Notes on Keto-enol Reports, Spring 2007

Try to keep the **Abstract** to less than one page. You do not need to include much (if any) analysis of the results – just stick to the purpose, method, numerical results (with uncertainties, percent error, etc.), and any additional conclusions that are non-numerical (there are not usually many of these).

Do not simply paraphrase the handout to write your **Introduction**. This is considered plagiarism, even if you reference the handout. Part of the goal of the experiment is for you to realize which parts of the background material are essential to what you have done and you should only include the important background and equations in the Introduction. For example, you do not need to go into gory detail on the effects of different types of substituents in the \( R_1, R_2, R_3 \) and \( R_4 \) positions on the position of the keto-enol equilibrium. It is sufficient to say that substituents of different sizes and in different positions may affect the position of the equilibrium and then say specifically what part of the molecule will be varied in your experiment. Also, since you did not use the molecular mechanics method for any of your calculations, you do not need to discuss it in the Introduction.

If you do quote directly from the handout, be sure you both reference it and put the quotation in quotation marks (““”). But, do not quote a section of the handout just because you don’t understand it – it is usually very obvious that you don’t have a clue what a particular sentence means when you quote it directly in this way. You will get a lot farther if you find out what that section means and then explain in your own words if it is something that is important enough to include in the Introduction.

Stick to one tense – either past or future, but do not switch back and forth. Many of you say things like, “The purpose of this experiment was to study keto-enol tautomerism. **This will be** done by NMR.”

Many of you are still not citing sources appropriately for your background material in the **Introduction**. If there is information that you are getting from the handout or the textbook, then you need to cite it. If all the information is stuff you already know before starting this experiment, then you wouldn’t need to cite the source unless it’s a specific quotation, literature value, etc., but since most of the background material is new to most of you for these experiments you need to acknowledge where you got your information.

Sources should also be numbered in the order that you cite them in the text, so the first endnote number encountered in the text should be #1, the second should be #2, etc. Then, if you need to refer to the same source again later use the same number that you used the first time. In your **References** section, the sources should appear in numerical order. There is a footnote/endnote feature in MSWord that makes this really easy and will automatically change the numbering if you go back and insert a new reference in the middle of the report. Go to **Insert → Reference → Footnote**, and then choose appropriate options. To cite the same reference a second time go to **Insert → Reference → Cross Reference** and then select **Endnote** (or **Footnote**) from the
left-hand dropdown list, choose the appropriate reference from the list that appears in the box below, and finally click **Insert**. This will insert the reference and link it to the original source so that if you add other references the numbers should automatically correct themselves (although you will frequently need to do a Print Preview to update the cross references). Whether or not you use the endnote feature, be sure when you proofread that your numbers in the text refer to the correct source.

The hydrogen bonds that form within one molecule are **intra**molecular. Between two molecules would be intermolecular. One important point in the **Introduction** is that the compounds you studied may have a stable enol form because of the stabilization from the intramolecular interaction.

Several of you have confused the rate constant \((k)\) with the equilibrium constant \((K)\). You were determining the equilibrium constant in this experiment. Also, be sure you give the chemical equation (in the **Introduction**) for which you’re determining the equilibrium constant.

You always determine a **change** in Gibbs energy (Gibbs energy of tautomerisation in this case). Also, Gibbs is the guy’s name, so it does not have an apostrophe in it (i.e. “Gibb’s” is incorrect).

In **Spartan**, semi-empirical calculations were used to find the lowest energy conformer for the different molecules, and then ab initio calculations were used to optimize the geometry and determine the energy for this conformer. The reason a few of you got different energies for the same molecules was that the semi-empirical calculations found different conformers depending on how you drew the molecules in the first place. To rectify this, a computational chemist would be sure to do every calculation several times, drawing the molecule differently each time. Then the absolute lowest energy conformer that was found out of all the calculations on that molecule would be the one that was used.

In the **Experimental** section, remember to give the maker (brand) and model number for the instruments you used (the NMR in this case). Also, computer programs used for data collection and analysis are essentially part of the equipment, too, so they should also be listed. In general, computer programs should also be cited in the references section (the first time you mention the program). You can usually get citation information from the **Help → About** menu in the program. Computer programs are copyrighted material, so it is improper not to cite them. You do not need to list Excel specifically in the Experimental section, because you’re really just using it like a glorified calculator, but all the other programs you use should be listed and cited.

One NMR is a **spectrum**; multiple NMR’s are spectra. **There is no such word as “spectrums” and if it appears in future reports you will lose points accordingly!**
Start your **Discussion** with a 1-2 sentence summary of what you did and how and why you did it. This puts the rest of the section into some sort of perspective. Also, you should include your percent errors as one of the things you discuss in this section.

Be careful of “seeing” what you want to in your data at the point you start writing the Discussion. Sometimes you’re expecting a certain result and you then read your numbers all the wrong way because that’s what’s necessary to agree with what you expect. If your results don’t agree with what you think you’re expecting, you just need to try to justify why they might differ. For instance, in at least one of the solutions the less polar form was increased in the more polar solvent. Several of you missed this fact (even though your data was correct) because it wasn’t what you were expecting, and you went on to justify the opposite of what you actually observed! When you write your **Discussion** be sure what your writing is actually justified by your data (and include the numbers to prove it).

**Read the handout!!!**