Problem Set 4
CHM102A

1. Calculate the radial distribution function $\{RDR = r^2R^2(r)\}$ for the 1s and 2s state of the hydrogen atom. Determine the locations (i.e. values of r) of its minima and maxima for both 1s and 2s in terms of a_0. What do these minima signify?

2. Find the total degeneracy of the energy level with $E = -\frac{13.6}{n^2} eV$ given the constraints: $m_1 = 0,\pm1,\pm2,...\pm l,\quad l = 0,1,2,3...(n-1)$ and $n = 1,2,3...$

3. The vibrations of the diatomic molecule $^1H^{35}Cl$ are better described by a Morse oscillator with the energy levels:

$$E_n = \tilde{\nu}\left(n+\frac{1}{2}\right) - \tilde{\nu}\,\tilde{x}\left(n+\frac{1}{2}\right)^2$$

With $\tilde{x} = \frac{hc\tilde{\nu}}{4D}$. The dissociation energy $D = 440.2\ kJ\ mol^{-1}$ and $\tilde{\nu} = 2886\ cm^{-1}$.
The energies are measured in cm^{-1}(wavenumbers).
   (i) Calculate the values of $\tilde{x}$ and hence $\tilde{\nu}\,\tilde{x}$.
   (ii) Estimate the zero-point energy (in wavenumbers).
   (iii) How many bound vibrational states are supported by this Morse oscillator?

4. The first ionization potential of Na is about 5.14 eV. Assume that the energy level of the outer electron (3s) can be represented by a hydrogen-like formula with some effective nuclear charge Z'. Calculate the value of Z'.

5. In case of the He atom, it is not possible to solve the Schrodinger equation exactly. Justify this statement by writing out the full Hamiltonian for the He-atom (in atomic units). What is the approximation made in the Hamiltonian so written to make the problem solvable?

6. Four, noninteracting, electrons are confined in a two-dimensional square box of length *L*=100 pm, which follow the Pauli exclusion principle, i.e. not more than two electrons are occupied in the same orbital.

   i. Calculate the ground state energy of the system (in *Joules*).
   ii. What is the longest wavelength transition (in *nm*)?
   iii. Suppose that the Pauli exclusion principle is ignored. Estimate the error that result in determining the longest wavelength.