

Class 5: advanced DFT and property calculations

1. Use `rdesktop` to login to the Windows Terminal Server at `minsc.oerc.ox.ac.uk` (use your supercomputer login credentials).
2. Use `ssh` from either the Linux host or from the terminal server to login to `orac.oerc.ox.ac.uk` and load the Gaussian module (`module load gaussian03`).
3. Compare the time it takes to run the energy calculation for toluene using SVWN and B3LYP exchange-correlation functionals in a 6-311G(d,p) basis set.
4. Try locating the bond breaking saddle point for hydrogen using CCSD/cc-pVTZ method. Set `opt=ts` to switch off the Hessian eigenvalue control and cause BFGS to converge to a saddle point. The starting point for the optimization should be your best guess for the transition state structure.
5. Optimize the geometry of cyclobutane and run a vibrational analysis job (use `freq` keyword). Visualize the resulting normal mode vibrations in GaussView.
6. Run the geometry optimization for benzene cation radical with an option to keep the checkpoint file (`%Chk=filename.chk`). Transform the checkpoint file into platform-independent ASCII (`fchk filename.chk`), and open the resulting `.fchk` file in GaussView. Generate the total electron density and spin density plots.
7. Optimize the geometry of cyclobutane with a non-gradient method (`opt=ef`). Observe the time taken.

Reminder: ORAC runscripts should look like this

```
#!/bin/bash
#PBS -l ncpus=8
#PBS -l walltime=24:00:00
#PBS -V

cd $PBS_O_WORKDIR
GAUSS_SCRDIR=$TMPDIR
export GAUSS_SCRDIR

g03 *****.com
g03 *****.com
g03 *****.com
```