Molecular Builders and Single Point Calculation

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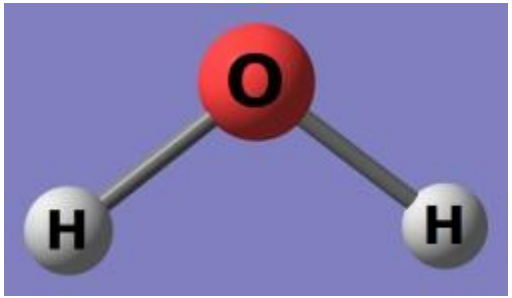
Molecular Structure Specification

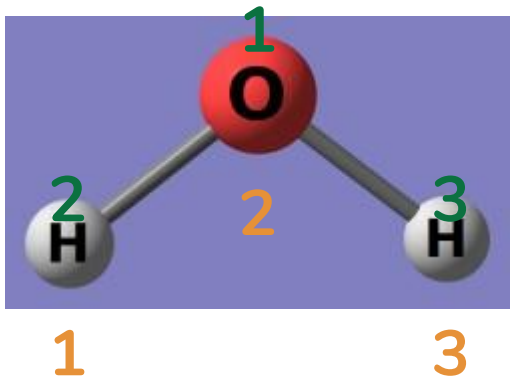
- Cartesian coordinates:

Molecule with N atoms → 3N Cartesian coordinates



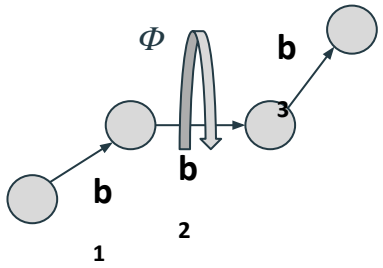
Element	X(Å)	Y(Å)	Z(Å)
O	-0.455432366	0.000000000	-1.763659097
H	-0.455432366	0.759337000	-1.167616097
H	-0.455432366	-0.759337000	-1.167616097

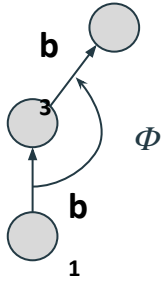
- Internal Coordinate: a systematic approach to build **Z-matrix** (***a list of internal coordinates***)
- nonlinear molecule: 3N-6 H_2O =3 internal coordinates (two bonds (**A**) and one angle (**B**))

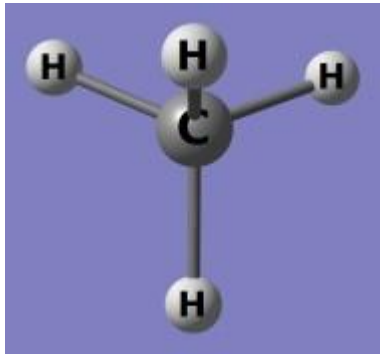


No.	Element	A	Bond length (Å)	B	Bond Angle (degrees)
1	O				
2	H	1	0.959		
3	H	1	0.959	2	103.9
1	H				
2	O	1	0.959		
3	H	2	0.959	1	103.9

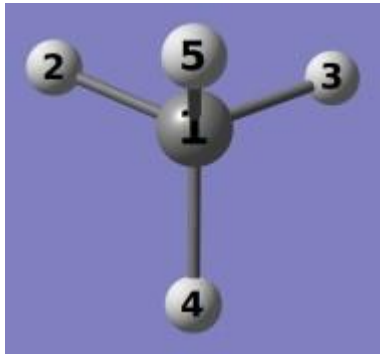
- For molecules if **N => 4,** there is an additional parameters called **dihedral (torsion) angle**.







No.	Element	A	Bond length (Å)	B	Bond angle (degrees)	D	Dihedral angle (degrees)
1	C						
2	H	1	1.089				
3	H	1	1.089	2	109.471		
4	H	1	1.089	2	109.471	3	120.000
5	H	1	1.089	2	109.471	3	-120.000



Builders in Wolf Computers

01	Avogadro	• Cross-platform (windows, Linux, Mac OS X) • Free, Open Source • Fast • https://avogadro.cc
02	Gaussview	• Comercial • Ability of generating specified parameters • https://gaussian.com/gv6main/
03	Nemesis	• Developed by Petr Kulhanek • https://nemesis.ncbr.muni.cz
04	Gabedit	• Free • Relatively slow • https://sites.google.com/site/allouchear/Home/gabedit

