

Chemistry 4000/5000/7001, Fall 2012, Assignment 2

Due: Friday, September 21, 4:00 p.m.

Total marks: 21

- (a) What are the units of \hbar ? [1 mark]
 - (b) Show that the units of $\omega = E/\hbar$ are appropriate units for a frequency. [1 marks]
- (a) Calculate the zero-point energy of an electron in a 1 nm box. [2 marks]
 - (b) Since there is no potential energy, the energy of a particle in a box is all kinetic. Calculate the speed of the electron. [2 marks]
 - (c) Calculate the absolute value of the momentum of the electron. [2 marks]
- (a) Calculate the reduced mass of a $^1\text{H}^{19}\text{F}$ molecule. Report your final answer in kg. [4 marks]
Note: You will need to look up the isotopic masses. You can use any source that gives reasonably accurate values. I recommend the NIST web site: <http://www.nist.gov/pml/data/comp.cfm>. Wherever you get your data, please cite your source.
 - (b) The force constant (k) in this molecule has the value 965.7 N/m. Calculate ω_0 . [2 marks]
4. How many normal modes would cyclobutane (C_4H_8) have? [2 marks]

Bonus: Would you describe any of the normal modes of cyclobutane as bending modes? If so, explain how you computed the normal modes (method/basis set), and report the frequency of the bending mode.

Note: There are basic instructions on using HyperChem on the course web site.

5. In our discussion of the time-dependent Schrödinger equation, we constructed superposition states

$$\Phi(x, t) = \Psi_1(x, t) + \Psi_2(x, t)$$

such that $E_1 \neq E_2$. What happens if $E_1 = E_2$? Why is this case not very interesting? [5 marks]