NAME

PDBCRD2ONIOM – Takes the coordinates from a PDB file, and puts them into a Gaussian ONIOM file

SYNOPSIS

pdbcrd2oniom [**−d?** (?:0˜3)] [**−g** *ONIOM_file_name*] [**−h**] [**−o** *output_ONIOM_file_name*] [**−pdb** *PDB_file_name*] [**−q**]

DESCRIPTION

This program generates a new Gaussian ONIOM input file from a Gaussian ONIOM input file with coordinates from a given PDB 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 the program is running.

−g *ONIOM_file_name*
: Gaussian ONIOM input file.

−h
−−help
: Print full PDBCRD2ONIOM documentation via perldoc. Cannot be used with other options.

−o *output_ONIOM_file_name*
: Output ONIOM file. Default name will be *output_ONIOM_file_name*_NEW.gjf.

−pdb *PDB_file_name*
: PDB file. Coordinates from this PDB file will be used to generate a new ONIOM input file using the given Gaussian ONIOM input file as a template.

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

EXAMPLES

pdbcrd2oniom
: Called without any parameters, PDBCRD2ONIOM will display usage information. If **−h** or **−−help** is passed then the full PDBCRD2ONIOM documentation is displayed via perldoc.

pdbcrd2oniom −g foo.gjf −pdb new.pdb −o foo_New.gjf
: PDBCRD2ONIOM reads a Gaussian ONIOM input file foo.gjf, then creates a new Gaussian ONIOM input file named foo_New.gjf using the coordinates from the PDB file new.pdb.

NOTES

PDBCRD2ONIOM is very different from PDB2ONIOM. PDB2ONIOM creates a new ONIOM input file using a PDB file. PDBCRD2ONIOM needs a PDB file and an existing Gaussian ONIOM input file as a template. These two files should have exactly the same number and types of atoms and in the exact same order. PDBCRD2ONIOM then takes ONLY coordinates from the given PDB file and replaces ONLY the coordinates in the given Gaussian ONIOM input file, nothing else.

The reason for developing this tool is that some users may find it easier to manipulate biomolecule structures when using PDB files. Using both PDBCRD2ONIOM and ONIOM2PDB, users can easily create a PDB file with an optimized geometry from a Gaussian ONIOM file using ONIOM2PDB, make some changes to the structure in the PDB file using their favorite tools (to create transition state or product, etc), and create a new ONIOM input file with modified coordinates using PDBCRD2ONIOM.

Please keep in mind that a PDB file only keeps 3 decimal places for the coordinate value. This is less than in a Gaussian ONIOM job file (6 decmial places).

VERSION

1.0

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