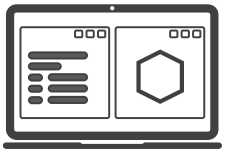

Introduction to Computational Chemistry
Handout Part 6

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1 Extracting data with `orca_mapspc`

For a full overview of the options you have, type

```
orca_mapspc
```

To extract the data from a spectrum with the name `dummy.out` as a text file, you can use

```
orca_mapspc dummy.out spectrumtype options
```

where instead of spectrum type you write the type you want (*e.g.*, IR or ABS) and add options such as the lineshape or the full-width at half-maximum height. You will receive two text files, which you can import into Excel or any other program you wish to use to plot the data.

2 IR

You can get the data for IR spectra with the `freq` or `numfreq` keywords (prefer `freq` if available). The IR spectrum and animations for the modes can be visualized in either Chemcraft or Avogadro, or you can use the `orca_mapspc` tool to plot the spectra yourself.
As we saw in Session 4, it is possible to calculate the vibrational modes with different isotopes. For this, add the mass of the isotope to the coordinates as shown below.

```
*xyz 0 1
H 0.0 0.0 0.0 # hydrogen (default)
H 0.0 0.0 0.7 M 2.00141 #  deuterium
*
```

You can also do this after a "normal" frequency calculation in combination with `!PrintThermoChem` by reading in the Hessian file (see Session 4 for details).

3 NMR

The minimal input to get NMR data is:

```
! Keywords NMR
#Resources
#Coordinates
```

You can ask for specific shifts or coupling constants by adding the `eprnmr` block **after** the coordinates.

```
#Rest of input
*xyzfile 0 1 coord.xyz
%eprnmr
Nuclei = All H {Shift, SSall}
end
```

In this example you will get all shifts and spin-spin coupling values for all H nuclei. You can add additional lines with more nuclei.

4 UV/Vis

To calculate excites states, you need to add the `tddft` block as shown below. You can choose the number of states by the number following `nroots`.

```
#Keywords
#Resources
%tddft
nroots 10
end
#Coordinates
```

The summary of the states is printed at the end of the `.out` file. You can use Chemcraft or Avogadro to view the UV/Vis spectrum or use the `orca_mapspc` tool to plot it yourself.

5 Excited State Calculation with STEOM-DLPNO-CCSD

Always run these calculation in the scratch directory as they produce a lot of temporary data. You can access your scratch directory by typing (on Euler)

```
cd /cluster/scratch/$USER/
```

or (on Grace)

```
cd /home/$USER/palmer_scratch
```

A model input file for an excited state calculation with this method is given below:

```
!STEOM-DLPNO-CCSD def2-TZVP def2-TZVP/C RIJCOSX def2/J tightscf
! CPCM(water) # add solvent if you want
#Resources - be sure to give enough
%mdci
Nroots 5 #The number of states you want
dorootwise true #Solves one root at a time
dosolv true #Include CPCM (if you have it)
end
#Coordinates
```

6 Useful Links

- ORCA tutorials for IR, NMR, and UV/VIS calculations
  `https://www.orcasoftware.de/tutorials/spec/IR.html`
  `https://www.orcasoftware.de/tutorials/spec/NMR.html`
  `https://www.orcasoftware.de/tutorials/spec/UVVis.html`
  `https://sites.google.com/site/orcainputlibrary/excited-state-calculations/tddft`
- A comprehensive review of spectroscopy with DFT
  F. Neese. *Coordination Chemistry Reviews* **2009**, *253*, 526563.
  `https://doi.org/10.1016/j.ccr.2008.05.014`
- Useful protocols and references for semi-automated NMR calculation. Requires other set of software than covered in this course.
  Patrick H Willoughby, Matthew J Jansma Thomas R Hoye. *Nature Protocols* **2014**, *9*, 643.
  `https://doi.org/10.1038/nprot.2014.042`