Laboratory 2: A Cool(ing) Can :Thermochemistry

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Introduction:

The concept of energy, while prevalent throughout the universe on both the microscopic and macroscopic levels, is still an elusive entity to define. However, parameters have been established around energy which seek to better quantify and describe it. One such field of study that achieves this is thermodynamics, or more specifically, the laws of thermodynamics (Olmsted et al., 2016, p. 117). The first law of thermodynamics, which relates to the law of conservation of mass states that energy is exchanged in only two ways: as heat or as work (Olmsted et al., 2016, p. 121). Using this principle, it is clear that energy is conserved as it changes forms in a chemical system.

Thermochemistry is the study of heat changes in a chemical reaction and this can be used to predict whether a reaction will release or absorb heat energy. Thermochemistry is also used to quantify the amount of energy that is gained or lost by a system. The equation used to determine the change in energy, in Joules, is:

$$q = mc\Delta T$$

Where:

- q is the heat, or the energy that is transferred by the substance, measured in joules (J)
- m is the mass of the substance in the system in grams (g)
- c is the specific heat capacity of the substance which is “the amount of heat needed to raise the temperature of 1 gram of substance by 1 ˚□”(Olmsted et al., 2016, p. 118). It is measured in units $Jg^{-1}{}^{\circ}C^{-1}$.
- ΔT is the change in temperature ($\Delta T = T_{final} - T_{inital}$).

The amount of heat transferred depends on the mass of material (m), “the identity of the material is expressed by the molar heat capacity” or c (Olmsted et al., 2016, p. 118), and on the change in temperature. If a substance absorbs heat, ΔT will be positive as will q. Likewise, if a substance releases heat, ΔT will be negative and so will q.

Enthalpy describes “the sum of the internal energy [of a system] and the product of the pressure and volume” (Silberberg et al., 2016, p. 205-208, G-7). It is an essential variable to consider when performing calorimetry. This value is typically measured in kJ/mol. When performing calorimetry the enthalpy of hydration, the lattice enthalpy, and the enthalpy of dissolution are commonly considered. The enthalpy of hydration is the energy released when one mole of gaseous ions are dissolved in water to form aqueous ions. The lattice enthalpy is the energy absorbed by one mole of a salt for it to vaporize and form gaseous ions. Finally, the enthalpy of dissolution is the net energy change of a reaction in which salt is dissolved in water. The enthalpy of dissolution can therefore be calculated by adding the enthalpy of hydration and lattice enthalpy of a reaction (Venkateswaran, 2016, p. 27-30).

The chemical reaction being observed is referred to as the system and everything else is referred as the surroundings. The heat lost by system is gained by the surroundings and vice versa.

$$q_{system} =- q_{surroundings}$$

$$m_{system}c_{system}\Delta T_{system} = - m_{surroundings}c_{surroundings}\Delta T_{surroundings}$$

In order to utilize these equations and concepts in an experimental context, chemists use calorimeters . A calorimeter “is a device used to measure heat flows that accompany chemical processes” It is insulated so the flow of heat is restricted between the calorimeter and its surroundings, maintaining accuracy of measured heat values. This is an example of an isolated system which “does not exchange either heat or matter with surroundings” (Braibanti, et al.,1998,p.254). However, in this experiment, the styrofoam calorimeter is considered a closed system rather than an isolated system since it "exchanges heat but not matter with the surroundings" (Braibanti, et al.,1998,p.254). "The styrofoam calorimeter is a constant-pressure calorimeter that functions by measuring the enthalpy of a solution in the cup, using a thermometer" (Olmsted et al., 2016, p. 135).

This experiment was designed to measure the temperature change of water with a dissolved chemical, in an assumed closed energy system of a styrofoam calorimeter. Using these variables, the heat of reaction could be determined and an ideal mass could be calculated.

