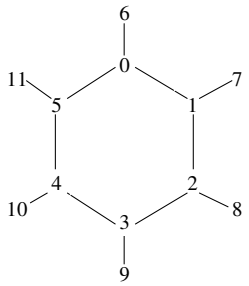
Day 5 Project: Energy of a benzene dimer from classical force field

The general theme of the project is to calculate different energy terms for a benzene dimer. Calculating the entire energy for the system is rather tedious so only certain values are considered. The files you need are:

- benz2.rst - An AMBER restart file with corrdinates
- benz2.prmtop - An AMBER parameter file to load the restart file into VMD
- benz_ene.py - A python script that reads in the restart file

The ordering of the atoms in the python script differ from that in the restart file, which will make handling indices more convinient. The coordinates are sorted with the following connectivity:



Here are a list of constants that you will need:

- Charges
  $q_C = -0.13011e$, $q_H = 0.13011e$
- Lennard-Jones parameters
  $r_{min,C-C} = 3.816\mathring{A}$, $\epsilon_{C-C} = 0.086kcal/mol$, $r_{min,H-C} = 3.367\mathring{A}$, $\epsilon_{H-C} = 0.036kcal/mol$,
  $r_{min,H-H} = 2.918\mathring{A}$, $\epsilon_{H-H} = 0.015kcal/mol$
- Bond equilibrium value and force constant
  $r_{min,C-C} = 1.387\mathring{A}$, $k_{C-C} = 956.8kcal/mol/\mathring{A}^2$
- Angle equilibrium value and force constant
  $\theta_{min,C-C-C} = 2.09457$, $k_{C-C-C} = 134.36kcal/mol$
- Dihedral force constant, phase and periodicity
  $k_{C-C-C-C} = 3.625kcal/mol$, $\phi_{C-C-C-C} = \pi$, $n_{C-C-C-C} = 2$

Questions:

1. Non-bonded interactions: Calculate the non-bonded energies (Coulombic, van der Waals) between atoms in different molecules.
2. Bonded interactions: Calculate the bonded energies (bond, angle, dihedral) for the carbon ring.
3. Which energy terms are we not calculating? What is the degeneracy of each type of interaction?