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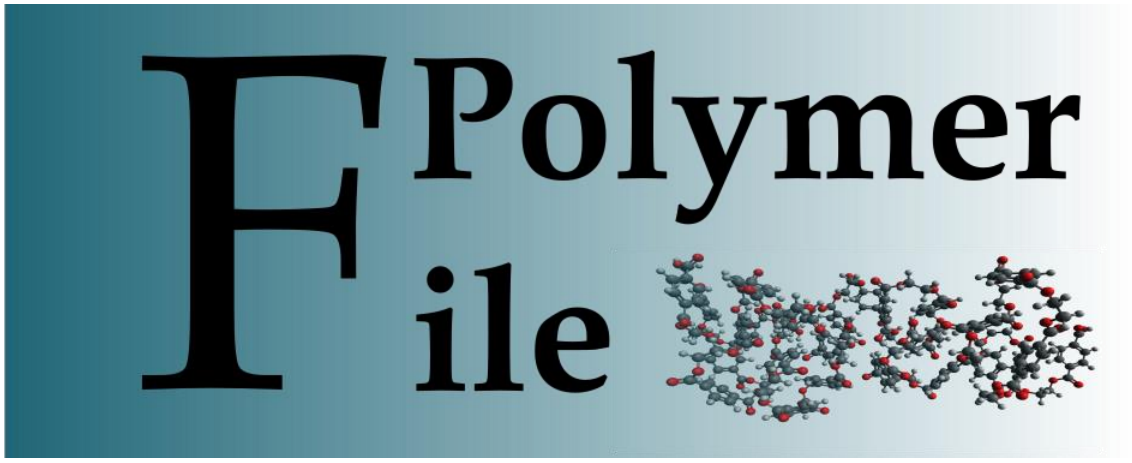


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# FPolymer

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A program for generating 3D structure files and OPLS topology of oligomers and polymers with high molecular mass

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**Version 1.0.0**

# User Guide

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# FPolymer 1.0.0

## Development team

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# Summary

# 1. INTRODUCTION

Polymers are the most used materials in the world and are present in virtually all segments. The great ease they present in being worked through process such as molding, and extrusion is one of the reasons that s makes it the best option for production from packaging to component and industrial equipment.

The word polymer originates from the Greek poly (many) and mere (repetition). Thus, a polymer is a substance composed of many repeating units that are called mere. The mere sums combine through covalent chemical bonds forming molecules of high home molecular weight and are usually considered compound polymers with molar mass MM>10000g·mol$^{-1}$, for substances with molar mass lower than this the correct term to be used is oligomer.

Due to their high size, the physical properties of polymers receive a greater contribution from intermolecular and intramolecular lures interactions, given that the larger the mass, the greater the number of repeating units and consequently the interaction energy. Because interaction energy is directly linked to macroscopic properties of polymers, molecular modeling techniques can be used to describe and predict polymer behaviors.

Molecular dynamics is a technique that uses the classical description for the atoms that make up a substance and, thus, has limitations, such as studies involving the electronic nature of matter. However, for studies involving problems that can be solved using classical methods, molecular dynamics is ideal mainly due to the possibility of working with systems of high size at a relatively low computational cost.

Despite the vast possibilities of work, study of polymeric systems using molecular dynamics, they are still not very common which can be attributed in parts because of the difficulty of creating the systems to undergo free programs capable of performing such calculations. Not many specific force fields for polymers are found, and the process

of parameterization of large molecules is unfeasible to be done manually and some existing programs for this purpose fail for large systems.

Thinking about it the FPolymer program was created to be an option for creating polymeric systems that can be used in the GROMACS program (https://www.gromacs.org/) which is a free use software and widely used for the treatment of biological systems that already has a range of results analysis tools.

## 2. OPERATING PRINCIPLES

The FPolymer program has a relatively simple function, it takes advantage of a property present in the very definition of polymers which is the fact that the polymer molecule is formed by a series of repetitions of a basic unit called mere. As the mere is repeated during the structure of the polymer all types of atoms present in the molecule can be found in this small unit. The exceptions are the atoms used to fetcher the valences of the beginning and end of the chain, to work around this problem and account in fact all can be used trimer structures where they will be present beyond the mere itself, the mere ending of the beginning and end of the structure.

In view of what has been said, the FPolymer program uses previously parameterized trimers available in its database and creates repetitions of the central mere of the trimer so that the final structure has the desired size. For this the program recalculates the coordinates of each atom to generate the <file>.pdb and adds all the connection information between the new meres in the file <file>.top. Thus, it is possible to obtain a representation capable of generating good results when submitted to a dynamic.

## 3. PROGRAM STRUCTURE

The FPolymer program is composed of a simple home screen where it is possible to indicate the parameters for generating the desired polymer structure. In your menu bar you can see three options where "tools" contain ferramenta such as adding new polymers to the

program database, "help" has a link to this manual and some quick information about problems and "the bout" presents a brief description of the program, researchers involved in its development and other information. Figure 1 shows the program interface.

