VaspForces_Demo

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1 VaspForces script Demo

VaspForces.sh is a bash script allows to extract forces and atoms position from VASP OUTCAR.
Script source

```
In [1]: %%bash
        ./VaspForces.sh -infos
```

```
This bash script allows to extract forces and atoms positions from OUTCAR VASP File.
The script takes three options :
        -outcar : Sets the outcar file name.
        -atom   : Sets the Atom number.
        -iter   : Sets the Iterations number.
        -out    : Sets the output file.
        -infos  : Prints infos

For helping : ./VaspForces.sh -h

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```

```
In [2]: %%bash
        ./VaspForces.sh -h
```

```
Usage of this script :
        -outcar : Sets the outcar file name.
        -atom   : Sets the Atom number default value : all atoms.
        -iter   : Sets the Iterations number default value : all iterations.
        -out    : Sets the output file.
        -h      : Print this message.

        Example:
                 VaspForces.sh -atom=4 -iter=all -outcar=OUTCAR
```

```
In [3]: %%bash
        ./VaspForces.sh -outcar=OUTCAR_test -iter=1
```

```
N_iteration :     1
```

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	0.00000	0.00000	-0.000000	0.000000	0.044726
3	1.40367	0.81041	2.34648	-0.000000	0.000000	0.087454
4	-0.00000	1.62082	4.65922	0.000000	-0.000000	-0.004325
5	0.00000	0.00000	6.96112	-0.000000	0.000000	-0.016941
6	1.40367	0.81041	9.25806	-0.000000	-0.000000	0.004007
7	-0.00000	1.62082	11.55613	-0.000000	0.000000	-0.002400
8	0.00000	0.00000	13.85529	-0.000000	0.000000	0.016958
9	1.40367	0.81041	16.15276	-0.000000	-0.000000	0.000512
10	-0.00000	1.62082	18.45244	-0.000000	0.000000	-0.000678
11	0.00000	0.00000	20.74969	-0.000000	0.000000	-0.005650
12	1.40367	0.81041	23.04695	0.000000	-0.000000	0.010209
13	-0.00000	1.62082	25.34662	-0.000000	0.000000	-0.008828
14	0.00000	0.00000	27.64409	-0.000000	0.000000	-0.011130
15	1.40367	0.81041	29.94325	-0.000000	0.000000	-0.012448
16	-0.00000	1.62082	32.24132	-0.000000	0.000000	-0.000735
17	0.00000	0.00000	34.53827	-0.000000	0.000000	0.016650
18	1.40367	0.81041	36.84016	0.000000	0.000000	-0.028154
19	-0.00000	1.62082	39.15291	0.000000	-0.000000	0.003737
20	0.00000	0.00000	41.49939	-0.000000	0.000000	-0.038777
21	1.40367	0.81041	43.56914	-0.000000	0.000000	0.039641
22	-0.00000	1.62082	45.41039	0.000000	-0.000000	0.010266
23	1.40367	0.81041	47.27455	0.000000	-0.000000	0.029564
24	-0.00000	1.62082	49.12012	0.000000	-0.000000	0.032760
25	1.40367	0.81041	50.96986	0.000000	0.000000	-0.045674
26	-0.00000	1.62082	52.81241	0.000000	-0.000000	0.013674
27	1.40367	0.81041	54.65496	-0.000000	0.000000	-0.023125
28	-0.00000	1.62082	56.49752	-0.000000	0.000000	0.039719
29	1.40367	0.81041	58.34007	0.000000	0.000000	0.020598
30	-0.00000	1.62082	60.18262	0.000000	0.000000	-0.043582
31	1.40367	0.81041	62.02517	0.000000	-0.000000	-0.015449
32	-0.00000	1.62082	63.86773	-0.000000	0.000000	-0.007666
33	1.40367	0.81041	65.71028	0.000000	-0.000000	0.009225
34	-0.00000	1.62082	67.55284	0.000000	-0.000000	-0.021633
35	1.40367	0.81041	69.39539	0.000000	-0.000000	0.067382
36	-0.00000	1.62082	71.24512	-0.000000	0.000000	0.019422
37	1.40367	0.81041	73.09069	-0.000000	-0.000000	-0.035805
38	-0.00000	1.62082	74.95485	-0.000000	0.000000	-0.012704

In [4]:
```
%%bash
./VaspForces.sh -outcar=OUTCAR_test -iter=1 -atom=4
```

```
N_iteration :     1
```

```
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.65922    0.000000    -0.000000    -0.004325
```

```
In [5]: %%bash
        ./VaspForces.sh -outcar=OUTCAR_test -iter=all -atom=4
```

```
N_iteration :     1
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.65922    0.000000    -0.000000    -0.004325

N_iteration :     2
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.65901    -0.000000    0.000000    0.017708

N_iteration :     3
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.65901    0.000000    -0.000000    0.017778

N_iteration :     4
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.65901    0.000000    -0.000000    0.017928

N_iteration :     5
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.65901    -0.000000    0.000000    0.018196

N_iteration :     6
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.65900    0.000000    -0.000000    0.018774

N_iteration :     7
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.65899    -0.000000    0.000000    0.019816

N_iteration :     8
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.65897    -0.000000    0.000000    0.022050

N_iteration :     9
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.65894    -0.000000    0.000000    0.026354

N_iteration :    10
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66025    -0.000000    0.000000    0.022689
```

```
N_iteration :    11
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66116    0.000000   -0.000000    0.020264

N_iteration :    12
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66257   -0.000000    0.000000    0.009298

N_iteration :    13
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66395    0.000000   -0.000000   -0.001224

N_iteration :    14
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66424   -0.000000    0.000000   -0.003422

N_iteration :    15
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66496    0.000000   -0.000000   -0.003867

N_iteration :    16
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66544    0.000000   -0.000000   -0.004232

N_iteration :    17
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66567   -0.000000    0.000000   -0.000063

N_iteration :    18
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66585    0.000000   -0.000000    0.003078

N_iteration :    19
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66591   -0.000000    0.000000    0.004140

N_iteration :    20
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66632   -0.000000    0.000000    0.004870

N_iteration :    21
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66671   -0.000000    0.000000    0.005475

N_iteration :    22
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66749   -0.000000    0.000000    0.006742
```

```
N_iteration :    23
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66708    0.000000    0.000000    0.006046

N_iteration :    24
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66793    0.000000   -0.000000   -0.000972

N_iteration :    25
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66855    0.000000   -0.000000   -0.006162

N_iteration :    26
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66858   -0.000000    0.000000    0.000093

N_iteration :    27
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66862   -0.000000    0.000000    0.007143

N_iteration :    28
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66883   -0.000000   -0.000000    0.005444

N_iteration :    29
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66945    0.000000    0.000000    0.000430

N_iteration :    30
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66956   -0.000000    0.000000   -0.000232

N_iteration :    31
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66983    0.000000   -0.000000   -0.001903

N_iteration :    32
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66985    0.000000    0.000000    0.002767

N_iteration :    33
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.66987   -0.000000    0.000000    0.008245

N_iteration :    34
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67042    0.000000   -0.000000    0.005559
```

```
N_iteration :    35
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67124    0.000000   -0.000000    0.001628

N_iteration :    36
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67192   -0.000000    0.000000    0.003026

N_iteration :    37
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67252   -0.000000   -0.000000    0.004125

N_iteration :    38
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67352   -0.000000    0.000000    0.001151

N_iteration :    39
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67416   -0.000000    0.000000   -0.000619

N_iteration :    40
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67508    0.000000   -0.000000   -0.001524

N_iteration :    41
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67556   -0.000000    0.000000   -0.001896

N_iteration :    42
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67612   -0.000000    0.000000    0.004701

N_iteration :    43
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67629    0.000000    0.000000    0.006700

N_iteration :    44
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67755   -0.000000    0.000000   -0.000189

N_iteration :    45
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67801   -0.000000    0.000000   -0.002585

N_iteration :    46
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67882    0.000000   -0.000000   -0.003447
```

```
N_iteration :    47
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67963    -0.000000    0.000000    -0.004311

N_iteration :    48
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67971     0.000000    -0.000000    0.002940

N_iteration :    49
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.67972     0.000000    0.000000     0.004065

N_iteration :    50
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.68010     0.000000    -0.000000    0.000924

N_iteration :    51
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.68021     0.000000    -0.000000    0.000039

N_iteration :    52
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.68048    -0.000000    0.000000    -0.001020

N_iteration :    53
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.68052    -0.000000    -0.000000   -0.001182

N_iteration :    54
 atom          X          Y          Z          Fx          Fy          Fz
    4   -0.00000    1.62082    4.68049    -0.000000    0.000000    0.000705
```

In [6]:
```
%%bash
./VaspForces.sh -outcar=OUTCAR_test -iter=all -atom=all
```

