

Cheat-Sheet for tools-for-g16.bash

(0.3.2, 2020-01-16)

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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 `##/##N/#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, see the manual for more detailed information.

Options for all scripts

All scripts have the following options available:

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

g16.prepare.sh

This tool reads a file with cartesian coordinates (Xmol, gjf, or Turbomole `coord` and writes a Gaussian inputfile with predefined keywords.

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)

g16.dissolve.sh

This tool reads a Gaussian 16 inputfile (of a preferably completed calculation) and adds relevant keywords for solvent corrections.¹

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)

g16.freqinput.sh

This tool reads in a Gaussian 16 inputfile (of a preferably completed calculation) and adds relevant keywords for a frequency calculation.¹

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)

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.¹

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>` Filename template 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)

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.¹

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)

¹Utilises the `%OldChk` directive and (if not specified otherwise) the `geom(check)/guess(read)` keywords.

-p <INT> Processors
-d <INT> disksize via MaxDisk (megabyte)

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.¹

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)

g16.nbo6prop.sh

This tool reads in a Gaussian 16 inputfile and writes a new inputfile for a subsequent NBO6 property calculation. It is not recommended to amend or overwrite the existing route section. This requires NBO6 to be installed additionally.¹

Usage: `g16.nbo6prop.sh [opt] <file>`

-o <ARG> Add ARG to the NBO6 input stack
-r <ARG> Add ARG to route section
-R <ARG> Overwrites route section with ARG
-t <ARG> Adds ARG to end of file (overwrites -o)
-f <ARG> Filename of generated input
-m <INT> Memory (megabyte)
-p <INT> Processors
-d <INT> disksize via MaxDisk (megabyte)

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>`

This script has only the common options available.

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.

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

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 (seperated by newline)
-1 Print only one line per 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

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

Author, Bugs, and the Rest

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