1. script 사용법 ( ir spectrum , radiative efficiency )

**1.1 generate ir spectrum from G16 output file. ( log file)**

tar –xvfz script.tgz

cd script

gfortran irspec\_scale.f –o irspec.x

**required : gauviblist.awk, gautoir , irspec\_scale.f**

example)

mol./gautoir mol\_0 -> generate ir spectrum from mol\_0.log

Output 1 : **mol\_0.ir**

- 1st line : number of normal modes,

- 2nd line: vib freq scale factor (values is 1,but don’t modify)

- 3rd line: intensity scale factor (values is 1, don’t modify)

- 4th line: FWHM of ir peak

- 5th line to final line : ir frequency and intensity (km/mol)

Output 2 : **mol\_0.prn (ir spectrum)**

Generated ir spectrum -> Radiative efficiency calculation , The IR spectrum can plot using plotting program.

Intensity of IR spectrum : (M-1 cm-1)

**1.2 Radiative efficiency calculation**

**Required : pinnock.txt (pinnock table), rad\_eff.f**

gfortran rad\_eff.f –o rad\_eff.x

./rad\_eff.x <mol\_0.prn >out

Final line of out : Radiative efficiency (unit W m−2 ppbv−1)

**1.3 Radaitive efficiency for GWP calculation**

RE unit (W m−2 ppbv−1) to RE unit (W m−2 kg−1)

Ma : average molecular weight of Air (28.97 g/mol)

Mi: molecular weight of molecule i

Tm : Total mass of atmosphere (5.1352Ⅹ1018)