```
N_iteration :     1
 atom          X          Y          Z          Fx          Fy          Fz
    1    0.00000    0.00000    0.00000     0.000000    0.000000    0.000000
    2    0.00000    0.00000    0.00000    -0.000000    0.000000    0.044726
    3    1.40367    0.81041    2.34648    -0.000000    0.000000    0.087454
    4   -0.00000    1.62082    4.65922     0.000000   -0.000000   -0.004325
    5    0.00000    0.00000    6.96112    -0.000000    0.000000   -0.016941
    6    1.40367    0.81041    9.25806    -0.000000   -0.000000    0.004007
    7   -0.00000    1.62082   11.55613    -0.000000    0.000000   -0.002400
    8    0.00000    0.00000   13.85529    -0.000000    0.000000    0.016958
    9    1.40367    0.81041   16.15276    -0.000000   -0.000000    0.000512
```

10	-0.00000	1.62082	18.45244	-0.000000	0.000000	-0.000678
11	0.00000	0.00000	20.74969	-0.000000	0.000000	-0.005650
12	1.40367	0.81041	23.04695	0.000000	-0.000000	0.010209
13	-0.00000	1.62082	25.34662	-0.000000	0.000000	-0.008828
14	0.00000	0.00000	27.64409	-0.000000	0.000000	-0.011130
15	1.40367	0.81041	29.94325	-0.000000	0.000000	-0.012448
16	-0.00000	1.62082	32.24132	-0.000000	0.000000	-0.000735
17	0.00000	0.00000	34.53827	-0.000000	0.000000	0.016650
18	1.40367	0.81041	36.84016	0.000000	0.000000	-0.028154
19	-0.00000	1.62082	39.15291	0.000000	-0.000000	0.003737
20	0.00000	0.00000	41.49939	-0.000000	0.000000	-0.038777
21	1.40367	0.81041	43.56914	-0.000000	0.000000	0.039641
22	-0.00000	1.62082	45.41039	0.000000	-0.000000	0.010266
23	1.40367	0.81041	47.27455	0.000000	-0.000000	0.029564
24	-0.00000	1.62082	49.12012	0.000000	-0.000000	0.032760
25	1.40367	0.81041	50.96986	0.000000	0.000000	-0.045674
26	-0.00000	1.62082	52.81241	0.000000	-0.000000	0.013674
27	1.40367	0.81041	54.65496	-0.000000	0.000000	-0.023125
28	-0.00000	1.62082	56.49752	-0.000000	0.000000	0.039719
29	1.40367	0.81041	58.34007	0.000000	0.000000	0.020598
30	-0.00000	1.62082	60.18262	0.000000	0.000000	-0.043582
31	1.40367	0.81041	62.02517	0.000000	-0.000000	-0.015449
32	-0.00000	1.62082	63.86773	-0.000000	0.000000	-0.007666
33	1.40367	0.81041	65.71028	0.000000	-0.000000	0.009225
34	-0.00000	1.62082	67.55284	0.000000	-0.000000	-0.021633
35	1.40367	0.81041	69.39539	0.000000	-0.000000	0.067382
36	-0.00000	1.62082	71.24512	-0.000000	0.000000	0.019422
37	1.40367	0.81041	73.09069	-0.000000	-0.000000	-0.035805
38	-0.00000	1.62082	74.95485	-0.000000	0.000000	-0.012704

N_iteration : 2

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	0.00216	0.000000	0.000000	-0.011709
3	1.40367	0.81041	2.35069	0.000000	-0.000000	0.036556
4	-0.00000	1.62082	4.65901	-0.000000	0.000000	0.017708
5	-0.00000	0.00000	6.96030	-0.000000	0.000000	-0.002862
6	1.40367	0.81041	9.25826	-0.000000	0.000000	0.004266
7	-0.00000	1.62082	11.55602	-0.000000	-0.000000	-0.000361
8	-0.00000	0.00000	13.85611	-0.000000	0.000000	-0.009035
9	1.40367	0.81041	16.15279	-0.000000	0.000000	0.004675
10	-0.00000	1.62082	18.45241	0.000000	-0.000000	-0.003294
11	-0.00000	0.00000	20.74942	-0.000000	0.000000	0.004669
12	1.40367	0.81041	23.04744	0.000000	-0.000000	-0.001598
13	-0.00000	1.62082	25.34619	-0.000000	0.000000	-0.000437
14	-0.00000	0.00000	27.64355	-0.000000	0.000000	0.011240
15	1.40367	0.81041	29.94265	0.000000	-0.000000	0.000903
16	-0.00000	1.62082	32.24129	0.000000	-0.000000	-0.005489

17	-0.00000	0.00000	34.53907	-0.000000	0.000000	-0.004897
18	1.40367	0.81041	36.83881	-0.000000	0.000000	0.000888
19	-0.00000	1.62082	39.15309	0.000000	0.000000	-0.011704
20	-0.00000	0.00000	41.49752	-0.000000	0.000000	0.017684
21	1.40367	0.81041	43.57105	0.000000	-0.000000	0.020172
22	-0.00000	1.62082	45.41089	0.000000	0.000000	-0.021201
23	1.40367	0.81041	47.27598	-0.000000	0.000000	-0.019684
24	-0.00000	1.62082	49.12170	0.000000	-0.000000	0.014534
25	1.40367	0.81041	50.96766	-0.000000	0.000000	-0.026034
26	-0.00000	1.62082	52.81307	-0.000000	0.000000	-0.010661
27	1.40367	0.81041	54.65385	-0.000000	-0.000000	0.012572
28	-0.00000	1.62082	56.49943	0.000000	-0.000000	-0.024668
29	1.40367	0.81041	58.34106	-0.000000	0.000000	-0.015650
30	-0.00000	1.62082	60.18052	-0.000000	0.000000	0.023239
31	1.40367	0.81041	62.02443	0.000000	-0.000000	0.001769
32	-0.00000	1.62082	63.86736	0.000000	0.000000	-0.002872
33	1.40367	0.81041	65.71073	0.000000	-0.000000	0.012044
34	-0.00000	1.62082	67.55180	0.000000	-0.000000	0.006293
35	1.40367	0.81041	69.39864	-0.000000	0.000000	0.025057
36	-0.00000	1.62082	71.24605	-0.000000	0.000000	-0.016930
37	1.40367	0.81041	73.08896	-0.000000	-0.000000	-0.001213
38	-0.00000	1.62082	74.95424	0.000000	0.000000	0.034144

N_iteration : 3

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	0.00216	0.000000	-0.000000	-0.011810
3	1.40367	0.81041	2.35071	0.000000	-0.000000	0.036388
4	-0.00000	1.62082	4.65901	0.000000	-0.000000	0.017778
5	-0.00000	0.00000	6.96030	0.000000	-0.000000	-0.002779
6	1.40367	0.81041	9.25826	0.000000	-0.000000	0.004290
7	-0.00000	1.62082	11.55602	-0.000000	0.000000	-0.000316
8	-0.00000	0.00000	13.85611	0.000000	-0.000000	-0.009063
9	1.40367	0.81041	16.15279	0.000000	-0.000000	0.004683
10	-0.00000	1.62082	18.45241	0.000000	-0.000000	-0.003357
11	-0.00000	0.00000	20.74942	0.000000	-0.000000	0.004655
12	1.40367	0.81041	23.04744	0.000000	-0.000000	-0.001632
13	-0.00000	1.62082	25.34619	0.000000	-0.000000	-0.000383
14	-0.00000	0.00000	27.64355	0.000000	-0.000000	0.011300
15	1.40367	0.81041	29.94265	-0.000000	-0.000000	0.000949
16	-0.00000	1.62082	32.24129	-0.000000	0.000000	-0.005457
17	-0.00000	0.00000	34.53907	0.000000	-0.000000	-0.004964
18	1.40367	0.81041	36.83880	0.000000	-0.000000	0.000966
19	-0.00000	1.62082	39.15309	0.000000	-0.000000	-0.011799
20	-0.00000	0.00000	41.49751	0.000000	-0.000000	0.017752
21	1.40367	0.81041	43.57106	0.000000	-0.000000	0.020104
22	-0.00000	1.62082	45.41089	0.000000	0.000000	-0.021250
23	1.40367	0.81041	47.27598	-0.000000	0.000000	-0.019693

24	-0.00000	1.62082	49.12171	0.000000	-0.000000	0.014538
25	1.40367	0.81041	50.96765	0.000000	-0.000000	-0.025994
26	-0.00000	1.62082	52.81307	0.000000	-0.000000	-0.010720
27	1.40367	0.81041	54.65385	-0.000000	0.000000	0.012683
28	-0.00000	1.62082	56.49944	0.000000	0.000000	-0.024676
29	1.40367	0.81041	58.34107	-0.000000	0.000000	-0.015696
30	-0.00000	1.62082	60.18051	-0.000000	-0.000000	0.023302
31	1.40367	0.81041	62.02443	-0.000000	0.000000	0.001763
32	-0.00000	1.62082	63.86735	-0.000000	0.000000	-0.002933
33	1.40367	0.81041	65.71073	0.000000	-0.000000	0.012022
34	-0.00000	1.62082	67.55179	-0.000000	0.000000	0.006360
35	1.40367	0.81041	69.39865	0.000000	-0.000000	0.024984
36	-0.00000	1.62082	71.24606	-0.000000	0.000000	-0.016987
37	1.40367	0.81041	73.08896	0.000000	-0.000000	-0.001199
38	-0.00000	1.62082	74.95423	-0.000000	0.000000	0.034153

N_iteration : 4

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	0.00218	0.000000	-0.000000	-0.012020
3	1.40367	0.81041	2.35073	0.000000	-0.000000	0.036134
4	-0.00000	1.62082	4.65901	0.000000	-0.000000	0.017928
5	-0.00000	0.00000	6.96030	0.000000	-0.000000	-0.002650
6	1.40367	0.81041	9.25826	0.000000	-0.000000	0.004307
7	-0.00000	1.62082	11.55601	0.000000	0.000000	-0.000271
8	-0.00000	0.00000	13.85612	0.000000	-0.000000	-0.009171
9	1.40367	0.81041	16.15279	0.000000	-0.000000	0.004686
10	-0.00000	1.62082	18.45241	0.000000	-0.000000	-0.003342
11	-0.00000	0.00000	20.74942	0.000000	-0.000000	0.004725
12	1.40367	0.81041	23.04744	0.000000	-0.000000	-0.001693
13	-0.00000	1.62082	25.34619	-0.000000	-0.000000	-0.000385
14	-0.00000	0.00000	27.64355	0.000000	-0.000000	0.011296
15	1.40367	0.81041	29.94265	0.000000	-0.000000	0.001022
16	-0.00000	1.62082	32.24129	0.000000	-0.000000	-0.005383
17	-0.00000	0.00000	34.53908	0.000000	-0.000000	-0.005042
18	1.40367	0.81041	36.83879	-0.000000	-0.000000	0.001077
19	-0.00000	1.62082	39.15309	-0.000000	0.000000	-0.011970
20	-0.00000	0.00000	41.49750	0.000000	-0.000000	0.017915
21	1.40367	0.81041	43.57107	0.000000	-0.000000	0.019987
22	-0.00000	1.62082	45.41089	0.000000	-0.000000	-0.021183
23	1.40367	0.81041	47.27599	-0.000000	0.000000	-0.019683
24	-0.00000	1.62082	49.12171	-0.000000	0.000000	0.014448
25	1.40367	0.81041	50.96764	-0.000000	0.000000	-0.025914
26	-0.00000	1.62082	52.81308	-0.000000	0.000000	-0.010823
27	1.40367	0.81041	54.65384	-0.000000	0.000000	0.012808
28	-0.00000	1.62082	56.49945	0.000000	-0.000000	-0.024742
29	1.40367	0.81041	58.34107	-0.000000	0.000000	-0.015729
30	-0.00000	1.62082	60.18050	-0.000000	-0.000000	0.023423

31	1.40367	0.81041	62.02442	-0.000000	-0.000000	0.001731
32	-0.00000	1.62082	63.86735	-0.000000	-0.000000	-0.002964
33	1.40367	0.81041	65.71073	0.000000	0.000000	0.012024
34	-0.00000	1.62082	67.55179	-0.000000	0.000000	0.006539
35	1.40367	0.81041	69.39866	-0.000000	0.000000	0.024862
36	-0.00000	1.62082	71.24606	0.000000	-0.000000	-0.017024
37	1.40367	0.81041	73.08895	0.000000	-0.000000	-0.001171
38	-0.00000	1.62082	74.95423	-0.000000	0.000000	0.033924

N_iteration : 5

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	0.00220	-0.000000	0.000000	-0.012381
3	1.40367	0.81041	2.35078	0.000000	-0.000000	0.035828
4	-0.00000	1.62082	4.65901	-0.000000	0.000000	0.018196
5	-0.00000	0.00000	6.96029	-0.000000	0.000000	-0.002576
6	1.40367	0.81041	9.25826	0.000000	0.000000	0.004174
7	-0.00000	1.62082	11.55601	-0.000000	0.000000	-0.000207
8	-0.00000	0.00000	13.85613	-0.000000	0.000000	-0.009279
9	1.40367	0.81041	16.15279	0.000000	-0.000000	0.004782
10	-0.00000	1.62082	18.45240	0.000000	0.000000	-0.003325
11	-0.00000	0.00000	20.74941	-0.000000	0.000000	0.004810
12	1.40367	0.81041	23.04745	-0.000000	0.000000	-0.001821
13	-0.00000	1.62082	25.34619	-0.000000	0.000000	-0.000359
14	-0.00000	0.00000	27.64354	-0.000000	0.000000	0.011269
15	1.40367	0.81041	29.94264	0.000000	-0.000000	0.001047
16	-0.00000	1.62082	32.24129	0.000000	0.000000	-0.005349
17	-0.00000	0.00000	34.53908	-0.000000	0.000000	-0.005236
18	1.40367	0.81041	36.83878	-0.000000	0.000000	0.001322
19	-0.00000	1.62082	39.15309	-0.000000	0.000000	-0.012196
20	-0.00000	0.00000	41.49748	-0.000000	0.000000	0.018224
21	1.40367	0.81041	43.57109	-0.000000	0.000000	0.019751
22	-0.00000	1.62082	45.41090	0.000000	-0.000000	-0.021130
23	1.40367	0.81041	47.27601	-0.000000	0.000000	-0.019732
24	-0.00000	1.62082	49.12173	0.000000	0.000000	0.014280
25	1.40367	0.81041	50.96761	-0.000000	-0.000000	-0.025677
26	-0.00000	1.62082	52.81308	-0.000000	-0.000000	-0.010983
27	1.40367	0.81041	54.65383	-0.000000	0.000000	0.012995
28	-0.00000	1.62082	56.49947	0.000000	0.000000	-0.024941
29	1.40367	0.81041	58.34108	-0.000000	-0.000000	-0.015854
30	-0.00000	1.62082	60.18048	0.000000	0.000000	0.023631
31	1.40367	0.81041	62.02441	-0.000000	0.000000	0.001730
32	-0.00000	1.62082	63.86735	-0.000000	0.000000	-0.002935
33	1.40367	0.81041	65.71074	0.000000	-0.000000	0.011974
34	-0.00000	1.62082	67.55178	0.000000	-0.000000	0.006740
35	1.40367	0.81041	69.39870	0.000000	-0.000000	0.024538
36	-0.00000	1.62082	71.24607	0.000000	-0.000000	-0.017070
37	1.40367	0.81041	73.08893	0.000000	-0.000000	-0.000953

38	-0.00000	1.62082	74.95422	-0.000000	0.000000	0.033827

N_iteration : 6

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	0.00225	-0.000000	0.000000	-0.013059
