## NAME

ONIOMRESP – Utility to assist in the RESP charge fitting process of ONIOM calculations

## SYNOPSIS

**oniomresp** [ **−d?** (?:0~3) ] [ **−m?** 1~3 ] [ **−q** ] [ **−h** ] [ **−mid** ] [ **−g** *Gaussian_file_name* ][ **−o** *output_file_name* ] [ **−#** number ] [ **−s** step_number ] [ **−qin** *charge_qout_file* ] [ **−p** *map_file* ] [ **−c** *charge_compare_file* ] [ **−list** *atom_list_file* ]

## DESCRIPTION

This program generates a Gaussian input file for an ESP calculation or a RESP fitting input file from a Gaussian log file or takes partial charges and adds them to an ONIOM input file.

There are three different tasks that ONIOMRESP can do, therefore, there are three modes (controlled by flag −m?) to run ONIOMRESP.

mode −m1
Generate a Gaussian input file for an ESP calculation from a Gaussian log file.

mode −m2
Generate a RESP input file from a Gaussian log file

mode −m3
Take the partial charges from a given charge file and add them to a Gaussian ONIOM 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 the program is running.

**−m?** (?:1~3) Running mode setup. There are three modes: −m1, −m2, −m3.
Default (either −m or no flag) is −m1.

mode −m1
Generate a Gaussian input file for an ESP calculation from a given Gaussian log file.
The reason for using a the Gaussian log file is that scaling factors
(listed in the log file on lines ‘‘ONIOM: Cut beween’’) for positioning
the hydrogen capping atoms are available in the log file.
usage:
oniomresp −m1 −g gaussianlogfile.log −o gaussianinput_4ESP.gjf

```
Default output file name is defined as following.
If no −o flag is given, then _4ESP.gjf will be added to the base of
 the given gaussian log file.
 e.g. gaussianlogfile_4ESP.gjf will be generated
      from gaussianlogfile.log
```

mode −m2
Generate a RESP setup.in file from a Gaussian log file
usage:
oniomresp −m2 −g gaussianlogfile.log −o respsetupfile.in

```
Default output file name is defined as following.
If no −o flag is given, then _RESP.in will be added to the
  base of the given gausian log file.
 e.g. gaussianlogfile_4ESP_RESP.in will be generated from
  gaussianlogfile_4ESP.log

This mode will take the log file and generate a RESP setup.in file.
```

mode −m3

Take the partial charges from given charge file and add them to a Gaussian ONIOM input file.
usage:
oniomresp −m3 −g oniomfilename.gjf −qin RESPchargefile.qout −o newoniomfile.gjf −c chargecomparefile.txt

```
Default output file name is defined as following.
If no −o flag is given, then _NEWchg.gjf will be added to the base of
  the given gaussian ONIOM input file.
 e.g. gaussianinput_NEWchg.gjf will be generated
   from gaussianinput.gjf

chargecomparefile.txt has both old and new partial charges
   for comparison purpose
Default output file name is defined as following.
If no −c flag is given, then _CompCHG.txt will be added to the base of
  the given gaussian ONIOM input file.
 e.g. gaussianinput_CompCHG.txt will be generated from gaussianinput.g
```

Please note that depending on which mode is specified, either a Gaussian ONIOM input file or Gaussian ONIOM log file is needed.

**−h**
**−−help** Print full ONIOMRESP documentation via perldoc. Can not be used with other options.

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

**−g** *Gaussian_file_name*
Gaussian file. This file can be either an ONIOM input file or a general log file depending on the −m flag. For −m1, an ONIOM log file will be used to generate an ESP single point calculation job input file. For −m2, a Gaussian log file will be used to generate a RESP input file. For −m3, an ONIOM input file will be used to generate a new input file with new charges on the QM atoms.

**−o** *Output_file_name*
Output file. This file can be either a Gaussian or RESP input file.

−# number number represents capping hydrogen atoms in the given Gaussian log file (from ESP calculation). With this option, additional input will be added in a RESP input file to add zero charge constraint on capping hydrogen atoms. The capping hydrogens are assumed to be the last atoms listed in the coordinates.

**−mid** Used in mode 1. When set, the middle layer (instead of the high layer) of a three-layer ONIOM job will be extracted with link atoms for further (RESP) calculations. By default the high layer (usually QM region) will be extracted with link atoms.

**−s** step_number When an optimization ONIOM log file is given, user can choose the structure along the optimization path that will be used for the RESP charge fitting. Default is the last geometry.

**−c** *charge_compare_file*
Charge comparison file. It will display old and new charges together for comparison purpose.

**−qin** *charge_qout_file*
Charge file that contains all the partial charges.

**−p** *map_file* map_file builds the mapping relationship between the atoms in the ONIOM input file and the atoms in the the partial charge file.

When this file is provided, ONIOMRESP will take the charge of each atom in a given charge file *charge_qout_file* and assign it to its corresponding ONIOM atom.

Example:

3450

...

3459

3582

3583

3584

3585

Partial charge 1 in *charge_qout_file* will be assigned to atom 3450 in the ONIOM input file "..." means partial charges of atoms 1 through 10 in the charge file will be assigned to atoms 3450 through 3459 in ONIOM input file. This option saves typing time.

If this file is not provided, ONIOMRESP will just take the partial charge of each atom from the partial charge file and assign it to the QM atom in the ONIOM input file in sequence.

**−list** *atom_list_file*

File contains the list of atoms that need to be extracted from the given ONIOM log file for the ESP charge calculation.

When this file is provided, ONIOMRESP will extract corresponding atoms from the given ONIOM log file and write them to a Gaussian input file for the ESP calculation.

Format:

AtomNumber

or

AtomNumber LinkHostNumber

or

AtomNumber LinkHostNumber ScalingFactor

or

AtomNumber LinkHostNumber ScalingFactor Element

For "AtomNumber LinkHostNumber" input, a hydrogen atom will be created as a link atom using a default scaling factor (0.723886, which is for a C−H bond scaled from a C−C bond) based on coordinates of AtomNumber and LinkHostNumber.

For "AtomNumber LinkHostNumber ScalingFactor" input, a hydrogen atom will be created as link using the given sacling factor based on coordinates of AtomNumber and LinkHostNumber.

For "AtomNumber LinkHostNumber ScalingFactor Element" input, a given Element atom will be created as a link atom using the given scaling factor based on the coordinates of AtomNumber and LinkHostNumber.

Example:

3450

...

3459

3582 3590

3583

3584 3587  0.761575 H

3585

4380

...

4390

4391

4392 4399 0.761575

4393

4394

## EXAMPLES

oniomresp

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

oniomresp −m1 −g foo.log −o foo_4ESP.in

ONIOMRESP reads a Gaussian ONIOM log file foo.log, then creates a Gaussian QM single point calculation file named foo_4ESP.in for the electrostatic potential calculation.

oniomresp −m2 −g foo.log −# 3 −o fooRESP.in

ONIOMRESP reads foo.log, then creates a RESP input file named fooRESP.in. The last three atoms will be treated as capping atoms with zero partial charge constraints.

oniomresp −m3 −g foo.gjf −qin fooRESP.qout −o fooNEWchg.gjf −c fooOldNewchg.txt

ONIOMRESP reads foo.gjf and fooRESP.qout, then takes charges from fooRESP.qout, assigns them to the QM atoms in foo.gjf, and saves fooNEWchg.gjf with new RESP charges on QM atoms. The old and new charges are listed together in fooOldNewchg.txt for the user's reference.

## NOTES

ONIOMRESP

## VERSION

1.0

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