H}_2 = (\Delta\hat{H}_f^{\circ})_{C_6H_5CH_3(g)} + \left[\int_{25}^{400} \overset{Table B.2}{\downarrow} \hat{C}_p\, dT\right]$

$= (+50 + 60.2)\ kJ/mol = \underline{110.2\ kJ/mol}$

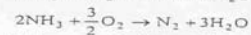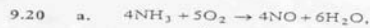$H_2(g,400°C)$: $\hat{H}_3 = \hat{H}_{H_2}(400°C) \overset{Table B.8}{\underset{\downarrow}{=}} \underline{10.89\ kJ/mol}$

c.

1 mol C_7H_{16} reacted $\Rightarrow \xi = 1$ mol

$Q = \Delta H = \xi \Delta\hat{H}_r^{\circ} + \sum_{out} n_i \hat{H}_i - \sum_{in} n_i \hat{H}_i$

$= \left\{(1)(237.8) + \left[(1)(60.2) + (4)(10.86) - (1)(104.1)\right]\right\}kJ = 237.3\ kJ$ (transferred to reactor)

d. $\Delta\hat{H}_r(400°C) = \dfrac{237.3\ kJ}{1\ mol\ C_7H_{16}\ react} = \underline{237.3\ kJ/mol}$

9.20 a. $4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$,

$2NH_3 + \dfrac{3}{2}O_2 \rightarrow N_2 + 3H_2O$

References: $N_2(g)$, $H_2(g)$, $O_2(g)$, at 25°C

Substance	$\dot{n}_{in}$ (mol/min)	$\hat{H}_{in}$ (kJ/mol)	$\dot{n}_{out}$ (mol/min)	$\hat{H}_{out}$ (kJ/mol)
NH_3	100	$\hat{H}_1$	–	–
Air	900	$\hat{H}_2$	–	–
NO	–	–	90	$\hat{H}_3$
H_2O	–	–	150	$\hat{H}_4$
N_2	–	–	716	$\hat{H}_5$
O_2	–	–	69	$\hat{H}_6$

$\hat{H}_i = \Delta\hat{H}_{fi}^o + \displaystyle\int_{25}^{T} C_{pi}\,dT$

$NH_3(g, 25°C)$: $\hat{H}_1 = (\Delta\hat{H}_f^o)_{NH_3} \overset{\text{Table B.1}}{=} \underline{-46.19 \text{ kJ/mol}}$

$Air(g, 150°C)$: $\hat{H}_2 \overset{\text{Table B.8}}{=} \underline{3.67 \text{ kJ/mol}}$

$NO(g, 700°C)$: $\hat{H}_3 = 90.37 + \displaystyle\int_{25}^{700} C_p\,dT \overset{\text{Table B.1, Table B.2}}{=} \underline{111.97 \text{ kJ/mol}}$

$H_2O(g, 700°C)$: $\hat{H}_4 \overset{\text{Table B.1, Table B.8}}{=} \underline{-216.91 \text{ kJ/mol}}$

$N_2(g, 700°C)$: $\hat{H}_5 \overset{\text{Table B.8}}{=} \underline{20.59 \text{ kJ/mol}}$

$O_2(g, 700°C)$: $\hat{H}_6 \overset{\text{Table B.8}}{=} \underline{21.86 \text{ kJ/mol}}$

b. $Q = \Delta H = \displaystyle\sum_{out} \dot{n}_i \hat{H}_i - \sum_{in} \dot{n}_i \hat{H}_i = -4890 \text{ kJ/min} \times (1 \text{ min}/60s) = \underline{-81.5 \text{ kW}}$

(heat transferred from the reactor)

c. If molecular species had been chosen as references for enthalpy calculations, the extents of each reaction would have to be calculated and Equation 9.5-1b used to determine ΔH. The value of Q would remain unchanged.