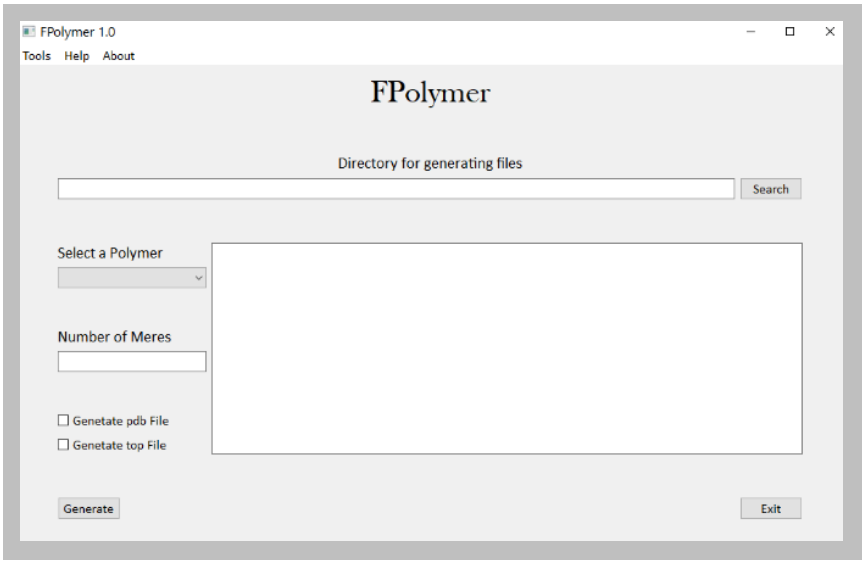


*Figure 1 - FPolymer program start screen*

## 4. ADDING A POLYMER TO THE DATABASE

FPolymer does not have polymers pre-added to its database (we are working on it for the next versions). However, there is the possibility to add the structure you want so that the program recognizes it and can generate the area work structures. For this it is necessary to get some.

### 4.1. GETTING THE FILES YOU NEED

To add new polymers, two. The first file is a coordinate file where data from the three-dimensional structure of a polymer trimer to be added is described. This file must be in PDB format and must be constructed following some criteria. For creation is recommended the use of the software AVOGADRO (https://avogadro.cc/). During the construction process, care should be taken to add the atoms in order so that the atoms belonging to the first mere are placed first (Figure 2 – A) and only after all the atoms of the central mere have been created (Figure 2 – B) and finally add the atoms of the

trimer terminal mere (Figure 2 – C). In addition, it is desirable that the trimer be oriented in space near the X axis otherwise problems may be encountered when generating structures from this data.

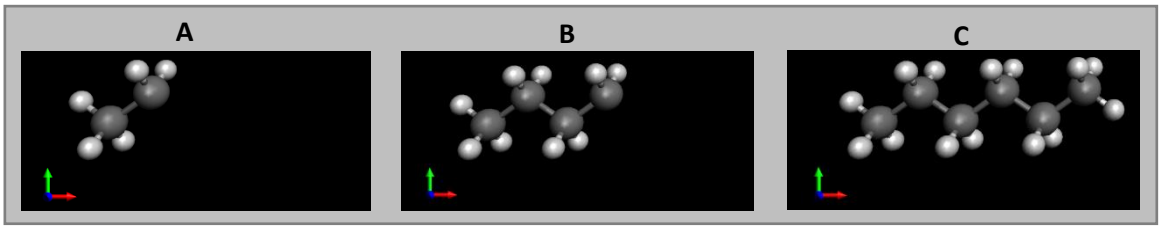


*Figure 2 - Steps for creating the trimer structures file to be added to FPolymer. "A" - Initial I was M; "B" - The addition of the central mere to the structure; "C" - The addition of the mere terminal of the trimer.*

The required file is generated through the trimer parameterization process. For now, FPolymer is not able to parameterize molecules (soon we will work on it), so to generate this file, it is recommended to use the PROGRAM ACPYPE (https://doi.org/10.1186/1756-0500-5-367). After parameterization, a file is generated <File>. itp with the description of all atoms of the molecule for the force field. This file needs to be adjusted manually and then can be added to the program's data lame.

A care that should be taken, is to ensure that the programs used for treatment and parameterization do not reheat the atoms. This can happen in cases of geometric optimization or other adjusting in other programs.

## 4.2. PREPARING FILES TO BE USED

The <File>.pdb does not require adjustments to be added to the program database, however, the <File>.itp must be adjusted. Initially this file has, in addition to the desired information, several lines of comments as can be seen in annex 1 of this manual. In this file all constants are indicated as comments by adding the character ";". For use, you must remove this character. All other comment lines should also be deleted, an example of how the file should look in Annex 2 of that manual. The final file must be saved as <file>.top.

## 4.3. PROCEDURE

To add new polymers to the database just click on the "tools -> add new Polymer" menu and a new window will open as shown in Figure 3.

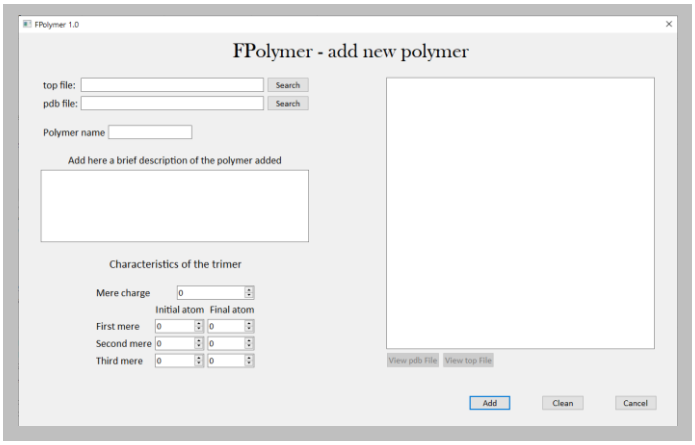


*Figure 3 - New polymer addition screen to the program database*

In this window, the first thing to do is to select the <File>.top and <File>.pdb referring to the polymer trimer that will be added. You can then view the contents of the files by clicking "View pdb file" or "View top file".

