Running TT-SOFT Calculations for Pyrazine on Omega

Sam Greene

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This document describes how to run TT-SOFT on Omega to calculate the photoabsorption spectrum of pyrazine using Matlab.

First, copy the TT-Toolbox directory, which can be found at Kenny/TT/newivan, to Omega. For the purposes of this document, I assume it is saved on Omega in your scratch directory, but you can save it anywhere and modify line 8 of the tt_SOFT.m script accordingly.

Next, copy all of the files in the Code subdirectory (which can be found in the directory in which this file is saved) to a single directory on Omega. Modify the fifth line of the submit.pbs script with your e-mail address. Then type "qsub submit.pbs" to submit the job to the ESI queue.

The job will produce several output files:

- **tt_SOFT.err** (a text file) will be empty unless there are issues with the job.
- The number of each propagation step is printed to **tt_SOFT.out** (a text file) as the job is running so you can check its status. Once finished, bottom of the file will also contain the total execution time.
- **overlap.mat** (a Matlab data file) contains the value of the autocorrelation function as a function of time, updated with each propagation step as the job is running.
- **ranks.mat** (a Matlab data file) contains the ranks of both nuclear wave functions as functions of time, updated every 5 propagation steps during execution.

Once execution finishes, copy the **overlap.mat** file back to your local computer. Import its contents into Matlab, which will give a variable "amp." Open the Matlab script Plot_24D.m and run it in the current directory (as it depends on the files Plotspec.m and ExptYama83.csv). This will plot the calculated photoabsorption spectrum in comparison to an experimental spectrum from *Faraday Discuss. Chem. Soc.*, 1983, **75**, 395–405.