HA 1, Date:14/02/2021

---

1. You must have studied and done experiments to calculate the UV-vis absorption spectra of molecules. There is also CD (circular dichroism) spectra which is used to check the chirality. The following two formulas are usually used to compute these spectra: For UV

$$\epsilon(\bar{\nu}) = \sum_{i=1}^{n} \left(1.3062974 \times 10^8 \times \frac{f_{osc}}{\sigma} \times exp\left[-\left(\frac{\bar{\nu} - \bar{\nu_i}}{\sigma} \right)^2 \right] \right)$$

and for CD

$$\Delta\epsilon(\bar{\nu}) = \{1/(2.296 \times 10^{-39} \times \sqrt{\pi}\sigma)\} \sum_{i=1}^{n} \bar{\nu_i} \times R^i_{str} exp\left[-\left(\frac{\bar{\nu} - \bar{\nu_i}}{\sigma} \right)^2 \right]$$

In these equations, $\bar{\nu}$, $\bar{\nu_i}$ and σ are in cm^{-1}. Attached is a file (filename=input.dat) containing 3 columns of data (40 rows). The first column is the wavelength (λ) in nm (nanometer), 2nd column contains the so-called oscillator strengths (denoted as f_{osc}, simple number without any unit) and the third column contains the rotatory strengths (denoted as R_{str}) in CGS units (10^{-40} erg-esu-cm/Gauss). Use these data to compute the full UV and CD spectra over 200 to 600 nm ($\Delta\lambda$=1 nm). Use σ=2480 cm^{-1}. You will upload two files: (1) the code showing UV and CD spectra, (2) the output file containing three columns, wavelength (in nm), ϵ and $\Delta\epsilon$, respectively. Check the units of various factors: ν is in cm^{-1}, wavelength is in nm, σ is in cm^{-1}.

2. Calculate the radial distribution function (RDF) for $1s$, $2s$ and $2p$ orbitals and then normalize the result so that maximum value of each RDF is one. The RDF is $4\pi\ r^2 \times \psi^2$. Let us say that $0.0 \leq r \leq 2.0$ with $\Delta r = 0.05$. The code will output r and RDF to a file which can be plotted. The wavefunctions are as follows:

   - 1s: $e^{-r/2}$
   - 2s: $32^{-1/2}(2 - r)e^{-r/2}$
   - 2p: $972^{-1/2}(6 - 6r + r^2)e^{-r/2}$

   Use modules and subroutines/functions. The main routine will only read in the orbital type we want, and accordingly, the code will enter the corresponding subroutine. You will be submitting the code only. When I check, I will enter the orbital index, and get the output file which I will plot and see.