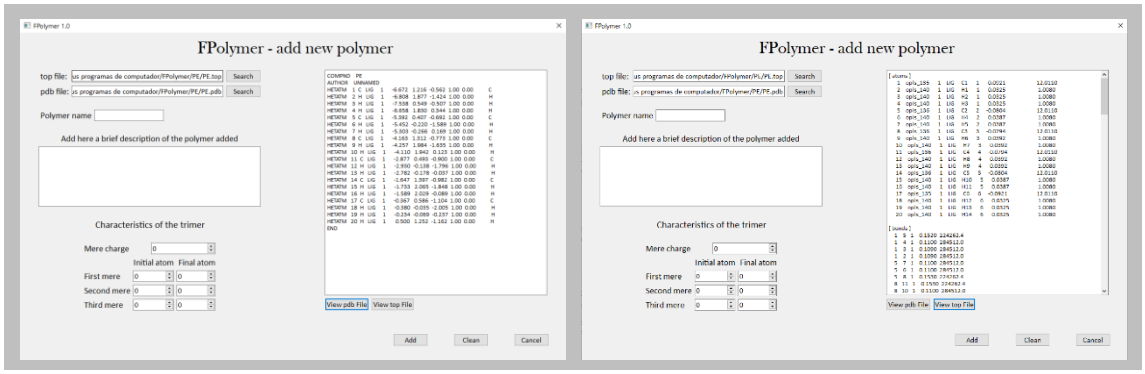


*Figure 4 - Display of the selected trimer files*

In the "Polymer name" field, the name of the polymer must be added. It is important that the name chosen is not equal to any other that has already been previously added otherwise an error message should be issued. The program also allows the addition of a brief description that will be displayed whenever the polymer is selected for creation.

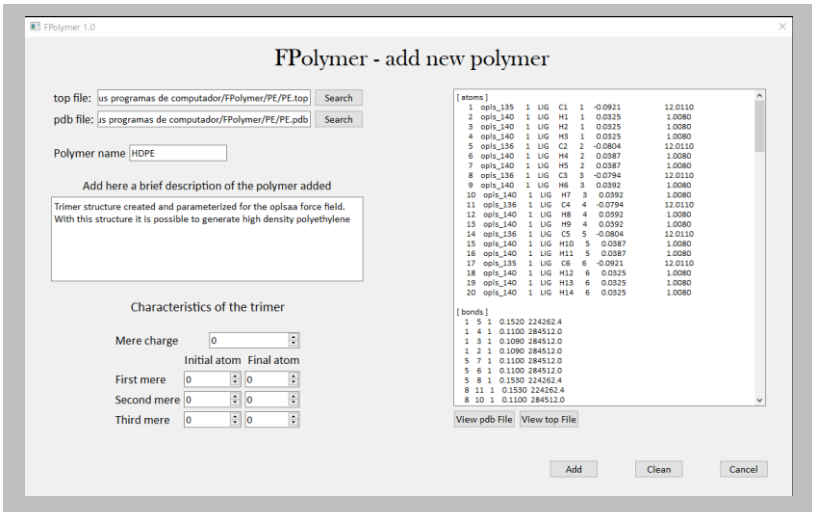


*Figure 5 - Insertion of the polymer name and desired description.*

Next, the load of a mere must be indicated, remembering that it is not the load of the trimer, but the load of a single mere that must be informed. With this information, some checks are made and if the load of the files is different from the reported an alert is issued.

The last step to add the polymer and indicate what are the initial and final atoms of each mere. To do this, the file view of the <File>.pdb by clicking "View pdb file" on the display screen you can manipulate the file without the seam changes saved. This allows you to separate the mere ones to make it easier to obtain the data.

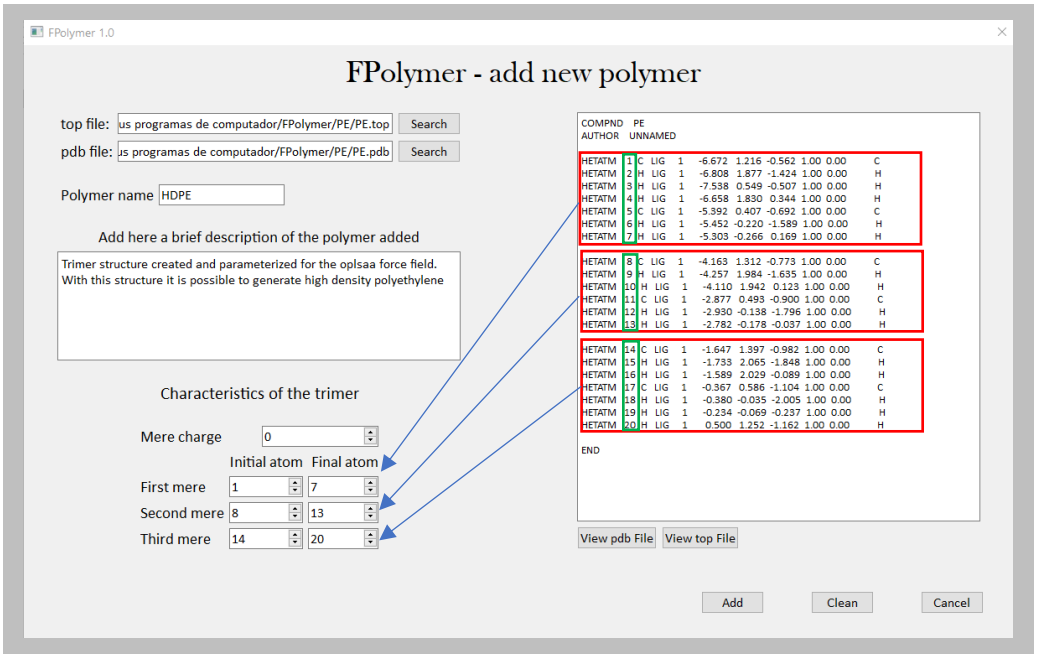


*Figure 6 - identification and indication of the initial and final atoms of each mere.*

After all the fields are filled in just click on the "add" button, polymer will be added to the database and then can be used to create structures of the desired size.

