CHEM356: Physical Chemistry II
Homework Set VI - due 21^{th} of May, 5.00 pm
Each problem is worth 5 points, 25 pts in total.

Instructor: Dr. Mateusz Marianski
Room#: HN-1321B
email: *mmarians@hunter.cuny.edu*
Office hours: Thu, 5-7 pm, HN-1321B

Problem I

A morse potential, given by $U(q) = D_e(1 - e^{-\beta(R-R_e)})^2$ is a good representation of the potential energy of diatomic molecule. Show that the force constant calculated for a Morse potential is given $k = 2D_e\beta^2$. Calculate the value of k for HCl, where $\beta = 1.83 \cdot 10^{10}$ m $^{-1}$ and $D_e = 7.31 \cdot 10^{-19}$ J. Compare it with k calculated from fundamental vibration 2990 cm^{-1}

Problem II

A vibronic transition consist of concerted electronic and vibrational excitations. First few vibronic excitations from zeroth to respectively $\theta = 2, 3, 4, 5$ states are given by $\bar{\nu}$= 12569.95, 13648.43, 14710.85 and 15757.50 cm^{-1}. Calcualte the values of $\bar{\nu}_e$ and $\bar{\nu}_e\bar{\chi}_e$.

Problem III

The follwoing data are obtained for the vib-rot spectrum of $H^{79}Br$. Determine $\bar{B}_0$, $\bar{B}_1$, $\bar{B}_e$ and $\bar{\alpha}_e$ and ν_e.

Line	Freq $[cm^{-1}]$
R(0)	2642.60
R(1)	2658.36
P(1)	2609.67
P(2)	2592.51

Probem IV

Using Jablonski diagram, explain fluorescence and phosphorescence processes. (I did not cover it during the lecture).

Problem V

The molecules $^{16}O^{12}C^{32}S$ and $^{16}O^{12}C^{34}S$ have B values of $6081.46 \cdot 10^6 s^{-1}$ and $5931.816 \cdot 10^6 s^{-1}$ respectively. Calculate the C-O and C-S bond distances.