Task (I)

Open Avogadro and Gaussview using the following commands:

Open a terminal (Ctrl+Alt+T)

$module add avogadro
$avogadro

- H_2O
- $CH_2CHCHCH_2$
- Benzylamine ($C_6H_5CH_2NH_2$)

$module add gaussview
$gv

- NH_2CH_3
- CH_3CH_2OH

Typical Gaussian input file for SP

```
%chk=<name>.chk
%mem=<int>gb
%nproc=<int>
# b3lyp/6-31g

Title Card Required

0 1
6       0.753169000     3.160531000    -2.318531000
6       1.979701000     2.378550000    -2.303684000
6       0.382563000     3.894249000    -1.178245000
6       2.803075000     2.378437000    -1.170502000
6       3.406284000     1.133090000    -0.722816000
6       3.269679000    -0.083775000    -1.462575000
6       3.422882000    -1.301939000    -0.725708000
6      -1.973088000     3.160186000    -1.432584000
....
```

wavefunction

Number of shared processor and the value of memory usage

Command line: opt or sp, function, basis set, other relevant commands

Charge and multiplicity (2S+1)

Cartesian coordination

Single Point (SP) Calculation

Workflow for Gaussian (https://gaussian.com)

- Create **input** file using any builders (for example: Gaussview or Avogadro)
- Specify the **method** (Function and basis set)
- For single point use **SP** in command line.
- Save the **.chk** file
- Specify the number of **cpus** and the **memory** value
- Save the input file as "**.com**" or "**.gjf**"
- if you don't specify the version of the software, automatically the latest version of the code will be added up.
- Prepare the file (for example run.sh) for job submission including the following commands:

```
#!/usr/bin/env infinity-env
module add gaussian:16.A3
g16 <inputfile>.gjf
```

- Submit the prepared job as follows:
  $**psubmit default run.sh ncpus=<int>,mem=<int>gb,walltime=<int>:<int>:<int> -y**

Logfile and .chk file

One can extract the energy, structure,and other relevant results using logfile.

.chk file is a binary file. In order to convert it into a human readable file, one can use the following command:

$ formchk -3 <name>.chk

The created <name>.fchk file can be used for analyzing of orbital, electron density.

SP calculation using Turbomole

- Prepare the **input file** using any builder
- Add turbomole module: $**module add turbomole**
- Convert the prepared input file to the turbomole input file using the command: **x2t <filename>.com > coord**
- execute define (as the interface between user and code) command: $**define**
- Two first items can be skipped.
- Molecular geometry specification:
  - Add atomic coordinate using **a <file>** command
  - Create internal coordinate using **ired** coomand
  - Terminate using * and go through the next step.
- Basis set specification:
  - Using **b** one can assign the basis set for all atoms like **b all def-SVP** or using b “atom nickname” def-SVP. For example: **b “cl” def-SVP**
  - **bl** can list the type of specified basis sets for each atom
  - Use * to terminate this section and keep continue.

- Initial guess using extended Huckel theory (**eht**) and carefully specified the item which you are being asked.
- Method specification:
  - Execute **dft** and specified the status of DFT options as follows:
    - Execute **on** in order to activate DFT method.
    - Specify function using **func** command.
    - Change the grid size using **grid** command.
    - Terminate this section using ***** and go through the next step.
  - **RI** parameters:
    - **On** command activates this option
    - **m** can change the usage memory for this item using for example **m 3000**
    - Terminate using *****.
  - **dsp** (Dispersion correction) :
    - **on** command to switch DFT-D3
    - Terminate using *****.

- After finishing all the mentioned commands, use * to complete the define section.
- One should provide **coord**, **control**, **mos**, **basis** and **auxbasis** files.
- submit the **run_turbo.sh** job including the following commands for **SP** calculation.

```
#!/usr/bin/env infinity-env
Module add turbomole
ridft > dft.out
```

- For normal geometry optimization, one should use **jobex** command as follows:

```
#!/usr/bin/env infinity-env
Module add turbomole
jobex -ri > dft.out
```

- http://www.turbomole-gmbh.com/32-newsmp/75-turbomole-version-74.html

Output files for Turbomole

- **job.start**: informs you about the current option
- **converged**: convergence is signalled by this file otherwise you should find not.converged file.
- **job.last**: last complete cycle
- **mos**: molecular orbitals
- **dft.out**: optimization procedure