Experiment 5: Enthalpy of Reaction

Post-Lab

CHE 347 TA: Alec Beaton

Student name:____

Introductory Information

1. What is a calorimeter?

2. Glycine:

   a. What is glycine?
   b. Where is it naturally found?
   c. Why is it important to study? (hint: does it have medicinal or therapeutic uses, and if so what are they?)

3. What equations will you need to turn the values recorded in your lab notebook into the main values (*i.e.*, meaningful physical quantities) that you wish to report?

4. What are the main values you are reporting?

5. Which of your main values are thermodynamic state functions?

Experimental Details

1. Name the chemicals used in this experiment. Provide the names and concentrations of solutions.

2. Report any additional observations during the course of the experiment.

Results

1. Plot your thermograms (temperature *vs.* time) for all three solutions in both Python and include the .png files in your post lab.

2. Measure

3. Report results in a formatted table (**must include units**) that includes:

   – Heats for each reaction (acidic, neutral, basic) (Q)
      - **Note:** The specific heat (C_p) for our calorimeter is 104.3908 J K^{-1}. For the solutions, please use the specific heat of water (4.1796 J g^{-1} K^{-1})

   – Enthalpies for each reaction (acidic, neutral, basic) (ΔH)

4. Report results in a separate formatted table (**must include units**):

   – Enthalpy of protonation of glycine (experimental)

- Enthalpy of protonation of glycine (literature)
- Enthalpy of deprotonation of glycine (experimental)
- Enthalpy of deprotonation of glycine (literature)
- Percent error comparison between experimental and literature values

5. Noting that the pKa of H_2Gly^+ is 2.350, determine the fraction of Glycine that is protonated when it is mixed with 0.3 M HCl

6. Describe how you arrived at this value for the enthalpy of protonation of glycine. Be sure to reference the relevant equations, and note that you must account for the incomplete protonation of glycine → see Ramette 1984 for more details.

7. In a similar fashion, describe how you arrived at the value for the enthalpy of deprotonation of glycine.

8. Describe how you arrived at the literature values for these enthalpies (be sure to reference relevant equations).

Discussion

1. How do your experimental results compare to literature? Which factors may have most contributed to any difference between the two?

2. We were interested in the enthalpy of protonation and deprotonation of glycine. Why was it not enough to monitor the temperature change/heat transfer of glycine in HCl and glycine in NaOH? In other words, what is the point of measuring the temperature change/heat transfer of glycine in NaCl?

3. If we had neglected the incomplete protonation of glycine, how would this have affected our results?

4. Which is more energetically favorable: the protonation of glycine or the deprotonation of glycine?

Experiment 8: Proton Exchange of Pyruvic Acid *via* NMR

Post-Lab

CHE 346 TA: Alec Beaton

Student name:____

Introductory Information:

1. What is NMR?
2. What are some uses and applications of NMR? Why is it important to study?
3. What is pyruvic acid? Where is it naturally found? Why is it important to study?
4. What is FWHM? How is it related to the values you will report?
5. What equations will you need to turn the values obtained in the actual experiments (in this case, the NMR spectra) into the main values (i.e., meaningful numbers) you wish to report?
6. What are the main values you are reporting?

Experimental Details:

1. Name the chemicals used in this experiment. Provide the names and concentrations of solutions.
2. Briefly describe the process of conducting an NMR experiment.

Results:

1. Plot linewidth vs $[H^+]$ for the pyruvic acid proton resonance at both 300 and 400 MHz. Provide a linear fit.
2. Plot linewidth vs $[H^+]$ for the 2,2-dihydroxypropanoic acid proton resonance at both 300 and 400 MHz. Provide a linear fit.
3. Report results in a formatted table (**must include units**)
    - Forward rate constant (k_f) at <u>both fields</u>
    - Reverse rate constant (k_r) at <u>both fields</u>
    - Equilibrium constant (K_{eq}) at <u>both fields</u>
    - Equilibrium constant (literature value)
    - Percent errors for equilibrium constant
4. Describe how you calculated $[H^+]$ for the sample preparation information
5. Describe how you arrived at your values for k_r
6. Describe how you arrived at your values for k_f

7. Describe how you arrived at your values for K_{eq}
8. Compare your value of K_{eq} to the literature value

Discussion:

1. How does the experimental result for K_{eq} compare to literature? Which factors may have most contributed to any difference between the two?
2. How does K_{eq} at 300 MHz compare to K_{eq} at 400 MHz? Do you expect this difference? Why or why not?
3. Suggest possible improvements for repeating this lab in the future.

Notes on completing post-lab

You all should have a functioning Lorentzian line-fitting jupyter notebook with 3 sets of data. The NMR data along with the line-fitting notebook should either be in a folder titled exp_8_bruker or exp_8_npz, as determined during the lab section.

You all should also have received an Excel sheet with two tables (proton_exchange_tables).

The data for the 400 MHz is in a green table. It should look very similar to `info_tables` in your jupyter notebook. **Carefully enter your linewidth values from your jupyter notebook into this table. You must also calculate the $[H^+]$ concentration from the sample preparation information provided.**

The data for the 300 MHz is in a blue table. The linewidths for these datasets have already been tabulated for you. **You must also calculate the $[H^+]$ concentration from the sample preparation information provided.**

The pre-lab reading by Sime contains all the information you will need to handle the data once your blue and green tables are complete. **You may disregard the sections of this reading that deal with temperature dependence and activation energy.**

The pre-lab reading by Griffiths and Socrates contains the **literature value** that you need.