After adding the polymer to the database, it is recommended to restart the program so that it appears in the list of polymers for generation. After restarting, you should create a structure of at least 10 meres and check for any problems in any of the files. Depending on the complexity of the polymer mere and the type of links involved, some manual adjustments may be required in the database files for error correction where the files generated by FPolymer have links between atoms that do not exist. If this occurs folder follow the following steps.

Using your file explorer, navigate to the FPolymer installation folder. There you will find the "structures" folder inside it there will be folders with the name of each polymer that has been added to the program. Find the folder with the name of the polymer that presented problem go to the folder. After accessing the folder you will find four files but what interests us at this time is the file <Polymer name>.conf. Open this file with a text editor of your choice and in item 30-Correction_factor, change the value from zero (0) to one (1), save the change restart the FPolymer and regenerate the file to see if the problem has been fixed. If p problem persists delete the polymer folder and reface the process of adding to the database.

## 5. CREATING A POLYMER FROM THE DATABASE

The process of generating files from the database is quite simple and intuitive. Simply select the folder where the files should be created, select the desired polymer name from a drop-down list to indicate the number of mere ones, and mark which files should be generated. Once this is done just click the "Generate" button and a message indicating the success of the operation will be issued and ready, your files will be generated and ready for use in Gromacs.

It is important to always check your topology to verify that there are no inconsistencies, especially when it is the first time that files are generated after they are added to the database.

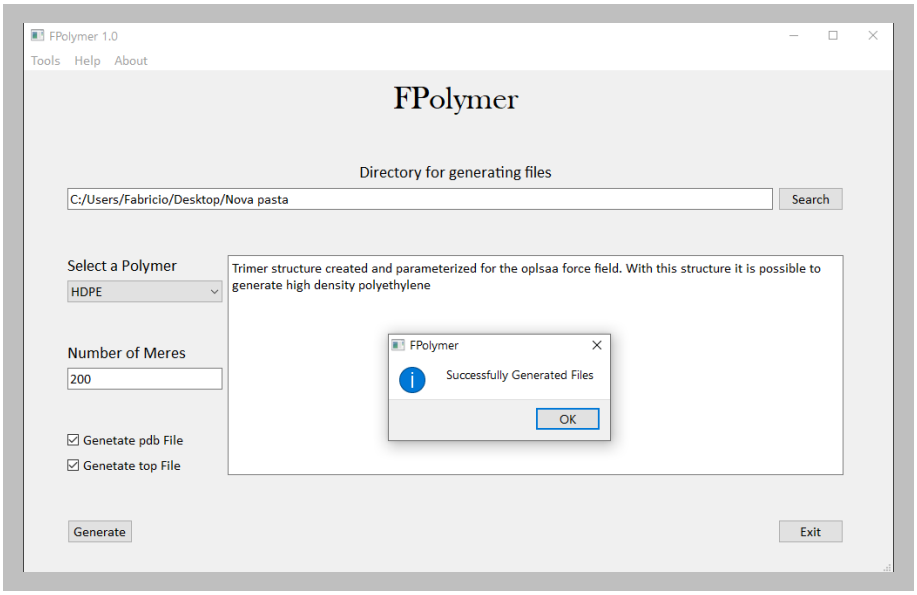


*Figure 7 - Example of file generation using the program database*

## 6. PROBLEMS AND SUGGESTIONS

We encourage you to submit information about problems encountered as well as are also open to suggestions to improve the program. Because it is a new project and without specific funding, we do not have a set schedule for the release of new versions. However, all messages sent by users will be considered and as soon as possible, new versions will be made available with the fixes as needed.

