Sample Formal Report

Writing a formal report is always a challenge, particularly when you are uncertain about what you should and should not include. The purpose of this sample report is to provide you with an example of a typical report. Like any example, of course, this report cannot anticipate every issue you might encounter during the semester; it does provide, however, a sense of how to construct a report. The comments below provide some additional thoughts and observations.

Abstract

There are four things to note about the abstract: it is short, it states the purpose of the experiment, it summarizes the experiment's two main results, and it compares one of the results to a theoretical value. As you prepare abstracts try to accomplish these three things.

Introduction

Your introduction must place the experiment within some context and define the experiment's goals. The context and goals, of course, are provided to you in the lab manual. For this experiment students were told that OCl^- is the active ingredient in bleach, that it is an oxidizing agent, and that its release into the environment poses a concern. The goal of the experiment was to determine the stoichiometry for the reaction between OCl^- and I^-. Students were given a copy of Job's paper on the method of continuous variations for metal-ligand complexes and asked to adapt that procedure to this experiment. In addition, because they had just completed a calorimetry experiment, the students were asked to use calorimetry in this experiment.

Note that this introduction accomplishes three things: it provides additional context for the experiment by citing references to the chemistry of OCl^- and relevant environmental concerns, and by discussing the difficulty of determining the stoichiometry of oxidation-reduction reactions (presumably the students did some research – note the references); it explains Job's method; and it clearly states the experiment's goals. Note, as well, that the first paragraph of the introduction begins with a "hook," which tells us why we should be interested in this research:

> "Although hypochlorite's reactivity with a wide variety of organic molecules is well known (*1*), particularly for organic dyes, its reactivity with inorganic ions has been studied less frequently. This is somewhat surprising given the significant release of OCl^- into the environment from household use (*2*)."

and that the final paragraph provides a transition to the rest of the report, telling the reader what is to come:

> "To evaluate the utility of the MCV as a method for studying oxidation-reduction chemistry, we present results for an analysis of the reaction between hypochlorite and iodide. A determination of the reaction's enthalpy provides further confirmation of the MCV results."

Procedure

The most striking observation about this procedure is the relative absence of numerical information. Note that the procedure makes no attempt to describe each individual experiment in detail. For example, examine carefully the first two sentences in the second para-

graph and contrast the general information provided there with the more specific details included in the results and conclusions section.

Results and Conclusions

There are five things to note here. First, the results and conclusions are organized so that the reader can follow the logic of the data analysis. Note the use of subheadings as a means of focusing the reader's attention. Second, good use is made of tables and figures. Note, as well, that only representative results are provided. Third, results are reported clearly, including both means and standard deviations. Fourth, the main conclusions for each part of the experiment are stated clearly. Fifth, and finally, an analysis of error is included.

References

Note that the references are provided in the correct format. By the way, the reference to the paper by Job is real, although its title is fictitious. The remainder of the references are fictitious; your references, of course, will be real!

Notes

Many journals include a notes section to provide a place for comments and other information that would only clutter the main body of your text. Here the notes are used effectively to present sample calculations.

Appendices

Be sure to indicate if any tables and figures in your Dropbox folder provide additional supporting information. Although I won't always look at them, I will if there are questions about your data.

A Thermodynamic Investigation
of the Reaction Between Hypochlorite and Iodide

Abstract

The method of continuous variations and a calorimetric determination of enthalpy were used to verify the stoichiometry for the reaction between hypochlorite, OCl^-, and iodide, I^-. Stoichiometric mixing occurred with a 3:1 mole ratio between OCl^- and I^-, suggesting that the reaction is

$$3OCl^-(aq) + I^-(aq) \rightleftharpoons IO_3^-(aq) + 3Cl^-(aq)$$
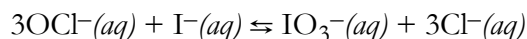
The experimentally determined value for ΔH of -344.4 kJ/mol_{rxn} compares favorably with the expected value of -346.4 kJ/ mol_{rxn}, providing further evidence that the proposed stoichiometry is correct.

Introduction

Hypochlorite ion, OCl^-, is a potent oxidizing agent commonly used in household bleaches. Although hypochlorite's reactivity with a wide variety of organic molecules is well known (*1*), particularly for organic dyes, its reactivity with inorganic ions has been studied less frequently. This is somewhat surprising given the significant release of OCl^- into the environment from household use (*2*).

