Potential Energy of Two MeOH Molecules

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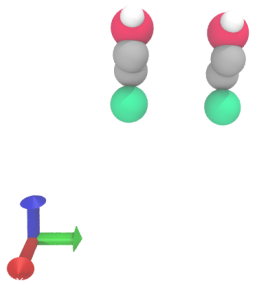
In this case we have two MeOH molecules separated by 5Å in the y direction.



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 (A)
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(interm_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=mapply(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
```

```
  interm_energies = mapply(coul_energy,charge_combos[,distances>=5][1,],charge_combos[,dista
  print(sum(interm_energies))
```

```
## [1] 0.5628225
```

The coulombic energy calculated here is:

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

1 Displace MeOH by 2A in Y Direction

```
  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))
  }
  S_2[4]=S_2[4]+1.
  C1_2[4]=C1_2[4]+1.
  C2_2[4]=C2_2[4]+1.
  O_2[4]=O_2[4]+1.
  H_2[4]=H_2[4]+1.
  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 6.0000000 6.5934259 6.2680691
##  [8] 7.2220004 7.6067082 1.5281953 1.4295471 1.9439588 6.5934259 6.0000000
## [15] 6.1915572 6.1679498 6.3070576 2.4154735 3.2437628 6.2680691 6.1915572
## [22] 6.0000000 6.4679604 6.8207036 0.9668987 7.2220004 6.1679498 6.4679604
## [29] 6.0000000 6.0774084 7.6067082 6.3070576 6.8207036 6.0774084 6.0000000
## [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]
  vdw_energy = sum(interm_energies)+2*-0.1406
  print(interm_energies)
```

```
##  [1] -0.17543077 -0.04574351 -0.06066907 -0.01568413  0.00000000
##  [6] -0.04574351 -0.03314609 -0.02783789 -0.01612032  0.00000000
## [11] -0.06066907 -0.02783789 -0.03314609 -0.01220641  0.00000000
## [16] -0.01568413 -0.01612032 -0.01220641 -0.00908311  0.00000000
## [21]  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
```

```
  sprintf("Total intermolecular Van der Waals Energy is: %4.8f kcal/mol",sum(interm_energies
```

```
## [1] "Total intermolecular Van der Waals Energy is: -0.60732869 kcal/mol"
```

```
  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=mapply(distance,charge_combos[1,],charge_combos[2,])
  print(distances)
```

```
##  [1] 2.4154735 3.2437628 6.0000000 6.4679604 6.8207036 0.9668987 6.4679604
##  [8] 6.0000000 6.0774084 6.8207036 6.0774084 6.0000000 2.4154735 3.2437628
## [15] 0.9668987
```

```
  interm_energies = mapply(coul_energy,charge_combos[,distances>=5][1,],charge_combos[,dista
  print(sum(interm_energies))
```

```
## [1] 0.26909
```

```
  coul_energy = sum(interm_energies)
  sprintf("Total intermolecular Coulombic Energy is: %4.8f kcal/mol",sum(interm_energies))
```

```
## [1] "Total intermolecular Coulombic Energy is: 0.26909000 kcal/mol"
```

$$\text{Total Energy} = -0.6194387 \text{ kcal/mol}$$