# Cheat-Sheet for `tools-for-g16.bash` (0.0.14, 2018-08-20)

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## Introduction

This accompanies the repository polyluxus/tools-for-g16.bash.
Various bash scripts to aid the use of the quantum chemistry software package Gaussian 16.

### Preliminary notes

The notation in brackets `[]` indicate optional arguments/inputs; arguments in angles `<>` require human input; a bar `|` indicates alternatives.
The following abbreviations will be used:

`opt` Short for option(s)
`ARG` String type argument
`INT` Positive integer
`NUM` Whole number
`FLT` Floating point number
`DUR` Duration in format `[[HH:]MM:]SS`

### g16.prepare.sh

This tool reads in a file containing a set of cartesian coordinates and writes a Gaussian inputfile with predefined keywords. The script interfaces to Xmol format, Turbomole/ GFN-xTB `coord` format, too.
Usage: `g16.prepare.sh [opt] <file>`

`-T <FLT>` Temperature (kelvin)
`-P <FLT>` Pressure (atmosphere)
`-r <ARG>` Add `<ARG>` to route section
`-R <ARG>` Specific route section `<ARG>`
`-l <INT>` Load predefined route section
`-l list` Show all predefined route sections
`-t <ARG>` Adds `<ARG>` to end of file
`-C <ARG>` Specify caption/title of job; Replacements: `%F` input filename, `%f` input filename without `.xyz`, `%s` like `%f`, also filtering `start`, `%j` jobname.
`-j <ARG>` Jobname
`-j %s` Jobname is filename filtering `start.xyz`
`-f <ARG>` Filename of generated input
`-c <NUM>` Charge
`-M <INT>` Multiplicity (not zero
`-U <INT>` Memory
`-m <INT>` Memory (megabyte)
`-p <INT>` Processors
`-d <INT>` disksize via MaxDisk (megabyte)
`-s` Silent script mode
`-h` Help file

### g16.testroute.sh

This tool parses a Gaussian 16 inputfile and tests the route section for syntax errors with the Gaussian 16 utility `testrt`.

`-s` Silent script mode
`-h` Help file

### g16.freqinput.sh

This tool reads in a Gaussian 16 inputfile and adds relevant keywords for a frequency calculation.
Usage: `g16.freqinput.sh [opt] <file>`

`-o <ARG>` Adds option `<ARG>` to the `freq` keyword.
`-R` Adds option `ReadFC` to the `freq` option list.
`-T <FLT>` Temperature (kelvin)
`-P <FLT>` Pressure (atmosphere)
`-r <ARG>` Add `<ARG>` to route section
`-t <ARG>` Adds `<ARG>` to end of file
`-m <INT>` Memory (megabyte)
`-p <INT>` Processors
`-d <INT>` disksize via MaxDisk (megabyte)
`-s` Silent script mode
`-h` Help file

### g16.submit.sh

This tool parses and then submits a Gaussian 16 inputfile to a queueing system.
Usage: `g16.submit.sh [opt] <file>`

`-m <INT>` Memory (megabyte)
`-p <INT>` Processors
`-d <INT>` disksize via MaxDisk (megabyte)
`-w <DUR>` Walltime limit
`-e <ARG>` Specify an environment variable, format `VAR=<value>`
`-j <INT>` Wait for job with ID `<INT>`
`-H` Submit with status hold (PBS) or `PSUSP` (BSUB)
`-k` Only create (keep) the jobscript, do not submit it.
`-Q <ARG>` Queue for which job script should be created (`pbs-gen/bsub-rwth`)
`-P <ARG>` Account to project (BSUB); if `<ARG>` is `default/0/''` presets are overwritten.
`-u <ARG>` set user email address (BSUB); if `<ARG>` is `default/0/''` presets are overwritten.
`-s` Silent script mode
`-h` Help file

### g16.getenergy.sh

This tool finds energy statements from Gaussian 16 calculations.
Usage: `g16.getenergy.sh [opt] [<file(s)>]`
If no files given, it finds energy statements from all log files in the current directory.

`-i <ARG>` Specify input suffix if processing directory
`-o <ARG>` Specify output suffix if processing directory
`-q` Silent script mode
`-h` Help file

### g16.getfreq.sh

This tool summarises a frequency calculation and extracts the thermochemistry data.
Usage: `g16.getfreq.sh [opt] <file(s)>`

`-v` Incrementally increase verbosity
`-V <INT>` Set level of verbosity directly, (0-4)
`-c` Separate values by comma (`-V0` or `-V1`)
`-O <ARG>` Write summary to file instead of screen
`-q` Silent script mode
`-h` Help file

### g16.chk2xyz.sh

A tool to convert a checkpoint file to an `xyz` file. This formats the `chk` first to a `fchk`.
Usage: `g16.chk2xyz.sh -f | <checkpointfile(s)>`

`-f` Formats all checkpointfiles that are found in the current directory
`-h` Help file

## Author, Bugs, and the Rest

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