FHI-aims Cheat Sheet: Harmonic Vibrations

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Computing the harmonic vibrations gives your access to several useful properties. The resulting vibrational spectrum can be compared to experimental infrared (IR) spectra and furthermore allows for a rough estimate of free energies.

How to begin?

First, you need to compile the FHI-aims binary:

```
make mpi
```

Second, compile the vibrations Perl script and diagonalizer (without a '`make clean`' in between):

```
make vibrations.mpi
```

Now the FHI-aims binary directory contains the files:

```
aims.[version].mpi.x
aims.vibrations.[version].mpi.pl
vibrations_diagonalizer.[version].mpi.x
```

The Perl script
`aims.vibrations.[version].mpi.pl` is to be copied into the working directory and some variables have to be checked and adapted, especially:

```
$AIMS_BINDIR    $EXE    $HESSIAN_DIAGONALIZATION_EXE
```

Geometry and calculation settings have to be specified in `geometry.in` and `control.in`, respectively.

Engage!

```
./aims.vibrations.[version].mpi.pl [name] [delta]
```

Giving the command line options `[name]` and `[delta]` overrides the defaults of 'basic' and '0.0025', respectively.

What do we get?

Visualize the vibrations, e.g. with `jmol`:

```
jmol basic.vib.xyz
```

Control the animation with *AtomSetChooser*.

Extract energies from the file `basic.vib.out`, you will find the zero-point energy and free energy at room temperature.

Characterize a stationary point as minimum if the vibrational modes 1 to 6 are close to zero.

Attention!

These cheat sheets are not intended to substitute for reading the manuals of the programs involved and the original literature cited therein!

With the task described here, some settings require your special attention:

The displacement δ defaults to 0.0025. This value strongly impacts on the vibrational modes 1 to 6 (translations and rotations).

The accuracy of the forces is crucial to obtain meaningful vibrational frequencies. Rather accurate settings are suggested for species defaults, convergence of the forces in the SCF cycle, and for the convergence of the geometry relaxation.

Have fun!