REB, The Course
Class 2 Practice Assignment Solution

2. The oxidation of ethanol to produce acetic acid is given in equation (1). Standard gas phase heats of formation at 298 K and heat capacities for the reagents are provided in Table 1. Generate an expression for the standard heat of reaction as a function of temperature and use it to calculate the standard heat of reaction at 300, 350, and 400 K.

$$C_2H_6O + O_2 \rightarrow C_2H_4O_2 + H_2O \qquad (1)$$

Reagent	$\Delta H_f\Big\vert_{298K}$ (kJ mol^{-1})	$\hat{C}_p$ (J mol^{-1} K^{-1})
C_2H_6O	-234	73.4
$C_2H_4O_2$	-443	71.7
H_2O	-242	33.9
O_2	0	29.7

Table 1. Thermodynamic data for question 2.

Calculate the standard heat of reaction at 298 K.

$$\Delta H_j^0\Big|_{T=298K} = \sum_i \left(\nu_{i,j} \Delta H_{f,i}^0\Big|_{T=298K} \right)$$

$$\Delta H_1^0\Big|_{T=298K} = \left(-\Delta H_{f,C_2H_6O}^0 - \Delta H_{f,O_2}^0 + \Delta H_{f,C_2H_4O_2}^0 + \Delta H_{f,H_2O}^0 \right)\Big|_{T=298K}$$

$$\Delta H_1^0\Big|_{T=298K} = \text{-441 kJ mol}^{-1}$$

Write the expression for the standard heat of reaction at temperature T.

$$\Delta H_j^0 = \Delta H_j^0\Big|_{T=298K} + \sum_i \left(\nu_{i,j} \int_{298\ \mathrm{K}}^{T} \hat{C}_{p,i} dT \right)$$

$$\Delta H_1^0 = \Delta H_1^0\Big|_{T=298K} + \int_{298K}^{T} \left(-\hat{C}_{p,C_2H_6O} - \hat{C}_{p,O_2} + \hat{C}_{p,C_2H_4O_2} + \hat{C}_{p,H_2O} \right) dT$$

$$\Delta H_1^0 = \Delta H_1^0\Big|_{T=298K} + \left(-\hat{C}_{p,C_2H_6O} - \hat{C}_{p,O_2} + \hat{C}_{p,C_2H_4O_2} + \hat{C}_{p,H_2O} \right) (T - 298K)$$

$$\Delta H_1^0 = \left(-441{,}000 + 2.5\,(T - 298K) \right) \text{ J mol}^{-1} \qquad (2)$$

Using equation (2), the standard heat of reaction is found to equal -441 kJ mol^{-1} at 300K, -440.9 kJ mol^{-1} at 350 K, and -440.7 kJ mol^{-1} at 400 K.