One of the challenges in studying any reaction is determining the products. This is particularly problematic for oxidation-reduction reactions, such as those involving hypochlorite, because of the large number of possible oxidation states available to the oxidizing and reducing agents. For example, the chlorine in OCl^-, with an oxidation state of $+1$, can be reduced to oxidation states of 0 in Cl_2 and -1 in Cl^-, or oxidized to oxidation states of $+3$ in ClO_2^-, $+5$ in ClO_3^- and $+7$ in ClO_4^-. Although the identity of the product can be determined through standard chemical testing, this usually requires isolating individual species before using a standard qualitative analysis scheme.

The method of continuous variations (MCV), first described by Job (*3*) for the stoichiometric analysis of metal-ligand complexation, may provide a simple method for determining the stoichiometry of an oxidation-reduction reaction. The basis of MCV involves combining solutions of two reactants, A and B, such that their combined moles, n_{tot}, remains constant in all experiments; thus

$$n_A + n_B = n_{tot}$$

where n_A and n_B are, respectively, the initial moles of A and B. The relative amount of each reactant can be expressed as a mole fraction, X

$$X_A = \frac{n_A}{n_{tot}}$$

$$X_B = 1 - X_A = \frac{n_B}{n_{tot}}$$

In a reaction between A and B, the extent of the reaction is determined by the limiting reagent. If an analytical signal is proportional to the limiting reagent, then a plot of that signal as a function of X_A will consist of two straight lines intersecting at a mole fraction for A, X_A, corresponding to the stoichiometric mixing of A and B. The mole ratio of A and B at this point is given by

$$\frac{n_A}{n_B} = \frac{X_A}{X_B} = \frac{X_A}{1 - X_A}$$

Figure 1 shows an MCV plot for a hypothetical reaction between the reactants A and B. The intersection at an X_A of 0.67 indicates that two moles of A stoichiometrically react with one mole of B, corresponding to a reaction of

$$2A + B \rightarrow \text{Products}$$
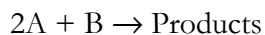
As noted by Job (*3*), there are three important limitations to the MCV: the reaction must involve only two reactants, there must be only one possible reaction, and the free energy for the reaction must be highly favorable.

To evaluate the utility of the MCV as a method for studying oxidation-reduction chemistry, we present results for an analysis of the reaction between hypochlorite and iodide. A determination of the reaction's enthalpy provides further confirmation of the MCV results.

Figure 1. Hypothetical MCV plot for the reaction of A and B showing a stoichiometric mixing when the mole ratio of A to B is 2:1.
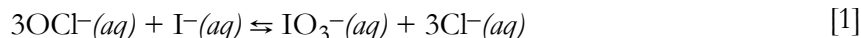
Procedure

All reactions were carried out in a locally designed cup calorimeter. Two small 8 oz. Styrofoam cups were nestled together and trimmed such that the inner cup did not protrude above the outer cup. The bottom of a 20 oz. Styrofoam cup was removed and used as a top. Two small holes were punched in the top to accommodate a digital thermometer connected to a LabQuest data interface (Vernier) and a small glass funnel for adding reagents. Data were analyzed using LoggerPro (Vernier).

The calorimeter's suitability was tested by measuring the change in temperature when reacting 1.00 M solutions of HCl (Fisher Scientific) and NaOH (Fisher Scientific). The calorimeter's constant was determined using the method of Joule (*4*), which is based on the thermal transfer of heat from hot water to cold water. In all calorimetric experiments, the temperature was monitored for several minutes both before and after adding the second solution to ensure that ΔT could be determined accurately by extrapolation.

Solutions of 0.213 M OCl⁻ and 0.213 M I⁻ were prepared from a commercial bleach (Kroger Brand) and reagent-grade KI (Fisher Scientific), respectively. The solution of KI was 0.1 M in NaOH (Fisher Scientific). Both solutions were tightly capped when not in use. Calorimetry experiments for reactions involving OCl⁻ and I⁻ were limited to a combined volume of 80 mL. The reagent with the larger volume was initially placed in the calorimeter and the reagent with the smaller volume was then added. For those experiments used to establish the reaction's stoichiometry only the solution volumes were reported; the mass of each solution was measured in experiments used to determine ΔH.

