Report 3 Guidelines for Written Portion Project 2
Experimental Chemistry I, CH 362 & 362H
Winter 2021—March 17

The written portion of Report 3 is due Wednesday of final's week, March 17, by5 pm. Please submit your report electronically via Canvas.

Remember there are two parts to this project: (1) the keto-enol solvent correlation study; (2) the 1 and 2 D NMR and MS experiments for the unknown. The key aspect of reporting each study is to have a thoughtful discussion that includes a succinct but informative overview of the problem that was studied, and an analysis of the results explained in scientific terms and within the framework of accepted theories. Of course, you may find it necessary to adapt current theory to describe your results and this is okay as long as any extensions you make are well founded and substantiated.

The first study concerns the keto-enol equilibrium of 2,4-pentanedione dissolved in different NMR solvents. The determination of K_{eq} for the eight solvents should include information you used to assign each peak in the spectrum. Any unusual or interesting aspects may be good for discussion. The aim is to find at least one, or possibly two, reasonable correlations between the K_{eq} (or some function thereof--hint!) and solvent parameter, and then to interpret the correlation in terms of the structures of the tautomers and the physical meaning of the correlating parameter (hint—what underlying physical property or behavior, in general, have you ever used K_{eq} measurements to find?). Note that there may be outliers from the correlation you find, but the exception(s) also call for physical interpretation.

The second study concerns the identification of an unknown disubstituted benzene on the basis of its mass spectrum and several NMR spectra (proton, carbon-13, COSY, HSQC, HMBC, and for some, fluorine). You should present at least one pathway to unambiguous identification of your compound—this will have been the core of your short oral report. In the written report you should assign all peaks in the proton and carbon-13 spectra. All 1D and 2D spectra should be considered, and we expect that you will use all the experiments to provide confirmatory evidence for your identification or assignments of your unknown. To the extent possible, you should measure and assign all ^{1}H-^{1}H coupling constants (and those with fluorine will need to measure and assign ^{1}H-^{19}F and ^{13}C-^{19}F coupling constants). We recognize that due to non-first order behavior and overlap, not all (or even any!) of the J values can be measured. Please use the standard numbering system for the carbons and hydrogens in your compound and assign a proper chemical name to the compound. You should use the lab manual appendices to guide you on making predictions about the behavior of the other regioisomer of your compound. Any unusual aspects (atypical chemical shifts or couplings, second-order effects, etc.) are candidates for additional discussion.

We look forward to reading what you have to say about the scientific analyses and the significance of your results.