## molfile qm basis t + num shells per atom + num prim per shell + basis + atomic number + angular momentum + shell symmetry

## molfile qm sysinfo t

- + nproc
- + memory
- + runtype
- + scftype
- + status
- + num electrons
- + totalcharge
- + num occupied A
- + num occupied B
- + nuc charge
- + basis\_string
- + runtitle

basis

- + geometry
- + version string

run

molfile\_qm\_t

+ hess + basis + run

## molfile qm hessian t

- + carthessian
- + imag\_modes
- + inthessian
- + wavenumbers
- + intensities
- + normalmodes

/ hess