

Cheat-Sheet for tools-for-g16.bash

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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 (including zero)

`NUM` Whole number (including zero)

`FLT` Floating point number

`DUR` Duration in format [[HH:]MM:]SS

Installation & Configuration

General settings for the scripts can be found in the file `g16.tools.rc`. Alternatively, settings can be stored in `.g16.toolsrc`, which always has precedence. Every script will check four different directories in the order 1. installation directory, 2. user's home, 3. `.config` in user's home, 4. parent working directory. It will load the last configuration file it finds.

Setting files can be generated with the `configure/configure.sh` script.

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; %c charge (with indicator `chrg`); %M multiplicity (with indicator `mult`); %U unpaired electrons (with indicator `uhf`).
- j <ARG> Jobname (derives filename of generated input; default: <file>)
- j %f Jobname is <file> filtering .xyz
- j %s Jobname is <file> filtering `start.xyz`
- f <ARG> Filename of generated input
- c <NUM> Charge (default: 0)
- M <INT> Multiplicity (default: 1; ≥ 1)
- U <INT> Unpaired electrons (unset; ≥ 0)
- m <INT> Memory (megabyte)
- p <INT> Processors
- d <INT> disksize via `MaxDisk` (megabyte)
- Close reading options
- s Silence script (incremental)
- 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`.

- Close reading options
- s Silence script (incremental)
- h Help file

g16.dissolve.sh

This tool reads in a Gaussian 16 inputfile (of a preferably completed calculation) and adds relevant keywords for solvent corrections. (Utilises the `%OldChk` directive and the `geom/ guess` keywords.)

Usage: `g16.dissolve.sh [opt] <file>`

- o <ARG> Adds option ARG to the `scrf` keyword.
- S <ARG> Adds option `solvent=ARG` to the `scrf` option list.
- O Runs an optimisation (preserves or adds OPT)
- r <ARG> Add ARG to route section
- t <ARG> Adds ARG to end of file
- f <ARG> Filename of generated input
- m <INT> Memory (megabyte)
- p <INT> Processors
- d <INT> disksize via `MaxDisk` (megabyte)

- Close reading options
- s Silence script (incremental)
- h Help file

g16.freqinput.sh

This tool reads in a Gaussian 16 inputfile (of a preferably completed calculation) and adds relevant keywords for a frequency calculation. (Utilises the `%OldChk` directive and the `geom/ guess` keywords.)

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
- f <ARG> Filename of generated input
- m <INT> Memory (megabyte)
- p <INT> Processors
- d <INT> disksize via `MaxDisk` (megabyte)
- Close reading options
- s Silence script (incremental)
- h Help file

g16.ircinput.sh

This tool reads in a Gaussian 16 inputfile from a (previously completed) frequency run and adds relevant keywords for two separate irc calculations. (Utilises the `%OldChk` directive and the `geom/ guess` keywords.)

Usage: `g16.ircinput.sh [opt] <file>`

- o <ARG> Adds option ARG to the `irc` keyword.
- r <ARG> Add ARG to route section
- t <ARG> Adds ARG to end of file
- f <ARG> Filenametemplate of generated input files; `jobname.suffix` produces `jobname.fwd.suffix` and `jobname.rev.suffix`
- m <INT> Memory (megabyte)
- p <INT> Processors
- d <INT> disksize via `MaxDisk` (megabyte)
- Close reading options
- s Silence script (incremental)
- h Help file

g16.optinput.sh

This tool reads in a Gaussian 16 inputfile preferably from a (previously completed) IRC run and writes and inputfile for a subsequent structure optimisation. (Utilises the %OldChk directive and the `geom/` `guess` keywords.)

Usage: `g16.optinput.sh [opt] <file>`

`-o <ARG>` Adds option `ARG` to the `opt` keyword.
`-r <ARG>` Add `ARG` to route section
`-t <ARG>` Adds `ARG` to end of file
`-f <ARG>` Filename of generated input
`-m <INT>` Memory (megabyte)
`-p <INT>` Processors
`-d <INT>` disksize via `MaxDisk` (megabyte)
`--` Close reading options
`-s` Silence script (incremental)
`-h` Help file

g16.spininput.sh

This tool reads in a Gaussian 16 inputfile and writes and inputfile for a subsequent calculation. It is possible to overwrite the existing route section, but still add the `geom/guess` directives to base it on. (Utilises the %OldChk directive.)

Usage: `g16.spininput.sh [opt] <file>`

`-r <ARG>` Add `ARG` to route section
`-R <ARG>` Overwrites route section with `ARG`
`-t <ARG>` Adds `ARG` to end of file
`-f <ARG>` Filename of generated input
`-m <INT>` Memory (megabyte)
`-p <INT>` Processors
`-d <INT>` disksize via `MaxDisk` (megabyte)
`--` Close reading options
`-s` Silence script (incremental)
`-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 `ARG` in format `<VAR=value>`
`-j <INT>` Wait for job with ID `INT`
`-H` Submit with status hold (PBS, SLURM) or PSUSP (BSUB)
`-k` Only create (keep) the jobscript, do not submit it.
`-Q <ARG>` Queue for which job script should be created `<queue>-<special>` (`<queue>`: `pbs`, `slurm`, `bsub`; `<special>`: `gen` [generic], `rwth`)
`-P <ARG>` Account to project (BSUB) or account (SLURM); if `ARG` is `default/0/''` presets are overwritten.
`-M <ARG>` Specify a machine type (only `bsub-rwth`); if `ARG` is `default/0/''` presets are overwritten.
`-u <ARG>` set user email address (SLURM, BSUB); if `ARG` is `default/0/''` presets are overwritten.
`--` Close reading options
`-s` Silence script (incremental)
`-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
`-L` Print the full file and path name (seperated by newline)
`--` Close reading options
`-s` Silence script (incremental)
`-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`)
`-f <ARG>` Write summary to file instead of screen
`--` Close reading options
`-s` Silence script (incremental)
`-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 [-s] -h | -a | <chk-file(s)>`

`-a` Formats all checkpointfiles that are found in the current directory
`--` Close reading options
`-s` Silence script (incremental)
`-h` Help file

Author, Bugs, and the Rest

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