Class 6: 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. Set up a potential energy scan with respect to the C=C bond stretch in ethylene using MP2/cc-pVDZ method with and without counterpoise BSSE correction. Observe the difference in the bond breaking profile.
4. Calculate the hyperfine couplings in benzene cation radical with and without SCI-PCM water. Observe the difference in 13C hyperfine couplings.
5. Use optimized methane geometry to perform a thermodynamic analysis (see the FREQ keyword documentation on Gaussian website).
6. Optimize methane geometry to a transition state with respect to the C-H bond breaking. Run the vibrational frequency calculation to demonstrate that the transition state is a saddle point.

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
```