3	1.40367	0.81041	2.35087	-0.000000	0.000000	0.035140
4	-0.00000	1.62082	4.65900	0.000000	-0.000000	0.018774
5	-0.00000	0.00000	6.96027	-0.000000	0.000000	-0.002441
6	1.40367	0.81041	9.25826	-0.000000	-0.000000	0.003879
7	-0.00000	1.62082	11.55601	-0.000000	0.000000	0.000006
8	-0.00000	0.00000	13.85615	-0.000000	0.000000	-0.009438
9	1.40367	0.81041	16.15279	-0.000000	0.000000	0.004907
10	-0.00000	1.62082	18.45240	0.000000	-0.000000	-0.003453
11	-0.00000	0.00000	20.74941	-0.000000	0.000000	0.004894
12	1.40367	0.81041	23.04746	-0.000000	0.000000	-0.002002
13	-0.00000	1.62082	25.34618	0.000000	0.000000	-0.000155
14	-0.00000	0.00000	27.64353	-0.000000	0.000000	0.011269
15	1.40367	0.81041	29.94263	-0.000000	0.000000	0.001036
16	-0.00000	1.62082	32.24128	0.000000	-0.000000	-0.005391
17	-0.00000	0.00000	34.53910	-0.000000	0.000000	-0.005685
18	1.40367	0.81041	36.83875	0.000000	0.000000	0.001888
19	-0.00000	1.62082	39.15310	-0.000000	0.000000	-0.012617
20	-0.00000	0.00000	41.49744	-0.000000	-0.000000	0.018947
21	1.40367	0.81041	43.57113	0.000000	-0.000000	0.019323
22	-0.00000	1.62082	45.41091	0.000000	-0.000000	-0.021002
23	1.40367	0.81041	47.27604	-0.000000	0.000000	-0.019902
24	-0.00000	1.62082	49.12177	-0.000000	0.000000	0.014030
25	1.40367	0.81041	50.96756	-0.000000	0.000000	-0.025144
26	-0.00000	1.62082	52.81310	0.000000	-0.000000	-0.011406
27	1.40367	0.81041	54.65380	0.000000	-0.000000	0.013317
28	-0.00000	1.62082	56.49951	0.000000	-0.000000	-0.025286
29	1.40367	0.81041	58.34110	0.000000	-0.000000	-0.016055
30	-0.00000	1.62082	60.18043	-0.000000	-0.000000	0.023946
31	1.40367	0.81041	62.02440	-0.000000	-0.000000	0.001737
32	-0.00000	1.62082	63.86734	-0.000000	0.000000	-0.002774
33	1.40367	0.81041	65.71075	0.000000	0.000000	0.011750
34	-0.00000	1.62082	67.55175	0.000000	-0.000000	0.007056
35	1.40367	0.81041	69.39877	0.000000	-0.000000	0.023985
36	-0.00000	1.62082	71.24609	-0.000000	0.000000	-0.017112
37	1.40367	0.81041	73.08889	-0.000000	0.000000	-0.000741
38	-0.00000	1.62082	74.95421	0.000000	-0.000000	0.033605

N_iteration : 7

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	0.00235	0.000000	-0.000000	-0.014644
3	1.40367	0.81041	2.35106	0.000000	0.000000	0.033531

4	-0.00000	1.62082	4.65899	-0.000000	0.000000	0.019816
5	-0.00000	0.00000	6.96023	-0.000000	0.000000	-0.001939
6	1.40367	0.81041	9.25827	-0.000000	-0.000000	0.003558
7	-0.00000	1.62082	11.55601	-0.000000	0.000000	0.000313
8	-0.00000	0.00000	13.85618	-0.000000	-0.000000	-0.010042
9	1.40367	0.81041	16.15279	-0.000000	0.000000	0.005148
10	-0.00000	1.62082	18.45240	-0.000000	0.000000	-0.003378
11	-0.00000	0.00000	20.74940	-0.000000	0.000000	0.005261
12	1.40367	0.81041	23.04748	-0.000000	0.000000	-0.002576
13	-0.00000	1.62082	25.34616	0.000000	-0.000000	-0.000043
14	-0.00000	0.00000	27.64351	-0.000000	0.000000	0.011316
15	1.40367	0.81041	29.94260	0.000000	-0.000000	0.001333
16	-0.00000	1.62082	32.24128	-0.000000	0.000000	-0.005236
17	-0.00000	0.00000	34.53914	-0.000000	-0.000000	-0.006582
18	1.40367	0.81041	36.83869	0.000000	-0.000000	0.002864
19	-0.00000	1.62082	39.15310	0.000000	-0.000000	-0.013562
20	-0.00000	0.00000	41.49735	0.000000	0.000000	0.020372
21	1.40367	0.81041	43.57122	-0.000000	-0.000000	0.018297
22	-0.00000	1.62082	45.41093	0.000000	0.000000	-0.020782
23	1.40367	0.81041	47.27610	0.000000	-0.000000	-0.020148
24	-0.00000	1.62082	49.12184	0.000000	0.000000	0.013312
25	1.40367	0.81041	50.96746	0.000000	-0.000000	-0.023925
26	-0.00000	1.62082	52.81313	-0.000000	0.000000	-0.011887
27	1.40367	0.81041	54.65375	0.000000	-0.000000	0.014064
28	-0.00000	1.62082	56.49960	-0.000000	0.000000	-0.026175
29	1.40367	0.81041	58.34115	0.000000	-0.000000	-0.016418
30	-0.00000	1.62082	60.18033	0.000000	-0.000000	0.024960
31	1.40367	0.81041	62.02436	-0.000000	0.000000	0.001568
32	-0.00000	1.62082	63.86732	-0.000000	0.000000	-0.002960
33	1.40367	0.81041	65.71077	-0.000000	0.000000	0.011536
34	-0.00000	1.62082	67.55171	0.000000	-0.000000	0.008200
35	1.40367	0.81041	69.39892	0.000000	-0.000000	0.022800
36	-0.00000	1.62082	71.24614	0.000000	0.000000	-0.017466
37	1.40367	0.81041	73.08881	0.000000	-0.000000	-0.000149
38	-0.00000	1.62082	74.95418	0.000000	-0.000000	0.032919

N_iteration : 8

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	0.00254	-0.000000	-0.000000	-0.017720
3	1.40367	0.81041	2.35145	-0.000000	0.000000	0.030465
4	-0.00000	1.62082	4.65897	-0.000000	0.000000	0.022050
5	-0.00000	0.00000	6.96016	-0.000000	0.000000	-0.001062
6	1.40367	0.81041	9.25829	-0.000000	-0.000000	0.002709
7	-0.00000	1.62082	11.55599	0.000000	-0.000000	0.001020
8	-0.00000	0.00000	13.85626	-0.000000	0.000000	-0.011006
9	1.40367	0.81041	16.15279	-0.000000	0.000000	0.005603
10	-0.00000	1.62082	18.45240	-0.000000	0.000000	-0.003583

11	-0.00000	0.00000	20.74937	-0.000000	0.000000	0.005813
12	1.40367	0.81041	23.04753	-0.000000	0.000000	-0.003514
13	-0.00000	1.62082	25.34612	-0.000000	0.000000	0.000412
14	-0.00000	0.00000	27.64346	-0.000000	0.000000	0.011275
15	1.40367	0.81041	29.94255	-0.000000	0.000000	0.001624
16	-0.00000	1.62082	32.24128	0.000000	-0.000000	-0.005004
17	-0.00000	0.00000	34.53921	-0.000000	0.000000	-0.008225
18	1.40367	0.81041	36.83856	-0.000000	0.000000	0.005000
19	-0.00000	1.62082	39.15312	-0.000000	0.000000	-0.015435
20	-0.00000	0.00000	41.49718	-0.000000	0.000000	0.023147
21	1.40367	0.81041	43.57139	0.000000	0.000000	0.016254
22	-0.00000	1.62082	45.41098	0.000000	-0.000000	-0.020235
23	1.40367	0.81041	47.27623	-0.000000	0.000000	-0.020459
24	-0.00000	1.62082	49.12198	0.000000	-0.000000	0.011953
25	1.40367	0.81041	50.96726	-0.000000	-0.000000	-0.021753
26	-0.00000	1.62082	52.81319	0.000000	-0.000000	-0.013006
27	1.40367	0.81041	54.65365	0.000000	-0.000000	0.015696
28	-0.00000	1.62082	56.49977	0.000000	0.000000	-0.027938
29	1.40367	0.81041	58.34124	-0.000000	0.000000	-0.017354
30	-0.00000	1.62082	60.18014	-0.000000	0.000000	0.026760
31	1.40367	0.81041	62.02430	0.000000	0.000000	0.001478
32	-0.00000	1.62082	63.86729	0.000000	0.000000	-0.002914
33	1.40367	0.81041	65.71081	0.000000	-0.000000	0.010868
34	-0.00000	1.62082	67.55161	0.000000	-0.000000	0.010094
35	1.40367	0.81041	69.39921	-0.000000	-0.000000	0.020403
36	-0.00000	1.62082	71.24622	-0.000000	0.000000	-0.017963
37	1.40367	0.81041	73.08866	0.000000	-0.000000	0.001220
38	-0.00000	1.62082	74.95413	0.000000	-0.000000	0.031594

N_iteration : 9

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	0.00293	0.000000	0.000000	-0.023656
3	1.40367	0.81041	2.35221	0.000000	0.000000	0.024259
4	-0.00000	1.62082	4.65894	-0.000000	0.000000	0.026354
5	-0.00000	0.00000	6.96001	-0.000000	0.000000	0.000739
6	1.40367	0.81041	9.25833	-0.000000	0.000000	0.001233
7	-0.00000	1.62082	11.55597	0.000000	-0.000000	0.002539
8	-0.00000	0.00000	13.85640	-0.000000	0.000000	-0.013022
9	1.40367	0.81041	16.15280	0.000000	-0.000000	0.006526
10	-0.00000	1.62082	18.45239	0.000000	-0.000000	-0.003822
11	-0.00000	0.00000	20.74932	-0.000000	0.000000	0.006997
12	1.40367	0.81041	23.04762	0.000000	0.000000	-0.005470
13	-0.00000	1.62082	25.34604	0.000000	-0.000000	0.001274
14	-0.00000	0.00000	27.64336	0.000000	0.000000	0.011337
15	1.40367	0.81041	29.94244	-0.000000	-0.000000	0.002341
16	-0.00000	1.62082	32.24127	0.000000	0.000000	-0.004565
17	-0.00000	0.00000	34.53936	-0.000000	0.000000	-0.011617

18	1.40367	0.81041	36.83832	-0.000000	0.000000	0.009092
19	-0.00000	1.62082	39.15315	-0.000000	0.000000	-0.019243
20	-0.00000	0.00000	41.49684	-0.000000	0.000000	0.028750
21	1.40367	0.81041	43.57174	-0.000000	0.000000	0.012328
22	-0.00000	1.62082	45.41107	-0.000000	0.000000	-0.019372
23	1.40367	0.81041	47.27649	-0.000000	-0.000000	-0.021159
24	-0.00000	1.62082	49.12227	0.000000	-0.000000	0.009456
25	1.40367	0.81041	50.96687	-0.000000	-0.000000	-0.017392
26	-0.00000	1.62082	52.81331	0.000000	-0.000000	-0.015519
27	1.40367	0.81041	54.65345	-0.000000	0.000000	0.018882
28	-0.00000	1.62082	56.50012	0.000000	-0.000000	-0.031104
29	1.40367	0.81041	58.34142	-0.000000	0.000000	-0.019007
30	-0.00000	1.62082	60.17976	0.000000	-0.000000	0.030286
31	1.40367	0.81041	62.02416	0.000000	-0.000000	0.001019
32	-0.00000	1.62082	63.86722	0.000000	-0.000000	-0.003164
33	1.40367	0.81041	65.71089	-0.000000	0.000000	0.009687
34	-0.00000	1.62082	67.55142	0.000000	-0.000000	0.014210
35	1.40367	0.81041	69.39980	-0.000000	0.000000	0.015955
36	-0.00000	1.62082	71.24639	-0.000000	0.000000	-0.018940
37	1.40367	0.81041	73.08834	0.000000	-0.000000	0.003431
38	-0.00000	1.62082	74.95402	-0.000000	-0.000000	0.028717

N_iteration : 10

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	0.00220	-0.000000	-0.000000	-0.019470
3	1.40367	0.81041	2.35442	-0.000000	0.000000	0.006227
4	-0.00000	1.62082	4.66025	-0.000000	0.000000	0.022689
5	-0.00000	0.00000	6.95986	0.000000	-0.000000	0.011251
6	1.40367	0.81041	9.25843	-0.000000	-0.000000	-0.000756
7	-0.00000	1.62082	11.55608	0.000000	-0.000000	-0.001488
8	-0.00000	0.00000	13.85592	0.000000	-0.000000	-0.003992
9	1.40367	0.81041	16.15314	0.000000	0.000000	-0.002264
10	-0.00000	1.62082	18.45219	0.000000	-0.000000	0.003155
11	-0.00000	0.00000	20.74962	0.000000	-0.000000	0.000654
12	1.40367	0.81041	23.04745	-0.000000	0.000000	-0.001741
13	-0.00000	1.62082	25.34601	-0.000000	0.000000	0.003474
14	-0.00000	0.00000	27.64383	0.000000	-0.000000	0.005373
15	1.40367	0.81041	29.94242	-0.000000	0.000000	0.004047
16	-0.00000	1.62082	32.24103	-0.000000	-0.000000	-0.004199
17	-0.00000	0.00000	34.53894	0.000000	-0.000000	-0.006746
18	1.40367	0.81041	36.83848	-0.000000	-0.000000	-0.001474
19	-0.00000	1.62082	39.15220	0.000000	-0.000000	-0.001579
20	-0.00000	0.00000	41.49791	-0.000000	-0.000000	0.016091
21	1.40367	0.81041	43.57281	0.000000	-0.000000	0.005273
22	-0.00000	1.62082	45.41018	-0.000000	0.000000	-0.009463
23	1.40367	0.81041	47.27572	0.000000	-0.000000	-0.015969
24	-0.00000	1.62082	49.12311	-0.000000	0.000000	-0.005687

25	1.40367	0.81041	50.96547	0.000000	-0.000000	-0.005046
26	-0.00000	1.62082	52.81266	-0.000000	0.000000	-0.012692
27	1.40367	0.81041	54.65417	-0.000000	-0.000000	0.004877
28	-0.00000	1.62082	56.49895	-0.000000	0.000000	-0.021781
29	1.40367	0.81041	58.34066	0.000000	-0.000000	-0.011492
30	-0.00000	1.62082	60.18085	0.000000	-0.000000	0.017150
31	1.40367	0.81041	62.02404	0.000000	-0.000000	0.003452
32	-0.00000	1.62082	63.86698	-0.000000	0.000000	0.002780
33	1.40367	0.81041	65.71149	-0.000000	0.000000	0.006817
34	-0.00000	1.62082	67.55192	0.000000	-0.000000	0.015285
35	1.40367	0.81041	69.40136	-0.000000	0.000000	0.003834
36	-0.00000	1.62082	71.24562	0.000000	-0.000000	-0.007457
37	1.40367	0.81041	73.08813	-0.000000	-0.000000	0.004795
38	-0.00000	1.62082	74.95536	0.000000	0.000000	0.007704

N_iteration : 11

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	0.00169	-0.000000	-0.000000	-0.017028
3	1.40367	0.81041	2.35594	-0.000000	0.000000	-0.006369
4	-0.00000	1.62082	4.66116	0.000000	-0.000000	0.020264
5	-0.00000	0.00000	6.95976	-0.000000	-0.000000	0.018690
6	1.40367	0.81041	9.25851	0.000000	-0.000000	-0.002097
7	-0.00000	1.62082	11.55615	-0.000000	-0.000000	-0.004285
8	-0.00000	0.00000	13.85558	-0.000000	-0.000000	0.002167
