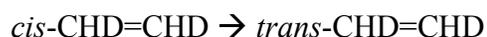


**10.675 Assignment #3**  
due 10/14/04

(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.



- (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.*