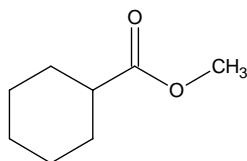
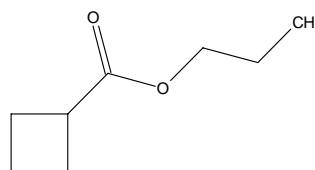


Pre-Lab assignments are due at 1 pm before lecture – Feb 10 TR Section; Feb 11 WF Section. Show all work and use proper significant figures.

1. (4 pts) Another isomeric ester to your ester is propyl cyclobutanecarboxylate ($C_8H_{14}O_2$). HyperChem is a computational chemistry software program that uses quantum mechanics to calculate the heat of formation from energy minimized structures. The following results for the heats of formation were obtained using a semi empirical quantum mechanical method.



Run1	-110.30542 (kcal/mol)
Run2	-109.66439
Run3	-110.31983
Run4	-110.84997



Run1	-89.74276 (kcal/mol)
Run2	-89.28332
Run3	-89.02535
Run4	-89.15217

Each run is an independent experiment based on a different minimized geometric structure for the compound. Determining the heat of formation using computational chemistry is an analogous experiment to measuring the heat of combustion that you are performing with the calorimeter in lab. By comparing the heat of formation for the most stable structure for the unstrained six membered ring of methyl cyclohexanecarboxylate with that for the most stable structure for the strained four membered ring of propyl cyclobutanecarboxylate, the strain energy in the cyclobutane ring can be estimated.

(a) Using the above data, determine the strain energy of the cyclobutane ring in kcal/mol. **Note: do not average the runs rather consider only the values for the most stable structure for each molecule based on the given data.**

(b) How does this calculated value compare to the reported literature value for the strain energy in a cyclobutane ring? You will find this data in your Organic text.