There were two potential chemicals for the product design: ammonium chloride (NH_4Cl) and ammonium nitrate (NH_4NO_3). The choice of the solute relied on four main factors: availability, cost, solubility, and the health and safety implications of the chemical. The solubility of ammonium chloride is 37.2g per 100g of water, with a cost of $62.50 per 500g. Ammonium nitrate has a solubility of 192g per100g of water, with the cost of $64.62 per 500g. Due to the small difference in cost this factor was relatively negligible. The safety factors for each chemical carried great weight in the selection of the chemical. Safety is an important factor to take into consideration as our product is associated with drinks that people will consume. According to the National Institute for Occupational Safety and Health (2015), NH_4Cl "irritates the eyes, the skin and the respiratory tract" and is nonflammable (NIOSH, "CDC-Ammonium chloride", 2015), whereas NH_4NO_3 "is irritating to the eyes, the skin and the respiratory tract. The substance may also cause effects on the blood, resulting in the formation of methemoglobin". It is "a strong oxidant and reacts with combustible and reducing materials". Also, "heating may cause violent combustion or explosion". Due to its explosive nature, ammonium nitrate is unavailable for purchases in large quantities (NIOSH, "CDC-Ammonium nitrate", 2015). Thus, NH_4Cl was the obvious choice as it passed Healthy and Safety regulations and is available in large quantities.

Materials/Apparatus:

- 65 g of ammonium chloride
- Distilled water (200 ml per trial)
- Aluminum can
- Styrofoam calorimeter
- Temperature probe
- LabQuest 2
- Scoopula for measuring the mass of ammonium chloride
- Two 150 mL beakers
- 50 mL graduated cylinder
- Analytical Scale
- Timer

Procedure:

1. In a 50 mL graduated cylinder, 100 mL of distilled water was measured by taking two measurements of 50 mL.
2. The two measurements of 50 mL of distilled water was added into the aluminum can.
3. Again, the 50 mL graduated cylinder was used, 100 mL of distilled water was measured by taking two measurements of 50 mL
4. This 100 mL of distilled water was poured into the styrofoam calorimeter.

5. The can containing the distilled water was placed inside the styrofoam calorimeter containing distilled water. It was ensured that the can was stable and it did not float. The lid of the styrofoam calorimeter was then placed on top to close the system.
6. The temperature probe was connected to labQuest and inserted into the hole on the calorimeter lid.
7. The initial temperature of the distilled water inside the can was recorded.
8. The mass of ammonium chloride was selected and was measured and weighed in a 150ml beaker using the analytical balance.
9. The lid of the calorimeter was removed and the sample of ammonium chloride was added into the styrofoam calorimeter (outside the can). The timer was started.
10. The lid (with the temperature probe attached) was placed on the calorimeter again and it was mixed by shaking the calorimeter against the table.
11. After 5 minutes, the the final temperature of the water in the can was recorded.
12. The ammonium chloride solution in the calorimeter was disposed into the waste container in the fume hood. The water in the can was disposed in the sink.
13. Repeat steps 2 - 12.

Data Table / Observations / Graph:

Table 1: The Changes in Temperature of Distilled Water in the Aluminium Can after 5 Minutes Relative to the Masses of Ammonium Chloride Used

Trial	Volume of Water in Calorimeter (mL)	Volume of Water in Can (mL)	Mass of NH4Cl (g)	Initial Temperature of Water in Can (˚C)	Final Temperature of Water in Can (˚C)	Change of Temperature of Water in Can (˚C)
1	100	100	11.16	24.0	20.4	- 3.6
2			12.08	24.5	20.3	- 4.2
3			13.11	24.7	20.2	- 4.5
4			14.2	24.8	19.8	- 5.0
5			15.01	24.6	19.7	- 4.9

Figure 1: The Correlation between the Change in Water Temperature in an Aluminum Can within 5 Minutes and the Amount of Dissolved Ammonium Chloride

