Two approaches to reaction enthalpy and entropy computations

Consider the reaction

$$aA + bB = cC$$

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 $\Delta H^{O}_{R,\,T}$ is then computed by either of the following methods. Note the arrow directions.

<u>Classroom Approach – Use this method that preserves the concept of state function</u>

	T	aA +	bB	cC
T ↑		↓	↓	↑
	298K	aA +	bB	⇒ cC

$$\Delta H^{O}_{R,\,T} = \Delta H^{O}_{R,\,298K} + a\int_{T}^{298} Cp_A dT + b\int_{T}^{298} Cp_B dT + c\int_{298}^{T} Cp_C dT$$

where

$$\Delta H^{O}_{R,\,298K} = c\Delta H^{O}_{f,\,298,\,C} - a\Delta H^{O}_{f,\,298,\,A} - b\Delta H^{O}_{f,\,298,\,B}$$

Therefore,

$$\Delta H^{O}_{R,\,T} = c\Delta H^{O}_{f,\,298,\,C} - a\Delta H^{O}_{f,\,298,\,A} - b\Delta H^{O}_{f,\,298,\,B} + a\int_{T}^{298} Cp_A dT + b\int_{T}^{298} Cp_B dT + c\int_{298}^{T} Cp_C dT$$

<u>Textbook Approach – Avoid this method except to make ThermoCalc®-type data tables</u>

	T	aA +	bB	⇒ cC
T ↑		↑	↑	↑
	298K	aA +	bB	cC

$$\Delta H^{O}_{R,\,T} = c\Delta H^{O}_{f,\,T,\,C} - a\Delta H^{O}_{f,\,T,\,A} - b\Delta H^{O}_{f,\,T,\,B}$$

where

$$\Delta H^{O}_{f,\,T,\,A} = a\Delta H^{O}_{f,\,298,\,A} + a\int_{298}^{T} Cp_A dT = a\Delta H^{O}_{f,\,298,\,A} - a\int_{T}^{298} Cp_A dT$$

$$\Delta H^{O}_{f,\,T,\,B} = b\Delta H^{O}_{f,\,298,\,B} + b\int_{298}^{T} Cp_B dT = b\Delta H^{O}_{f,\,298,\,B} - b\int_{T}^{298} Cp_B dT$$

$$\Delta H^{O}_{f,\,T,\,C} = c\Delta H^{O}_{f,\,298,\,C} + c\int_{298}^{T} Cp_C dT$$

Therefore,

$$\Delta H^{O}_{R,\,T} = c\Delta H^{O}_{f,\,298,\,C} - a\Delta H^{O}_{f,\,298,\,A} - b\Delta H^{O}_{f,\,298,\,B} + a\int_{T}^{298} Cp_A dT + b\int_{T}^{298} Cp_B dT + c\int_{298}^{T} Cp_C dT$$