# ANNEXES

# Annex 1 - Example of acpype-generated itp file for a Polyethylene trimer

```
; pe_GMX_OPLS.itp created by acpype (Rev: 373) on Wed Jul 14 21:42:36 2021

; For OPLS atomtypes manual fine tuning
; AC_at:OPLS_at:OPLScode: Possible_Aternatives (see ffoplsaa.atp and ffoplsaanb.itp)
; c3:CT:opls_135: ['136', '137', '149', '157', '158', '206', '209', '210', '223B', '224B', '245', '246', '274', '283', '284', '285', '292', '292B', '293B', '296', '307', '308', '505']
; hc:HC:opls_140: []

[ moleculetype ]
;name            nrexcl
 on the 3rd

[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge      mass       ; qtot   bond_type
     1 opls_135 1 THE C1 1 -0.093100 12.01100 ; qtot -0.093 ct
     2 opls_140 1 THE HH1 2 0.032700 1.00800 ; qtot -0.060 HC
     3 opls_140 1 IT H1 3 0.032700 1.00800 ; qtot -0.028 HC
     4 opls_140 1 IT H2 4 0.032700 1.00800 ; qtot 0.005 HC
     5 opls_135 1 THE C2 5 -0.080400 12.01100 ; qtot -0.075 ct
     6 opls_140 1 THE HH2 6 0.038700 1.00800 ; qtot -0.037 HC
     7 opls_140 1 IT H3 7 0.038700 1.00800 ; qtot 0.002 HC
     8 opls_135 1 THE C3 8 -0.079400 12.01100 ; qtot -0.077 ct
     9 opls_140 1 IT HH3 9 0.038700 1.00800 ; qtot -0.039 HC
    10 opls_140 1 IT H4 10 0.038700 1.00800 ; qtot 0.000 hc
    11 opls_135 1 THE C4 11 -0.079400 12.01100 ; qtot -0.079 ct
    12 opls_140 1 THE HH4 12 0.038700 1.00800 ; qtot -0.041 HC
    13 opls_140 1 IT H5 13 0.038700 1.00800 ; qtot -0.002 HC
    14 opls_135 1 THE C5 14 -0.080400 12.01100 ; qtot -0.082 ct
    15 opls_140 1 THE HH5 15 0.038700 1.00800 ; qtot -0.044 HC
    16 opls_140 1 IT H6 16 0.038700 1.00800 ; qtot -0.005 HC
    17 opls_135 1 THE C6 17 -0.093100 12.01100 ; qtot -0.098 ct
    18 opls_140 1 THE HH6 18 0.032700 1.00800 ; qtot -0.065 HC
    19 opls_140 1 IT H7 19 0.032700 1.00800 ; qtot -0.033 HC
    20 opls_140 1 IT H8 20 0.032700 1.00800 ; qtot 0.000 hc

[ bonds ]
;   you aj funct r k
     1 2 1 ;   1.0920e-01 2.8225e+05 ;    C1 - HH1 CT - HC
     1 3 1 ;   1.0920e-01 2.8225e+05 ;    C1 - H1 CT - HC
     1 4 1 ;   1.0920e-01 2.8225e+05 ;    C1 - H2 CT - HC
     1 5 1 ;   1.5350e-01 2.5363e+05 ;    C1 - C2 CT - CT
     5 6 1 ;   1.0920e-01 2.8225e+05 ;    C2 - HH2 CT - HC
     5 7 1 ;   1.0920e-01 2.8225e+05 ;    C2 - H3 CT - HC
     5 8 1 ;   1.5350e-01 2.5363e+05 ;    C2 - C3 CT - CT
     8 9 1 ;   1.0920e-01 2.8225e+05 ;    C3 - HH3 CT - HC
     8 10 1 ;   1.0920e-01 2.8225e+05 ;    C3 - H4 CT - HC
     8 11 1 ;   1.5350e-01 2.5363e+05 ;    C3 - C4 CT - CT
    11 12 1 ;   1.0920e-01 2.8225e+05 ;    C4 - HH4 CT - HC
    11 13 1 ;   1.0920e-01 2.8225e+05 ;    C4 - H5 CT - HC
    11 14 1 ;   1.5350e-01 2.5363e+05 ;    C4 - C5 CT - CT
    14 15 1 ;   1.0920e-01 2.8225e+05 ;    C5 - HH5 CT - HC
    14 16 1 ;   1.0920e-01 2.8225e+05 ;    C5 - H6 CT - HC
    14 17 1 ;   1.5350e-01 2.5363e+05 ;    C5 - C6 CT - CT
    17 18 1 ;   1.0920e-01 2.8225e+05 ;    C6 - HH6 CT - HC
    17 19 1 ;   1.0920e-01 2.8225e+05 ;    C6 - H7 CT - HC
    17 20 1 ;   1.0920e-01 2.8225e+05 ;    C6 - H8 CT - HC

[ pairs ]
;   you aj funct
     1     9     1 ;    C1 - HH3
     1    10     1 ;    C1 - H4
     1    11     1 ;    C1 - C4
     2     6     1 ;   HH1 - HH2
     2     7     1 ;   HH1 - H3
     2     8     1 ;   HH1 - C3
     3     6     1 ;    H1 - HH2
     3     7     1 ;    H1 - H3
     3     8     1 ;    H1 - C3
     4     6     1 ;    H2 - HH2
     4     7     1 ;    H2 - H3
     4     8     1 ;    H2 - C3
     5    12     1 ;    C2 - HH4
     5    13     1 ;    C2 - H5
     5    14     1 ;    C2 - C5
     6     9     1 ;   HH2 - HH3
     6    10     1 ;   HH2 - H4
     6    11     1 ;   HH2 - C4
     7     9     1 ;   H3 - HH3
     7    10     1 ;    H3 - H4
     7    11     1 ;    H3 - C4
     8    15     1 ;    C3 - HH5
     8    16     1 ;    C3 - H6
     8    17     1 ;    C3 - C6
     9    12     1 ;   HH3 - HH4
     9    13     1 ;   HH3 - H5
     9    14     1 ;   HH3 - C5
    10    12     1 ;    H4 - HH4
    10    13     1 ;    H4 - H5
    10    14     1 ;    H4 - C5
    11    18     1 ;    C4 - HH6
    11    19     1 ;    C4 - H7
    11    20     1 ;    C4 - H8
    12    15     1 ;   HH4 - HH5
    12    16     1 ;   HH4 - H6
    12    17     1 ;   HH4 - C6
    13    15     1 ;    H5 - HH5
    13    16     1 ;    H5 - H6
    13    17     1 ;    H5 - C6
    15    18     1 ;   HH5 - HH6
    15    19     1 ;   HH5 - H7
```

```
   15    20     1 ;   HH5 - H8
   16    18     1 ;   H6 - HH6
   16    19     1 ;   H6 - H7
   16    20     1 ;   H6 - H8

[ angles ]
;   ai if funct theta cth
