Molecular Modeling in Process Engineering

2023/2024

Project 7

Preliminary steps
Login and configure Cineca following the instructions in the ppt on Webeep

Since you do not have a licence for gaussian16 (g16), you must therefore use gaussian09 with the following command:

sbatch /g100_work/pMI24_ChiCa/bincc/rung09 geom.com

where geom.com is the input file

NMR shift estimation
The purpose is to compute the NMR shift of the following molecule:

Acetic acid, ethanol, acetaldehyde, dimethyl ether, acetone

Each student must perform calculations for a single molecule. Organize yourself so that you do not calculate the same.

To determine the shift, it is first necessary to make the optimization and the NMR calculation for the standard molecule: tetramethylsilane (TMS). It is suggested to use Molden's Zmat editor tool to construct the z-matrix for optimization. Use the GIAO method for NMR calculations. The output of interest is the magnetic shielding in ppm of isotropic H.

Subsequently, perform the same calculations as for TMS for the molecule whose NMR shift is to be calculated. The calculations must be performed at the same level of theory. The shift is the difference between the two magnetic shielding.
Compare results with data reported in: https://www.chemicalbook.com/

Please refer to the Gaussian manual for writing the input.