

Question 5

Potential energy of system of water molecules

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The total Potential energy of a system is the sum of pairwise potentials.

The pairwise potential for a pair of molecules a,b:

$$E_{ab} = \sum_i^{\text{on } a} \sum_j^{\text{on } b} \frac{k_C q_i q_j}{r_{ij}^2} + \frac{A}{r_{\text{OO}}^{12}} - \frac{B}{r_{\text{OO}}^6},$$

We use periodic boundary conditions to calculate the answer.

Given Lx=23.623; Ly=22.406; Lz=27.1759.

Take the charges information from the psf file and configuration of the molecules from the pdb file.

After parsing the data, calculate the potentials.

Pseudo code:

```

for i in range(1296):
    energy = 0
    Q = q[i]
    x = X[i]
    y = Y[i]
    z = Z[i]
    num_of_mmol = num_mols[i]
    for j in range(i+1,1296):
        ch = q[j]
        xc = X[j]
        yc = Y[j]
        zc = Z[j]
        r = calc_dist(x, y, z, xc, yc, zc)

        mn = num_mols[j]
        if mn == num_of_mmol:
            continue

        DIST.append(r)
        energy += calc_q(Q, ch, r)

        if mols[j] == mols[i] and mols[i] == 'OT':
            energy += ((A/(r**12)) - (B/(r**6)))
    E += energy

```

Where 1296 is the number of molecules in the system

By summing the pairwise potentials:

Total Potential Energy of system: -4559.667472442068