Excercise 1: H-H Bond Dissociation of H_2 Molecule with Different Methods

Use *Gaussian* to do a PES (Potential Energy Surface) scan for the dissociation of a H_2 molecule. That is, do a sequence of single point energy calculations with different bond lengths. CCSD/cc-pVQZ should be used (**find the last "E(CORR)=" of each step**), which also generates the results of SCF (RHF), MP2 and MP3 (locate the word "Summary"). T**he acronym refers to *Coupled Clusters with Singles and Doubles*** which is a method similar to CISD. **The keywords are *#T CCSD/cc-pVQZ Scan Test*.** Please read the *Gaussian03 user's reference* for using the **keyword *Scan***. Do the scan in the range of H-H bond lengths between [0.24Å, 1.14Å] with a step size of 0.1Å and in the range [1.14Å, 5.74Å] with the step size of 0.5Å.

Do it again with UHF. **Add the keyword *Guess=Mix* t**o destroy alpha-beta and spatial symmetries, otherwise the result is exactly the same as RHF. Plot your data from RHF, UHF, MP2, MP3 and CCSD in one picture. Print out both the data file and the plot. Explain the differences among the curves. You can use *xmgr* to plot the data. Prepare your data file such that the first column contains the H-H distance and all other columns contain the energies obtained with the different methods. The first line of the file may look like this:

0.2400 -0.32380 -0.23028 -0.35752 -0.36182 -0.36287513586D+00

After you have prepared the data file, run the command

$xmgr -nxy <data_file>

to plot it.

Exercise 2: Elimination Transition State Optimization

The purpose of this exercise is to show you that *Gaussian* can also deal with chemical reactions (It can not only predict the TS, but also follow reaction paths. **The keyword *IRC*** can be used to do that). So no conclusion is required for this exercise. **Please print out the TS structure and explain the input file and output file.**

Predict the structure of the transition state for the following reaction:

$CH_3Br+Cl^- \rightarrow CH_3Cl + Br^-$

What are the predicted Si-H and H-H bond lengths for the departing H atoms?

备注：

由于机房没有 Gaussian 程序，所以以上作业中的运算过程已由助教跑好。所有的输入文件和输出文件都放在文件夹 exercise2 中。同学们依据里面的文件完成以上作业。