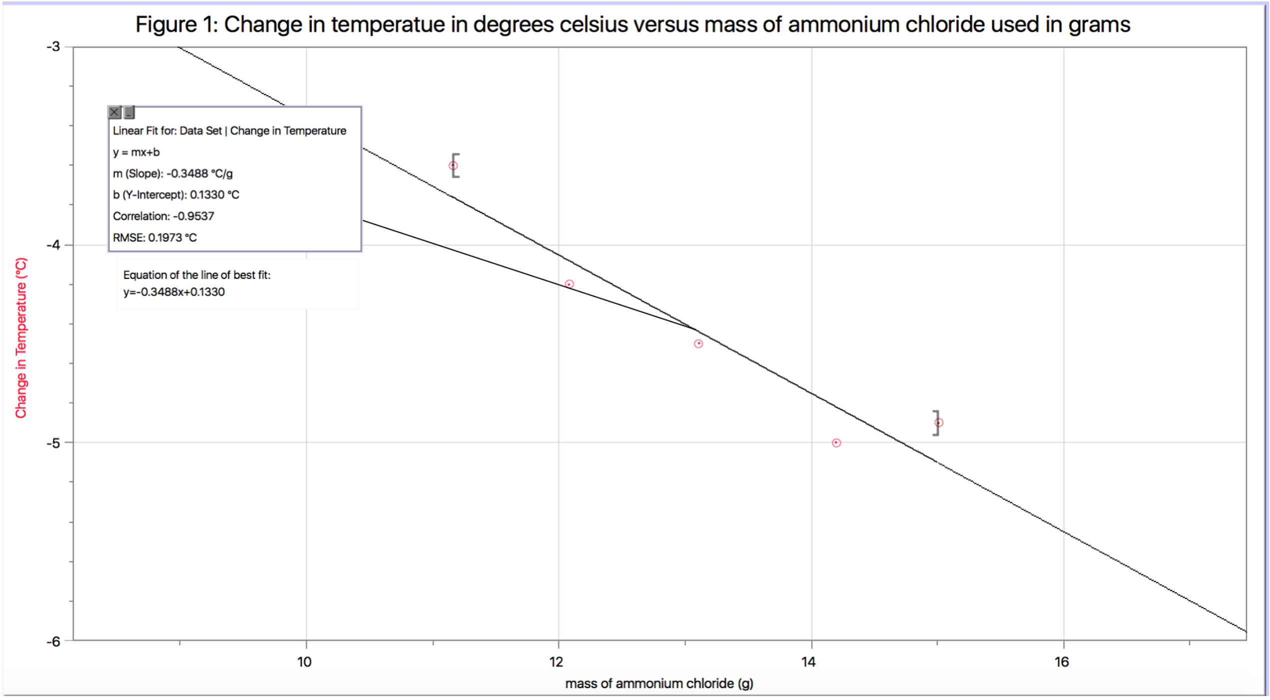
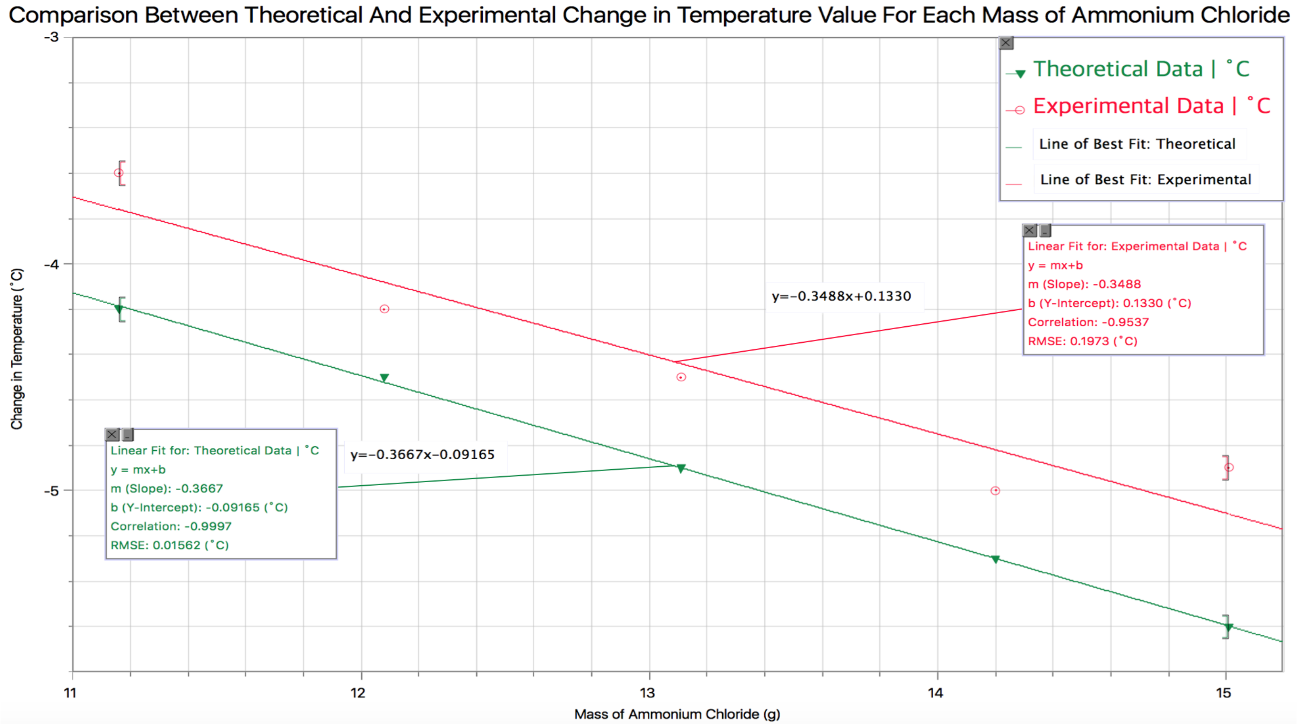


