

# 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;  $\geq 1$ )  
-U <INT> Unpaired electrons (unset;  $\geq 0$ )  
-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 [-s] -h | -a | <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  
-- Close reading options  
-s Silence script (incremental)  
-h Help file

## Author, Bugs, and the Rest

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