Results and Conclusions

Evaluation of Calorimeter. The calorimeter's suitability for experiments based on the method of continuous variations was evaluated by measuring the temperature change upon mixing 40.0 mL of 1.00 M HCl with 40.0 mL of 1.00 M NaOH. Since $\Delta H°$ for the reaction
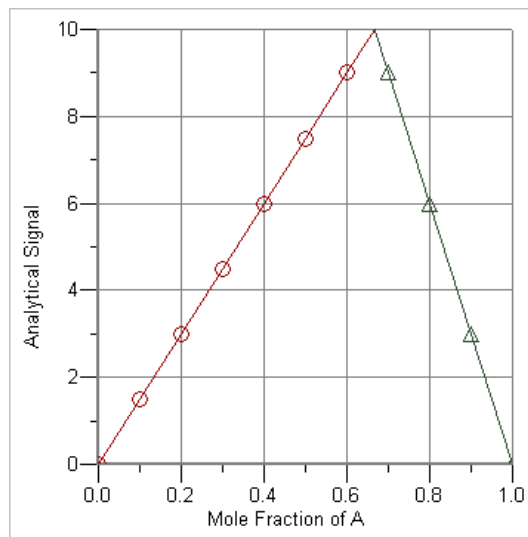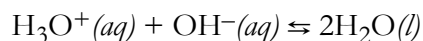
$$\text{H}_3\text{O}^+(aq) + \text{OH}^-(aq) \rightleftharpoons 2\text{H}_2\text{O}(l)$$

is -55.836 kJ/mol$_{rxn}$, the expected change in temperature is approximately 6.7°C (Note 1). A typical result is shown in Figure 2 with ΔT being 6.9°C. The mean ΔT for five trials was 6.8°C with a standard deviation of 0.16°C. The close agreement between the expected and experimental ΔT suggests that the change in temperature is a suitable means for studying the reaction.

Method of Continuous Variations. To establish the reaction's stoichiometry by the method of continuous variations, a series of calorimetry experiments were carried out in which the relative amounts of OCl$^-$ and of I$^-$ were changed while maintaining a constant combined volume. Temperature-time curves for these experiments were similar to that shown in Figure 2 and are not included here. Table 1 and Figure 3 provide a summary of typical data.

(11.2, 27.211)

Figure 2. Temperature-time curve for 40 mL of hot water mixed with 40 mL of cold water.

Table I. Measurement of ΔT for Mixtures of OCl$^-$ and I$^-$

mL OCl$^-$	mL I$^-$	ΔT
10	70	0.7
20	60	1.5
30	50	2.2
40	40	2.9
50	30	3.7
60	20	4.4
70	10	2.2

Figure 3, which is a variation of the traditional MCV plot, shows that a stoichiometric mixing was achieved for the reaction of 60 mL of 0.213 M OCl$^-$ with 20 mL of 0.213 M I$^-$. This corresponds to 1.28×10^{-2} mol OCl$^-$ and 4.26×10^{-3} mol I$^-$, or a 3:1 molar ratio.

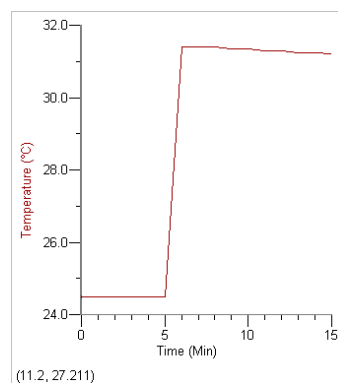Because iodine in I$^-$ is in its most negative oxidation state, it must undergo oxidation. The chlorine in OCl$^-$ must be reduced to either Cl$_2$ or Cl$^-$. If Cl$_2$ is the product, then a total of three electrons are needed to reduce the chlorine in the three OCl$^-$ ions from oxidation states of +1 to 0. This requires the single I$^-$ to experience a three electron oxidation from its initial oxidation state of –1 to a final oxidation state +2; however, no such oxidation state for iodine exists. If Cl$^-$ is the reduction product, then a total of six electrons are needed to reduce the chlorine in the three OCl$^-$ ions from oxidation states of +1 to –1. Oxidation of I$^-$ to IO$_3^-$ provides the necessary electrons. The proposed balanced redox reaction for this system is

Figure 3. MCV plot showing that stoichiometric mixing occurs at 60 mL of hypochlorite and 20 mL of iodide.

