Cheat-Sheet for `tools-for-g16.bash` (0.1.2, 2019-02-07)

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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
`-j %f` Jobname is filename filtering `.xyz`
`-j %s` Jobname is filename filtering `start.xyz`
`-f <ARG>` Filename of generated input
`-c <NUM>` Charge
`-M <INT>` Multiplicity (≥ 1)
`-U <INT>` Unpaired electrons (≥ 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 and adds relevant keywords for solvent corrections.

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
`-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 and adds relevant keywords for a frequency calculation.
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
`-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 frequency run and adds relevant keywords for two separate irc calculations.
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
`-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 an IRC run and writes and inputfile for a subsequent structure optimisation.

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.

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) or `PSUSP` (BSUB)
`-k` Only create (keep) the jobscript, do not submit it.
`-Q <ARG>` Queue for which job script should be created (`pbs-gen/bsub-rwth`)
`-P <ARG>` Account to project (BSUB); if `ARG` is `default/0/''` presets are overwritten.
`-M <ARG>` Specify a machine type (BSUB); if `ARG` is `default/0/''` presets are overwritten.
`-u <ARG>` set user email address (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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