Coding Project - PetitJean Index

This coding project is a team work of 2 students. The goal is to write a python script to calculate the PetitJean index of a set of molecules (minimum of 5). PetitJean index is a popular topological descriptor, which is a type of shape descriptor that is calculated from the connection matrix/table of a molecular structure.

I have uploaded the original paper of the PetitJean Index on Blackboard to help/guide you in your coding project.

The program, which should be very well commented, takes as an input a directory containing multiple molecule structures in molfile format or a single sdf file encoding the multiple chemical structures. The input should be provided as a command line argument to your script.

The output will be the name of the molecule and the value of its PetitJean index. Adding a graphical user interface to your program will be a plus.

You will be graded according to the below criteria:

1. Content: Code reflects understanding (and synthesis) of the subject
2. Execution: program works in the way the student intended (functional and refined with extra features)
3. Code: Program is well organized, easy to read and understand (commented, variables with useful names)

The deadline for this project is **November 12th 2020** by midnight and it must be respected. A student failing to meet the deadline will get 20% of the grade deducted per day late.

You should upload on Blackboard an archive containing your python script and the set of molecules (minimum of 5 and maximum of 20) you have used to test your code.