NAME

ONIOMLOG − Gaussian ONIOM job monitoring tool.

SYNOPSIS

oniomlog [**−d?** (?:0˜3)] [**−fn** number] [**−fo** *filename*] [**−g**] [**−h**] [**−−help**] [**−ha**] [**−i** *filename*] [**−l** [123]] [**−o**] [**−oi**] [**−q**] [**−r**] [**−s** *filename*] [**−t** *filename*]

DESCRIPTION

This program is a summary and extraction tool for Gaussian ONIOM jobs. Its main purpose is to monitor and analyze running and finished Gaussian ONIOM jobs.

OPTIONS

Command line option specifications are processed from left to right and may be specified more than once. If conflicting options are specified, later specifications override earlier ones. The input filename passed to ONIOMLOG must be a Gaussian ONIOM log file (partial or complete).

−d? (?:0˜3)	Turn on debug printing. The printing level can be controlled by a given number. The larger the number, the more information will be printed when the program is running.
−fn number	Specify the structrue from geometry optimization job log file. Default is the last output structure (0).
−fo *filename*	Write a Gaussian ONIOM input file with the new coordinates. Default is newONIOMinput.gjf.
−g	Extract atoms which are allowed to move during the optimization.
−h **−−help**	Print usage information. Cannot be used with other options.
−ha	Using absolute (not relative) energies in hatree for optimization path output
−i *filename*	Gaussian ONIOM log file.
−l [123]	Choose layers for structure extraction. 1: H layer, 2: M layer, 3: L layer. It can be any combination of 123 in any order:1, 2, 3, 12, 213, 13, 23, etc. Default is 0 when −g is used. If −l or −g are not used, level will be set to 1 (QM region). In this way, users have more flexibility to choose any part of the system.
−o	Energy of each optimized step will be extracted and printed out. If both −s and −o are used, structures along the optimization path will also be extracted and saved to the file (file name given by −s flag). The structure file can be loaded by a common visualization program (VMD for example) and played as a movie.
−oi	Write a new Gaussian ONIOM input file. This provides a method to quickly create a Gaussian input file based on a template input file and Gaussian log file. It takes coordinates from the Guassian log file and replaces the coordinates in the template file with those from the log file. In this way, the setup of the old input file (atom type, partial charges, link atoms, flag for freeze etc.) can be kept.
−q	Run in quiet mode and do not print progress messages.
−r	When used, all raw figures from Gaussian log file are displayed. By default, energies are displayed up to six decimal places. Dipole moments are displayed up to four decimal places. Partial charges are displayed up to six decimal places.
−s *filename*	Specifies the portion of the structure to be extracted and output (as XYZ file) to a file with the given file name. When this flag is not used, no structure will be extracted. When flag −s is used, a filename must be provided.
−t *filename*	Gaussian ONIOM input file to be used as a template.

EXAMPLES

oniomlog
> Called without any parameters, ONIOMLOG will display usage information. If −**h** or −−**help** is passed then the full ONIOMLOG documentation is displayed via perldoc.

oniomlog −i long.log
> Check the energy of a Gaussian ONIOM job

oniomlog −o −i long.log
> Check the energies of a Gaussian ONIOM job with optimization information

oniomlog −s oniomqm.xyz −o −i oniom.log
> Extract QM region geometries for all of the structures along an optimization from a Gaussian ONIOM job (oniom.log). and save to oniom.xyz. The ONIOM setup information is taken from the Gaussian ONIOM log file (oniom.log).

oniomlog −s oniom.xyz −t oniominput.gjf −g −i oniom.log
> Extract all the moving parts from the last structure in a Gaussian ONIOM job (oniom.log) and save to oniom.xyz. The ONIOM setup information is taken from the Gaussian ONIOM input file (oniominput.gjf). oniominput.gjf will be used as a template for the Gaussian ONIOM job setup (e.g. the moving flag). If the flag −t is not used to provide a template file, the Gaussian ONIOM job setup information will be obtained from oniom.log.

oniomlog −s oniom.xyz −l 2 −t oniominput.gjf −g −o −i oniom.log
> Extract only layer 2 for all of the structures along the optimization from a Gaussian ONIOM job (oniom.log) and save to oniom.xyz.

oniomlog −oi −t oniominput.gjf −fo new.gjf −i oniom.log
> Create a new Gaussian ONIOM input file (new.gjf) from a Gaussian job (oniom.log). A Gaussian ONIOM input file (oniominput.gjf) is needed as a template.

oniomlog −oi −fn 3 −t oniominput.gjf −fo new3.gjf −i oniom.log
> Create a new Gaussian ONIOM input file (new.gjf) using the third structure along the optimization from a Gaussian job (oniom.log). A Gaussian ONIOM input file (oniominput.gjf) is needed as a template.

VERSION
1.0

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