Documentation for Auto_THERM

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Auto_THERM is a python program that can calculate all the inputs needed to find thermodynamic properties of a chemical species using THERM, a software which uses group additivity method. This program can also perform group additivity using the group databases in THERM.

1 System Requirements

- OS : Ubuntu or Windows. (This document is written for Ubuntu)
- Python 2.7
- RDKit - an open-source package.

2 Installation

- Python is default in Ubuntu.
- Installing RDKit : Open terminal. Type : 'sudo apt-get install python-rdkit'

3 Initial setup

This is a program that acts as a preprocessing tool for THERM. Hence, if THERM is present in the system, its path needs to be provided to this program. Because, this program can perform the group additivity on its own, using the group database of THERM, and can create an output file with extension .LST, which can be directly input to THERM for fitting the NASA polynomial. Hence, for obtaining thermodynamic properties of a species, what user has to essentially do is to provide this .LST file as input to THERM than typing in all the values provided by this program into THERM.

If THERM is not present, this program still gives output as those input values needed to run THERM, and these values can be input to THERM manually after installing THERM.

- Copy all files into one folder.
- Open 'therm.config' file and edit these entries (as applicable) :
  - $PATH\_TO\_THERM$ = Absolute path to THERM ($/home/path\_to\_therm/$)
  - $HC\_GROUPS\_FILENAME$ = Hydrocarbon group filename in THERM
  - $HCO\_GROUPS\_FILENAME$ = Hydrocarbon-oxygen group filename in THERM
  - $INT\_GROUPS\_FILENAME$ = Steric interacion groups filename in THERM
  - $BD\_GROUPS\_FILENAME$ = Bond dissociation groups filename in THERM
  - $OUTPUT\_FOLDER$ = Absolute path to output folder, where all the output files should be created.
  - $WAIT\_TIME$ = Time in seconds, the code will wait for manual input of bond dissociation group.

- R = Universal gas constant value (cal/molK)
- hf_H = Standard heat of formation of hydrogen radical at 298K (kcal/mol)

therm.config : This is a text file which is very important in the working of this program. Comments can be provided in this file by putting a '#' before that line. Blank lines can also be provided. It should be taken care that the format of this file should not be changed, i.e. the spaces or tabs present in this file should not be removed. Also, the keys written in this file (mentioned above) should not be changed. Only, value of each keys should be changed.

4 Running the program

After initial setup,

- Open terminal and change directory to the folder where all the files were copied.
- Make the file 'Auto_THERM.py' executable. Type in terminal :
  $chmod\ +x\ Auto\_THERM.py$
- Now, the file 'Auto_THERM.py' can be run by giving inputs as arguments.

5 Input Arguments

Input arguments to 'Auto_THERM.py' can be specified using flags :
In one run of the program, among -s, -sf and -mf, only one should be given as argument.

-s	Specifying SMILES of a species.
-sf	Providing SMILES of many species written in a text file.
-mf	Providing molfile of a species as input to the program.
-o	Specifying output filename for .LST file.
-doc	Specifying output filename for .DOC file.

5.1 -s flag

This is to input SMILES of one species. Its syntax is :

-s <"SMILES"> <"Name_of_species">

Here, SMILES and Name_of_species should be enclosed in single or double quotes. Name_of_species is an optional argument. If it is not specified, by default the name of the species will be taken as "Molecule".
P.S. Length of name of the species should not exceed nine characters because, THERM support only names with maximum of nine characters. If user is writing a name with more than nine characters, first nine characters of that name will be taken as the name of the species.

5.2 -sf flag

This is to provide many species at a time as input to the program. A text file containing SMILES of many species can be created.

Format of the text file: In the text file, a line should contain only one SMILES and also, it should be the first entry in that line. Second entry should be the name of the species. This is an optional argument. If name is not specified, by default name of that species will be "Mol*", where * will be the number of that species in that text file. Third entry should be the bond dissociation group if the species is a radical. This is also an optional argument and if it is not specified, bond dissociation group will be found out by the program and user will have an option to change if he is not satisfied with that group while running the program. Hence, one line in SMILES text file will look like :

<SMILES> <Name> <BD_group>

If user has to provide bond dissociation group without providing name of the species, then, in place of name of the species, '*' can be written. Example :

<SMILES> * <BD_group>

In this text file, blank lines are allowed and also, lines can be commented out by providing a '#' in front.

To provide this file as an input to the program, syntax is :

-sf <Path_to_text_file>

Here, path can be absolute or relative.
P.S. Length of name of the species should not exceed nine characters because, THERM support only names with maximum of nine characters. If user is writing a name with more than nine characters, first nine characters of that name will be taken as the name of the species.

5.3 -mf flag

This is to provide molfile of the species as input to the program. Syntax :

-mf <Path_to_molfile> <"Name_of_species">

Here, path can be absolute of relative and name of the species should be written within single or double quotes.
P.S. Length of name of the species should not exceed nine characters because, THERM support only names with maximum of nine characters. If user is writing a name with more than nine characters, first nine characters of that name will be taken as the name of the species.

5.4 -o flag

This is used to provide name of .LST file which is created after performing group additivity. This .LST file will be created only if this flag is provided. This file can be given as input to THERMFIT, which is a feature in THERM that fits the NASA polynomials. While providing the name of the file, extension should not be given. For example, name can be given as THERMO, but not THERMO.LST, because, the extension .LST will be filled by the program, by default. This file will be created at the location provided at the OUTPUT_FOLDER key in 'therm.config' file. Syntax :

-o <Name_of_file>

If this flag is provided, group additivity will be done by the program and hence if the species is a radical the program will find a bond dissociation group and will ask the user if he/she wants to change it. Program will wait for that much amount of time specified in the WAIT_TIME key in 'therm.config' file. If within this time, there was no press of Enter key, program will continue its calculation with the bond dissociation group evaluated by the program. However, if Enter key was pressed within this wait time, user will be asked to enter new bond dissociation group and that group will be used for further calculations.

5.5 -doc flag

This is used to provide the name of .DOC file, which contains the input values needed for THERM about a species. It essentially writes the terminal output to a text file with extension .DOC. Here also, similar to the .LST file, name should not be written with extension. Extension .DOC will be filled by the program, by default. This file will also be created at the location specified at the OUTPUT_FOLDER key in 'therm.config' file. Syntax :

-doc <Name_of_file>