    1     5     6     1 ;   1.1005e+02   3.8802e+02 ;    C1 - C2  - HH2     CT -  CT - HC
    1     5     7     1 ;   1.1005e+02   3.8802e+02 ;    C1 - C2  - H3      CT -  CT - HC
    1 5 8 1 ;   1.1063e+02 5.2894e+02 ;    C1 - C2 - C3 CT - CT - CT
    2     1     3     1 ;   1.0835e+02   3.2995e+02 ;   HH1 - C1  - H1      HC -  CT - HC
    2     1     4     1 ;   1.0835e+02   3.2995e+02 ;   HH1 - C1  - H2      HC -  CT - HC
    2     1     5     1 ;   1.1005e+02   3.8802e+02 ;   HH1 - C1  - C2      HC -  CT - CT
    3     1     4     1 ;   1.0835e+02   3.2995e+02 ;    H1 - C1  - H2      HC -  CT - HC
    3     1     5     1 ;   1.1005e+02   3.8802e+02 ;    H1 - C1  - C2      HC -  CT - CT
    4     1     5     1 ;   1.1005e+02   3.8802e+02 ;    H2 - C1  - C2      HC -  CT - CT
    5     8     9     1 ;   1.1005e+02   3.8802e+02 ;    C2 - C3  - HH3     CT -  CT - HC
    5     8    10     1 ;   1.1005e+02   3.8802e+02 ;    C2 - C3  - H4      CT -  CT - HC
    5 8 11 1 ;   1.1063e+02 5.2894e+02 ;    C2 - C3 - C4 CT - CT - CT
    6     5     7     1 ;   1.0835e+02   3.2995e+02 ;   HH2 - C2  - H3      HC -  CT - HC
    6     5     8     1 ;   1.1005e+02   3.8802e+02 ;   HH2 - C2  - C3      HC -  CT - CT
    7     5     8     1 ;   1.1005e+02   3.8802e+02 ;    H3 - C2  - C3     HC -  CT - CT
    8    11    12     1 ;   1.1005e+02   3.8802e+02 ;    C3 - C4  - HH4     CT -  CT - HC
    8    11    13     1 ;   1.1005e+02   3.8802e+02 ;    C3 - C4  - H5      CT -  CT - HC
    8 11 14 1 ;   1.1063e+02 5.2894e+02 ;    C3 - C4 - C5 CT - CT - CT
    9     8    10     1 ;   1.0835e+02   3.2995e+02 ;   HH3 - C3  - H4      HC -  CT - HC
    9     8    11     1 ;   1.1005e+02   3.8802e+02 ;   HH3 - C3  - C4      HC -  CT - CT
   10     8    11     1 ;   1.1005e+02   3.8802e+02 ;    H4 - C3  - C4     HC -  CT - CT
   11    14    15     1 ;   1.1005e+02   3.8802e+02 ;    C4 - C5  - HH5     CT -  CT - HC
   11    14    16     1 ;   1.1005e+02   3.8802e+02 ;    C4 - C5  - H6      CT -  CT - HC
   11 14 17 1 ;   1.1063e+02 5.2894e+02 ;    C4 - C5 - C6 CT - CT - CT
   12    11    13     1 ;   1.0835e+02   3.2995e+02 ;   HH4 - C4  - H5      HC -  CT - HC
   12    11    14     1 ;   1.1005e+02   3.8802e+02 ;   HH4 - C4  - C5      HC -  CT - CT
   13    11    14     1 ;   1.1005e+02   3.8802e+02 ;    H5 - C4  - C5     HC -  CT - CT
   14    17    18     1 ;   1.1005e+02   3.8802e+02 ;    C5 - C6  - HH6     CT -  CT - HC
   14    17    19     1 ;   1.1005e+02   3.8802e+02 ;    C5 - C6  - H7      CT -  CT - HC
   14    17    20     1 ;   1.1005e+02   3.8802e+02 ;    C5 - C6  - H8      CT -  CT - HC
   15    14    16     1 ;   1.0835e+02   3.2995e+02 ;   HH5 - C5  - H6      HC -  CT - HC
   15    14    17     1 ;   1.1005e+02   3.8802e+02 ;   HH5 - C5  - C6      HC -  CT - CT
   16    14    17     1 ;   1.1005e+02   3.8802e+02 ;    H6 - C5  - C6     HC -  CT - CT
   18    17    19     1 ;   1.0835e+02   3.2995e+02 ;   HH6 - C6  - H7      HC -  CT - HC
   18    17    20     1 ;   1.0835e+02   3.2995e+02 ;   HH6 - C6  - H8      HC -  CT - HC
   19    17    20     1 ;   1.0835e+02   3.2995e+02 ;    H7 - C6  - H8     HC -  CT - HC

[ dihedrals ] ; Next
; treated as RBs in GROMACS to use combine multiple AMBER torsions per quartet
;   i j k l func C0 C1 C2 C3 C4 C5
    1     5     8     9     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   C1-   C2-   C3-   HH3     CT-  CT-  CT-  HC
    1     5     8    10     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   C1-   C2-   C3-   H4      CT-  CT-  CT-  HC
    1     5     8    11     3 ;   3.68192   3.09616  -2.09200  -3.01248   0.00000   0.00000 ;   C1-   C2-   C3-   C4      CT-  CT-  CT-  CT
    2     1     5     6     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   HH1-  C1-   C2-   HH2     HC-  CT-  CT-  HC
    2     1     5     7     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   HH1-  C1-   C2-   H3      HC-  CT-  CT-  HC
    2     1     5     8     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   HH1-  C1-   C2-   C3      HC-  CT-  CT-  CT
    3     1     5     6     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H1-   C1-   C2-   HH2     HC-  CT-  CT-  HC
    3     1     5     7     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H1-   C1-   C2-   H3      HC-  CT-  CT-  HC
    3     1     5     8     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   H1-   C1-   C2-   C3      HC-  CT-  CT-  CT
    4     1     5     6     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H2-   C1-   C2-   HH2     HC-  CT-  CT-  HC