9	1.40367	0.81041	16.15338	-0.000000	0.000000	-0.008367
10	-0.00000	1.62082	18.45205	0.000000	0.000000	0.008004
11	-0.00000	0.00000	20.74983	-0.000000	-0.000000	-0.003690
12	1.40367	0.81041	23.04733	-0.000000	0.000000	0.000838
13	-0.00000	1.62082	25.34599	0.000000	-0.000000	0.004949
14	-0.00000	0.00000	27.64415	-0.000000	-0.000000	0.001236
15	1.40367	0.81041	29.94241	-0.000000	0.000000	0.005245
16	-0.00000	1.62082	32.24086	-0.000000	0.000000	-0.003915
17	-0.00000	0.00000	34.53865	-0.000000	-0.000000	-0.003372
18	1.40367	0.81041	36.83859	0.000000	-0.000000	-0.008879
19	-0.00000	1.62082	39.15154	0.000000	-0.000000	0.010452
20	-0.00000	0.00000	41.49864	-0.000000	0.000000	0.007521
21	1.40367	0.81041	43.57355	-0.000000	0.000000	0.000206
22	-0.00000	1.62082	45.40956	-0.000000	0.000000	-0.002660
23	1.40367	0.81041	47.27519	-0.000000	0.000000	-0.012294
24	-0.00000	1.62082	49.12370	0.000000	0.000000	-0.016176
25	1.40367	0.81041	50.96450	0.000000	-0.000000	0.003348
26	-0.00000	1.62082	52.81220	0.000000	-0.000000	-0.010734
27	1.40367	0.81041	54.65467	-0.000000	-0.000000	-0.004697
28	-0.00000	1.62082	56.49814	-0.000000	0.000000	-0.015319
29	1.40367	0.81041	58.34014	0.000000	-0.000000	-0.006374
30	-0.00000	1.62082	60.18161	-0.000000	0.000000	0.007978
31	1.40367	0.81041	62.02396	0.000000	-0.000000	0.005110

32	-0.00000	1.62082	63.86680	0.000000	0.000000	0.006961
33	1.40367	0.81041	65.71190	0.000000	-0.000000	0.004906
34	-0.00000	1.62082	67.55227	0.000000	-0.000000	0.016298
35	1.40367	0.81041	69.40244	0.000000	-0.000000	-0.004329
36	-0.00000	1.62082	71.24509	-0.000000	0.000000	0.000644
37	1.40367	0.81041	73.08798	-0.000000	0.000000	0.005922
38	-0.00000	1.62082	74.95629	-0.000000	0.000000	-0.007475

N_iteration : 12

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	0.00057	0.000000	-0.000000	-0.005549
3	1.40367	0.81041	2.35594	0.000000	-0.000000	-0.002994
4	-0.00000	1.62082	4.66257	-0.000000	0.000000	0.009298
5	-0.00000	0.00000	6.96084	0.000000	-0.000000	0.013446
6	1.40367	0.81041	9.25840	-0.000000	0.000000	0.004137
7	-0.00000	1.62082	11.55592	-0.000000	0.000000	-0.001991
8	-0.00000	0.00000	13.85562	0.000000	-0.000000	-0.002796
9	1.40367	0.81041	16.15294	0.000000	0.000000	0.000361
10	-0.00000	1.62082	18.45248	0.000000	-0.000000	-0.001491
11	-0.00000	0.00000	20.74966	0.000000	-0.000000	0.001400
12	1.40367	0.81041	23.04735	0.000000	-0.000000	0.001306
13	-0.00000	1.62082	25.34628	0.000000	-0.000000	0.002520
14	-0.00000	0.00000	27.64430	0.000000	-0.000000	0.003278
15	1.40367	0.81041	29.94272	-0.000000	-0.000000	0.000598
16	-0.00000	1.62082	32.24059	-0.000000	-0.000000	-0.000275
17	-0.00000	0.00000	34.53838	0.000000	-0.000000	-0.004880
18	1.40367	0.81041	36.83810	0.000000	-0.000000	-0.001341
19	-0.00000	1.62082	39.15200	0.000000	-0.000000	0.005358
20	-0.00000	0.00000	41.49926	0.000000	-0.000000	0.003693
21	1.40367	0.81041	43.57374	-0.000000	0.000000	-0.000196
22	-0.00000	1.62082	45.40926	-0.000000	0.000000	-0.001984
23	1.40367	0.81041	47.27433	-0.000000	0.000000	-0.009402
24	-0.00000	1.62082	49.12289	0.000000	-0.000000	-0.013357
25	1.40367	0.81041	50.96447	-0.000000	0.000000	-0.001981
26	-0.00000	1.62082	52.81146	0.000000	-0.000000	-0.006800
27	1.40367	0.81041	54.65452	-0.000000	0.000000	-0.009951
28	-0.00000	1.62082	56.49704	-0.000000	-0.000000	-0.008506
29	1.40367	0.81041	58.33964	0.000000	0.000000	-0.003745
30	-0.00000	1.62082	60.18226	-0.000000	0.000000	0.001164
31	1.40367	0.81041	62.02425	-0.000000	-0.000000	0.006072
32	-0.00000	1.62082	63.86717	-0.000000	0.000000	0.007818
33	1.40367	0.81041	65.71229	-0.000000	0.000000	0.006605
34	-0.00000	1.62082	67.55331	0.000000	-0.000000	0.008994
35	1.40367	0.81041	69.40245	0.000000	-0.000000	-0.000548
36	-0.00000	1.62082	71.24500	0.000000	-0.000000	0.003128
37	1.40367	0.81041	73.08830	-0.000000	0.000000	0.002318
38	-0.00000	1.62082	74.95608	0.000000	-0.000000	-0.006487

N_iteration : 13

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	-0.00053	-0.000000	0.000000	0.005567
3	1.40367	0.81041	2.35593	-0.000000	0.000000	0.000301
4	-0.00000	1.62082	4.66395	0.000000	-0.000000	-0.001224
5	-0.00000	0.00000	6.96189	-0.000000	0.000000	0.008426
6	1.40367	0.81041	9.25830	0.000000	-0.000000	0.010287
7	-0.00000	1.62082	11.55569	0.000000	0.000000	0.000207
8	-0.00000	0.00000	13.85567	-0.000000	0.000000	-0.007781
9	1.40367	0.81041	16.15252	0.000000	0.000000	0.008762
10	-0.00000	1.62082	18.45291	0.000000	0.000000	-0.010691
11	-0.00000	0.00000	20.74950	-0.000000	0.000000	0.006448
12	1.40367	0.81041	23.04737	-0.000000	0.000000	0.001749
13	-0.00000	1.62082	25.34656	-0.000000	0.000000	0.000072
14	-0.00000	0.00000	27.64444	-0.000000	0.000000	0.005203
15	1.40367	0.81041	29.94302	-0.000000	0.000000	-0.003931
16	-0.00000	1.62082	32.24033	0.000000	0.000000	0.003368
17	-0.00000	0.00000	34.53812	-0.000000	0.000000	-0.006292
18	1.40367	0.81041	36.83762	-0.000000	0.000000	0.005941
19	-0.00000	1.62082	39.15244	-0.000000	0.000000	0.000363
20	-0.00000	0.00000	41.49987	-0.000000	0.000000	-0.000015
21	1.40367	0.81041	43.57392	-0.000000	0.000000	-0.000641
22	-0.00000	1.62082	45.40896	0.000000	-0.000000	-0.001532
23	1.40367	0.81041	47.27350	-0.000000	0.000000	-0.006449
24	-0.00000	1.62082	49.12210	-0.000000	0.000000	-0.010343
25	1.40367	0.81041	50.96443	0.000000	-0.000000	-0.007228
26	-0.00000	1.62082	52.81074	-0.000000	0.000000	-0.003251
27	1.40367	0.81041	54.65436	-0.000000	0.000000	-0.015257
28	-0.00000	1.62082	56.49597	0.000000	-0.000000	-0.001835
29	1.40367	0.81041	58.33915	-0.000000	0.000000	-0.001059
30	-0.00000	1.62082	60.18289	0.000000	-0.000000	-0.005405
31	1.40367	0.81041	62.02452	0.000000	-0.000000	0.007019
32	-0.00000	1.62082	63.86753	0.000000	0.000000	0.008646
33	1.40367	0.81041	65.71267	-0.000000	0.000000	0.008306
34	-0.00000	1.62082	67.55432	-0.000000	0.000000	0.001935
35	1.40367	0.81041	69.40245	0.000000	-0.000000	0.003130
36	-0.00000	1.62082	71.24492	0.000000	-0.000000	0.005521
37	1.40367	0.81041	73.08860	0.000000	-0.000000	-0.001272
38	-0.00000	1.62082	74.95587	0.000000	-0.000000	-0.005418

N_iteration : 14

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	0.00000	-0.00076	0.000000	-0.000000	0.007881
3	1.40367	0.81041	2.35593	0.000000	-0.000000	0.000948
4	-0.00000	1.62082	4.66424	-0.000000	0.000000	-0.003422

5	-0.00000	0.00000	6.96211	0.000000	-0.000000	0.007517
6	1.40367	0.81041	9.25828	0.000000	0.000000	0.011590
7	-0.00000	1.62082	11.55564	0.000000	-0.000000	0.000581
8	-0.00000	0.00000	13.85568	0.000000	-0.000000	-0.008824
9	1.40367	0.81041	16.15243	0.000000	-0.000000	0.010559
10	-0.00000	1.62082	18.45300	0.000000	0.000000	-0.012602
11	-0.00000	0.00000	20.74947	0.000000	-0.000000	0.007518
12	1.40367	0.81041	23.04737	-0.000000	-0.000000	0.001869
13	-0.00000	1.62082	25.34661	0.000000	-0.000000	-0.000442
14	-0.00000	0.00000	27.64447	0.000000	-0.000000	0.005601
15	1.40367	0.81041	29.94308	0.000000	-0.000000	-0.004863
16	-0.00000	1.62082	32.24027	-0.000000	-0.000000	0.004117
17	-0.00000	0.00000	34.53806	0.000000	-0.000000	-0.006594
18	1.40367	0.81041	36.83751	-0.000000	-0.000000	0.007492
19	-0.00000	1.62082	39.15253	-0.000000	0.000000	-0.000669
20	-0.00000	0.00000	41.49999	0.000000	-0.000000	-0.000793
21	1.40367	0.81041	43.57396	-0.000000	-0.000000	-0.000733
22	-0.00000	1.62082	45.40890	-0.000000	0.000000	-0.001349
23	1.40367	0.81041	47.27333	-0.000000	0.000000	-0.005844
24	-0.00000	1.62082	49.12193	0.000000	-0.000000	-0.009924
25	1.40367	0.81041	50.96442	0.000000	-0.000000	-0.008407
26	-0.00000	1.62082	52.81059	-0.000000	0.000000	-0.002346
27	1.40367	0.81041	54.65433	-0.000000	0.000000	-0.016271
28	-0.00000	1.62082	56.49574	-0.000000	0.000000	-0.000529
29	1.40367	0.81041	58.33904	0.000000	-0.000000	-0.000580
30	-0.00000	1.62082	60.18303	-0.000000	0.000000	-0.006770
31	1.40367	0.81041	62.02458	-0.000000	0.000000	0.007276
32	-0.00000	1.62082	63.86761	0.000000	-0.000000	0.008843
33	1.40367	0.81041	65.71275	-0.000000	0.000000	0.008593
34	-0.00000	1.62082	67.55454	-0.000000	0.000000	0.000500
35	1.40367	0.81041	69.40245	-0.000000	0.000000	0.003995
36	-0.00000	1.62082	71.24490	-0.000000	0.000000	0.006029
37	1.40367	0.81041	73.08866	0.000000	-0.000000	-0.002059
38	-0.00000	1.62082	74.95582	0.000000	-0.000000	-0.005318

N_iteration : 15

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	-0.00096	-0.000000	-0.000000	0.008623
3	1.40367	0.81041	2.35599	-0.000000	0.000000	0.003600
4	-0.00000	1.62082	4.66496	0.000000	-0.000000	-0.003867
5	0.00000	-0.00000	6.96339	-0.000000	-0.000000	0.000897
6	1.40367	0.81041	9.25905	0.000000	-0.000000	0.009489
7	-0.00000	1.62082	11.55552	-0.000000	0.000000	0.002759
8	-0.00000	-0.00000	13.85507	-0.000000	-0.000000	0.000940
9	1.40367	0.81041	16.15290	-0.000000	0.000000	-0.003537
10	-0.00000	1.62082	18.45238	0.000000	-0.000000	0.001122
11	0.00000	0.00000	20.74990	-0.000000	-0.000000	-0.001079

12	1.40367	0.81041	23.04752	0.000000	-0.000000	0.003961
13	-0.00000	1.62082	25.34678	-0.000000	-0.000000	0.001882
14	0.00000	-0.00000	27.64498	-0.000000	-0.000000	-0.000699
15	1.40367	0.81041	29.94294	-0.000000	0.000000	0.000984
16	-0.00000	1.62082	32.24038	-0.000000	0.000000	-0.002653
17	-0.00000	-0.00000	34.53740	-0.000000	-0.000000	0.003863
18	1.40367	0.81041	36.83772	0.000000	0.000000	0.002322
19	-0.00000	1.62082	39.15280	-0.000000	0.000000	-0.000463
20	-0.00000	0.00000	41.50036	-0.000000	0.000000	-0.003352
21	1.40367	0.81041	43.57404	0.000000	-0.000000	-0.001349
22	-0.00000	1.62082	45.40859	-0.000000	0.000000	-0.002458
23	1.40367	0.81041	47.27232	-0.000000	0.000000	-0.003495
24	-0.00000	1.62082	49.12065	0.000000	-0.000000	-0.005630
25	1.40367	0.81041	50.96379	0.000000	-0.000000	-0.011661
26	-0.00000	1.62082	52.80991	-0.000000	0.000000	-0.004828
27	1.40367	0.81041	54.65304	-0.000000	0.000000	-0.011184
28	-0.00000	1.62082	56.49495	0.000000	-0.000000	-0.000170
29	1.40367	0.81041	58.33866	-0.000000	0.000000	-0.000761
30	-0.00000	1.62082	60.18298	0.000000	-0.000000	-0.005255
31	1.40367	0.81041	62.02530	-0.000000	-0.000000	0.004671
32	-0.00000	1.62082	63.86850	-0.000000	0.000000	0.007517
33	1.40367	0.81041	65.71364	0.000000	-0.000000	0.007497
34	-0.00000	1.62082	67.55529	-0.000000	0.000000	-0.000588
35	1.40367	0.81041	69.40275	-0.000000	0.000000	0.005984
36	-0.00000	1.62082	71.24527	0.000000	0.000000	0.004245
37	1.40367	0.81041	73.08873	0.000000	0.000000	-0.002857
38	-0.00000	1.62082	74.95529	0.000000	-0.000000	-0.001878

N_iteration : 16

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	-0.00109	-0.000000	0.000000	0.009151
3	1.40367	0.81041	2.35604	-0.000000	0.000000	0.005365
4	-0.00000	1.62082	4.66544	0.000000	-0.000000	-0.004232
5	0.00000	-0.00000	6.96425	-0.000000	0.000000	-0.003550
6	1.40367	0.81041	9.25956	-0.000000	0.000000	0.008031
7	-0.00000	1.62082	11.55544	-0.000000	0.000000	0.004194
8	0.00000	-0.00000	13.85466	-0.000000	0.000000	0.007499
9	1.40367	0.81041	16.15321	-0.000000	0.000000	-0.012993
10	-0.00000	1.62082	18.45197	-0.000000	0.000000	0.010259
11	0.00000	-0.00000	20.75019	-0.000000	0.000000	-0.006839
12	1.40367	0.81041	23.04762	0.000000	-0.000000	0.005412
13	-0.00000	1.62082	25.34689	-0.000000	-0.000000	0.003467
14	0.00000	-0.00000	27.64533	-0.000000	0.000000	-0.004932
