input file:

check 1: length and angles

0	1	2	3	4	5
atoms id	water moleeule	type	xsu	ysu	zsu
1	1	2	x_1	y_1	z_1
	1	1			
2	1	1	x_2	y_2	z_2
3	2	2	x_3	y_3	z_3
⋮	2	1		⋮	
⋮	2	1		⋮	
⋮	⋮	⋮		⋮	
⋮	1000	2		⋮	
⋮	1000	1		⋮	
3000	1000	1	x_{3000}	y_{3000}	z_{3000}

---

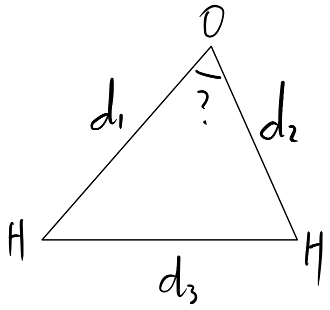
define subfunction to calculate distance and angle

distance$(x_1, y_1, z_1, x_2, y_2, z_2)$:

$$L=\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}$$

angle(d_1, d_2, d_3)

$$\frac{d_1^2+d_2^2-d_3^2}{2d_1d_2}=\cos\theta$$



angle = math.acos(θ).

a = a*180/math.pi (radians to degree)

Length and angle of each water molecule.

```
list_out=[[ ] for i in range(1000)]

while i <= 3000 (3*num_mole):
    j = i+1
    k = i+2
    dd1 = distance( list[i][4], list[i][5], list[j][6],
                    list[j][4]. list[j][5]. list[j][6].
    dd2 = distance( list[i][4], list[i][5], list[j][6],
                    list[k][4]. list[k][5]. list[k][6].
    dd3 = distance( list[j][4], list[j][5], list[j][6],
                    list[k][4]. list[k][5]. list[k][6].
    list_out[i].append(dd1)
    list_out[i].append(dd2)
    list-out[i].append(angle(dd1, dd2, dd3))
    i = i+3
```

average value:

```
    for i in range(1000):
        sum1 = sum1 + list_out[i][0]
        sum2 = sum2 + list_out[i][1]

    avg1 = sum1/1000
    avg2 = sum2/1000
    avg12 = (avg1 + avg2)/2
```

deviation:

```
    list_dev = [[] for i in range 1000]
    for i in range(1000):
        for j in range(2):
        list_dev[i].append(list_out[i][j] - avg3)
```

find the largest deviation:

```
    max = 0
    ilist = []
    for i in range(1000):
        for j in range(2):
```

```
if list_dev[i][j] > max
    max = list_dev[i][j]
    ilist.append(i)
```

ilist[-1]: the largest one.

bond connection

bond number:	bond type		
1	1	1	2
2	1	1	3
3	1	4	5
4	1	4	6
⋮	⋮	7	8
⋮	⋮	7	9
⋮	⋮	⋮	
2000	1		

if:

list[i][3] - list[i][2] = 1

list[i+1][3] - list[i+1][2] = 2

check 3 : angles

angle number	angle type			
1	1	2	1	3
2	1	5	4	6
3	1	8	7	9
4	1	11	10	12
⋮	⋮	14	13	15
1000	1			

if:

list[i][4] = list[i][3]+2

list[i][2] = list[i][3]+1