Figure 2: Comparison Between Theoretical and Experimental Change in Temperature Value for Each Mass of Ammonium Chloride



Qualitative Observations:

The distilled water was a clear liquid with no colour or odour. The ammonium chloride on the other hand was a solid, white, opaque powder .When measuring the initial temperature, it took several moments for the temperature to stabilize. When pouring out the ammonium chloride from the beaker and into the calorimeter, there were a few grains of NH_4Cl stuck to the bottom of the beaker thus making it difficult to get all of the powder into the calorimeter. There was a bit of water leaking out from the Styrofoam calorimeter. When stirring the Styrofoam calorimeter, a longer stirring period correlated with a greater temperature change. During the reaction, the temperature would increase and decrease regularly. The stopper attached to the temperature probe and the hole in the lid was loose and fell into the cup for the first run of Trial 3. After the 5 minutes of Trial 1 and 2, the solution in the calorimeter became foggy if it was not stirred for a long time. However, when stirred for a longer time, the solution was clearer. The end product of Trials 1 and 2 were found to be a foggy, translucent solution. Throughout all trials, the temperature was observed to fluctuate (increase and decrease) at certain intervals during the 5 minute time period, but the overall result always resulted in a decrease in temperature of the water.

Theoretical Calculations for the Mass of Ammonium Chloride:

1. To find the change in temperature of the water in the can for Trial 1:

$\Delta T = T_{Final} - T_{Initial}$

$\Delta T = 20.4^\circ C - 24.0^\circ C$

$\Delta T = -3.6\ ^\circ C$

2. a) To find the total volume of water to be used in all trials:

$V_{Total} = V_{Calorimeter} + V_{Can}$

$V_{Total} = 100\ mL + 100\ mL$

$V_{Total} = 200\ mL$

2. b) Total mass of water used in all trials (using density):

$m_{Water} = (200mL)(1.00g\ mL^{-1})$

$m_{Water} = 200\ g$

2. c) To find the mass required to decrease the temperature of the deionized water by 5˚C, the equation for the heat of reaction must be rearranged to suit the situation. Since the change in temperature will be the same for all the components of the equation, and the specific heat capacity of water is a constant, the mass of the water in the can and calorimeter can be taken as a sum as one variable to form the equation:

$q_{system} = m_{H2O}c_{H2O}\Delta T_{H2O} + m_{Can}c_{Can}\Delta T_{Can}$

$q_{system} = (200\ g)(4.18\ J\ g^{-1}\ ℃^{1})(-5.0\ ℃) + (9.72\ g)(0.90J\ g^{-1}\ ℃^{1})(-5.0\ ℃)$

$q_{system} = -4180J - 43.74$

$q_{system} = -4223.74J$

$q_{system} = 4.2x10^{3}J$ * with sig figs

2. d) Enthalpy of the ammonium chloride is a positive value since its surroundings lose energy.

$\Delta E_{NH4Cl} = -q_{system}$

$\Delta E_{NH4Cl} = 4223.74J$ * using exact values for further calculations

3. a) Once the enthalpy is calculated (q), the number of moles required to generate this heat of reaction can be found using the equation: $n_{NH4Cl} = \Delta E_{NH4Cl} / \Delta E_{Molar}$

Where:

- ΔE is the enthalpy of the reaction (q)

- ΔE_{Molar} is the enthalpy of dissolution for one mole of solute (calculated in Pre-lab)

  $n_{NH4Cl} = 4223.74 \text{ J} / 17000 \text{ J mol}^{-1}$

  $n_{NH4Cl} = 0.248455 \text{ mol}$

  $n_{NH4Cl} = 2.5 \times 10^{-1} \text{ mol}$

3\. b) To find the molar mass of ammonium chloride.

$M_{NH4Cl} = M_N + M_{4(H)} + M_{Cl}$

$M_{NH4Cl} = (14.01 \text{ g mol}^{-1}) + 4(1.008 \text{ g mol}^{-1}) + (35.45 \text{ g mol}^{-1})$

$M_{NH4Cl} = 53.492 \text{ g mol}^{-1}$

$M_{NH4Cl} = 53.49 \text{ g mol}^{-1}$

3\. c) To find the required mass of ammonium chloride.