15	1.40367	0.81041	29.94284	-0.000000	-0.000000	0.004907
16	-0.00000	1.62082	32.24046	0.000000	-0.000000	-0.007169
17	0.00000	-0.00000	34.53695	-0.000000	0.000000	0.010904
18	1.40367	0.81041	36.83786	0.000000	-0.000000	-0.001134

19	-0.00000	1.62082	39.15298	0.000000	-0.000000	-0.000373
20	0.00000	-0.00000	41.50061	-0.000000	0.000000	-0.005102
21	1.40367	0.81041	43.57409	0.000000	-0.000000	-0.001747
22	-0.00000	1.62082	45.40838	-0.000000	0.000000	-0.003131
23	1.40367	0.81041	47.27164	0.000000	-0.000000	-0.001978
24	-0.00000	1.62082	49.11980	0.000000	-0.000000	-0.002882
25	1.40367	0.81041	50.96336	0.000000	0.000000	-0.013802
26	-0.00000	1.62082	52.80946	-0.000000	-0.000000	-0.006342
27	1.40367	0.81041	54.65218	-0.000000	0.000000	-0.007741
28	-0.00000	1.62082	56.49442	0.000000	-0.000000	-0.000069
29	1.40367	0.81041	58.33840	-0.000000	0.000000	-0.000967
30	-0.00000	1.62082	60.18295	0.000000	0.000000	-0.004056
31	1.40367	0.81041	62.02578	0.000000	0.000000	0.003063
32	-0.00000	1.62082	63.86911	-0.000000	-0.000000	0.006445
33	1.40367	0.81041	65.71424	0.000000	-0.000000	0.006650
34	-0.00000	1.62082	67.55579	0.000000	-0.000000	-0.001204
35	1.40367	0.81041	69.40295	0.000000	-0.000000	0.007270
36	-0.00000	1.62082	71.24553	0.000000	-0.000000	0.002896
37	1.40367	0.81041	73.08877	0.000000	-0.000000	-0.003423
38	-0.00000	1.62082	74.95493	-0.000000	0.000000	0.000681

N_iteration : 17

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	-0.00059	0.000000	-0.000000	0.003632
3	1.40367	0.81041	2.35647	-0.000000	-0.000000	0.004557
4	-0.00000	1.62082	4.66567	-0.000000	0.000000	-0.000063
5	0.00000	-0.00000	6.96494	0.000000	-0.000000	-0.003374
6	1.40367	0.81041	9.26070	-0.000000	0.000000	-0.000223
7	-0.00000	1.62082	11.55565	-0.000000	0.000000	0.009440
8	0.00000	-0.00000	13.85475	-0.000000	-0.000000	0.003613
9	1.40367	0.81041	16.15263	-0.000000	-0.000000	-0.003452
10	-0.00000	1.62082	18.45225	-0.000000	-0.000000	0.001695
11	0.00000	-0.00000	20.75002	0.000000	-0.000000	0.000386
12	1.40367	0.81041	23.04812	-0.000000	0.000000	0.000483
13	-0.00000	1.62082	25.34725	0.000000	-0.000000	0.002297
14	0.00000	-0.00000	27.64535	-0.000000	-0.000000	-0.001256
15	1.40367	0.81041	29.94308	0.000000	-0.000000	-0.000944
16	-0.00000	1.62082	32.24003	-0.000000	0.000000	0.001591
17	-0.00000	-0.00000	34.53724	0.000000	-0.000000	0.004880
18	1.40367	0.81041	36.83793	0.000000	-0.000000	0.000945
19	-0.00000	1.62082	39.15314	0.000000	-0.000000	-0.002269
20	0.00000	-0.00000	41.50051	-0.000000	-0.000000	-0.003847
21	1.40367	0.81041	43.57402	-0.000000	0.000000	-0.003758
22	-0.00000	1.62082	45.40794	0.000000	-0.000000	-0.003579
23	1.40367	0.81041	47.27076	-0.000000	-0.000000	-0.001256
24	-0.00000	1.62082	49.11866	0.000000	0.000000	-0.002256
25	1.40367	0.81041	50.96191	-0.000000	0.000000	-0.010931

26	-0.00000	1.62082	52.80851	-0.000000	0.000000	-0.009740
27	1.40367	0.81041	54.65068	-0.000000	0.000000	-0.002158
28	-0.00000	1.62082	56.49384	0.000000	-0.000000	-0.002812
29	1.40367	0.81041	58.33805	-0.000000	0.000000	-0.001724
30	-0.00000	1.62082	60.18263	0.000000	-0.000000	0.000475
31	1.40367	0.81041	62.02653	0.000000	-0.000000	0.000298
32	-0.00000	1.62082	63.87022	-0.000000	-0.000000	0.003833
33	1.40367	0.81041	65.71537	0.000000	-0.000000	0.003766
34	-0.00000	1.62082	67.55626	0.000000	-0.000000	0.002502
35	1.40367	0.81041	69.40368	-0.000000	0.000000	0.005329
36	-0.00000	1.62082	71.24601	-0.000000	0.000000	0.000775
37	1.40367	0.81041	73.08858	0.000000	0.000000	-0.000994
38	-0.00000	1.62082	74.95459	-0.000000	0.000000	0.002265

N_iteration : 18

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	-0.00018	0.000000	-0.000000	-0.000772
3	1.40367	0.81041	2.35681	0.000000	-0.000000	0.003885
4	-0.00000	1.62082	4.66585	0.000000	-0.000000	0.003078
5	0.00000	-0.00000	6.96550	0.000000	-0.000000	-0.003365
6	1.40367	0.81041	9.26162	-0.000000	-0.000000	-0.006887
7	-0.00000	1.62082	11.55582	0.000000	0.000000	0.013759
8	0.00000	-0.00000	13.85482	0.000000	-0.000000	0.000494
9	1.40367	0.81041	16.15217	0.000000	-0.000000	0.004216
10	-0.00000	1.62082	18.45247	0.000000	0.000000	-0.005290
11	0.00000	-0.00000	20.74988	0.000000	-0.000000	0.006207
12	1.40367	0.81041	23.04852	0.000000	0.000000	-0.003449
13	-0.00000	1.62082	25.34755	-0.000000	-0.000000	0.001343
14	0.00000	-0.00000	27.64537	0.000000	-0.000000	0.001624
15	1.40367	0.81041	29.94328	0.000000	-0.000000	-0.005773
16	-0.00000	1.62082	32.23969	0.000000	-0.000000	0.008690
17	-0.00000	-0.00000	34.53748	0.000000	-0.000000	0.000178
18	1.40367	0.81041	36.83798	0.000000	-0.000000	0.002687
19	-0.00000	1.62082	39.15328	-0.000000	0.000000	-0.003939
20	0.00000	-0.00000	41.50044	0.000000	-0.000000	-0.002879
21	1.40367	0.81041	43.57397	-0.000000	-0.000000	-0.005285
22	-0.00000	1.62082	45.40758	-0.000000	0.000000	-0.003630
23	1.40367	0.81041	47.27005	-0.000000	0.000000	-0.000729
24	-0.00000	1.62082	49.11774	0.000000	-0.000000	-0.001937
25	1.40367	0.81041	50.96075	0.000000	-0.000000	-0.008768
26	-0.00000	1.62082	52.80774	-0.000000	0.000000	-0.012509
27	1.40367	0.81041	54.64948	-0.000000	0.000000	0.002641
28	-0.00000	1.62082	56.49336	0.000000	-0.000000	-0.004650
29	1.40367	0.81041	58.33776	0.000000	0.000000	-0.002309
30	-0.00000	1.62082	60.18237	-0.000000	0.000000	0.003869
31	1.40367	0.81041	62.02713	-0.000000	0.000000	-0.002093
32	-0.00000	1.62082	63.87112	-0.000000	0.000000	0.001661

33	1.40367	0.81041	65.71628	-0.000000	0.000000	0.001667
34	-0.00000	1.62082	67.55663	-0.000000	0.000000	0.005877
35	1.40367	0.81041	69.40427	0.000000	-0.000000	0.003471
36	-0.00000	1.62082	71.24640	-0.000000	0.000000	-0.001291
37	1.40367	0.81041	73.08842	0.000000	-0.000000	0.001131
38	-0.00000	1.62082	74.95431	-0.000000	-0.000000	0.003689

N_iteration : 19

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	-0.00004	0.000000	0.000000	-0.002275
3	1.40367	0.81041	2.35693	0.000000	-0.000000	0.003627
4	-0.00000	1.62082	4.66591	-0.000000	0.000000	0.004140
5	0.00000	-0.00000	6.96569	-0.000000	-0.000000	-0.003381
6	1.40367	0.81041	9.26193	-0.000000	0.000000	-0.009226
7	-0.00000	1.62082	11.55588	-0.000000	-0.000000	0.015195
8	0.00000	-0.00000	13.85484	-0.000000	-0.000000	-0.000570
9	1.40367	0.81041	16.15201	-0.000000	-0.000000	0.006819
10	-0.00000	1.62082	18.45255	-0.000000	0.000000	-0.007633
11	0.00000	-0.00000	20.74983	-0.000000	0.000000	0.008222
12	1.40367	0.81041	23.04865	-0.000000	0.000000	-0.004762
13	-0.00000	1.62082	25.34765	0.000000	-0.000000	0.001032
14	0.00000	-0.00000	27.64538	0.000000	0.000000	0.002672
15	1.40367	0.81041	29.94335	0.000000	-0.000000	-0.007320
16	-0.00000	1.62082	32.23957	0.000000	-0.000000	0.011074
17	-0.00000	-0.00000	34.53756	-0.000000	0.000000	-0.001571
18	1.40367	0.81041	36.83800	0.000000	-0.000000	0.003149
19	-0.00000	1.62082	39.15332	-0.000000	0.000000	-0.004434
20	0.00000	-0.00000	41.50041	-0.000000	0.000000	-0.002468
21	1.40367	0.81041	43.57395	0.000000	-0.000000	-0.005775
22	-0.00000	1.62082	45.40745	0.000000	-0.000000	-0.003742
23	1.40367	0.81041	47.26981	0.000000	0.000000	-0.000517
24	-0.00000	1.62082	49.11742	-0.000000	-0.000000	-0.001607
25	1.40367	0.81041	50.96035	0.000000	-0.000000	-0.008035
26	-0.00000	1.62082	52.80748	-0.000000	-0.000000	-0.013523
27	1.40367	0.81041	54.64906	0.000000	-0.000000	0.004293
28	-0.00000	1.62082	56.49320	0.000000	-0.000000	-0.005344
29	1.40367	0.81041	58.33767	-0.000000	0.000000	-0.002517
30	-0.00000	1.62082	60.18228	-0.000000	0.000000	0.005242
31	1.40367	0.81041	62.02734	-0.000000	-0.000000	-0.002802
32	-0.00000	1.62082	63.87143	0.000000	-0.000000	0.000806
33	1.40367	0.81041	65.71659	-0.000000	0.000000	0.000764
34	-0.00000	1.62082	67.55676	-0.000000	-0.000000	0.006878
35	1.40367	0.81041	69.40447	0.000000	-0.000000	0.002954
36	-0.00000	1.62082	71.24653	0.000000	-0.000000	-0.001839
37	1.40367	0.81041	73.08837	-0.000000	0.000000	0.001802
38	-0.00000	1.62082	74.95421	-0.000000	0.000000	0.004086

N_iteration : 20

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.00026	-0.000000	0.000000	-0.002612
3	1.40367	0.81041	2.35748	-0.000000	0.000000	0.001455
4	-0.00000	1.62082	4.66632	-0.000000	0.000000	0.004870
5	0.00000	-0.00000	6.96608	-0.000000	0.000000	-0.002993
6	1.40367	0.81041	9.26237	0.000000	-0.000000	-0.005878
7	-0.00000	1.62082	11.55688	0.000000	-0.000000	0.005769
8	0.00000	-0.00000	13.85488	-0.000000	0.000000	0.004496
9	1.40367	0.81041	16.15189	-0.000000	0.000000	0.007013
10	-0.00000	1.62082	18.45237	-0.000000	-0.000000	-0.004224
11	0.00000	-0.00000	20.75014	-0.000000	0.000000	0.004210
12	1.40367	0.81041	23.04881	0.000000	-0.000000	-0.002347
13	-0.00000	1.62082	25.34801	-0.000000	0.000000	-0.001440
14	0.00000	-0.00000	27.64554	-0.000000	0.000000	0.001700
15	1.40367	0.81041	29.94316	0.000000	0.000000	-0.002347
16	-0.00000	1.62082	32.23981	0.000000	-0.000000	0.007592
17	-0.00000	-0.00000	34.53771	-0.000000	0.000000	-0.000580
18	1.40367	0.81041	36.83823	-0.000000	0.000000	0.000670
19	-0.00000	1.62082	39.15322	0.000000	-0.000000	-0.002966
20	0.00000	-0.00000	41.50020	-0.000000	0.000000	-0.002971
21	1.40367	0.81041	43.57358	-0.000000	-0.000000	-0.005966
22	-0.00000	1.62082	45.40688	-0.000000	0.000000	-0.003456
23	1.40367	0.81041	47.26905	0.000000	-0.000000	-0.001304
24	-0.00000	1.62082	49.11639	0.000000	-0.000000	-0.002781
25	1.40367	0.81041	50.95871	-0.000000	0.000000	-0.004243
26	-0.00000	1.62082	52.80597	-0.000000	0.000000	-0.011173
27	1.40367	0.81041	54.64805	0.000000	-0.000000	0.003180
28	-0.00000	1.62082	56.49243	-0.000000	-0.000000	-0.005125
29	1.40367	0.81041	58.33724	-0.000000	0.000000	-0.001934
30	-0.00000	1.62082	60.18230	0.000000	-0.000000	0.005538
31	1.40367	0.81041	62.02781	-0.000000	0.000000	-0.002903
32	-0.00000	1.62082	63.87239	-0.000000	0.000000	-0.001709
33	1.40367	0.81041	65.71756	-0.000000	-0.000000	-0.000746
34	-0.00000	1.62082	67.55752	0.000000	-0.000000	0.007620
35	1.40367	0.81041	69.40524	-0.000000	0.000000	0.001102
36	-0.00000	1.62082	71.24683	0.000000	-0.000000	-0.001617
37	1.40367	0.81041	73.08830	-0.000000	-0.000000	0.003635
38	-0.00000	1.62082	74.95415	0.000000	0.000000	0.005074

N_iteration : 21

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.00054	-0.000000	-0.000000	-0.002889
3	1.40367	0.81041	2.35801	0.000000	-0.000000	-0.000528
4	-0.00000	1.62082	4.66671	-0.000000	0.000000	0.005475
5	0.00000	-0.00000	6.96644	0.000000	0.000000	-0.002650

6	1.40367	0.81041	9.26280	-0.000000	0.000000	-0.002584
7	-0.00000	1.62082	11.55782	0.000000	-0.000000	-0.003079
8	0.00000	-0.00000	13.85492	0.000000	0.000000	0.009463
9	1.40367	0.81041	16.15178	0.000000	-0.000000	0.007279
10	-0.00000	1.62082	18.45219	-0.000000	-0.000000	-0.001054
11	0.00000	-0.00000	20.75042	0.000000	-0.000000	0.000292
12	1.40367	0.81041	23.04895	0.000000	-0.000000	0.000024
13	-0.00000	1.62082	25.34835	0.000000	-0.000000	-0.003800
14	0.00000	-0.00000	27.64569	0.000000	-0.000000	0.000624
15	1.40367	0.81041	29.94297	0.000000	0.000000	0.002393
16	-0.00000	1.62082	32.24005	-0.000000	0.000000	0.004502
17	-0.00000	-0.00000	34.53786	-0.000000	0.000000	0.000481
18	1.40367	0.81041	36.83845	-0.000000	0.000000	-0.001810
19	-0.00000	1.62082	39.15313	0.000000	-0.000000	-0.001572
20	0.00000	-0.00000	41.50000	-0.000000	-0.000000	-0.003329
