

Due Fri. Oct. 20 at 5pm (sharp) in Prof. Ginger's mailbox

Key will be posted online at 5pm

Put CHEM 455 at the top of your HW.

Circle your answers. Submit your problems in order. Staple your work together.

Textbook

P7.1 zero point and vibrational energies of HF

P7.8 $\langle x^2 \rangle$ (mean squared displacement) for H.O.

Additional

1) Review your spherical polar coordinates and 3D integrals by finding the volume of a sphere of radius a by integrating the spherical volume element $dV = r^2 \sin(\theta) dr d\theta d\phi$ in spherical polar coordinates from $r=0$ to $r=a$ (Pay attention, some texts switch theta and phi. In our book [and class] theta is the angle the radius vector makes with the z-axis, and the limits on theta run from 0 to π).

2) Read problem 7.3. You should *know* that the H.O. wavefunctions will be orthonormal. In 1-2 sentences explain how and why you know this (and not just because the textbook said so).

3) The infrared spectrum of H^{79}Br shows an intense line at 2600 cm^{-1} . Calculate the force constant of H^{79}Br and the period of vibration of H^{79}Br .

4) A function that looks like a realistic molecular potential is the Morse Potential. (see eqn 8.4 in the text): $V(x) = D_e(1 - e^{-\beta x})^2$ Expand $V(x)$ in a Taylor series about $x=0$ to obtain

$U(x) = D_e \beta^2 x^2 - D_e \beta^3 x^3 + \dots$ Given that, for HCl, $D_e = 7.31 \times 10^{-19} \text{ J/molecule}$, and $\beta = 1.82 \times 10^{10} \text{ m}^{-1}$, calculate the force constant for HCl.

5) In 2-3 sentences, explain why we encounter the harmonic oscillator potential so frequently in chemistry and physics problems? Comment on the suitability of the harmonic oscillator potential to the HCl molecule using your calculations of 7.13 as a reference, *in particular comment on what situations you think the H.O. would be a bad approximation?*