

Cheat-Sheet for tools-for-g16.bash

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Martin C Schwarzer, March 26, 2019

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

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 `##/##/##P/##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.

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 `scrfl` keyword.

`-S <ARG>` Adds option `solvent=ARG` to the `scrfl` 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.spinput.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.spinput.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 queuing 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.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.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

Martin C Schwarzer ≡ Martin-マーチン ☯ polyluxus

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