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School of Advanced Sciences and Languages, Chemistry

Introduction to Computational Chemistry

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Practical 7: Frequency calculation of Molecules

Aim

To perform frequency calculation of a molecule by computational chemistry tools.

Theory:

Frequency calculation is a crucial step in molecular modeling, which helps in predicting the vibrational spectrum of a molecule. This involves calculating the frequencies of various modes of vibrations of a molecule and their corresponding energies. The vibrations of a molecule can be divided into three types: stretching, bending, and torsional. The stretching mode is associated with the stretching of bonds between atoms in the molecule, the bending mode with the bending of bonds, and the torsional mode with the rotation of atoms around a bond.

To get the vibrational structure of the molecule, Hessian calculation is performed. Hessian is the second order energy derivative with respect to the nuclear coordinate. It represents the curvature of the energy surfaces. The eigen value of Hessian matrix leads to the vibrational frequencies and eigen-vector leads to the vibrational mode of the molecules. The Hessian gives important information of the molecules whether it is minimum or not? If the all eigen-values is positive, then the molecule is present at one of the minima. Therefore, to confirm the minima structure of molecule, Hessian calculation is important. Additionally, after getting the vibrations of the molecule, Infrared spectra can also be simulated.

In this session, we generate the vibrational frequencies, vibrational mode and IR spectra of the water molecule.

Procedure:

- Build the water molecule in Chemcompute or any other software.
- Perform energy optimization of the water molecule at B3LYP/6-31G level of theory.
- Set up the calculation for the Frequency calculation using the optimized geometry.
- Submit the job.
- Under the Vibrationals visualizations, choose the vibrational frequencies to animate the three vibrational mode.

Results:

Draw the following molecules and generate its Vibrational frequencies. Report the four vibrational frequencies.

- CO_2
- CH_4