Molecular Modeling in Process Engineering

2023/2024

Project 3

Quantum Chemical Calculation of the energies of atomic hydrogen and molecular hydrogen

The purpose is to determine the energies of atomic and molecular hydrogen solving numerically the Schrodinger equation using the g09 code. The manual page of g09 can be found at:

https://gaussian.com/man/

To carry out the project you must:

- write the input for H and successively H2
- start the optimization
- examine the output file

Once you have run the calculation, you must:

1. try to understand what has been done in the calculation and which thermodynamic properties have been determined

2. find the energy in the output file and save it. (Energies are reported in Hartrees, the conversion to kcal/mol is 1 Hartree = 627.5 kcal/mol)

3. compare the energies of H and H2 and try to determine the energy of the reaction: $H_2 \rightarrow 2H$

4. Determine the energy of H2 at fixed H-H distances (frozen coordinate) and construct a table of H2 energies as a function of the distance. (You must find out how to do that looking at the gaussian manual)

5. If you are really successful and find this easy, try to do the same using the molpro code.

6. If you have mastered all the previous points, you can move forward with the next project by carrying out the optimisation for the following molecules: H_2O, CO, NO_2