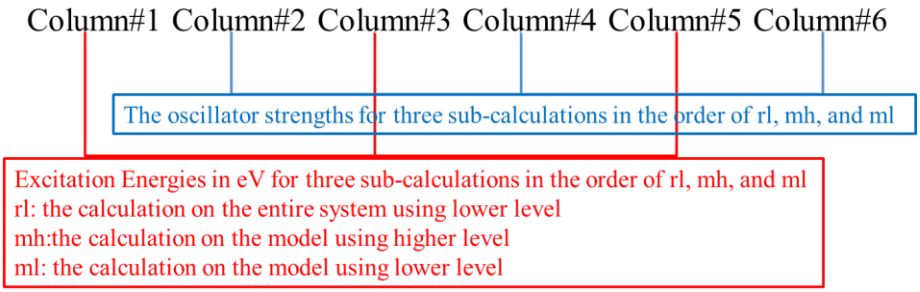
User Reference

I. **Executing command:** The code can be executed by `perl filename.plx` followed by other input file names and output file names.

II. **Input file options:** The program is usable for both Gaussian and non-Gaussian users, and accepts three input formats:

1. One Gaussian output file from two-layered ONIOM excited calculation. For this input option, the executing command is `perl filename.plx inputfile.log outputfile.txt`
   in which a preferred output file name should be given by the user for the program to write in data.
2. Three Gaussian output files, which are the sub-calculations of two-layered ONIOM done as three separate excited state calculations. The three input files should be given in the sequence of real low, model high, and model low. For this input option, the executing command is
   `perl filename.plx inputfile_rl.log inputfile_mh.log inputfile_ml.log outputfile.txt`
3. One txt file containing excitation energies and oscillator strengths. The txt file should be constructed using as follow:



   For this input option, the executing command is `perl filename.plx inputfile.txt outputfile.txt`
   Notice that only one space should be added between columns.

III. **Additional parameters:** A list of parameters should be specified for the program, and those can be added to the end or the beginning of input file, regardless of which input format is used. User should follow the following format:

```
extn 2
sdrl yes
sdmh yes
sdml yes
sigma 0.4
sdt 0.1
```

extn: number of states to extrapolate

sdrl sdmh sdml: turning shoulder detection option on/off. To turn off shoulder detection, "yes" should be replaced by "no". The default is shoulder detection on for all three sub-calculations.

sigma: the band width parameter for Gaussians. The default is 0.4 eV.

sdt: the shoulder detection threshold. Setting this value small would be able to detect smaller shoulders. The default is 0.2 eV.

If the second input option is used, those parameters can only be added to the first input file. Those parameters can be adjusted accordingly to get better extrapolation for specific cases.

IV. **Output files:** The program gives out four output files: outrl.txt outmh.txt outml.txt and another file (outfile.txt) with the name specified by the user.

outrl.txt outmh.txt outml.txt contain data for real low, model high, and model low spectra, respectively.

outfile.txt contains data for the extrapolated spectra

For all output files, the first column is the excitation energies (eV), and the second column is the ε, which is the intensity.