$$3OCl^-(aq) + I^-(aq) \rightleftharpoons IO_3^-(aq) + 3Cl^-(aq) \qquad [1]$$

Calorimetric Determination of ΔH. To provide further evidence that the stoichiometry shown in Equation 1 is correct, additional experiments were run to determine the reaction's enthalpy, ΔH. The careful calorimetric measurement of a reaction's ΔH requires determining the amount of heat absorbed by the calorimeter, q_{cal}. If the calorimeter's heat capacity, C_{cal}, is known then q_{cal} is given by

$$q_{cal} = C_{cal}\Delta T_{cal} \qquad [2]$$

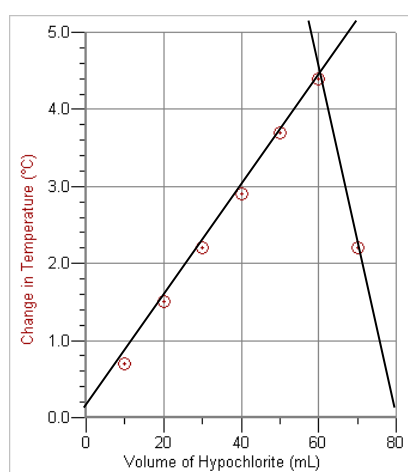where ΔT_{cal} is the calorimeter's change in temperature.

To evaluate the calorimeter's heat capacity approximately 40 g of room temperature water was placed in the calorimeter and the temperature monitored for several minutes to establish the initial temperature for both the water and the calorimeter. Approximately 40 g of hot water was then added to the calorimeter and the mixture's temperature monitored for several minutes. Conservation of energy requires that any heat lost by the hot water is absorbed by the room temperature water and the calorimeter; thus

$$-q_{hot} = q_{room} + q_{cal} \qquad [3]$$

Substituting Equation 2 and the equation for the heat flow for a solution into Equation 3 gives

$$-m_{hot}S_{hot}\Delta T_i = m_{rt}S_{rt}\Delta T_{rt} + C_{cal}\Delta T_{cal}$$

where m is the water's mass and S is water's specific heat. Results for a typical run are shown in Figure 4, yielding a value of 31.5 J/°C for C_{cal} (Note 2). The average value of C_{cal} was found to be 31.4 J/oC with a standard deviation of 0.56 J/oC for three trials.

To determine ΔH_{rxn}, additional calorimetry experiments were run using 60.00 mL of 0.213 M OCl⁻ and 20.00 mL of 0.213 M I⁻. Results of these experiments are shown in Table 2.

The resulting mean and standard deviation for ΔH_{rxn} are −341 kJ/mol$_{rxn}$ and 4.62 kJ/mole$_{rxn}$, respectively (Note 3). The theoretical value for ΔH_{rxn} is −346.4 kJ/mol$_{rxn}$, which gives an error of −1.8%. Because ΔT is known to two significant figures only, the expected uncertainty in ΔH_{rxn} is ±10 kJ/mol$_{rxn}$, or a relative uncertainty of 2.8%. The experimental error of +1.8%, therefore, is reasonable and suggests that there are no significant problems with the experiment.
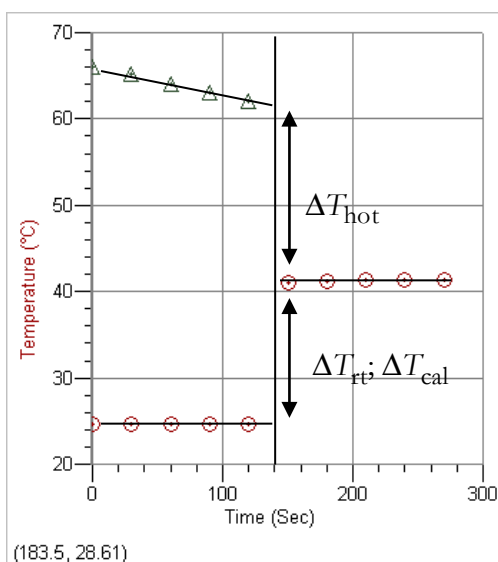

(183.5, 28.61)

Figure 4. Typical temperature-time curve used to determine the calorimeter's constant.

Table 2. Calorimetry Results for the Reaction of 60.00 mL of 0.213 M OCl⁻ with 20.00 mL of 0.213 M I⁻

mass of solution (g)	ΔT (°C)	ΔH (kJ/mol$_{rxn}$)
82.409	3.9	−344
82.616	3.8	−336
82.195	3.9	−344

References

1. Ajax, V. *The Chemistry of Bleach*, Comet Press: New York, 1999.

2. "Environmentalist Expresses Concern Over Excessive Release of Bleach to Big Walnut Creek", http://www.bannergraphic.com/9.17.04/Bleach (accessed August 2014).

