Cheat-Sheet for `tools-for-g16.bash` (0.2.2, 2019-04-04)

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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.

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 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>` Overwites 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.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

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