10.675 Assignment #3
due 10/14/04

(Note: Do not wait until the day before to start these runs.)

(1) Pose a simple problem to address using G03, and solve it.

(2) Using the same methods that you used in Assignment 2, for the isomerization reaction below, use transition-state theory in G03 to compute the barrier height for reaction. Confirm that you have only one complex mode (negative frequency) and visualize it to get the pathway for isomerization.

\[ \text{cis-CHD=CHD} \rightarrow \text{trans-CHD=CHD} \]

(3) Compare the results from (2) to the experimental data (at 770 K), \( \log A = 13 \text{ s}^{-1} \), and \( E = 65 \text{ kcal/mol} \) (JCP, 23, 315 (1955)).

Note that each assignment should be done individually, even though several may be using the same methods.