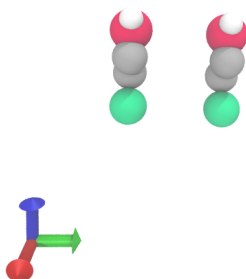


Turning Off Atoms in a Two MeOH System

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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 (Å)
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=mapapply(distance,atom_combos[1,],atom_combos[2,])
interm_energies = mapapply(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:

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

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(C2,0,C2_2,0_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[,distances>=5][2,])
print(sum(interm_energies))

## [1] 1.159854

```

The coulombic energy calculated here is:

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