Turning Off Atoms in a Two MeOH System

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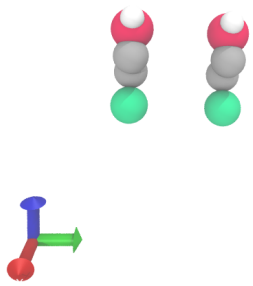
In this case we have two MeOH molecules separated by 5Å in the y direction.



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)
```

If we turn off 1 atom then we now have 9 atoms this gives a total number of combinations of:

$$\binom{9}{2} - \binom{4}{2} - \binom{5}{2} + 2 = 22$$

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

1 Turning off one H atom

Calculating the energies of all possible combinations when we turn off a hydrogen atom (H) 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,S_2,C1_2,C2_2,O_2,H_2)
  atom_combos = combn(atoms,2)
  distances=mapply(distance,atom_combos[1,],atom_combos[2,])
  interm_energies = mapply(energy,atom_combos[,distances>=5][1,],atom_combos[,distances>=5]
  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"
```

Adding in the intramolecular energy of -0.2812 we get a total Van der Waals energy of:

$$\boxed{\text{Total Van der Waals Energy} = -1.3898847 + -0.2812 = -1.6710847 \text{ kcal/mol}}$$

The total coulombic energy when we turn off 1 hydrogen atom is:

```
  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,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 5.0000000 5.5528832 5.9600333 5.5528832 5.0000000 5.0926312
##  [8] 2.4154735 3.2437628 0.9668987
```

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

```
## [1] 1.159854
```

The coulombic energy calculated here is:

$$\boxed{\text{Total Coulombic Energy} = 1.1598538 \text{ kcal/mol}}$$

2 Turning off O and H

Calculating the energies of all possible combinations when we turn off a hydrogen atom (H) and an oxygen atom (O) 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,S_2,C1_2,C2_2,O_2,H_2)
  atom_combos = combn(atoms,2)
  distances=mapply(distance,atom_combos[1,],atom_combos[2,])
  interm_energies = mapply(energy,atom_combos[,distances>=5][1,],atom_combos[,distances>=5]
  sprintf("Total intermolecular Van der Waals Energy is: %4.4f kcal/mol",sum(interm_energies
```

```
## [1] "Total intermolecular Van der Waals Energy is: -1.2597 kcal/mol"
```

Adding in the intramolecular energy of -0.1406 we get a total Van der Waals energy of:

$$\boxed{\text{Total Van der Waals Energy} = -1.2597423 + -0.1406 = -1.4003423 \text{ kcal/mol}}$$

The total coulombic energy when we turn off a hydrogen and an oxygen atom is:

```
  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,C2_2,O_2,H_2)
  charge_combos = combn(charged_atoms,2)
  distances=mapply(distance,charge_combos[1,],charge_combos[2,])
  print(distances)
```

```
## [1] 5.0000000 5.5528832 5.9600333 2.4154735 3.2437628 0.9668987
```

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

```
## [1] 0.01201865
```

The coulombic energy calculated here is:

$$\boxed{\text{Total Coulombic Energy} = 0.0120187 \text{ kcal/mol}}$$

3 Turning off C_2, O, and H

Calculating the energies of all possible combinations when we turn off a hydrogen atom (H), oxygen atom (O) and C2 atom (C) 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,S_2,C1_2,C2_2,O_2,H_2)
```

```
  atom_combos = combn(atoms,2)
  distances=mapply(distance,atom_combos[1,],atom_combos[2,])
  interm_energies = mapply(energy,atom_combos[,distances>=5][1,],atom_combos[,distances>=5]
  sprintf("Total intermolecular Van der Waals Energy is: %4.4f kcal/mol",sum(interm_energies
```

```
## [1] "Total intermolecular Van der Waals Energy is: -0.9395 kcal/mol"
```

Adding in the intramolecular energy of -0.1406 we get a total Van der Waals energy of:

$$\boxed{\text{Total Van der Waals Energy} = -0.9395268 + -0.1406 = -1.0801268 \text{ kcal/mol}}$$

The total coulombic energy when we turn off a hydrogen, an oxygen atom, and a carbon is:

```
  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_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 0.9668987
```

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

```
## list()
```

The intermolecular coulombic energy calculated here is 0 since the charged atoms on the other molecule are turned off. Given that the intramolecular coulombic energy is 0 we then have that the total coulombic energy is:

$$\boxed{\text{Total Coulombic Energy} = 0 \text{ kcal/mol}}$$

4 Turning off C_1, C_2, O, and H

Calculating the energies of all possible combinations when we turn off a hydrogen atom (H), oxygen atom (O), C2 atom (C), and the C1 atom 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,S_2,C1_2,C2_2,O_2,H_2)
  atom_combos = combn(atoms,2)
  distances=mapply(distance,atom_combos[1,],atom_combos[2,])
  interm_energies = mapply(energy,atom_combos[,distances>=5][1,],atom_combos[,distances>=5]
  sprintf("Total intermolecular Van der Waals Energy is: %4.4f kcal/mol",sum(interm_energies
```

```
## [1] "Total intermolecular Van der Waals Energy is: -0.6457 kcal/mol"
```

Adding in the intramolecular energy of -0.1406 we get a total Van der Waals energy of:

$$\boxed{\text{Total Van der Waals Energy} = -0.6456932 + -0.1406 = -0.7862932 \text{ kcal/mol}}$$

The intermolecular coulombic energy calculated here is 0 since the charged atoms on the other molecule are turned off. Given that the intramolecular coulombic energy is 0 we then have that the total coulombic energy is:

$$\boxed{\text{Total Coulombic Energy} = 0 \text{ kcal/mol}}$$

5 Turning off S, C_1, C_2, O, and H

```
  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_2,C1_2,C2_2,O_2,H_2)
  atom_combos = combn(atoms,2)
  distances=mapply(distance,atom_combos[1,],atom_combos[2,])
```

```
  interm_energies = mapply(energy,atom_combos[,distances>=5][1,],atom_combos[,distances>=5]
  sprintf("Total intermolecular Van der Waals Energy is: %4.4f kcal/mol",length(interm_energ

## [1] "Total intermolecular Van der Waals Energy is: 0.0000 kcal/mol"
```

Adding in the intramolecular energy of -0.1406 we get a total Van der Waals energy of:

$$\boxed{\text{Total Van der Waals Energy} = 0 + -0.1406 = -0.1406 \text{ kcal/mol}}$$

The intermolecular coulombic energy calculated here is 0 since the charged atoms on the other molecule are turned off. Given that the intramolecular coulombic energy is 0 we then have that the total coulombic energy is:

$$\boxed{\text{Total Coulombic Energy} = 0 \text{ kcal/mol}}$$