

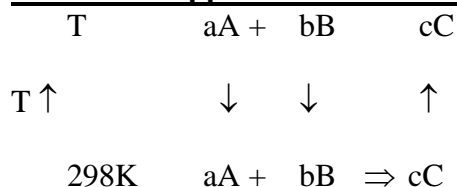
Two approaches to reaction enthalpy and entropy computations

Consider the reaction



at temperature T with enthalpy (or entropy) data stated at 298 K as well as Cp data from 298 K to T for all components. The $\Delta H_{R,T}^{\circ}$ is then computed by either of the following methods. Note the arrow directions.

Classroom Approach – Use this method that preserves the concept of state function



$$\Delta H_{R,T}^{\circ} = \Delta H_{R,298K}^{\circ} + a \int_T^{298} C_{p_A} dT + b \int_T^{298} C_{p_B} dT + c \int_{298}^T C_{p_C} dT$$

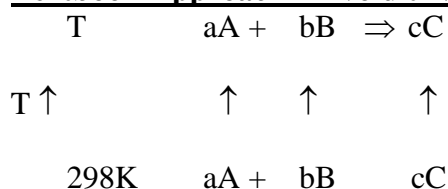
where

$$\Delta H_{R,298K}^{\circ} = c\Delta H_{f,298,K}^{\circ}, C - a\Delta H_{f,298,K}^{\circ}, A - b\Delta H_{f,298,K}^{\circ}, B$$

Therefore,

$$\Delta H_{R,T}^{\circ} = c\Delta H_{f,298,K}^{\circ}, C - a\Delta H_{f,298,K}^{\circ}, A - b\Delta H_{f,298,K}^{\circ}, B + a \int_T^{298} C_{p_A} dT + b \int_T^{298} C_{p_B} dT + c \int_{298}^T C_{p_C} dT$$

Textbook Approach – Avoid this method except to make ThermoCalc[®]-type data tables



$$\Delta H_{R,T}^{\circ} = c\Delta H_{f,T,K}^{\circ}, C - a\Delta H_{f,T,K}^{\circ}, A - b\Delta H_{f,T,K}^{\circ}, B$$

where

$$\Delta H_{f,T,K}^{\circ}, A = a\Delta H_{f,298,K}^{\circ}, A + a \int_{298}^T C_{p_A} dT = a\Delta H_{f,298,K}^{\circ}, A - a \int_T^{298} C_{p_A} dT$$

$$\Delta H_{f,T,K}^{\circ}, B = b\Delta H_{f,298,K}^{\circ}, B + b \int_{298}^T C_{p_B} dT = b\Delta H_{f,298,K}^{\circ}, B - b \int_T^{298} C_{p_B} dT$$

$$\Delta H_{f,T,K}^{\circ}, C = c\Delta H_{f,298,K}^{\circ}, C + c \int_{298}^T C_{p_C} dT$$

Therefore,

$$\Delta H_{R,T}^{\circ} = c\Delta H_{f,298,K}^{\circ}, C - a\Delta H_{f,298,K}^{\circ}, A - b\Delta H_{f,298,K}^{\circ}, B + a \int_T^{298} C_{p_A} dT + b \int_T^{298} C_{p_B} dT + c \int_{298}^T C_{p_C} dT$$