Instruction for Case Studies in Chapter 1

Case Study 1

Since we have illustrated all keywords needed for Case Study 1, this instruction will only show you how to obtain the results you want from the Gaussian output (.log or .out) file.

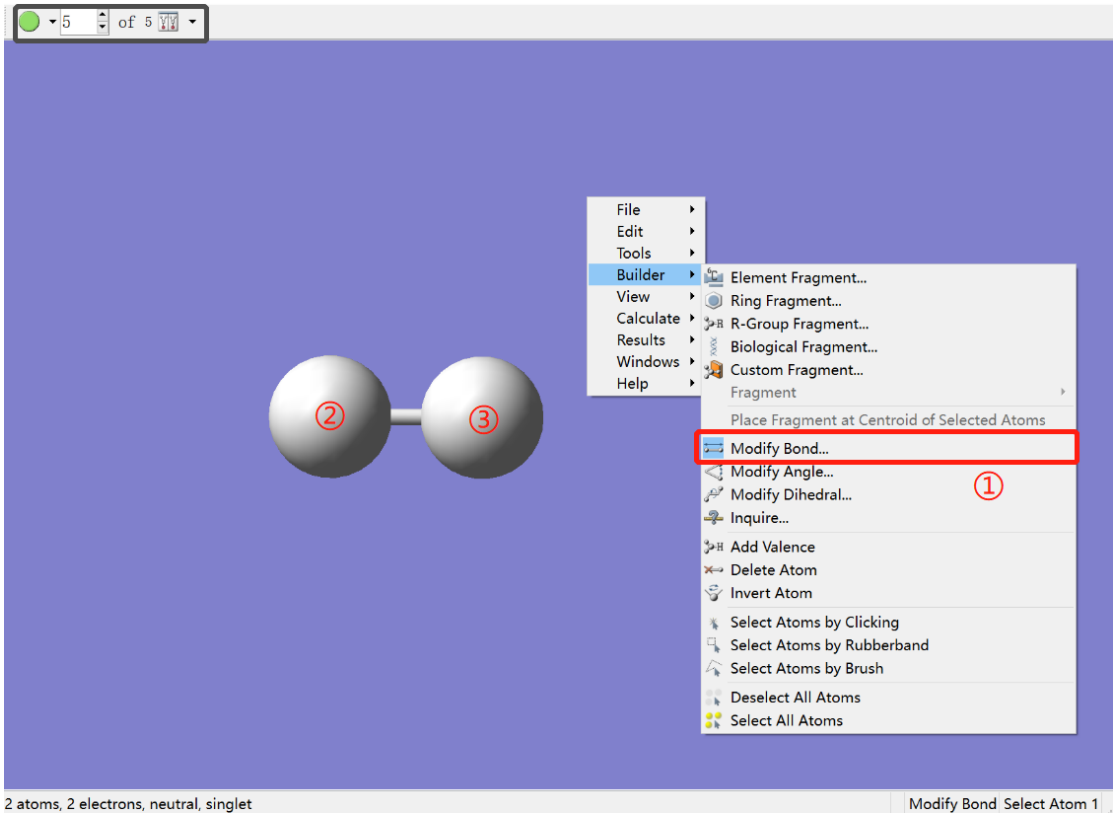
For Case Study 1, various optimized bond lengths of hydrogen molecule (H_2) at different computational levels are compared to see the influence of different methods and basis sets. Hence, we need to locate the position of the final optimized geometry in the output file. There are two ways to obtain the final optimized geometry.

The first one is to open the output file with a text editor (for example, Notepad++ for Windows or Vim for Linux), search for the keyword “Coordinates (Angstroms)” and locate the last one. The final optimized geometry is presented in the following form:

```
(Enter /share/apps/g16/A03/l202.exe)
                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          1           0        4.701736    0.031991    0.473076
     2          1           0        3.959114    0.031991    0.473076
---------------------------------------------------------------------
Stoichiometry    H2
Framework group  D*H[C*(H.H)]
Deg. of freedom     1
Full point group                 D*H     NOp   8
RotChk:  IX=0 Diff= 1.12D-16
Largest Abelian subgroup         D2H     NOp   8
Largest concise Abelian subgroup C2      NOp   2
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          1           0        0.000000    0.000000    0.371311
     2          1           0        0.000000    0.000000   -0.371311
---------------------------------------------------------------------
```

As we can see, the coordinates in the “Input orientation” section are the geometry in the input file, and the coordinates in the “Standard orientation” section are the optimized geometry for each step, which is the final optimized geometry here since we locate the last “Coordinates (Angstroms)”. From the coordinates listed here, we can calculate the bond length.

The second one is to open the output file with GaussView software. Once you open the output file, you can see the interface like this:



The optimized geometry of every step can be checked by the controller in the black box in the upper-left corner. One can right-click on the background and follow the instruction by the numbers in red to check the bond length of every step.

Case Study 2

For Case Study 2, one need to calculate the optimized geometry of the molecule or ion at the DFT level with the ωB97XD functional and 6-31G(d) basis set, whose input files are ended with "-opt". Then do a single point calculation on the optimized geometry at the restricted open-shell MP2 (ROMP2)/cc-pVDZ level, whose input files are ended with "-energy". So, we need to get the optimized geometry and the single point energy in two output files, respectively.

Once the geometry optimization is done, one can check the final optimized geometry in two way mentioned above. However, it can be very cumbersome if we copy the final optimized coordinates in the "-opt" output file to the "-energy" input file one by one. You might noticed that there is another output file ended with the extension

".chk" for every calculation. The .chk file contains the wavefunction and the geometry (final optimized geometry for geometry optimization calculation) information. So, instead of copying the coordinates, one can simply copy the .chk file to the same dictionary of the "-energy" input file, and add "%oldchk=" with your .chk file of the previous calculation in the beginning of the "-energy" input file, add the keywords "guess=read" and "geom=check", which tells the program to read the initial guess and the geometry from the old .chk files, and remove the coordinates section. The program will use the geometry in the old .chk file to do the calculation. The third line in each "-energy" input file "%mem=20gb" is to determine how many memory will be used for this calculation.

When the calculation is finished, one will need to get the converged energy from the output file. Open the output file with a text editor, search for the keyword "SCF Done" and locate the last one, where you can find the converged HF (or ROHF in this case) energy, search for the keyword "EUMP2" and locate the last one, where you can find the converged MP2 (or ROMP2 in this case) energy, as shown follow:

```
SCF Done:  E(ROHF) =  -39.5596130257     A.U. after    9 cycles
E2 =    -0.1308605492D+00 EUMP2 =    -0.39690473574942D+02
```