C7800 Introduction to molecular modelling - exercise
TSM Modeling of molecular structures

Section Modelling
Programs for molecular modelling II

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Exercise 1

1. In a text editor, create a file in the xyz format describing the water model with the following parameters. The length of OH bonds will be 1 Å. The HOH bond angle will be 90°. Save it to your home directory as "**water.xyz**".

2. Load the created file into the VMD program.

3. Verify the actual bond length and the size of the HOH angle. (VMD Main > Mouse > Label, VMD Main > Graphics > Labels)

4. Display the water molecule in the following models: Lines, CPK, Licorice, VDW.

OpenBabel

Open Babel is a chemical toolbox designed to speak the many languages of chemical data. It's an open, collaborative project allowing anyone to search, convert, analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas.

http://openbabel.org/wiki/Main_Page

Format conversion by openbabel:

```
$ module add openbabel
$ babel input.xyz output.mol2

alternatively:

$ babel -ixyz input.txt -omol2 output.out
```

List supported formats:

```
$ babel -L formats
```

Help:

```
$ babel -H
```

capital H

Exercise 2

1. Activate the module openbabel.
2. List the formats that the installed version openbabel supports.
3. Convert the file **water.xyz** to the format Sybyl Mol2 format and save it as **water.mol2**.
4. Open the file **water.mol2** in a text editor and discuss the meaning of its contents.
5. Convert the file **water.xyz** to the format InChI and save it as **water.txt**.
6. Open the file **water.txt** in a text editor and discuss the meaning of its contents.

Exercise 3

1. Load into the program **Avogadro** molecule from the file **water.xyz**.
2. Optimize its geometry. What is the optimal bond length and bond angle?
3. Display the molecule in various graphical representations.
4. Load the file **water.xyz** into the program **Nemesis** (Import Structure -> OpenBabel)
5. Display the molecule in various graphical representations.
6. Optimize its geometry. What is the optimal bond length and bond angle? Compare with results obtained in Avogadro. Explain any differences.

Exercise 4

1. In Sketch Structure project in the program **Nemesis,** draw the structure of benzoic acid.

2. Convert the molecule to a 3D representation (Structure > Convert to 3D). Rate the quality of the conversion.

3. Repeat the same procedure for cyclohexane.

Exercise 5

1. Build C_{60} in Avogadro using SMILES.

2. Find "Buckminsterfullerene" topic in Wikipedia and get SMILES representation of the molecule.

3. Build the model (Build > Insert > SMILES …).

4. Optimize and polish the model if necessary.