Assignment 6 **BCH5887**
Due 03/30/10

Please put your programs in new directory called assignment6 in your homework directory. Please also include your name as a comment on the second line of your program.

Starting with the algorithms you developed in assignment5, develop a module that you can import that contains functions that will read and parse a pdb file, write a formatted pdb, calculate the center of geometry and center of mass for a pdb file, and calculate the Root Mean Squared Deviation (RMSD) between two PDB structures. Remember, the center of mass is given by:

$$\frac{\sum m_i r_i}{\sum m_i}$$

where m specifies the mass of a given atom and r is the coordinates for a given atom

and RMSD is given by:

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(v_{ix}-w_{ix})^2+(v_{iy}-w_{iy})^2+(v_{iz}-w_{iz})^2}$$

where v and w represent the set of coordinates for two different pdb files.

Use the module you have developed to write two different programs. In the first program, write a script that will center a pdb based on the user's choice of center of mass or center of geometry. In the second program, write a script that will calculate the RMSD between "5tnc_move.pdb" and "5tnc_move2.pdb" that are located at /home.local/bch5887-01/.