3. Job, P. "The Method of Continuous Variations for Studying Metal-Ligand Complexation" *Ann. Chim.*, **1928**, *9*, 113.

4. Joule, K. J. "Establishing the Calorimeter Constant by the Thermal Transfer of Energy From Hot to Cold Water" *J. Therm.* **1945**, *8*, 134.

Notes

1. The value of approximately 7°C was determined as follows:

   a. Because equal moles of HCl and NaOH are mixed, either reagent can be used as the limiting reagent. The moles of HCl used is 0.0400 moles.

   b. The amount of heat released, q_{rxn}, is

   $$\frac{-55.836 \text{ kJ}}{\text{mol}_{rxn}} \times \frac{1 \text{ mol}_{rxn}}{\text{mol HCl}} \times 0.0400 \text{ mol HCl} \times \frac{1000 \text{ J}}{\text{kJ}} = -2233 \text{ J}$$

   c. The heat absorbed by the calorimeter, q_{cal}, is $-qr_{xn}$, or +2233 J.

   d. The change in temperature is $q_{cal} = mS\Delta T$. Assuming the combined solution has a density of 1.00 g/mL, the solution's mass is 80 g. Taking the specific heat as 4.184 J/g°C, we have

   $$+2233 \text{ J} = (80 \text{ g}) \times (4.184 \text{ J/g°C}) \times \Delta T$$

   gives ΔT as 6.7°C. Note that no correction for the calorimeter's heat capacity was made as its influence is expected to be insignificant given the limit of one significant figure for the approximate temperature change.

2. The data in Figure 4 were obtained using 40.133 g of room temperature water and 39.168 g of hot water. Extrapolating the three temperature-time curves to the point of mixing gives the initial temperature of the room temperature water and calorimeter as 24.7°C, the initial temperature of the hot water as 61.5°C, and the mixture's final temperature as 41.3°C. Thus, we find that ΔT_{rt} and ΔT_{cal} are 16.6°C and ΔT_{hot} is -20.2°C. Assuming that the solution's density is 1.00 g/mL and that the specific heat is 4.184 J/g°C, we have

   $$-(39.168 \text{ g})(4.184 \text{ J/g°C})(-20.2°C) = (40.133 \text{ g})(4.184 \text{ J/g°C})(16.6°C) + C_{cal}(16.6°C)$$

   which gives C_{cal} as 31.50 J°C.

3. Outlined here are results for the data in the first row of Table 2. Applying the conservation of energy requires that

   $$-q_{rxn} = q_{soln} + q_{cal}$$

   where q_{rxn} is the heat supplied by the exothermic reaction and q_{soln} is the heat gained by the solution in the calorimeter; thus

   $$-q_{rxn} = m_{soln}S_{soln}\Delta T_{soln} + C_{cal}\Delta T_{cal}$$

   Assuming that the solution's specific heat is the same as water gives

   $$-q_{rxn} = (82.409 \text{ g})(4.184 \text{ J/g°C})(3.9°C) + (31.50 \text{ J/g°C})(3.9°C) = -1470 \text{ J}$$

Because this is a stoichiometric mixture, the enthalpy change can be calculated using either OCl^- or I^-. Using OCl^-, for example, gives

$$\Delta H = q_{rxn}/n = -1470 \text{ J}/\{(0.213 \text{ M})(0.0600 \text{ L})\} \times 1 \text{ kJ}/1000 \text{ J} = -115 \text{ kJ/mol } OCl^-$$

where n is the moles of OCl^-. Accounting for hypochlorite's stoichiometry gives ΔH_{rxn} as

$$\Delta H_{rxn} = \Delta H \times (n\text{LR})/\text{mol}_{rxn}$$

$$\Delta H_{rxn} = (3 \text{ mol } OCl^-/\text{mol}_{rxn})(-115 \text{ kJ/mol } OCl^-) = -340 \text{ kJ/mol}_{rxn}$$

Appendices
The following supplemental information is available in our group's Dropbox folder:

- four additional temperature-time curves validating the calorimeter's performance

- four additional temperature-time curves for determining the calorimeter's constant

- data tables for the data in each figure appearing in this report or the appendix