Dear Fellow Chemists,

To use this program, please simply execute the python file ewt.py as “python ewt.py”

Now, chose the option carefully and give inputs are directed.

**If you want to debug or modify :**

First of all, you seem to be a brave kid :D

Let me brief you with the algorithm and direct you to the right files for them.

1. The program finds the cummulants first, and sends the “rest” of the operators again through a recursive call to the function make\_c. (this is done in make\_c.py file)
2. When we have required number of cummulannts, it forms contractions, through recursive call to function fix\_uv, as the name suggest it fixes the operators to be used in contractions (this is done in make\_c.py and in fix\_uv.py)
3. When it has the required number of contactions and cummulants, it prints them and the remaining string in latex format in tec.txt file.

Now let me brief you to some important data structure that have important role in the program.

1. For cummulants, there is a list of list in make\_c.py - I\_forgot\_the\_name\_of\_list = [ ]. Each element in this list contains all the operators, so when we have to pick a cummulant, we simply pick the first element from each list. Then check it and delete it when not required.
2. For contractions, we have a better data structure - “poss” (abbreviated to possibility of forming contraction). This list is ordered with the position of operator in the original operator list (full = [ ]).Each element contains all possible operators that can contract with the corresponding element.

Now you are aware of the most important elements of the program. Go ahead and make all the modifications that you want (and curse me for using stupid variable names ). Also, if you think that the coding style is stupid, sorry but I am relatively new to python and am not aware of the cool things that it can do.

If you don’t want to go into details of modifying, just drop me a mail at [ayushasthana15@gmail.com](mailto:ayushasthana15@gmail.com) and I will be happy to do that for you.