

Guidance on Report 2 CH 463 & CH 463H

Write about the significance of your results in the spectroscopy, photophysics and photochemistry part of the lab. This should be journal style and about 750 words.

Complete the Jablonski diagrams for the two types of transitions, both the $n\pi^*$ and the $\pi\pi^*$ transitions (remember you may have several $\pi\pi^*$). See the web form on the Experiment 1 page for downloadable diagrams that you can fill in on line and print out. Include all the values you have data for and include units if needed. Report values to three (3) significant figures. Discuss how the photophysical parameters differ or agree for different types of transitions. Is there a trend among different types of transitions in the same solvent? How can you use the parameters to prove that a transition is strongly allowed or weakly allowed (symmetry forbidden) or strongly forbidden (symmetry and spin forbidden)? Experimental oscillator strengths can be compared with calculated values from quantum mechanics using HyperChem (for example.) If you have information from the literature compare to your experimental values. Discuss the qualitative photochemistry experiment (in sunlight) and report the mp if you were lucky enough to get some benzpinacol. Did you see the yellow color of the intermediate LAT? What is the phosphorescence efficiency for your ketone compare to regular benzophenone? If you have a value for Φ_{ph} and the ketone is not 100% efficient at phosphorescence, what other processes might be going on?

If you did the solvent study, discuss the experiment and what you hope to find out about the nature of the transitions in different solvents. Are all modes equally affected by a change in solvent polarity? How does this information help you to label the type of transitions as $n\pi^*$ or $\pi\pi^*$? Did you see any CT states? If you did, how do you explain this behavior?

If you did the quantitative photochemistry experiment to determine a value for Φ_{red} , discuss the experiment. How did you analyze the data? What is the significance for the photoreduction quantum efficiency? If it is not 100% efficient, what else is happening after the sample is irradiated? Show plots and give linear regression for: calibration curve of area vs. concentration of ketone. What peak(s) did you select as a gauge for the ketone concentration? Any idea what modes these are (carbonyl stretch, aromatic stretch, etc.?) Show a plot of moles of benzophenone reacted vs. moles of photons irradiated. Report Φ_{red} . Based on this result, should your ketone be good starting material for the photo-synthesis of the substituted benzpinacol on a commercial basis?