Removing imaginary vibrational frequencies

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Often, a geometry optimization will lead to an undesirable number (i.e. > 0) of imaginary vibrational frequencies. This may be corrected by making a small displacement along the coordinates of the undesired mode and restarting the optimization. We have a script called **run_qchem_rem_imag_modes** that will iterate this displacement/reoptimization procedure until no imaginary frequencies remain. To use it, open a command-line terminal on an MGCF workstation and go to the directory containing the pertinent optimization+frequency calculation. The script is run as

run_qchem_rem_imag_modes file.in ncpu

where **file.in** is your q-chem input file and **ncpu** is the number of cpu's you want to use. The input file can have several calculations in tandem, but the final part of the file must contain an optimization calculation followed by a frequency calculation, like this:

```
$molecule
 ⋮
$end


$rem
jobtype opt
 ⋮
$end


@@@


$molecule
 read
$end

$rem
jobtype freq
 ⋮
```

$end

The freq calculation must use “read” in the $molecule section. If the calculation has imaginary modes, the script will proceed with new calculations titled file_iter1.in, file_iter2.in, etc. (assuming the original input file is called file.in), until no imaginary modes are found. The script will detect if any optimization has failed and if so, it will exit the process, because there’s no sense in continuing the process in that case. When this happens, the script will print out a message saying an optimization failed and that it’s exiting; this error message will be found in the file.job.o### file, so always check this file for any such message.

It’s ok to use scf_guess = read, because the script will run all the calculations in a single scratch directory, so that orbitals will be saved after each calculation.

See here for an example input file. The input file “h2o2_lin.in” contains 3 tandem calculations. The first one is just a single-point calculation at a different spin state, whose orbitals will be read into the 2nd calculation, which is an optimization, and after that, the geometry and orbitals are read into the 3rd calculation, i.e. the freq calculation. This illustrates that any number of preliminary calculations can be placed before the final opt+freq. Often we need to use preliminary calculations to set up the right orbitals or starting geometry.