21	1.40367	0.81041	43.57323	-0.000000	0.000000	-0.006032
22	-0.00000	1.62082	45.40633	0.000000	0.000000	-0.003228
23	1.40367	0.81041	47.26833	0.000000	-0.000000	-0.002083
24	-0.00000	1.62082	49.11541	0.000000	-0.000000	-0.004087
25	1.40367	0.81041	50.95716	-0.000000	0.000000	-0.001312
26	-0.00000	1.62082	52.80453	0.000000	-0.000000	-0.009379
27	1.40367	0.81041	54.64710	0.000000	-0.000000	0.002296
28	-0.00000	1.62082	56.49170	0.000000	-0.000000	-0.004739
29	1.40367	0.81041	58.33683	-0.000000	0.000000	-0.001363
30	-0.00000	1.62082	60.18231	-0.000000	0.000000	0.005649
31	1.40367	0.81041	62.02825	-0.000000	0.000000	-0.003219
32	-0.00000	1.62082	63.87331	-0.000000	0.000000	-0.003782
33	1.40367	0.81041	65.71849	0.000000	-0.000000	-0.001714
34	-0.00000	1.62082	67.55824	0.000000	-0.000000	0.008477
35	1.40367	0.81041	69.40597	0.000000	0.000000	-0.000712
36	-0.00000	1.62082	71.24712	-0.000000	0.000000	-0.001378
37	1.40367	0.81041	73.08824	0.000000	-0.000000	0.005644
38	-0.00000	1.62082	74.95409	-0.000000	0.000000	0.005826

N_iteration : 22

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.00110	0.000000	-0.000000	-0.003347
3	1.40367	0.81041	2.35905	-0.000000	0.000000	-0.004589
4	-0.00000	1.62082	4.66749	-0.000000	0.000000	0.006742
5	-0.00000	-0.00000	6.96718	0.000000	0.000000	-0.001892
6	1.40367	0.81041	9.26364	-0.000000	-0.000000	0.003861
7	-0.00000	1.62082	11.55971	-0.000000	0.000000	-0.020966
8	0.00000	-0.00000	13.85500	0.000000	-0.000000	0.019223
9	1.40367	0.81041	16.15157	0.000000	-0.000000	0.007595
10	-0.00000	1.62082	18.45185	-0.000000	-0.000000	0.005386
11	0.00000	-0.00000	20.75100	0.000000	0.000000	-0.007258
12	1.40367	0.81041	23.04924	0.000000	-0.000000	0.004703

13	-0.00000	1.62082	25.34904	0.000000	0.000000	-0.008533
14	-0.00000	-0.00000	27.64600	0.000000	0.000000	-0.001379
15	1.40367	0.81041	29.94261	0.000000	-0.000000	0.011831
16	-0.00000	1.62082	32.24051	0.000000	-0.000000	-0.001966
17	-0.00000	-0.00000	34.53815	0.000000	0.000000	0.002416
18	1.40367	0.81041	36.83888	0.000000	-0.000000	-0.006600
19	-0.00000	1.62082	39.15294	0.000000	-0.000000	0.001239
20	0.00000	-0.00000	41.49960	0.000000	0.000000	-0.004252
21	1.40367	0.81041	43.57254	0.000000	0.000000	-0.006321
22	-0.00000	1.62082	45.40525	-0.000000	0.000000	-0.002769
23	1.40367	0.81041	47.26689	0.000000	-0.000000	-0.003383
24	-0.00000	1.62082	49.11345	-0.000000	-0.000000	-0.006253
25	1.40367	0.81041	50.95406	-0.000000	0.000000	0.005202
26	-0.00000	1.62082	52.80165	0.000000	-0.000000	-0.005422
27	1.40367	0.81041	54.64518	-0.000000	0.000000	0.000445
28	-0.00000	1.62082	56.49023	0.000000	0.000000	-0.004030
29	1.40367	0.81041	58.33602	-0.000000	0.000000	-0.000183
30	-0.00000	1.62082	60.18234	0.000000	-0.000000	0.006087
31	1.40367	0.81041	62.02914	-0.000000	0.000000	-0.003739
32	-0.00000	1.62082	63.87515	-0.000000	0.000000	-0.008432
33	1.40367	0.81041	65.72034	0.000000	-0.000000	-0.003964
34	-0.00000	1.62082	67.55967	-0.000000	-0.000000	0.010052
35	1.40367	0.81041	69.40742	0.000000	-0.000000	-0.004498
36	-0.00000	1.62082	71.24769	-0.000000	0.000000	-0.000996
37	1.40367	0.81041	73.08811	-0.000000	0.000000	0.009092
38	-0.00000	1.62082	74.95397	-0.000000	-0.000000	0.007539

N_iteration : 23

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.00080	0.000000	-0.000000	-0.003052
3	1.40367	0.81041	2.35850	0.000000	-0.000000	-0.002449
4	-0.00000	1.62082	4.66708	0.000000	0.000000	0.006046
5	0.00000	-0.00000	6.96679	0.000000	-0.000000	-0.002277
6	1.40367	0.81041	9.26319	0.000000	-0.000000	0.000522
7	-0.00000	1.62082	11.55871	0.000000	0.000000	-0.011414
8	0.00000	-0.00000	13.85496	0.000000	-0.000000	0.014068
9	1.40367	0.81041	16.15168	-0.000000	-0.000000	0.007369
10	-0.00000	1.62082	18.45203	0.000000	-0.000000	0.001896
11	0.00000	-0.00000	20.75069	0.000000	-0.000000	-0.003237
12	1.40367	0.81041	23.04909	0.000000	-0.000000	0.002314
13	-0.00000	1.62082	25.34867	0.000000	-0.000000	-0.006011
14	-0.00000	-0.00000	27.64584	0.000000	-0.000000	-0.000344
15	1.40367	0.81041	29.94280	0.000000	-0.000000	0.006816
16	-0.00000	1.62082	32.24026	-0.000000	-0.000000	0.001454
17	-0.00000	-0.00000	34.53800	0.000000	-0.000000	0.001381
18	1.40367	0.81041	36.83865	-0.000000	0.000000	-0.004029
19	-0.00000	1.62082	39.15304	-0.000000	0.000000	-0.000203

20	0.00000	-0.00000	41.49981	0.000000	-0.000000	-0.003714
21	1.40367	0.81041	43.57291	-0.000000	-0.000000	-0.006069
22	-0.00000	1.62082	45.40582	-0.000000	0.000000	-0.002820
23	1.40367	0.81041	47.26765	-0.000000	-0.000000	-0.002825
24	-0.00000	1.62082	49.11449	-0.000000	0.000000	-0.005206
25	1.40367	0.81041	50.95570	0.000000	-0.000000	0.001638
26	-0.00000	1.62082	52.80318	-0.000000	0.000000	-0.007704
27	1.40367	0.81041	54.64620	-0.000000	0.000000	0.001200
28	-0.00000	1.62082	56.49101	-0.000000	0.000000	-0.004532
29	1.40367	0.81041	58.33645	0.000000	-0.000000	-0.000880
30	-0.00000	1.62082	60.18233	0.000000	-0.000000	0.005887
31	1.40367	0.81041	62.02867	-0.000000	0.000000	-0.003281
32	-0.00000	1.62082	63.87418	-0.000000	0.000000	-0.005853
33	1.40367	0.81041	65.71936	-0.000000	0.000000	-0.002735
34	-0.00000	1.62082	67.55891	0.000000	-0.000000	0.009289
35	1.40367	0.81041	69.40665	0.000000	-0.000000	-0.002344
36	-0.00000	1.62082	71.24738	-0.000000	0.000000	-0.001159
37	1.40367	0.81041	73.08818	-0.000000	-0.000000	0.007035
38	-0.00000	1.62082	74.95403	-0.000000	-0.000000	0.006586

N_iteration : 24

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.00087	-0.000000	0.000000	0.001681
3	1.40367	0.81041	2.35886	-0.000000	-0.000000	-0.000902
4	-0.00000	1.62082	4.66793	0.000000	-0.000000	-0.000972
5	0.00000	-0.00000	6.96700	-0.000000	0.000000	0.003363
6	1.40367	0.81041	9.26367	-0.000000	0.000000	-0.003778
7	-0.00000	1.62082	11.55884	-0.000000	0.000000	-0.003204
8	0.00000	-0.00000	13.85603	-0.000000	0.000000	0.004062
9	1.40367	0.81041	16.15212	-0.000000	-0.000000	0.008737
10	-0.00000	1.62082	18.45199	-0.000000	0.000000	0.005422
11	0.00000	-0.00000	20.75075	-0.000000	0.000000	-0.002257
12	1.40367	0.81041	23.04941	-0.000000	0.000000	-0.002154
13	-0.00000	1.62082	25.34858	-0.000000	0.000000	-0.002012
14	0.00000	-0.00000	27.64597	-0.000000	0.000000	-0.000659
15	1.40367	0.81041	29.94312	0.000000	-0.000000	0.005965
16	-0.00000	1.62082	32.24061	0.000000	-0.000000	0.000688
17	-0.00000	-0.00000	34.53825	-0.000000	0.000000	-0.000260
18	1.40367	0.81041	36.83857	-0.000000	0.000000	-0.002320
19	-0.00000	1.62082	39.15292	-0.000000	0.000000	-0.001815
20	0.00000	-0.00000	41.49933	-0.000000	0.000000	-0.003591
21	1.40367	0.81041	43.57210	-0.000000	-0.000000	-0.004676
22	-0.00000	1.62082	45.40505	0.000000	-0.000000	-0.003630
23	1.40367	0.81041	47.26670	0.000000	0.000000	-0.003779
24	-0.00000	1.62082	49.11309	-0.000000	0.000000	-0.003972
25	1.40367	0.81041	50.95422	0.000000	-0.000000	0.001165
26	-0.00000	1.62082	52.80112	-0.000000	0.000000	-0.000808

27	1.40367	0.81041	54.64529	-0.000000	0.000000	-0.003367
28	-0.00000	1.62082	56.48992	0.000000	-0.000000	-0.001237
29	1.40367	0.81041	58.33597	-0.000000	0.000000	0.000529
30	-0.00000	1.62082	60.18277	0.000000	-0.000000	0.000822
31	1.40367	0.81041	62.02889	-0.000000	0.000000	-0.001826
32	-0.00000	1.62082	63.87469	0.000000	-0.000000	-0.005211
33	1.40367	0.81041	65.72011	0.000000	0.000000	-0.001865
34	-0.00000	1.62082	67.56034	0.000000	-0.000000	0.002285
35	1.40367	0.81041	69.40723	0.000000	-0.000000	-0.000801
36	-0.00000	1.62082	71.24759	0.000000	-0.000000	0.002178
37	1.40367	0.81041	73.08863	0.000000	-0.000000	0.006407
38	-0.00000	1.62082	74.95445	-0.000000	0.000000	0.006894

N_iteration : 25

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.00092	-0.000000	0.000000	0.005193
3	1.40367	0.81041	2.35912	-0.000000	-0.000000	0.000245
4	-0.00000	1.62082	4.66855	0.000000	-0.000000	-0.006162
5	0.00000	-0.00000	6.96716	-0.000000	0.000000	0.007488
6	1.40367	0.81041	9.26401	0.000000	-0.000000	-0.006750
7	-0.00000	1.62082	11.55894	-0.000000	0.000000	0.003017
8	0.00000	-0.00000	13.85682	-0.000000	0.000000	-0.003153
9	1.40367	0.81041	16.15243	-0.000000	0.000000	0.009656
10	-0.00000	1.62082	18.45197	-0.000000	0.000000	0.007944
11	0.00000	-0.00000	20.75079	-0.000000	0.000000	-0.001516
12	1.40367	0.81041	23.04965	0.000000	-0.000000	-0.005329
13	-0.00000	1.62082	25.34852	0.000000	-0.000000	0.000918
14	0.00000	-0.00000	27.64607	-0.000000	0.000000	-0.000955
15	1.40367	0.81041	29.94334	-0.000000	0.000000	0.005280
16	-0.00000	1.62082	32.24086	-0.000000	0.000000	0.000174
17	-0.00000	-0.00000	34.53844	-0.000000	0.000000	-0.001326
18	1.40367	0.81041	36.83852	0.000000	-0.000000	-0.001007
19	-0.00000	1.62082	39.15284	-0.000000	0.000000	-0.003001
20	0.00000	-0.00000	41.49898	-0.000000	0.000000	-0.003458
21	1.40367	0.81041	43.57151	0.000000	0.000000	-0.003393
22	-0.00000	1.62082	45.40449	-0.000000	0.000000	-0.004079
23	1.40367	0.81041	47.26601	0.000000	0.000000	-0.004998
24	-0.00000	1.62082	49.11207	-0.000000	0.000000	-0.003316
25	1.40367	0.81041	50.95314	0.000000	-0.000000	0.000569
26	-0.00000	1.62082	52.79963	0.000000	-0.000000	0.003856
27	1.40367	0.81041	54.64464	-0.000000	0.000000	-0.006896
28	-0.00000	1.62082	56.48912	0.000000	0.000000	0.001101
29	1.40367	0.81041	58.33562	-0.000000	0.000000	0.001466
30	-0.00000	1.62082	60.18310	0.000000	-0.000000	-0.002780
31	1.40367	0.81041	62.02905	0.000000	-0.000000	-0.000625
32	-0.00000	1.62082	63.87507	0.000000	-0.000000	-0.004661
33	1.40367	0.81041	65.72066	-0.000000	0.000000	-0.001050

34	-0.00000	1.62082	67.56138	0.000000	-0.000000	-0.002666
35	1.40367	0.81041	69.40765	-0.000000	0.000000	0.000439
36	-0.00000	1.62082	71.24775	0.000000	-0.000000	0.004561
37	1.40367	0.81041	73.08897	0.000000	0.000000	0.005738
38	-0.00000	1.62082	74.95476	0.000000	-0.000000	0.007190

N_iteration : 26

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.00140	0.000000	-0.000000	0.005054
3	1.40367	0.81041	2.35937	-0.000000	0.000000	0.000010
4	-0.00000	1.62082	4.66858	-0.000000	0.000000	0.000093
5	0.00000	-0.00000	6.96793	-0.000000	-0.000000	-0.003721
6	1.40367	0.81041	9.26375	0.000000	-0.000000	0.003387
7	-0.00000	1.62082	11.55928	-0.000000	-0.000000	-0.000657
8	0.00000	-0.00000	13.85726	-0.000000	-0.000000	0.000654
9	1.40367	0.81041	16.15353	0.000000	-0.000000	0.002992
10	-0.00000	1.62082	18.45261	0.000000	-0.000000	0.006429
11	0.00000	-0.00000	20.75070	-0.000000	-0.000000	0.001944
12	1.40367	0.81041	23.04940	0.000000	-0.000000	-0.003049
13	-0.00000	1.62082	25.34854	-0.000000	0.000000	-0.001071
14	0.00000	-0.00000	27.64608	-0.000000	-0.000000	0.003321
15	1.40367	0.81041	29.94400	0.000000	0.000000	-0.001192
16	-0.00000	1.62082	32.24110	0.000000	-0.000000	0.001836
17	-0.00000	-0.00000	34.53849	-0.000000	-0.000000	-0.001416
18	1.40367	0.81041	36.83839	-0.000000	0.000000	-0.001190
19	-0.00000	1.62082	39.15251	0.000000	-0.000000	-0.003331
20	0.00000	-0.00000	41.49838	0.000000	-0.000000	-0.003116
21	1.40367	0.81041	43.57070	0.000000	0.000000	-0.002672
22	-0.00000	1.62082	45.40365	-0.000000	0.000000	-0.004661
23	1.40367	0.81041	47.26497	0.000000	0.000000	-0.004640
24	-0.00000	1.62082	49.11088	0.000000	-0.000000	-0.001514
25	1.40367	0.81041	50.95223	-0.000000	0.000000	-0.001022
26	-0.00000	1.62082	52.79861	0.000000	-0.000000	0.003665
