Physical Chemistry II
Problem Set 1—due Friday, February 8, 2008 (at 4 p.m.)
Total Number of Points = 68

Notes: (1) Write all numbers with the correct number of significant figures and units. Avoid rounding errors by writing intermediate results with additional subscripted non-significant figures. (2) Assume all zeroes to the left of the decimal place are significant (unless told otherwise). For example, 100 V has three significant figures (and should therefore have been written by Atkins and de Paula as 100. V or 1.00×10^2 V). (3) The answers to most of these problems are in the back of the book. However, you must justify your answers to receive credit.

1. (2 points) Atkins and de Paula Exercise 20.4b. Assume a first-order reflection (that is, $n = 1$.) Report the wavelength in Å.

2. (9 points) Atkins and de Paula Exercise 8.8b.

3. (7 points) Atkins and de Paula Exercise 8.10b. Do parts (a) and (c) only. Report the wavelengths in Å. Also, note that the answer in the back of the book for part (c) is wrong!

4. (10 points) Bohr Model Problem:
   (a) Calculate the numerical value of the Bohr radius, $a_o = \frac{\varepsilon_o h^2}{\pi e^2 m}$, in Å to four significant figures.
   (b) Starting from the equation for the total energy of a one-electron atom, $E = \frac{1}{2}mv^2 - \frac{Ze^2}{4\pi\varepsilon_o r}$, derive the equation $E = -R\left(\frac{Z^2}{n^2}\right)$. Your derivation must include an expression for R (the Rydberg constant) in terms of fundamental physical constants.

5. (5 points) Atkins and de Paula Exercise 8.12b. Since the diameter of an atom is only approximately 100 pm, let us assume we know the length to only one significant figure.

6. (12 points) Atkins and de Paula Problem 8.4.
   - Start by sketching the wavefunction and by confirming (via integration) that it is normalized.
   - Then do only parts (b), (d), and (e).
   - No points off for significant figures here (unless you're being ridiculous).
   - Answers: (b) Probability = 0.0069; (d) Probability = 0.609.

7. (12 points) Atkins and de Paula Problem 8.14.
   - Do only part (a) (the normalization) and treat only wavefunction (ii)
   - Use the hint in Problem 8.13.
   - Anticipate the need to invoke a fundamental trigonometric identity and using a trigonometric substitution to perform an integral. Alternatively, you can look up the integral in a CRC Handbook.
   - Final answer: $N = \sqrt{\frac{1}{32\pi a_o^5}}$

8. (7 points) Atkins and de Paula Problem 8.15.

9. (7 points) Atkins and de Paula Problem 8.17.