Multi State Extrapolation Program
User Reference

The **msextra.plx** program extrapolates UV/Vis spectra from QM/QM excited state calculations. It requires three sub-calculations as in the ONIOM method. The program first builds the spectrum for each sub-calculation as an envelop of Gaussian functions assigned to each transition. Then, the program recognizes all bands in each sub-calculation, and extrapolates the bands position, eight, and half-width. The extrapolated spectrum is built by assigning and summing a Gaussian function to each extrapolated band.

I. **Input file options:** The program is usable directly with GAUSSIAN output files, or with simple text files:

1. One GAUSSIAN output file from two-layered ONIOM excited calculation. For this input option, the executing command is: **perl msextra.plx inputfile.log outputfile.txt**
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. Note that the three sub-calculations do not need to include the same number of excited states. For this input option, the executing command is:
   perl msextra.plx inputfile_rl.log inputfile_mh.log inputfile_ml.log outputfile.txt
3. One txt file containing excitation energies (ω) in eV and oscillator strengths (f). Each state is reported on a different line as follows:
   ω _rl,f_rl, ω _mh,f_mh, ω _ml,f_ml
   where rl: real low, mh: model high; ml: model low. Note that there must be no space between numbers. However, the number of excited states in the file may be different for each sub-calculation. In that case, the column with less data should have an empty space between commas, e.g.:
   ω _rl,f_rl, , , ω _ml,f_ml
   For this input option, the executing command is: **perl msextra.plx inputfile.txt outputfile.txt**

II. **Additional parameters:** A list of parameters may be specified for the program, and those can be added to the end or the beginning of the input file, regardless of which input format is used. These parameters can be adjusted to get better extrapolation for specific cases. The format is:

extn,2
sigma,0.4
sdtrl,0.1
sdtmh,0.1
sdtml,0.1

extn: number of bands to extrapolate. The default is 3.

sdtrl sdtmh sdtml: shoulder detection threshold for each sub-calculation. Setting this parameter to a small value allows detecting smaller shoulders. The default is 0.1.

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

If the second input option is used, those parameters need only be added to the first input file.

III. **Output files:** The program produces five output files: outbands.txt, outrl.txt, outmh.txt, outml.txt, and outputfile.txt (only the latter's name can be specified by the user).

outbands.txt contains the information about the bands detected in each sub-calculation: position, height, and half-width. If it is a shoulder, the band to which the shoulder belongs is also reported.

outrl.txt outmh.txt outml.txt contain the spectra for the real low, model high, and model low sub-calculations, respectively.

outputfile.txt contains the extrapolated spectrum.

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

The example files report a calculation with 100 states/sub-calculation with input method 3 for 1,3-decadiene (in Å). In the table below, the column "Layer" reports the atoms in the low layer, and "Link Atom" reports the atom center replaced by a link atom. The file "data3.txt" reports the input data, and the file "method3.txt" reports the extrapolated spectrum. The other files are as explained in **III**.

	Layer	Link Atom
C -4.48032 -0.39878 -0.27457		
C -5.54644 -0.66634 0.47609		
H -4.52445 -0.57955 -1.34601		
H -6.45865 -1.06072 0.0467		
H -5.53911 -0.49824 1.54789		
C -3.22393 0.13161 0.23791		
C -2.1622 0.40238 -0.52039		
C -0.85697 0.93784 -0.02284		
C 0.32266 0.00645 -0.31921	L	H
H -0.66215 1.90883 -0.49505		
H -0.92123 1.12197 1.05407		
H 0.14224 -0.96176 0.15977	L	
H 0.36622 -0.1894 -1.39686	L	
H -3.17327 0.3124 1.31001		
H -2.22705 0.21402 -1.59155		
C 1.66154 0.56877 0.1476	L	
H 1.83382 1.53968 -0.33218	L	
H 1.61514 0.76673 1.22508	L	
C 2.84089 -0.35379 -0.144	L	
H 2.66763 -1.32546 0.33379	L	
H 2.88941 -0.55073 -1.22172	L	
C 4.18144 0.20409 0.32495	L	
H 4.35461 1.17459 -0.15294	L	
H 4.13282 0.40044 1.40162	L	
C 5.35294 -0.72612 0.02876	L	
H 6.29882 -0.30164 0.37227	L	
H 5.22353 -1.69249 0.52354	L	
H 5.44404 -0.91528 -1.04427	L	