NAME

CHECKCONNECT − Searches for isolated atoms and atoms with multiple connections in an Gaussian ONIOM input file.

SYNOPSIS

checkconnect [−**c** number] [−**d?** (?:0˜3)] [−**g** *Gaussian_job_file_name*] [−**h**] [−**q**]

DESCRIPTION

This program looks through the connectivity table of the given Gaussian input file and searches for isolated atoms and atoms with multiple connections as sanity check for 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.

−**c** number   Any atoms with the same or more connections are printed. If this option is not used, then all the atoms with the most connections are printed.

−**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.

−**g** Gaussian_job_file_name
        Gaussian ONIOM input file.

−**h**
−−**help**   Print full CHECKCONNECT documentation via perldoc. Cannot be used with other options.

−**q**   Run in quiet mode and do not print progress messages.

EXAMPLES

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

checkconnect −g foo.gjf
    CHECKCONNECT reads foo.gif, then finds any isolated atoms and atoms with the most connections.

checkconnect −g foo.gjf −c 5
    CHECKCONNECT reads foo.gif, then finds any isolated atoms and atoms with connections equal to or larger than 5.

NOTES

CHECKCONNECT

VERSION

1.0

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