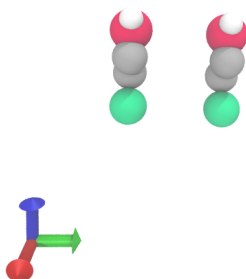


Potential Energy of Two MeOH Molecules

May 25, 2017

In this case we have two MeOH molecules separated by 5\AA in the y direction.



Our MeOH molecules have the following coordinates:

S (0.138, 0.0, -1.654)	S' (0.138, 5.0, -1.654)
$C1$ (0.474, 0.0, 1.059)	$C1'$ (0.474, 5.0, 1.059)
$C2$ (-0.621, 0.0, -0.007)	$C2'$ (-0.621, 5.0, -0.007)
O (-0.125, 0.0, 2.357)	O' (-0.125, 5.0, 2.357)
H (0.598, 0.0, 2.999)	H' (0.598, 5.0, 2.999)

```
S=c(2,0.0,0.138,0.0,-1.654)
C1=c(1,0.0,0.474,0.0,1.059)
C2=c(1,0.265,-0.621,0.0,-0.007)
O=c(3,-0.700,-0.125,0.0,2.357)
H=c(4,0.435,0.598,0.0,2.999)
S_2=c(2,0.0,0.138,5.0,-1.654)
C1_2=c(1,0.0,0.474,5.0,1.059)
C2_2=c(1,0.265,-0.621,5.0,-0.007)
```

```
O_2=c(3,-0.700,-0.125,5.0,2.357)
H_2=c(4,0.435,0.598,5.0,2.999)
```

Based on the number of atoms the total number of pairwise interactions are:

$$\binom{N_{atoms}}{2} = \binom{10}{2} = 45$$

Subtracting off the excluded intramolecular forces we have:

$$\binom{N_{atoms}}{2} - 2 \cdot \binom{N_{atoms}/2}{2} + 2 = \binom{10}{2} - 2 \cdot \binom{5}{2} + 2 = 27$$

The LJ Parameters are:

Elements	Epsilons (kcal/mol)	Sigmas (Å)
C	0.118	3.905
S	0.397	4.250
O	0.200	2.850
H	0.000	1.780

Calculating the energies of all possible combinations we get:

```
distance=function(atom1,atom2){
  return(norm(atom1[3:5]-atom2[3:5],type="2"))
}
energy=function(atom1,atom2){
  r=distance(atom1,atom2)
  sigma = (sigmas[atom1[1]]+sigmas[atom2[1]])/2
  epsilon = sqrt(epsilons[atom1[1]]*epsilons[atom2[1]])
  return(4*epsilon*((sigma/r)^12-(sigma/r)^6))
}
atoms = list(S,C1,C2,O,H,S_2,C1_2,C2_2,O_2,H_2)
atom_combos = combn(atoms,2)
distances=mapply(distance,atom_combos[1,],atom_combos[2,])
print(distances)

## [1] 2.7337273 1.8134746 4.0196132 4.6756827 5.0000000 5.6985318 5.3187113
## [8] 6.4153948 6.8455832 1.5281953 1.4295471 1.9439588 5.6985318 5.0000000
## [15] 5.2283249 5.2003466 5.3646040 2.4154735 3.2437628 5.3187113 5.2283249
## [22] 5.0000000 5.5528832 5.9600333 0.9668987 6.4153948 5.2003466 5.5528832
## [29] 5.0000000 5.0926312 6.8455832 5.3646040 5.9600333 5.0926312 5.0000000
## [36] 2.7337273 1.8134746 4.0196132 4.6756827 1.5281953 1.4295471 1.9439588
## [43] 2.4154735 3.2437628 0.9668987

interm_energies = mapply(energy,atom_combos[,distances>=5][1,],atom_combos[,distances>=5])
print(interm_energies)
```

```
## [1] -0.37343756 -0.10065368 -0.14015464 -0.03144736 0.00000000
## [6] -0.10065368 -0.08280619 -0.06771469 -0.04265897 0.00000000
## [11] -0.14015464 -0.06771469 -0.08280619 -0.02953994 0.00000000
## [16] -0.03144736 -0.04265897 -0.02953994 -0.02649616 0.00000000
## [21] 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000

sprintf("Total intermolecular Van der Waals Energy is: %4.4f kcal/mol",sum(inter_m_energies))
## [1] "Total intermolecular Van der Waals Energy is: -1.3899 kcal/mol"
```

Therefore the total energy is given as the total intermolecular energy plus the intramolecular energy of the two MeOHs:

$$\begin{aligned}\text{Total Van der Waals Energy} &= \text{Intermolecular Energy} + \text{Intramolecular Energy} \\ &= -1.3898847 + -0.2812 = -1.6710847 \text{ kcal/mol}\end{aligned}$$

Now we use the following code to calculate the total coulombic energy:

```
coul_energy=function(atom1,atom2){
  r=distance(atom1,atom2)
  k=0.2
  return(332.0636*((atom1[2]*atom2[2])/r)*exp(-k*r))
}
charged_atoms = list(C2,O,H,C2_2,O_2,H_2)
charge_combos = combn(charged_atoms,2)
distances=mapapply(distance,charge_combos[1,],charge_combos[2,])
print(distances)

## [1] 2.4154735 3.2437628 5.0000000 5.5528832 5.9600333 0.9668987 5.5528832
## [8] 5.0000000 5.0926312 5.9600333 5.0926312 5.0000000 2.4154735 3.2437628
## [15] 0.9668987

inter_m_energies = mapapply(coul_energy,charge_combos[,distances>=5][1,],charge_combos[,distances>=5][2,])
print(sum(inter_m_energies))

## [1] 0.5628225
```

The coulombic energy calculated here is:

$\text{Total Coulombic Energy} = 0.5628225 \text{ kcal/mol}$
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