Introduction to Computational Chemistry
Handout Part 3

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1 The xyz file format

The xyz file is a file that lists the Cartesian coordinates of a compound in Ångstroms. The general structure is as follows:

```
<number of atoms>
Comment line; can be just an empty line
<element symbol> X Y Z
<element symbol> X Y Z
...
```

Most programs will read in the number of atoms specified in the first line. Any additional atoms in the xyz file will be ignored—therefore, it is important to make sure this number is correct. If you generate the xyz with some program (Avogadro, Chemcraft, Open Babel, . . .), this is not usually an issue.

2 Visualizing structures

Note that the xyz files do not contain any information about chemical bonds—most visualization programs show bonds based on distances between atoms (i.e., the visualized bonds do not result from a quantum mechanical calculation).

Chemcraft/Avogadro

- Use your file browser (MobaXterm or FileZilla) to navigate to the directory of the xyz file
- Right-click on the file and choose “Open with. . . ” (MobaXterm) or “View/Edit” and then “Use custom program” (FileZilla)
- Choose either Chemcraft or Avogadro (this step is automatic if they are the default programs for xyz)

In Chemcraft, you can change the visualization options under the “Display” menu. You can also create your own visualization style. To save the selected style as default, do Display-Customize-Save all-Close.

In Avogadro, you can change the visualization settings by opening the “Display Settings. . . ” (or “Display types" in Avogadro 2) tab. The changes are saved automatically.

Molden (if available)

- Call Molden on an xyz file:

  ```
  molden xyzfile.xyz
  ```

- Exit by the skull icon or `Ctrl-C` in the terminal

For Mac and Windows users: if you use any other terminal but MobaXterm, you need to install an X11 forwarding application to visualize Graphical User Interfaces (GUIs), such as Molden. For example, XQuartz for Macs or Xming for Windows. Additionally, you need to use the `-Y` flag with the `ssh` command when accessing Euler:

```
ssh -Y username@euler.ethz.ch
```

3 Interactive jobs

In case you want to interactively work on calculations that are too intensive for the login node, you can request an interactive bash terminal on a compute node. With the `x11` flag, you can also run graphical software from the interactive node.

3.1 Euler

```
srun --pty --x11 bash
```

You will then be put in the queue for the requested resources. You can use the usual `sbatch` options to ask for specific resources. For example, you can ask for 4 cores by:

```
srun --pty --x11 -n 4 bash
```

See `https://scicomp.ethz.ch/wiki/X11_forwarding_batch_interactive_jobs` for more information.

3.2 Grace

```
salloc --x11
```

You will then be put in the queue for the requested resources. You can use the usual `sbatch` options to ask for specific resources. For example, you can ask for 4 cores and 4 GB of RAM for 4 hours by:

```
salloc --x11 -n 4 --mem=4G -t 4:00:00
```

See `https://docs.ycrc.yale.edu/clusters-at-yale/job-scheduling/#interactive-jobs` for more information.

3.3 General

The `-x11` flag enables graphics forwarding, so you can use graphical software (like Molden or plotting tools). If you don't wish to use any graphical software during the interactive job, you can skip the `-x11` flag.

Once your interactive job is accepted, you will be able to use the terminal to run commands on the compute node for the specified amount of time. Once you are done with the calculations, you should stop the interactive job to free up the resources. To stop the interactive job, type:

```
exit
```

You can check the current node you're on by:

```
hostname
```

If the resulting name includes “login” in it (Euler) or “graceX.grace" (Grace), you're on a login node.

4 Optimizing geometries

You can optimize any xyz file with `xtb` to find the closest minimum energy structure on the potential energy surface. You can check the available `xtb` keywords by typing:

```
xtb -h
```

For optimizing the structure starting from an xyz file called filename.xyz, the usage is as follows:

```
xtb filename.xyz --opt
```

This will run the default optimization procedure. If you want the structure to be optimized according to more stringent convergence criteria, you can add the respective keyword like this:

```
xtb filename.xyz --opt verytight
```

This can be important to get good starting geometries for large non-covalent assemblies and organometallic systems.

In case of ions, the charge has to be additionally specified. For example, for a singly charged anion:

```
xtb filename.xyz --opt verytight --chrg -1
```

For large compounds, it may be reasonable to submit the calculations to the queue instead of running them interactively. You can use the `sbatch` command:

```
sbatch --wrap="xtb filename.xyz --opt verytight --chrg -1"
```

This will print the output of the calculation into the slurm output file. You can redirect the output with:

```
sbatch --wrap="xtb filename.xyz --opt verytight --chrg -1 > filename.out"
```

If you wish to calculate large systems, you might also want to ask for different resources than the default ones. Take a look at the `xtb` manual referenced in Section 7 for more information on this, and don't forget to change the `sbatch` flags accordingly.

The calculation will produce the following files:

File	Description
`charges`	atomic partial charges
`wbo`	Wiberg bond orders
`xtbopt.log`	trajectory of the optimization
`xtbopt.xyz`	the optimized structure
`xtbrestart`	file for restarting calculations
`xtbtopo.mol`	xtb-specific topology file

Important: as the files are always given the same name, they will be overwritten if you run several calculations in the same directory. You should either change the filenames in between calculations or have a separate directory for each calculation.

The `xtbopt.xyz` file is the most relevant file—this contains the xyz coordinates of the optimized structure. If you want to keep the output that is by default printed on the screen, you have to redirect it to an output file as already shown above.

5 Generating structures

5.1 From a SMILES string

- Copy the SMILES string of a ChemDraw drawing
  - Select Edit-Copy as-SMILES, or
  - Press `Alt-Ctrl-C` or `Opt-Cmd-C` (Mac)
- Use Avogadro to convert the SMILES string by selecting Build-Insert-SMILES... or
- Call the `smi2xyz.sh` script on the SMILES string (*between quotation marks*):

  ```
  smi2xyz.sh "SMILES"
  ```

To see the usage guide for additional options, type:

```
smi2xyz.sh
```

5.2 Avogadro

- Prepare the structure using the drawing tools
- Optional: optimize the structure with the Avogadro optimization tool
- Save the XYZ file, or if Avogadro 1:
- Select the structure (`Ctrl-A`) and copy it (`Ctrl-C`)
- Paste the coordinates into a text file and save as `.xyz`

5.3 Chemcraft

- Prepare the structure using the fragment (`Ctrl-F`) and atom (`Ctrl-A`) adding tools
- Optional: adjust the positions/angles/dihedrals
- Open the “Coord” tab, select “Coords format – XMOL format (symbol X Y Z)”, and press “Copy”
- Paste the coordinates into a text file and save as `.xyz`

6 Common errors

- The SMILES conversion fails because of stereochemistry in fused rings or undefined valencies (mostly with organometallics).
- The result files are overwritten when optimizing several structures in the same directory.
- The `xtb` output stream is not saved into a file (important if the information is required later on).

7 Useful links

- xTB manual:
  `https://xtb-docs.readthedocs.io/en/latest/contents.html`
- Avogadro manual:
  `https://avogadro.cc/docs/`
- References for xTB:
  `https://pubs.acs.org/di/10.1021/acs.jctc.7b00118`
  `https://pubs.acs.org/doi/10.1021/acs.jctc.8b01176`
  `https://doi.org/10.1002/wcms.1493`
- Reference for Open Babel:
  `https://doi.org/10.1186/1758-2946-3-33`
- A short description of SMILES:
  `https://www.daylight.com/dayhtml/doc/theory/theory.smiles.html`
- Documentation for CREST (for conformer sampling; not covered in the workshop)
  `https://crest-lab.github.io/crest-docs/`