NAME

EXTRACTCHARGE − Extracts extracts atomic charges from a Gaussian log file and save them to a file in RESP format.

SYNOPSIS

extractcharge [**−c?** (?:1~3)] [**−d?** (?:0~3)] [**−g** *filename*] [**−h**] [**−o** *filename*] [**−q**]

DESCRIPTION

This program is an extraction tool for Gaussian output files. Its main purpose is to extract the charges of specified atoms from a Gaussian log 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.

−c? (?:1~3)   Type of charges that will be extracted from the given Gaussian log file. Currently available charge types: 1 for Mulliken charges, 2 for atomic polar tensor (APT) charges, 3 for natural population analysis (NPA) charges. Default is Mulliken charges.

−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 *filename*   Guassian log file from which the charges will be extracted.

−h
−−help   Print usage information. Cannot be used with other options.

−o *filename*   Output file which will contain extracted charges in the following format:

```
0.494560 −0.595262  0.442097  0.071576  0.220557 −0.114917 −0.521308
0.084777 −0.048257
```

Default file name is Chargefile.dat

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

EXAMPLES

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

extractcharge −c3 −g foo.log −o foo.qout
    EXTRACTCHARGE extracts NPA charges from foo.log file and writes them to foo.qout.

VERSION

1.0

AUTHOR

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

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