

## C455A - Homework 4 Due Mon 4/28

Note: You might want to work some of these problems BEFORE midterm #1. Those have been starred for you (mostly we have worked similar problems in class already!)

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

### Textbook

\*P6.17 Commutator for  $x$  and  $p_x$  (and vice versa)

\*P7.23 Zero point energy and IR absorptions of HF

P7.5 HI vibration and rotational transitions

P7.6 Linear combinations of spherical harmonics

\*P7.12 Orthogonality of energy eigenfunctions of harmonic oscillator

P7.13 Comparing mean square displacement with bond length.

### 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 Pi).

\*2) Before you worked problem 7.12 you should have *known* that the H.O. wavefunctions would 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  $\text{H}^{79}\text{Br}$  shows an intense line at  $2600 \text{ cm}^{-1}$ . Calculate the force constant of  $\text{H}^{79}\text{Br}$  and the period of vibration of  $\text{H}^{79}\text{Br}$ .

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. Use Excel or another computer package to plot the Morse potential and the corresponding H.O. potential on the same graph. (in other words, make your own Fig. 7.1).

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?*