Quantum Mechanics and Spectroscopy
CHEM 3PA3
Assignment 4 **Name:** _____

1. The force constant of $^{35}Cl^{35}Cl$ is 319 $N{\cdot}m^{-1}$. Calculate the fundamental vibrational frequency and the zero-point energy of Cl_2.

2. The Hamiltonian for the quantum harmonic oscillator is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2.$$

You are told that its ground-state wavefunction is

$$\Psi_0(x) = A\exp\left(-\frac{\sqrt{km}}{2\hbar}x^2\right)$$

(a) What is the normalization constant for this wavefunction?

(b) What is the zero-point energy for this wavefunction?

(c) What is the kinetic energy for this wavefunction?

(d) What is the expectation value of $\hat{p}^2$ for this wavefunction?

(e) The Heisenberg Uncertainty Principle says that $\sigma_x\sigma_{p_x} \geq \frac{1}{2}\hbar$. Show that this is true for the Harmonic oscillator. What is the interpretation of the Heisenberg Uncertainty Principle.

(f) The Heisenberg Uncertainty principle can be derived from the (usually stronger) Schrödinger Uncertainty relationship, $\sigma_x^2\sigma_{p_x}^2 \geq \left|\frac{1}{2}\langle x\hat{p}+\hat{p}x\rangle - \langle\hat{p}\rangle\langle\hat{x}\rangle\right|^2 + \left|\frac{1}{2i}\langle x\hat{p}-\hat{p}x\rangle\right|^2$. Show that this principle is also satisfied by the harmonic oscillator.