CHM 3411, Dr. Chatfield, Spring 2018
Problem Set 5
Suggested completion date: Friday, Feb 16

This problem set is NOT to be turned in. However, the material covered on it will be on Exam 1. Solutions will be posted on Friday, Feb. 16. It is strongly suggested that you work through this problem set as preparation for Exam 1.

Suggested "warmups": Rotational motion: Discussion questions 8C.3; Exercises [all (b)] 8C.1,5-8.

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These problems explore angular momentum.

1. Exercise 8C.4b

2. Exercise 8C.5b

3. Exercise 8C.6b. (The wording of the exercise is ambiguous. Calculate the magnitude of the angular momentum when the molecule is rotating with energy = $\frac{\hbar^2}{I}$ ).

4. Exercise 8C.7b

5. We stated in class that the quantum mechanical operator $\hat{l}_z$ for the z-component of the angular momentum expressed in Cartesian coordinates, is:

$$\hat{l}_z = x\hat{p}_y - y\hat{p}_x$$

Show that when we convert to polar coordinates, the operator $\hat{l}_z$ becomes:

$$\hat{l}_z = \frac{\hbar}{i}\frac{d}{d\phi}$$

6. By integration, show explicitly that the spherical harmonics $Y_{0,0}$ and $Y_{1,0}$ (given in Table 8C.1) are orthonormal (i.e., that each is normalized and that they are orthogonal to each other). Be careful with the two-dimensional volume element in the integration; it is $d\tau = \sin\theta \, d\theta \, d\phi$.

7. The quantization of angular momentum is sometimes hard to grasp, particularly since its spatial representation is so counterintuitive. This problem attempts to make the concept clearer.
   a) For a particle on a sphere, derive an expression for the angle that the angular momentum vector makes with the z-axis for the spherical harmonic $Y_{l,m_l}$. The angle should be expressed in terms of $l$ and $m_l$.
   b) Calculate the allowed angles when $l$ is 1, 2, and 3 and show that the minimum angle approaches zero as $l$ approaches infinity.

8. Spartan problem. This problem requires you to calculate an electrostatic potential map of the surface of a molecule. The map indicates which regions of the molecule are electron deficient (positive potential, colored blue) and which are electron abundant (negative potential; colored red). Your instructor will demonstrate how to calculate the electrostatic potential map.

Problem: Calculate the electrostatic potential for HF, $H_2O$, $NH_3$, and one other molecule of your choice. Cut and paste the Spartan graphics to display the maps on your homework. Be sure that the color scale is the same for all the molecules. From the results, answer these questions: (a) Is the electrostatic potential map correlated with acidity? (b) If so, can you explain why? [Use the B3LYP/6-31G* method, and perform an Equilibrium Geometry calculation before you calculate the electrostatic potential map.]

Hints on Spartan: After optimizing, click the "surfaces" icon (looks like fat daisy with blue edges and red center). Surfaces window pops up: click on "Add" and choose "electrostatic potential map." To see the values associated with the colors, right click on the molecule and choose "properties." Surfaces properties window appears. Adjust ranges etc. as needed. Make note of the maximum value. Play around, clicking on different parts of the molecule. The value of the electrostatic potential at that point will show in the Surface Properties window.