

## NAME

TRANSGEOM – Transfers optimized geometry from a model system to a production run input

## SYNOPSIS

**Transgeom** [ **-d?** (? : 0~3) ] [ **-h** ] [ **-q** ] [ **-atmp** ] [ **-atmtyp** ] [ **-chgp** ] [ **-coordp** ] [ **-layerp** ] [ **-movep** ] [ **-t** tolerance ] *filename*

## DESCRIPTION

This program extracts the atomic setup information from calculations of a model system and prepares a production run input

## 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.
- h**  
**--help** Print full TRANSGEOM documentation via perldoc. Cannot be used with other options.
- q** Run in quiet mode and do not print progress messages.
- atmp** If set, use the element information from the production ONIOM input file. Default uses model system input file.
- atmtyp** If set, use the atom type information from the production ONIOM input file. Default uses model system input file.
- chgp** If set, use the partial charges information from the production ONIOM input file. Default uses model system input file.
- coordp** If set, use the coordinate information from the production ONIOM input file. Default uses model system input file.
- movep** If set, use the move flag information from the production ONIOM input file. Default uses model system input file.
- layerp** If set, use the layer setup information from the production ONIOM input file. Default uses model system input file.
- t** tolerance Tolerance to decide if an atom has been moved during the optimization. Default is 0.00001;

*filename*

Format :

Modelgjf	ONIOM input file name for model system
Modelonb	ONIOM ONB file for model system
Productiongjf	ONIOM input file name for production run system
Productiononb	ONIOM ONB file for production run system
Productioninput	New ONIOM input file for production run system (Default)

These files can be specified in any order.

The parameter filename must be the last command line argument when running transgeom.

## EXAMPLES

transgeom

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

transgeom foo.in

TRANSGEOM reads foo.in, then creates a production run input. Please note that there is no flag needed before setup file name in command line. Sample foo.in

Modelgif      ONIOMmodelinput.gif  
Modelonb      ONIOMmodelinput.onb  
Productiongif    ONIOMproductioninput.gif  
Productiononb    ONIOMproductioninput.onb  
Productioninput   ONIOMproductioninputwithmodelgeom.gif

## **NOTES**

The model system is not necessary smaller than the production system. A full protein model can be used as a model system, and a reduced size model for the same protein can be used as the production system. TRANSGEOM will extract corresponding portion of the geometry from the full size model and build a partial model.

## **VERSION**

1.1

## **AUTHOR**

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

## **COPYRIGHT**

Copyright (c) 2009~2010 by Peng Tao