27	1.40367	0.81041	54.64347	0.000000	-0.000000	-0.003629
28	-0.00000	1.62082	56.48850	-0.000000	-0.000000	0.001035
29	1.40367	0.81041	58.33542	0.000000	-0.000000	0.000352
30	-0.00000	1.62082	60.18316	-0.000000	0.000000	-0.004132
31	1.40367	0.81041	62.02913	0.000000	0.000000	-0.001142
32	-0.00000	1.62082	63.87501	0.000000	-0.000000	-0.002119
33	1.40367	0.81041	65.72107	0.000000	0.000000	-0.001802
34	-0.00000	1.62082	67.56208	0.000000	0.000000	-0.005437
35	1.40367	0.81041	69.40807	0.000000	-0.000000	0.002014
36	-0.00000	1.62082	71.24827	-0.000000	0.000000	0.005735
37	1.40367	0.81041	73.08975	-0.000000	0.000000	0.004828
38	-0.00000	1.62082	74.95565	-0.000000	0.000000	0.005532

N_iteration : 27

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.00194	0.000000	-0.000000	0.005014
3	1.40367	0.81041	2.35966	-0.000000	0.000000	-0.000205
4	-0.00000	1.62082	4.66862	-0.000000	0.000000	0.007143
5	-0.00000	-0.00000	6.96880	0.000000	-0.000000	-0.016514
6	1.40367	0.81041	9.26346	-0.000000	0.000000	0.014900
7	-0.00000	1.62082	11.55966	0.000000	0.000000	-0.004680
8	0.00000	-0.00000	13.85775	0.000000	-0.000000	0.005031
9	1.40367	0.81041	16.15477	-0.000000	-0.000000	-0.004509
10	-0.00000	1.62082	18.45334	0.000000	-0.000000	0.004759
11	-0.00000	-0.00000	20.75060	0.000000	-0.000000	0.005856
12	1.40367	0.81041	23.04913	0.000000	0.000000	-0.000542
13	-0.00000	1.62082	25.34856	0.000000	-0.000000	-0.003275
14	0.00000	-0.00000	27.64609	0.000000	-0.000000	0.008217
15	1.40367	0.81041	29.94473	0.000000	0.000000	-0.008613
16	-0.00000	1.62082	32.24137	-0.000000	0.000000	0.003635
17	-0.00000	-0.00000	34.53855	0.000000	-0.000000	-0.001499
18	1.40367	0.81041	36.83824	0.000000	0.000000	-0.001435
19	-0.00000	1.62082	39.15214	0.000000	-0.000000	-0.003725
20	0.00000	-0.00000	41.49769	0.000000	0.000000	-0.002795
21	1.40367	0.81041	43.56978	0.000000	0.000000	-0.001897
22	-0.00000	1.62082	45.40269	-0.000000	0.000000	-0.005319
23	1.40367	0.81041	47.26379	0.000000	-0.000000	-0.004150
24	-0.00000	1.62082	49.10953	-0.000000	-0.000000	0.000541
25	1.40367	0.81041	50.95119	-0.000000	0.000000	-0.002690
26	-0.00000	1.62082	52.79746	-0.000000	0.000000	0.003626
27	1.40367	0.81041	54.64214	-0.000000	0.000000	0.000129
28	-0.00000	1.62082	56.48780	0.000000	-0.000000	0.000894
29	1.40367	0.81041	58.33521	-0.000000	0.000000	-0.001011
30	-0.00000	1.62082	60.18323	-0.000000	0.000000	-0.005762
31	1.40367	0.81041	62.02923	-0.000000	-0.000000	-0.001653
32	-0.00000	1.62082	63.87495	-0.000000	-0.000000	0.000897
33	1.40367	0.81041	65.72152	0.000000	-0.000000	-0.002600
34	-0.00000	1.62082	67.56288	-0.000000	0.000000	-0.008474
35	1.40367	0.81041	69.40854	-0.000000	0.000000	0.003780
36	-0.00000	1.62082	71.24886	0.000000	-0.000000	0.006776
37	1.40367	0.81041	73.09063	-0.000000	0.000000	0.003480
38	-0.00000	1.62082	74.95665	0.000000	0.000000	0.003596

N_iteration : 28

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.00235	-0.000000	0.000000	0.004036
3	1.40367	0.81041	2.35981	0.000000	-0.000000	0.001602
4	-0.00000	1.62082	4.66883	-0.000000	-0.000000	0.005444
5	-0.00000	-0.00000	6.96881	-0.000000	0.000000	-0.013771
6	1.40367	0.81041	9.26370	0.000000	-0.000000	0.012193

7	-0.00000	1.62082	11.55974	-0.000000	0.000000	-0.001631
8	0.00000	-0.00000	13.85814	-0.000000	0.000000	0.003912
9	1.40367	0.81041	16.15529	0.000000	-0.000000	-0.005193
10	-0.00000	1.62082	18.45384	-0.000000	-0.000000	0.002489
11	-0.00000	-0.00000	20.75070	-0.000000	0.000000	0.006779
12	1.40367	0.81041	23.04898	-0.000000	0.000000	0.001382
13	-0.00000	1.62082	25.34848	-0.000000	0.000000	-0.002065
14	0.00000	-0.00000	27.64631	-0.000000	0.000000	0.005785
15	1.40367	0.81041	29.94488	0.000000	-0.000000	-0.007443
16	-0.00000	1.62082	32.24161	-0.000000	0.000000	0.001624
17	-0.00000	-0.00000	34.53854	-0.000000	0.000000	-0.000652
18	1.40367	0.81041	36.83812	-0.000000	0.000000	-0.001911
19	-0.00000	1.62082	39.15185	0.000000	-0.000000	-0.003415
20	0.00000	-0.00000	41.49727	-0.000000	0.000000	-0.002751
21	1.40367	0.81041	43.56925	-0.000000	0.000000	-0.001858
22	-0.00000	1.62082	45.40205	0.000000	-0.000000	-0.005041
23	1.40367	0.81041	47.26307	0.000000	0.000000	-0.003559
24	-0.00000	1.62082	49.10886	0.000000	-0.000000	0.000759
25	1.40367	0.81041	50.95058	-0.000000	0.000000	-0.002713
26	-0.00000	1.62082	52.79697	-0.000000	0.000000	0.002643
27	1.40367	0.81041	54.64147	-0.000000	0.000000	0.002269
28	-0.00000	1.62082	56.48746	0.000000	-0.000000	0.000503
29	1.40367	0.81041	58.33507	0.000000	-0.000000	-0.001948
30	-0.00000	1.62082	60.18311	0.000000	-0.000000	-0.005477
31	1.40367	0.81041	62.02924	0.000000	-0.000000	-0.001988
32	-0.00000	1.62082	63.87494	0.000000	0.000000	0.001488
33	1.40367	0.81041	65.72169	0.000000	-0.000000	-0.003072
34	-0.00000	1.62082	67.56307	0.000000	-0.000000	-0.007895
35	1.40367	0.81041	69.40888	-0.000000	0.000000	0.003646
36	-0.00000	1.62082	71.24934	0.000000	-0.000000	0.006361
37	1.40367	0.81041	73.09118	0.000000	0.000000	0.003268
38	-0.00000	1.62082	74.95725	0.000000	0.000000	0.002631

N_iteration : 29

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.00359	0.000000	0.000000	0.000866
3	1.40367	0.81041	2.36023	0.000000	0.000000	0.006901
4	-0.00000	1.62082	4.66945	0.000000	0.000000	0.000430
5	-0.00000	-0.00000	6.96884	0.000000	0.000000	-0.005447
6	1.40367	0.81041	9.26443	-0.000000	0.000000	0.004184
7	-0.00000	1.62082	11.55996	0.000000	0.000000	0.007457
8	-0.00000	-0.00000	13.85930	0.000000	0.000000	0.000517
9	1.40367	0.81041	16.15684	0.000000	-0.000000	-0.007112
10	-0.00000	1.62082	18.45535	-0.000000	0.000000	-0.004234
11	-0.00000	-0.00000	20.75101	0.000000	0.000000	0.009352
12	1.40367	0.81041	23.04852	0.000000	0.000000	0.006912
13	-0.00000	1.62082	25.34825	0.000000	0.000000	0.001681

14	-0.00000	-0.00000	27.64698	0.000000	0.000000	-0.001235
15	1.40367	0.81041	29.94533	-0.000000	0.000000	-0.003961
16	-0.00000	1.62082	32.24232	-0.000000	-0.000000	-0.004538
17	-0.00000	-0.00000	34.53852	0.000000	0.000000	0.001885
18	1.40367	0.81041	36.83777	-0.000000	0.000000	-0.003437
19	-0.00000	1.62082	39.15099	-0.000000	0.000000	-0.002489
20	-0.00000	-0.00000	41.49599	0.000000	0.000000	-0.002553
21	1.40367	0.81041	43.56769	0.000000	-0.000000	-0.001807
22	-0.00000	1.62082	45.40016	0.000000	-0.000000	-0.004355
23	1.40367	0.81041	47.26093	-0.000000	0.000000	-0.001644
24	-0.00000	1.62082	49.10682	0.000000	-0.000000	0.001684
25	1.40367	0.81041	50.94877	0.000000	-0.000000	-0.002716
26	-0.00000	1.62082	52.79549	0.000000	-0.000000	-0.000297
27	1.40367	0.81041	54.63944	-0.000000	-0.000000	0.008811
28	-0.00000	1.62082	56.48646	-0.000000	0.000000	-0.000729
29	1.40367	0.81041	58.33465	-0.000000	0.000000	-0.004707
30	-0.00000	1.62082	60.18275	-0.000000	0.000000	-0.004599
31	1.40367	0.81041	62.02927	-0.000000	0.000000	-0.003137
32	-0.00000	1.62082	63.87491	0.000000	-0.000000	0.003182
33	1.40367	0.81041	65.72218	-0.000000	0.000000	-0.004704
34	-0.00000	1.62082	67.56362	-0.000000	0.000000	-0.006330
35	1.40367	0.81041	69.40990	-0.000000	0.000000	0.003499
36	-0.00000	1.62082	71.25079	-0.000000	-0.000000	0.005396
37	1.40367	0.81041	73.09281	0.000000	-0.000000	0.002639
38	-0.00000	1.62082	74.95908	-0.000000	0.000000	-0.000342

N_iteration : 30

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.00380	0.000000	-0.000000	0.002559
3	1.40367	0.81041	2.36059	-0.000000	0.000000	0.004700
4	-0.00000	1.62082	4.66956	-0.000000	0.000000	-0.000232
5	-0.00000	-0.00000	6.96861	0.000000	-0.000000	-0.000305
6	1.40367	0.81041	9.26471	0.000000	-0.000000	0.001382
7	-0.00000	1.62082	11.56031	0.000000	-0.000000	0.006259
8	-0.00000	-0.00000	13.85948	0.000000	-0.000000	-0.000064
9	1.40367	0.81041	16.15676	-0.000000	0.000000	-0.004916
10	-0.00000	1.62082	18.45538	-0.000000	-0.000000	-0.002527
11	-0.00000	-0.00000	20.75145	0.000000	-0.000000	0.005517
12	1.40367	0.81041	23.04875	0.000000	-0.000000	0.007262
13	-0.00000	1.62082	25.34829	0.000000	-0.000000	0.002887
14	-0.00000	-0.00000	27.64702	0.000000	-0.000000	-0.002297
15	1.40367	0.81041	29.94522	-0.000000	0.000000	-0.003017
16	-0.00000	1.62082	32.24222	0.000000	-0.000000	-0.003480
17	-0.00000	-0.00000	34.53859	0.000000	-0.000000	-0.000915
18	1.40367	0.81041	36.83758	-0.000000	0.000000	-0.001914
19	-0.00000	1.62082	39.15076	-0.000000	0.000000	-0.002591
20	-0.00000	-0.00000	41.49570	0.000000	-0.000000	-0.002421

21	1.40367	0.81041	43.56739	0.000000	0.000000	-0.002275
22	-0.00000	1.62082	45.39971	-0.000000	0.000000	-0.003119
23	1.40367	0.81041	47.26055	-0.000000	-0.000000	-0.001397
24	-0.00000	1.62082	49.10661	-0.000000	0.000000	0.000365
25	1.40367	0.81041	50.94840	-0.000000	0.000000	-0.001540
26	-0.00000	1.62082	52.79527	-0.000000	-0.000000	0.000218
27	1.40367	0.81041	54.63953	0.000000	-0.000000	0.006408
28	-0.00000	1.62082	56.48628	-0.000000	0.000000	-0.000243
29	1.40367	0.81041	58.33440	-0.000000	0.000000	-0.004070
30	-0.00000	1.62082	60.18251	0.000000	-0.000000	-0.003834
31	1.40367	0.81041	62.02914	0.000000	-0.000000	-0.002725
32	-0.00000	1.62082	63.87505	-0.000000	0.000000	0.001043
33	1.40367	0.81041	65.72205	-0.000000	0.000000	-0.003680
34	-0.00000	1.62082	67.56343	0.000000	-0.000000	-0.003790
35	1.40367	0.81041	69.41019	-0.000000	0.000000	0.002094
36	-0.00000	1.62082	71.25122	-0.000000	0.000000	0.003932
37	1.40367	0.81041	73.09316	-0.000000	0.000000	0.002637
38	-0.00000	1.62082	74.95932	0.000000	-0.000000	0.000559

N_iteration : 31

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	0.00434	-0.000000	-0.000000	0.006675
3	1.40367	0.81041	2.36149	0.000000	0.000000	-0.001236
4	-0.00000	1.62082	4.66983	0.000000	-0.000000	-0.001903
5	-0.00000	-0.00000	6.96803	-0.000000	0.000000	0.013223
6	1.40367	0.81041	9.26543	0.000000	-0.000000	-0.005492
7	-0.00000	1.62082	11.56120	-0.000000	0.000000	0.002967
8	-0.00000	-0.00000	13.85996	-0.000000	-0.000000	-0.001844
9	1.40367	0.81041	16.15654	0.000000	0.000000	0.000927
10	-0.00000	1.62082	18.45546	-0.000000	-0.000000	0.002196
11	-0.00000	-0.00000	20.75258	-0.000000	0.000000	-0.004324
12	1.40367	0.81041	23.04933	-0.000000	0.000000	0.007873
13	-0.00000	1.62082	25.34839	-0.000000	0.000000	0.005928
14	0.00000	-0.00000	27.64712	-0.000000	-0.000000	-0.004885
15	1.40367	0.81041	29.94495	0.000000	-0.000000	-0.000600
16	-0.00000	1.62082	32.24198	-0.000000	0.000000	-0.000959
17	-0.00000	-0.00000	34.53879	-0.000000	-0.000000	-0.008219
18	1.40367	0.81041	36.83708	-0.000000	-0.000000	0.001990
19	-0.00000	1.62082	39.15018	-0.000000	-0.000000	-0.002749
20	-0.00000	-0.00000	41.49497	-0.000000	-0.000000	-0.001957
21	1.40367	0.81041	43.56663	-0.000000	0.000000	-0.003490
22	-0.00000	1.62082	45.39855	-0.000000	0.000000	-0.000201
23	1.40367	0.81041	47.25961	-0.000000	0.000000	-0.000729
24	-0.00000	1.62082	49.10606	0.000000	-0.000000	-0.002920
25	1.40367	0.81041	50.94745	-0.000000	0.000000	0.001935
26	-0.00000	1.62082	52.79471	0.000000	0.000000	0.001740
27	1.40367	0.81041	54.63976	0.000000	-0.000000	-0.000032

28	-0.00000	1.62082	56.48584	-0.000000	0.000000	0.001035
29	1.40367	0.81041	58.33374	0.000000	-0.000000	-0.002293
30	-0.00000	1.62082	60.18188	0.000000	-0.000000	-0.001886
31	1.40367	0.81041	62.02880	0.000000	-0.000000	-0.001888