    4     1     5     7     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H2-   C1-   C2-   H3      HC-  CT-  CT-  HC
    4     1     5     8     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   H2-   C1-   C2-   C3      HC-  CT-  CT-  CT
    5     8    11    12     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   C2-   C3-   C4-   HH4     CT-  CT-  CT-  HC
    5     8    11    13     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   C2-   C3-   C4-   H5      CT-  CT-  CT-  HC
    5     8    11    14     3 ;   3.68192   3.09616  -2.09200  -3.01248   0.00000   0.00000 ;   C2-   C3-   C4-   C5      CT-  CT-  CT-  CT
    6     5     8     9     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   HH2-  C2-   C3-   HH3     HC-  CT-  CT-  HC
    6     5     8    10     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   HH2-  C2-   C3-   H4      HC-  CT-  CT-  HC
    6     5     8    11     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   HH2-  C2-   C3-   C4      HC-  CT-  CT-  CT
    7     5     8     9     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H3-   C2-   C3-   HH3     HC-  CT-  CT-  HC
    7     5     8    10     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H3-   C2-   C3-   H4      HC-  CT-  CT-  HC
    7     5     8    11     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   H3-   C2-   C3-   C4      HC-  CT-  CT-  CT
    8    11    14    15     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   C3-   C4-   C5-   HH5     CT-  CT-  CT-  HC
    8    11    14    16     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   C3-   C4-   C5-   H6      CT-  CT-  CT-  HC
    8    11    14    17     3 ;   3.68192   3.09616  -2.09200  -3.01248   0.00000   0.00000 ;   C3-   C4-   C5-   C6      CT-  CT-  CT-  CT
    9     8    11    12     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   HH3-  C3-   C4-   HH4     HC-  CT-  CT-  HC
    9     8    11    13     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   HH3-  C3-   C4-   H5      HC-  CT-  CT-  HC
    9     8    11    14     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   HH3-  C3-   C4-   C5      HC-  CT-  CT-  CT
   10     8    11    12     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H4-   C3-   C4-   HH4     HC-  CT-  CT-  HC
   10     8    11    13     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H4-   C3-   C4-   H5      HC-  CT-  CT-  HC
   10     8    11    14     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   H4-   C3-   C4-   C5      HC-  CT-  CT-  CT
   11    14    17    18     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   C4-   C5-   C6-   HH6     CT-  CT-  CT-  HC
   11    14    17    19     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   C4-   C5-   C6-   H7      CT-  CT-  CT-  HC
   11    14    17    20     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   C4-   C5-   C6-   H8      CT-  CT-  CT-  HC
   12    11    14    15     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   HH4-  C4-   C5-   HH5     HC-  CT-  CT-  HC
   12    11    14    16     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   HH4-  C4-   C5-   H6      HC-  CT-  CT-  HC
   12    11    14    17     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   HH4-  C4-   C5-   C6      HC-  CT-  CT-  CT
   13    11    14    15     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H5-   C4-   C5-   HH5     HC-  CT-  CT-  HC
   13    11    14    16     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H5-   C4-   C5-   H6      HC-  CT-  CT-  HC
   13    11    14    17     3 ;   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000 ;   H5-   C4-   C5-   C6      HC-  CT-  CT-  CT
   15    14    17    18     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   HH5-  C5-   C6-   HH6     HC-  CT-  CT-  HC
   15    14    17    19     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   HH5-  C5-   C6-   H7      HC-  CT-  CT-  HC
   15    14    17    20     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   HH5-  C5-   C6-   H8      HC-  CT-  CT-  HC
   16    14    17    18     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H6-   C5-   C6-   HH6     HC-  CT-  CT-  HC
   16    14    17    19     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H6-   C5-   C6-   H7      HC-  CT-  CT-  HC
   16    14    17    20     3 ;   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000 ;   H6-   C5-   C6-   H8      HC-  CT-  CT-  HC
```

