

## NAME

PARMLOOKUP – Looks up missing force field parameters for an ONIOM calculation.

## SYNOPSIS

**parmlookup** [ **-d?** (? : 0~3) ] [ **-g** *Gaussian\_ONIOM\_log\_file* ] [ **-h** ] [ **-q** ] [ **-o** *parmfilename* ]

## DESCRIPTION

This program looks up missing AMBER force field parameters for ONIOM calculations based on a given Gaussian output and AMBER parameters files. It goes through the AMBER force field parameter file for amino acids first, then the GAFF (General AMBER Force Field).

## 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 the program is running.

**-g** *Gaussian\_ONIOM\_log\_file*  
Gaussian log file. The missing parameter messages should be located at the end of this file. Other information obtained from this file includes all the atoms and their types.

**-h**

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

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

**-o** *parmfilename* Output file containing missing parameters. Default is NewParm.txt.

## EXAMPLES

parmlookup

Called with no parameters at all, PARMLOOKUP will display usage information. If **-h** or **--help** is passed, then the full PARMLOOKUP documentation is displayed via perldoc.

parmlookup -g foo.log -o fooparm.txt

PARMLOOKUP reads foo.log, then looks up missing parameters in the AMBER Force Field files and saves them to fooparm.txt.

## NOTES

If PARMLOOKUP cannot find a parameter in the AMBER force field files, a zero value is displayed. A user can estimate values for parameters that cannot be found by looking up corresponding parameters for atoms with similar atom types.

## VERSION

1.0

## AUTHOR

Peng Tao, <tao.21@osu.edu>

## COPYRIGHT

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