Handout for NMR Analysis (B):
NMR Determination of a Keto-Enol Equilibrium Constant

Procedure:


Each student shall conduct the experiment on one of the following solutions:

Solution 1: 0.20 mole fraction acetylacetone in solvent A
Solution 2: 0.20 mole fraction acetylacetone in solvent B
Solution 3: 0.20 mole fraction ethyl acetoacetate in solvent A
Solution 4: 0.20 mole fraction ethyl acetoacetate in solvent B
Solution 5: 0.20 mole fraction diethyl malonate in solvent A
Solution 6: 0.20 mole fraction diethyl malonate in solvent B

Solvent A: carbon tetrachloride (CCl₄), spectrochemical grade (or HPLC grade) with 5% (v/v) tetramethylsilane (TMS) added.
Solvent B: methanol (CH₃OH), spectrochemical grade (or HPLC grade) with 5% (v/v) tetramethylsilane (TMS) added

Report:

This report will be done as a full journal style paper. Students are to write a report that will focus on the use of NMR data to investigate the influence of molecular structure and solvent on keto-enol equilibria.