## Annex 2 - Example of top file generated through manual modification performed in an itp file for a polyethylene trimer

```
[ atoms ]
    1 opls_135 1 IT C1 1 -0.093100 12.01100
    2 opls_140 1 IT HH1 2 0.032700 1.00800
    3 opls_140 1 IT H1 3 0.032700 1.00800
    4 opls_140 1 IT H2 4 0.032700 1.00800
    5 opls_135 1 IT C2 5 -0.080400 12.01100
    6 opls_140 1 IT HH2 6 0.038700 1.00800
    7 opls_140 1 IT H3 7 0.038700 1.00800
    8 opls_135 1 THE C3 8 -0.079400 12.01100
    9 opls_140 1 IT HH3 9 0.038700 1.00800
   10 opls_140 1 IT H4 10 0.038700 1.00800
   11 opls_135 1 IT C4 11 -0.079400 12.01100
   12 opls_140 1 IT HH4 12 0.038700 1.00800
   13 opls_140 1 IT H5 13 0.038700 1.00800
   14 opls_135 1 IT C5 14 -0.080400 12.01100
   15 opls_140 1 IT HH5 15 0.038700 1.00800
   16 opls_140 1 IT H6 16 0.038700 1.00800
   17 opls_135 1 IT C6 17 -0.093100 12.01100
   18 opls_140 1 IT HH6 18 0.032700 1.00800
   19 opls_140 1 IT H7 19 0.032700 1.00800
   20 opls_140 1 IT H8 20 0.032700 1.00800

[ bonds ]
    1 2 1 1.0920e-01 2.8225e+05
    1 3 1 1.0920e-01 2.8225e+05
    1 4 1 1.0920e-01 2.8225e+05
    1 5 1 1.5350e-01 2.5363e+05
    5 6 1 1.0920e-01 2.8225e+05
    5 7 1 1.0920e-01 2.8225e+05
    5 8 1 1.5350e-01 2.5363e+05
    8 9 1 1.0920e-01 2.8225e+05
    8 10 1 1.0920e-01 2.8225e+05
    8 11 1 1.5350e-01 2.5363e+05
   11 12 1 1.0920e-01 2.8225e+05
   11 13 1 1.0920e-01 2.8225e+05
   11 14 1 1.5350e-01 2.5363e+05
   14 15 1 1.0920e-01 2.8225e+05
   14 16 1 1.0920e-01 2.8225e+05
   14 17 1 1.5350e-01 2.5363e+05
   17 18 1 1.0920e-01 2.8225e+05
   17 19 1 1.0920e-01 2.8225e+05
   17 20 1 1.0920e-01 2.8225e+05

[ angles ]
    1 5 6 1 1.1005e+02 3.8802e+02
    1 5 7 1 1.1005e+02 3.8802e+02
    1 5 8 1 1.1063e+02 5.2894e+02
    2 1 3 1 1.0835e+02 3.2995e+02
    2 1 4 1 1.0835e+02 3.2995e+02
    2 1 5 1 1.1005e+02 3.8802e+02
    3 1 4 1 1.0835e+02 3.2995e+02
    3 1 5 1 1.1005e+02 3.8802e+02
    4 1 5 1 1.1005e+02 3.8802e+02
    5 8 9 1 1.1005e+02 3.8802e+02
    5 8 10 1 1.1005e+02 3.8802e+02
    5 8 11 1 1.1063e+02 5.2894e+02
    6 5 7 1 1.0835e+02 3.2995e+02
    6 5 8 1 1.1005e+02 3.8802e+02
    7 5 8 1 1.1005e+02 3.8802e+02
    8 11 12 1 1.1005e+02 3.8802e+02
    8 11 13 1 1.1005e+02 3.8802e+02
    8 11 14 1 1.1063e+02 5.2894e+02
    9 8 10 1 1.0835e+02 3.2995e+02
    9 8 11 1 1.1005e+02 3.8802e+02
   10 8 11 1 1.1005e+02 3.8802e+02
   11 14 15 1 1.1005e+02 3.8802e+02
   11 14 16 1 1.1005e+02 3.8802e+02
```

```
11 14 17 1 1.1063e+02 5.2894e+02
12 11 13 1 1.0835e+02 3.2995e+02
12 11 14 1 1.1005e+02 3.8802e+02
13 11 14 1 1.1005e+02 3.8802e+02
14 17 18 1 1.1005e+02 3.8802e+02
14 17 19 1 1.1005e+02 3.8802e+02
14 17 20 1 1.1005e+02 3.8802e+02
15 14 16 1 1.0835e+02 3.2995e+02
15 14 17 1 1.1005e+02 3.8802e+02
16 14 17 1 1.1005e+02 3.8802e+02
18 17 19 1 1.0835e+02 3.2995e+02
18 17 20 1 1.0835e+02 3.2995e+02
19 17 20 1 1.0835e+02 3.2995e+02

[ dihedrals ]
  1   5   8   9   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
  1   5   8  10   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
  1   5   8  11   3   3.68192   3.09616  -2.09200  -3.01248   0.00000   0.00000
  2   1   5   6   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  2   1   5   7   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  2   1   5   8   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
  3   1   5   6   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  3   1   5   7   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  3   1   5   8   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
  4   1   5   6   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  4   1   5   7   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  4   1   5   8   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
  5   8  11  12   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
  5   8  11  13   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
  5   8  11  14   3   3.68192   3.09616  -2.09200  -3.01248   0.00000   0.00000
  6   5   8   9   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  6   5   8  10   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  6   5   8  11   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
  7   5   8   9   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  7   5   8  10   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  7   5   8  11   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
  8  11  14  15   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
  8  11  14  16   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
  8  11  14  17   3   3.68192   3.09616  -2.09200  -3.01248   0.00000   0.00000
  9   8  11  12   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  9   8  11  13   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
  9   8  11  14   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
 10   8  11  12   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
 10   8  11  13   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
 10   8  11  14   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
 11  14  17  18   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
 11  14  17  19   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
 11  14  17  20   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
 12  11  14  15   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
 12  11  14  16   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
 12  11  14  17   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
 13  11  14  15   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
 13  11  14  16   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
 13  11  14  17   3   0.66944   2.00832   0.00000  -2.67776   0.00000   0.00000
 15  14  17  18   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
 15  14  17  19   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
 15  14  17  20   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
 16  14  17  18   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
 16  14  17  19   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000
 16  14  17  20   3   0.62760   1.88280   0.00000  -2.51040   0.00000   0.00000

[ pairs ]
  1   9   1
  1  10   1
  1  11   1
  2   6   1
  2   7   1
  2   8   1
  3   6   1
  3   7   1
  3   8   1
  4   6   1
  4   7   1
  4   8   1
  5  12   1
  5  13   1
```

```
5  14   1
6   9   1
6  10   1
6  11   1
7   9   1
7  10   1
7  11   1
8  15   1
8  16   1
8  17   1
9  12   1
9  13   1
9  14   1
10  12   1
10  13   1
10  14   1
11  18   1
11  19   1
11  20   1
12  15   1
12  16   1
12  17   1
13  15   1
13  16   1
13  17   1
15  18   1
15  19   1
15  20   1
16  18   1
16  19   1
16  20   1
```