Problem 2

Trans-cycloalkenes in larger rings are normal, stable alkenes. Trans-cyclooctene has been isolated, but it is rather more reactive that the typical alkene. Trans-cycloheptene has been detected by nmr at low temperature but never isolated. Trans-cyclohexene has been detected by flash photolysis and has a microsecond lifetime at room temperature.

a. Using the AM1 Hamiltonian, carry out appropriate energy calculations for the three trans-cycloalkenes mentioned and their corresponding cis isomers. Determine the energy differences.

b. Using ab initio techniques, repeat your calculation for trans- and cis-cyclohexene. Use the 3-21G basis and the 6-31G* basis.

c. Tabulate your three cis-trans energy differences for trans- and cis-cyclohexene. Which do you expect to be the more likely to be accurate? Why?

d. Trans-cyclohexene is exceptionally reactive toward acid. Your task in this section is to discover and explain why this is so. To that end, perform calculations on trans-cyclohexene and at least two other model compounds which will allow for appropriate comparison. [Hint: a model alkene known or expected to be unreactive to acid and a compound such as an amine, known to be a base, would be useful.] Use your knowledge of Spartan's surface tools to make a convincing presentation. [Hint: both orbital(s) and electrostatic potential maps might be useful.] You will be graded on the clarity and cogency of your presentation as well as its scientific soundness.