1 Data Collection

1.1 Raw Data

The collected experimental data is shown in a tabular format below.

1.2 Qualitative Observations

The coffee cup calorimeter was visibly colder to the touch after the reaction compared to before. Furthermore, after certain trials, there were still small pieces of ammonium nitrate visibly left in the container.

2 Data Processing

The data processing procedure is demonstrated through the use of a sample calculation. The data used in the following calculations are the trial one raw data collected for the temperature at 303K. Based on the experimental value for the enthalpy of reaction and using the theoretical entropy of reaction value, the Gibbs Free Energy of the reaction can be determined.

2.1 Corrected Final Temperature (T_{final})

2.2 Calculation of Temperature Change (ΔT)

The temperature change (ΔT) can be determined by finding the difference between the final temperature (T_{final}) and the initial temperature ($T_{initial}$).

$$
\begin{aligned}
\Delta T &= T_{final} - T_{initial} \\
&= 299.67 \pm 0.01K - 303.02 \pm 0.01K \\
&= -3.35 \pm 0.02K
\end{aligned}
\tag{1}
$$

2.3 Calculation of Enthalpy of Reaction ($\Delta H_{experimental}$)

Based on the calculated temperature change, the enthalpy of reaction ($\Delta H_{theoretical}$) can be calculated through the calorimetric process based on the quantity of heat transferred (q) between the reaction to the distilled water. The heat transfer is calculated as the product between the mass of the water (m), specific heat capacity of water (c_p) and temperature change (ΔT).

$$
\begin{aligned}
q &= mc_p\Delta T \\
&= 100.0mL \times 1g/mL \times 4.18J/gK \times (-3.35K \pm 0.6\%) \\
&= -1.4kJ \pm 0.6\% \\
\Delta H_{experimental} &= -q \\
&= (-1.4kJ \pm 0.6\%) \\
&= 1.4kJ \pm 0.6\%
\end{aligned}
\tag{2}
$$

2.4 Calculation of Theoretical Entropy of Reaction ($\Delta S_{theoretical}$)

In order to determine the Gibbs Free Energy of the reaction, the entropy of reaction at 303K must be determined. The entropy of reaction can be determined based on the the literature value for the specific heat capacity (c_p) of ammonium nitrate, which is (139.30J/molK) (Stephenson et al., 1955) and the number of moles (n). The final temperature (T_2) and the temperature of the literature value under standard conditions (T_1)are also required

$$
\begin{aligned}
\Delta S_{change} &= nc_p \ln \frac{T_2}{T_1} \\
\Delta S_{theoretical_{T_2}} &= \Delta S_{theoretical_{T_1}} + nc_p \ln \frac{T_2}{T_1} \\
&= 108.7J/molK + 139.30J/molK \times \ln \frac{303.02K}{298.15K} \\
&= 110.96J/molK
\end{aligned}
\tag{3}
$$

2.5 Calculation of Gibbs Free Energy ($\Delta G_{\text{experimental}}$)

From the previously calculated enthalpy of reaction (ΔH) and entropy of reaction (ΔS) values, and the absolute temperature of the reaction is known (T), the Gibbs Free Energy (ΔG) of the reaction can be calculated.

$$
\begin{aligned}
\Delta G &= \Delta H_{\text{experimental}} - T\Delta S_{\text{theoretical}} \\
&= 1.4 \pm 0.6\%\text{kJ} - 303.02\text{K} \times \frac{5.00\text{g}}{80.06\text{g/mol}} \times 110.96\text{J/molK} \\
&= -0.70 \pm 0.6\%\text{kJ/mol}
\end{aligned}
\tag{4}
$$

2.6 Calculation of Theoretical Enthalpy of Reaction ($\Delta H_{\text{theoretical}}$)

In order to determine the theoretical Gibbs Free Energy ($\Delta G_{\text{theoretical}}$) at the specific temperature value, the theoretical enthalpy of reaction ($\Delta H_{\text{theoretical}}$) must first be determined.

$$
\begin{aligned}
\Delta H_{\text{theoretical}_{T_2}} &= \Delta H_{\text{theoretical}_{T_1}} + c_p(T_2 - T_1) \\
&= 25.69\text{kJ/mol} + 139.30\text{J/molK}(303.02\text{K} - 298.15\text{K}) \\
&= 26.37\text{kJ/mol}
\end{aligned}
\tag{5}
$$

2.7 Calculation of Theoretical Gibbs Free Energy ($\Delta G_{\text{theoretical}}$)

Utilizing the previously calculated theoretical enthalpy of reaction ($\Delta H_{\text{theoretical}}$), the theoretical Gibbs Free Energy ($\Delta H_{\text{theoretical}}$) can be calculated using the Gibbs-Helmholtz equation.

$$
\begin{aligned}
\Delta G_{\text{theoretical}_{T_2}} &= \Delta G_{\text{theoretical}_{T_1}} - \int_{T_1}^{T_2} \frac{\Delta H}{T^2} dT \\
&= \Delta G_{\text{theoretical}_{T_1}} - \int_{T_1}^{T_2} \frac{\Delta H_{\text{theoretical}_{T_2}} - \Delta H_{\text{theoretical}_{T_1}}}{(T_2 - T_1)^2} dT \\
&= -6.72\text{kJ/mol} - \int_{298.15\text{K}}^{303.02\text{K}} \frac{26.37\text{kJ} - 25.69\text{kJ}}{(303.02\text{K} - 298.15\text{K})^2} \times \frac{5.00\text{g}}{80.06\text{g/mol}} \\
&= -7.4\text{kJ/mol} \times \frac{5.00\text{g}}{80.06\text{g/mol}} \\
&= -0.46\text{kJ/mol}
\end{aligned}
\tag{6}
$$

2.8 Calculation of Percentage Error (%Error)

$$
\begin{aligned}
\%\text{Error} &= \frac{|\Delta G_{\text{experimental}} - \Delta G_{\text{theoretical}}|}{|\Delta G_{\text{theoretical}}|} \times 100\% \\
&= \frac{|-0.70\text{kJ} - 0.46\text{kJ}|}{|-0.46\text{kJ}|} \\
&= 52.2\%
\end{aligned}
\tag{7}
$$

3 Processed Data

The raw data can be processed using the procedure demonstrated in the previous section and the correlation between absolute temperature and the Gibbs Free Energy of reaction can be shown as follows.

3.1 Tabular Representation of Processed Data

4 Evaluation of Data

The experimental data can be compared to the theoretical Gibbs Free Energy at the respective data values.

References

Stephenson, C., Bentz, D., & Stevenson, D. (1955). The heat capacity of ammonium nitrate from 15 to 315° k. *Journal of the American Chemical Society, 77*(8), 2161–2164.

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