$m_{NH4Cl} = (n_{NH4Cl})(M_{NH4Cl})$

$m_{NH4Cl} = (0.248455 \text{ mol})(53.492 \text{ g mol}^{-1})$

$m_{NH4Cl} = 13.29 \text{ g}$

$m_{NH4Cl} = 13.3 \text{ g}$

Sample Calculation of the Theoretical Change in Temperature for Trial 1 (m=11.16g)

1. Find number of moles of NH_4Cl used:

   $n_{NH4Cl} = (11.16\text{g})/(53.491\text{g/mol})$

   $n_{NH4Cl} = 0.2086\text{mol of } NH_4Cl$

   $= 0.209\text{mol } NH_4Cl$

2. Heat energy (q)

   $q = n\Delta H$

   $q = (0.2086 \text{ mol})(+17\text{kJ/mol})$

$q = 3546\ \text{J}$

$q = 3500\ \text{J}$

3. Change in Temperature of Water

*Assume components of system have same change in temperature

$q= (m_{canwater}+m_{calorimeterwater})c_{water}\Delta T_{water} + m_{can}c_{can}\Delta T_{can}$

$3546\ \text{J}= (200\text{g})(4.18\ \text{J g}^{-1}\ ℃^{-1})\Delta T+(9.72\text{g})(0.90\text{J g}^{-1}\ ℃^{-1})\Delta T$

$3546\ \text{J}=836\Delta T+8.748\Delta T$

$\Delta T=-4.2^\circ\text{C}$ *negative value as temperature final temperature is lower than initial temperature

Calculation for Experimental Mass using Slope

The slope of the graph shows the change in temperature with respect to the mass of ammonium chloride. The rate of change from Figure 1, -0.3488 ℃ g^{-1}, and the y-intercept, 0.1330 ℃ g^{-1}, can be used to form the equation to calculate the required mass for a decrease in temperature by 5˚C:

$-5.00℃= (-0.3488\ ℃\text{g}^{-1})(m_{NH4Cl}) + 0.1330\ ℃\text{g}^{-1}$

$m_{NH4Cl} = (-5.00\ ℃- 0.1330\ ℃) / -0.3488℃\text{g}^{-1}$

$m_{NH4C} = 14.71\text{g}$

$=14.7\text{g}$

Discussion:

In any experiment, when drafting a chemical procedure and executing an experiment there are many factors that must be considered. For instance, potential sources of error must be identified and evaluated as well as any hazards toward the general safety of consumers.

In this experiment, the goal was to develop a product that was capable of cooling drinkable water by 5˚C in less than 5 minutes. The product was designed to be similar to a coffee cup calorimeter or a styrofoam calorimeter, operating at a constant pressure. In “constant pressure calorimetry the pressure of the system is fixed” (Olmsted et al., 2016, p. 135). The product would consist of two cans or layers. The outer layer, or the outer can, would act as a calorimeter, and would contain 100 mL of deionized water and an ionic compound. The inner can would contain the drinkable water. After shaking the product, the ionic compound would be hydrated by the deionized water to create an endothermic reaction. Heat from the water in the inner can would be absorbed by the reaction. Since the chemicals are absorbing heat “is positive and the reaction is endothermic. The calorimeter loses this heat (is negative), and the temperature of the calorimeter falls” (Olmsted et al., 2016, p.134). In other words, the heat flows from the inner can with the drinkable water to the outer can where the reaction between the chemicals and deionized water absorbs the heat. Thus, the temperature of the drinkable water would decrease due to the endothermic reaction between the deionized water and the chemical.

The temperature change of the water in the can is dependent on the mass of ammonium chloride that is dissolved in the water in the calorimeter, as shown by the equation $q = mc\Delta T$. An increase in mass of the ammonium chloride would result in the increase in the change of temperature. This ultimately signifies a greater enthalpy of reaction. The approximate value of solute of ammonium chloride needed for the temperature to decrease by 5˚C was calculated to be approximately 13.3 grams before the experiment started. Thus, the selected masses were based on values close to 13.3 grams. The data revealed that a higher mass of 14.7 grams was required in order for the desired temperature change to occur.

