

## Pre-lab for Experimental and Computational Study of N,N-dimethylacetamide

1. Sketch the structure and an approximate proton NMR spectrum for a) N,N-dimethylacetamide assuming free rotation about C-N bond. b) N,N-dimethylacetamide assuming no rotation about C-N bond (i.e., that the methyl groups on the N are distinct). c) Ethylene glycol.
2. Read “Computational Study of Formamide Internal Rotation.” Focus on the abstract and first few sections. Answer the following questions on paper:
  - a. What do they find from their computations to be the barrier to isomerization?
  - b. Why is it useful to look at the changes in C-N and C-O bond length upon isomerization?
3. Read “J of Chem Ed Article – NMR Determination of Rotational Barrier in N,N-DMA”. Answer the following questions (Hint: check tables and figures!):
  - a. Sketch the effect of exchange of chemically equivalent nuclei as a function of rate of exchange.
  - b. Tabulate  $E_a$ ,  $\Delta G^\ddagger$ ,  $\Delta H^\ddagger$ , and  $\Delta S^\ddagger$  from this study and that of Reeves et al.
4. Write out equations 28.72, 28.78, and 28.73 from McQuarrie and Simon. Explain how you would find  $\Delta G^\ddagger$ ,  $\Delta H^\ddagger$ ,  $\Delta S^\ddagger$ , from these equations and the parameters ( $k(T)$ ,  $E_a$ ) you’ll obtain in lab. ( $c^\circ$  is  $1 \text{ mol}\cdot\text{L}^{-1}$ .)