

# 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 $\text{Cu}_3\text{Au}$

## 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**