Figure 1 displays a positive correlation for the change in temperature versus the mass of ammonium chloride. From the line of best fit it is deducible that as more mass of ammonium chloride is added to the calorimeter, the calculated change in temperature increases in magnitude. This linear, proportional relationship between both variables was expected. The experimental mass of ammonium chloride calculated from the slope was 14.7 grams whereas the theoretical mass was 13.3 grams. Experimental sources of error that accounts for this discrepancy are the mass of ammonium chloride lost during its direct transfer and the calorimeter itself, which is a closed system. As a result, these errors caused the values of mass and recorded temperature change to become lower respectively, which would ultimately lower the slope of the graph. Since the experimental mass calculation had temperature being divided by the slope, the experimental mass would appear larger than it should be. This means that more mass of ammonium chloride would have to be used relative to the theoretical value in order to experimentally obtain the same temperature deduction of 5˚C.

Figure 2 displays a strong, negative correlation for both theoretical and experimental data. As seen in Figure 2, the slope between the theoretical line of best fit and the experimental line of best fit are relatively similar. The line of the experimental data is slightly less steep, having a rate of change of -0.3488, whereas the theoretical line of best fit has a rate of change of -0.3667. Instead, it seems as though the line of the theoretical data was shifted upward by a number of units to form the line of the experimental data. Therefore there was a constant factor that would always affect each of the recorded values during our measurements in the lab, presenting a systematic source of error. This affected the accuracy of the data collection. Heat exiting the system would result in a smaller temperature change than predicted as seen in Figure 2. Figure 2 also has one data point which does not follow the trend of the line of best fit, which would be Trial 5 (m=15.01g). This error may be due to the assumption that the calorimeter was a closed system, meaning that no heat was no transfer of heat in or out of the system and that it was at a constant pressure. In reality, the temperature of the surroundings will attempt to reach thermal equilibrium with water which explains the fluctuations in temperature during the experiment (Pearson Canada, 2008). Also, the calorimeter had to be opened to put in the solute. Thus, at this time the system was not closed, and pressure was not always constant. To ensure that both the reactants, ammonium chloride and water, reacted with each other, the calorimeter was swirled while being pressed to the table. If a stirring rod was used, like the very first draft of the procedure called for, this would have increased the time the system was open. Therefore this would have impacted our results by posing a greater source of error to the lab. Lastly, the calorimeter used was made of styrofoam which provided better insulation to isolate the system from the surroundings. If the quality of the calorimeter increased to provide better insulation, the potential for heat loss would have been decreased. While some errors such as heat loss can be predicted, many are unpredictable.

An unforeseen error occurred during the initial run of Trial 3. The stopper piece that closed the hole between the outside edge of the temperature probe and the inside of the calorimeter fell through into the calorimeter itself. This meant that the temperature actually began to increase, as the system was no longer closed. After noticing the piece had fell through the trial was deemed an error. Thus, trial 3 was stopped and repeated.

As stated in the qualitative observations, small amounts of ammonium chloride were left in the beaker. This was a recurring issue during the experiment; ensuring all the measured ammonium chloride was deposited from the beaker into the outer layer of the calorimeter. Often it was difficult for the entirety of ammonium chloride to fall out of the beaker. Also, throughout the experiment, the solution was leaking from the calorimeter. Both these sources of error affected the dependent variable, the change in temperature. The loss in ammonium chloride led to a smaller change in temperature than expected. Due to these factors, more mass of ammonium chloride was needed to cool the water by 5˚C than the mass that was experimentally calculated.

For Trials 1 and 2, the end product was observed to be a foggy, translucent solution. This means all the solute did not react with the solvent. If all the solute does not dissolve into the solvent, then there is a smaller amount of solute reacting, resulting in a smaller change in temperature as observed in the lab. The calorimeter cup was swirled while pressed to the lab bench in attempt to cause all of the ammonium chloride to dissolve in the solution. However, this did not occur as fluctuations of temperature were still observed. In reality, not all the ammonium chloride reacted at the same time causing an increase in temperature as the solution attempts to reach thermal equilibrium with the water (Pearson Canada, 2008). When the ammonium chloride ended up reacting at a different time interval, subsequently there would be another decrease in temperature. During our experiment, several small clumps of ammonium chloride with each trial were observed. The entire dissolution of ammonium chloride will occur faster if all the ammonium chloride entered the water as a powder as there is a greater surface area.

To ameliorate the results of this experiment, one can use a higher quality calorimeter, increase the surface area of the solute, and decrease the assumptions made throughout an experiment but monitoring various factors such as pressure.

Conclusion

Despite sources of error, the experiment was able to determine the mass. The mass of ammonium chloride needed to cool the can by 5˚C is 14.7 grams.