

NAME

CHARGESUM – Provides a summary of the partial charge information for an ONIOM output or input file.

SYNOPSIS

chargesum [**-d?** (? : 0 ~ 3)] [**-g** *Gaussian_ONIOM_file*] [**-h**] [**-q**] [**-r**]

DESCRIPTION

This program provides a summary of the partial charge information for an ONIOM output or input file.

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.

-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 program is running.

-g *Gaussian_ONIOM_file*
Gaussian ONIOM file, either input or output file.

-h

--help Print full CHARGESUM documentation via perldoc. Cannot be used with other options.

-q

Run in quiet mode and do not print progress messages.

-r

When used, all raw values from the Gaussian file are displayed. By default, energies are displayed with up to six decimal places. Dipole moments are displayed with up to four decimal places. Partial charges are displayed with up to six decimal places.

EXAMPLES

chargesum

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

chargesum -g foo.gjf

CHARGESUM reads foo.gjf, then sums the total partial charges of each layer of the ONIOM calculation.

NOTES

CHARGESUM can treat both two-layer and three-layer ONIOM calculations. Please interpret results based on the setup of your system.

VERSION

1.1

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