

Thermodynamics project

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1 Introduction

some blurb on report, results and analysis

talk about why finding entropy change is useful

1.1 Order-disorder transitions in Cu_3Au

1.2 Heat capacities

1.3 Measuring C_P

Practically, C_P is much easier to measure than C_V . Recall definition:

$$C_P = \frac{dQ_p}{dT} = \left(\frac{dH}{dT} \right)_p$$

where state function H is the enthalpy. Since $H = U + PV$:

$$dH = TdS + VdP$$

and dividing by dT :

$$\frac{dH}{dT} = T \frac{dS}{dT} + V \frac{dP}{dT}.$$

If $\Delta P = 0$ then:

$$C_P(T) = T \left(\frac{dS}{dT} \right)_P.$$

Rearranging and integrating gives us the change in entropy:

$$\Delta S = \int_{(1)}^{(2)} \frac{C_P(T)}{T} dT.$$

1.4 Ideal entropy of mixing

Consider a box with separator, containing n_A moles at V_A of gas A on one side and n_B moles at V_B of gas B on the other. We set $\Delta T = 0$, $\Delta P = 0$ and proceed to mix gases A and B.

The **entropy of mixing** is:

$$\begin{aligned} \Delta S &= \Delta S_A + \Delta S_B \\ &= n_i R \ln \left(\frac{V_f}{V_i} \right) \\ &= n_A R \ln \left(\frac{V_A + V_B}{V_A} \right) + n_B R \ln \left(\frac{V_A + V_B}{V_B} \right), \end{aligned}$$

Since P and T are fixed, the ideal state equation $PV = nRT$ implies that:

$$\frac{V_A + V_B}{V_A} = \frac{n_A + n_B}{n_A}$$

and so we define **inverse mole fractions** as:

$$x_A = \frac{n_A}{n_A + n_B}$$

and

$$x_B = \frac{n_B}{n_A + n_B}.$$

After substituting and dividing through by $n_A + n_B$ we find the **molar specific entropy of mixing**:

$$\Delta s_{mix} = -R(x_A \ln x_A + x_B \ln x_B).$$

2 Data analysis

2.1 Methodology and visualisations

2.2 Numerical integration scheme

3 Interpretation of results

3.1 Comparison with ideal entropy of mixing

3.2 Physical interpretations

3.3 Conclusions