

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 for this cheat-sheet

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 *or* INT[D|H|M]

General notes on the processed files

The scripts in this repository use *input* files as templates to write new input files. Route sections of these input files will only be recognised, if they contain a start pattern `##/##/##/##T` followed by a space, even though a valid Gaussian input does not necessitate this.

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, see the manual for more detailed information.

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.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 an 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 an 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.testroute.sh

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

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

`--` 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. For details on the extended mail interface see the manual.

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.wrapper.sh

This tool provides a Gaussian 16 environment to execute utilities interactively.

Usage: `g16.wrapper.sh [opt] <utility commandline>`

`-m <INT>` Memory (megabyte)
`-p <INT>` Processors
`--` Close reading options
`-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
`-R` Recurse into directories
`-L` Print the full file and path name (separated by newline)
`-1` Print only one line per file
`--` 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`)
`-c <ARG>` Separate values by `ARG` (`-V0` or `-V1`); arguments: `space`, `comma`, `semicolon`, `colon`, `slash`, `pipe`,
`-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 [opt] [<chk-file(s)>]`

`-a` Formats all checkpointfiles that are found in the current directory
`-A` Formats almost all checkpointfiles that are found in the current directory (same as `-aS`)
`-B` Create backup files in cases where it would overwrite them (default)
`-F` Forces files to be overwritten
`-S` Skips files in cases where it would overwrite them
`-R` Recurse through directories
`-P` Print; dry run
`--` Close reading options
`-s` Silence script (incremental)
`-h` Help file

Author, Bugs, and the Rest

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