ESCUELA DE POSGRADO
MAESTRÍA EN QUÍMICA

PROGRAMA CURSO QUI729MODULAR DE SÍNTESIS QUÍMICA 1

MODELAMIENTO MOLECULAR

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3 A 6 DE DICIEMBRE DE 2012 (5 A 9 PM)

[1] Drawing with HYPERCHEM

Creating a molecule from scratch
Optimization with the elementary builder

Creating a [Hyperchem] HIN file
Reading the HIN file with a TextEditor [Notepad]
Transforming the HIN format to other important formats [PDB / MOL ...]

Various options for Rendering [Wire / Balls & Sticks ...]

Duplicating a molecule [to create a dimer]

Volume & Surface of a molecule
Dipolar Electric Moment

[2] HYPERCHEM without HYPERCHEM but with the following KEY freewares :

- AVOGADRO
- MERCURY
- Open-BABEL

[3] Geometry Optimization

using 3 different methods :

===> on a small molecule

- Fully classical [Molecular Force Field] : MM+
- Semi-empirical [Quantum Mechanical in part] : AM1 / PM3 / ZINDO-1
- Ab-Initio [Fully Quantum Mechanical] : STO-3G / 3-21G

===> on a much larger molecule

- Builder ===> MM+ ===> PM3 or ZINDO/1

[4] Vibration Analysis & IR spectrum

1. Draw a molecule
2. Open the LOG file [an easily readable TXT file with a wealth of Chemical Information]
3. Single Point calculation
4. Geometry Optimization
5. Calculations of all vibration modes [IR + not IR active]
6. The IR spectrum [frequencies , intensities , eigenvectors , visualization]
7. Saving the LOG file
8. Exporting / Saving the IR spectrum
9. Step-by-step detailed study of what is listed in the LOG file

[5] Looking for conformers with Monte-Carlo / Molecular Dynamics

The case of Biphenyl [The stable configuration is not planar !]
... Start from a planar molecule and find the lowest energy form ...
Heat - Search - Cool to the stable form
Manual computation of Energy versus Torsion angle to find the minimal energy conformation.

[6] Same thing as [5] using a SCRIPT

The purpose of this session is to learn how to write scripts for automatic searches and/or procedures.
More about scripts.

[7] Molecular Orbital Calculations

Use semi-empirical calculations to compute :
- the electrostatic potential
- the total charge density
- the molecular orbitals
- atomic charges

... for a simple molecule : Water

[8] Summary : what have you learned that is really important ?
can you do it all by yourself ?

Investigate the dimer of a simple carboxylic acid :

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Part I : A single acid molecule
- draw it
- optimize its geometry with [1] the builder (classic rules of Chemistry)
[2] the MM+ classical force field
[3] the PM3 semi-classical method
- compute the EDM [Electric Dipole Moment]
- visualize the EDM and finds its three components.
- export the result in [1] HIN (Hyperchem) format
[2] PDB format
[3] MOL format
- make sure you can read the PDB and MOL format into MERCURY
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Part II : Create and optimize the carboxylic dimer
using the builder , MM+ and PM3.
Compute the vibrational spectrum.
Can you visualize some of the IR low frequency vibrations ?
..... some of the IR high frequency vibrations ?
Compare your results with published results.
- compute the EDM [Electric Dipole Moment]
- visualize the EDM and finds its three components.
Could you create the hyperchem.LOG file ?
Can you open it with Notepad ?
Can you find all the relevant quantitative information in it ?
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