32	-0.00000	1.62082	63.87538	0.000000	-0.000000	-0.004910
33	1.40367	0.81041	65.72172	0.000000	0.000000	-0.001179
34	-0.00000	1.62082	67.56294	0.000000	-0.000000	0.002730
35	1.40367	0.81041	69.41094	0.000000	-0.000000	-0.001509
36	-0.00000	1.62082	71.25233	-0.000000	0.000000	0.000405
37	1.40367	0.81041	73.09403	0.000000	-0.000000	0.003177
38	-0.00000	1.62082	74.95994	-0.000000	0.000000	0.002846

N_iteration : 32

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	0.00492	-0.000000	-0.000000	0.004426
3	1.40367	0.81041	2.36182	0.000000	-0.000000	-0.001890
4	-0.00000	1.62082	4.66985	0.000000	0.000000	0.002767
5	-0.00000	-0.00000	6.96847	-0.000000	0.000000	0.007814
6	1.40367	0.81041	9.26546	-0.000000	0.000000	0.000379
7	-0.00000	1.62082	11.56174	-0.000000	0.000000	-0.003006
8	-0.00000	-0.00000	13.86007	-0.000000	0.000000	-0.000038
9	1.40367	0.81041	16.15650	-0.000000	0.000000	0.002929
10	-0.00000	1.62082	18.45561	0.000000	-0.000000	0.001550
11	-0.00000	-0.00000	20.75284	-0.000000	-0.000000	-0.002283
12	1.40367	0.81041	23.04999	0.000000	-0.000000	0.003582
13	-0.00000	1.62082	25.34874	-0.000000	-0.000000	0.004431
14	0.00000	-0.00000	27.64691	-0.000000	0.000000	-0.001017
15	1.40367	0.81041	29.94481	-0.000000	-0.000000	-0.001125
16	-0.00000	1.62082	32.24183	-0.000000	0.000000	-0.002169
17	-0.00000	-0.00000	34.53844	-0.000000	0.000000	-0.005526
18	1.40367	0.81041	36.83697	-0.000000	-0.000000	-0.001333
19	-0.00000	1.62082	39.14978	0.000000	-0.000000	-0.001099
20	-0.00000	-0.00000	41.49455	-0.000000	-0.000000	-0.002257
21	1.40367	0.81041	43.56612	0.000000	-0.000000	-0.002997
22	-0.00000	1.62082	45.39804	0.000000	-0.000000	0.000230
23	1.40367	0.81041	47.25916	0.000000	-0.000000	-0.000775
24	-0.00000	1.62082	49.10568	-0.000000	0.000000	-0.002818
25	1.40367	0.81041	50.94715	0.000000	-0.000000	0.002514
26	-0.00000	1.62082	52.79456	-0.000000	0.000000	0.002008
27	1.40367	0.81041	54.63986	0.000000	0.000000	-0.002392
28	-0.00000	1.62082	56.48571	0.000000	0.000000	0.000660
29	1.40367	0.81041	58.33333	-0.000000	0.000000	-0.000922
30	-0.00000	1.62082	60.18151	-0.000000	-0.000000	-0.001191
31	1.40367	0.81041	62.02856	-0.000000	-0.000000	-0.001977
32	-0.00000	1.62082	63.87527	-0.000000	0.000000	-0.005801
33	1.40367	0.81041	65.72151	0.000000	-0.000000	0.000024
34	-0.00000	1.62082	67.56287	0.000000	-0.000000	0.003793

35	1.40367	0.81041	69.41118	-0.000000	0.000000	-0.001728
36	-0.00000	1.62082	71.25282	0.000000	-0.000000	-0.000850
37	1.40367	0.81041	73.09457	-0.000000	0.000000	0.002140
38	-0.00000	1.62082	74.96035	0.000000	0.000000	0.003385

N_iteration : 33

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	0.00561	0.000000	0.000000	0.001729
3	1.40367	0.81041	2.36220	0.000000	-0.000000	-0.002825
4	-0.00000	1.62082	4.66987	-0.000000	0.000000	0.008245
5	-0.00000	-0.00000	6.96899	0.000000	-0.000000	0.001563
6	1.40367	0.81041	9.26548	0.000000	-0.000000	0.007641
7	-0.00000	1.62082	11.56238	-0.000000	0.000000	-0.010074
8	-0.00000	-0.00000	13.86019	0.000000	-0.000000	0.002110
9	1.40367	0.81041	16.15644	-0.000000	0.000000	0.005290
10	-0.00000	1.62082	18.45579	-0.000000	0.000000	0.000685
11	-0.00000	-0.00000	20.75315	0.000000	-0.000000	0.000041
12	1.40367	0.81041	23.05078	-0.000000	0.000000	-0.001484
13	-0.00000	1.62082	25.34916	0.000000	-0.000000	0.002733
14	0.00000	-0.00000	27.64666	0.000000	-0.000000	0.003581
15	1.40367	0.81041	29.94463	0.000000	-0.000000	-0.001806
16	-0.00000	1.62082	32.24165	0.000000	-0.000000	-0.003684
17	-0.00000	-0.00000	34.53804	0.000000	-0.000000	-0.002343
18	1.40367	0.81041	36.83684	-0.000000	0.000000	-0.005214
19	-0.00000	1.62082	39.14931	0.000000	-0.000000	0.000884
20	-0.00000	-0.00000	41.49405	0.000000	-0.000000	-0.002729
21	1.40367	0.81041	43.56551	0.000000	-0.000000	-0.002551
22	-0.00000	1.62082	45.39744	0.000000	-0.000000	0.000673
23	1.40367	0.81041	47.25862	-0.000000	0.000000	-0.000611
24	-0.00000	1.62082	49.10521	0.000000	-0.000000	-0.002593
25	1.40367	0.81041	50.94678	0.000000	-0.000000	0.003037
26	-0.00000	1.62082	52.79438	0.000000	-0.000000	0.002124
27	1.40367	0.81041	54.63997	0.000000	-0.000000	-0.005142
28	-0.00000	1.62082	56.48554	-0.000000	0.000000	0.000422
29	1.40367	0.81041	58.33285	0.000000	0.000000	0.000886
30	-0.00000	1.62082	60.18107	-0.000000	-0.000000	-0.000362
31	1.40367	0.81041	62.02827	-0.000000	0.000000	-0.002164
32	-0.00000	1.62082	63.87514	0.000000	-0.000000	-0.006921
33	1.40367	0.81041	65.72127	-0.000000	0.000000	0.001397
34	-0.00000	1.62082	67.56279	-0.000000	0.000000	0.004919
35	1.40367	0.81041	69.41147	-0.000000	0.000000	-0.002250
36	-0.00000	1.62082	71.25342	-0.000000	0.000000	-0.002310
37	1.40367	0.81041	73.09522	-0.000000	0.000000	0.001340
38	-0.00000	1.62082	74.96085	-0.000000	-0.000000	0.004116

N_iteration : 34

atom	X	Y	Z	Fx	Fy	Fz

1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	0.00630	0.000000	0.000000	-0.001819
3	1.40367	0.81041	2.36234	-0.000000	-0.000000	0.002442
4	-0.00000	1.62082	4.67042	0.000000	-0.000000	0.005559
5	-0.00000	-0.00000	6.96953	0.000000	-0.000000	0.001713
6	1.40367	0.81041	9.26600	0.000000	-0.000000	0.003761
7	-0.00000	1.62082	11.56226	0.000000	-0.000000	-0.003923
8	-0.00000	-0.00000	13.86044	0.000000	-0.000000	-0.000056
9	1.40367	0.81041	16.15674	-0.000000	-0.000000	0.004316
10	-0.00000	1.62082	18.45598	0.000000	-0.000000	0.001761
11	-0.00000	-0.00000	20.75341	0.000000	-0.000000	0.001489
12	1.40367	0.81041	23.05134	-0.000000	-0.000000	-0.003465
13	-0.00000	1.62082	25.34969	-0.000000	0.000000	-0.000124
14	0.00000	-0.00000	27.64669	0.000000	-0.000000	0.004932
15	1.40367	0.81041	29.94437	-0.000000	0.000000	-0.000885
16	-0.00000	1.62082	32.24126	0.000000	-0.000000	-0.003658
17	-0.00000	-0.00000	34.53754	0.000000	-0.000000	-0.001487
18	1.40367	0.81041	36.83639	0.000000	-0.000000	-0.004768
19	-0.00000	1.62082	39.14898	0.000000	-0.000000	-0.001094
20	-0.00000	-0.00000	41.49346	0.000000	-0.000000	-0.001562
21	1.40367	0.81041	43.56484	0.000000	0.000000	-0.001447
22	-0.00000	1.62082	45.39698	-0.000000	-0.000000	-0.000213
23	1.40367	0.81041	47.25814	0.000000	-0.000000	-0.000492
24	-0.00000	1.62082	49.10466	-0.000000	0.000000	-0.000460
25	1.40367	0.81041	50.94667	-0.000000	0.000000	0.001557
26	-0.00000	1.62082	52.79436	-0.000000	-0.000000	0.000608
27	1.40367	0.81041	54.63974	-0.000000	0.000000	-0.004081
28	-0.00000	1.62082	56.48544	-0.000000	0.000000	-0.000838
29	1.40367	0.81041	58.33251	-0.000000	0.000000	0.001547
30	-0.00000	1.62082	60.18068	-0.000000	-0.000000	-0.000090
31	1.40367	0.81041	62.02789	-0.000000	0.000000	-0.002411
32	-0.00000	1.62082	63.87458	-0.000000	0.000000	-0.004249
33	1.40367	0.81041	65.72116	0.000000	-0.000000	0.001011
34	-0.00000	1.62082	67.56304	-0.000000	0.000000	0.002548
35	1.40367	0.81041	69.41157	0.000000	-0.000000	-0.000676
36	-0.00000	1.62082	71.25376	0.000000	-0.000000	-0.001837
37	1.40367	0.81041	73.09585	0.000000	-0.000000	-0.000033
38	-0.00000	1.62082	74.96152	0.000000	-0.000000	0.003163

N_iteration : 35

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	0.00732	-0.000000	-0.000000	-0.007136
3	1.40367	0.81041	2.36255	0.000000	-0.000000	0.010243
4	-0.00000	1.62082	4.67124	0.000000	-0.000000	0.001628
5	-0.00000	-0.00000	6.97032	0.000000	-0.000000	0.001897
6	1.40367	0.81041	9.26676	0.000000	-0.000000	-0.002067
7	-0.00000	1.62082	11.56209	-0.000000	-0.000000	0.005306

8	-0.00000	-0.00000	13.86080	0.000000	-0.000000	-0.003196
9	1.40367	0.81041	16.15718	0.000000	-0.000000	0.002809
10	-0.00000	1.62082	18.45626	0.000000	-0.000000	0.003295
11	-0.00000	-0.00000	20.75380	0.000000	-0.000000	0.003640
12	1.40367	0.81041	23.05218	-0.000000	0.000000	-0.006310
13	-0.00000	1.62082	25.35047	0.000000	-0.000000	-0.004267
14	0.00000	-0.00000	27.64672	0.000000	-0.000000	0.006949
15	1.40367	0.81041	29.94398	-0.000000	-0.000000	0.000409
16	-0.00000	1.62082	32.24068	-0.000000	0.000000	-0.003613
17	-0.00000	-0.00000	34.53681	0.000000	-0.000000	-0.000139
18	1.40367	0.81041	36.83573	0.000000	-0.000000	-0.004133
19	-0.00000	1.62082	39.14849	0.000000	0.000000	-0.004101
20	0.00000	-0.00000	41.49258	0.000000	-0.000000	0.000123
21	1.40367	0.81041	43.56385	-0.000000	-0.000000	0.000248
22	-0.00000	1.62082	45.39629	-0.000000	0.000000	-0.001566
23	1.40367	0.81041	47.25743	-0.000000	-0.000000	-0.000461
24	-0.00000	1.62082	49.10384	-0.000000	0.000000	0.002672
25	1.40367	0.81041	50.94651	0.000000	-0.000000	-0.000685
26	-0.00000	1.62082	52.79434	-0.000000	-0.000000	-0.001663
27	1.40367	0.81041	54.63939	-0.000000	0.000000	-0.002307
28	-0.00000	1.62082	56.48528	0.000000	-0.000000	-0.002552
29	1.40367	0.81041	58.33200	0.000000	0.000000	0.002492
30	-0.00000	1.62082	60.18010	-0.000000	0.000000	0.000173
31	1.40367	0.81041	62.02733	0.000000	-0.000000	-0.002900
32	-0.00000	1.62082	63.87376	-0.000000	0.000000	-0.000247
33	1.40367	0.81041	65.72099	0.000000	-0.000000	0.000608
34	-0.00000	1.62082	67.56341	0.000000	-0.000000	-0.000891
35	1.40367	0.81041	69.41171	-0.000000	0.000000	0.001600
36	-0.00000	1.62082	71.25427	-0.000000	0.000000	-0.001185
37	1.40367	0.81041	73.09677	0.000000	-0.000000	-0.002128
38	-0.00000	1.62082	74.96253	-0.000000	0.000000	0.001751

N_iteration : 36

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	0.00752	-0.000000	-0.000000	0.000271
3	1.40367	0.81041	2.36342	0.000000	-0.000000	0.005654
4	-0.00000	1.62082	4.67192	-0.000000	0.000000	0.003026
5	-0.00000	-0.00000	6.97101	-0.000000	0.000000	0.000215
6	1.40367	0.81041	9.26715	0.000000	-0.000000	-0.001020
7	-0.00000	1.62082	11.56234	-0.000000	0.000000	0.004454
8	-0.00000	-0.00000	13.86082	-0.000000	0.000000	0.001261
9	1.40367	0.81041	16.15769	-0.000000	0.000000	-0.000777
10	-0.00000	1.62082	18.45669	0.000000	-0.000000	0.004503
11	-0.00000	-0.00000	20.75433	-0.000000	0.000000	0.000517
12	1.40367	0.81041	23.05231	-0.000000	0.000000	-0.003020
13	-0.00000	1.62082	25.35071	-0.000000	-0.000000	-0.002974
14	0.00000	-0.00000	27.64724	-0.000000	0.000000	0.000484

15	1.40367	0.81041	29.94374	0.000000	-0.000000	0.002517
16	-0.00000	1.62082	32.24002	-0.000000	0.000000	-0.000285
17	-0.00000	-0.00000	34.53630	-0.000000	0.000000	-0.002669
18	1.40367	0.81041	36.83498	0.000000	-0.000000	-0.001889
19	-0.00000	1.62082	39.14785	0.000000	-0.000000	-0.004659
20	0.00000	-0.00000	41.49198	-0.000000	0.000000	-0.000363
21	1.40367	0.81041	43.56318	0.000000	-0.000000	0.000884
22	-0.00000	1.62082	45.39571	0.000000	-0.000000	-0.001774
23	1.40367	0.81041	47.25690	-0.000000	0.000000	-0.000171
24	-0.00000	1.62082	49.10347	0.000000	-0.000000	0.002888
25	1.40367	0.81041	50.94635	-0.000000	0.000000	-0.001690
26	-0.00000	1.62082	52.79421	0.000000	0.000000	-0.002808
27	1.40367	0.81041	54.63898	0.000000	0.000000	-0.000469
28	-0.00000	1.62082	56.48499	-0.000000	-0.000000	-0.002355
29	1.40367	0.81041	58.33182	-0.000000	0.000000	0.000716
30	-0.00000	1.62082	60.17972	-0.000000	0.000000	-0.000071
31	1.40367	0.81041	62.02674	0.000000	-0.000000	-0.001432
32	-0.00000	1.62082	63.87317	0.000000	-0.000000	0.001979
33	1.40367	0.81041	65.72092	0.000000	-0.000000	-0.000423
34	-0.00000	1.62082	67.56360	-0.000000	0.000000	-0.002388
35	1.40367	0.81041	69.41192	0.000000	-0.000000	0.001757
36	-0.00000	1.62082	71.25454	0.000000	-0.000000	0.000031
37	1.40367	0.81041	73.09726	0.000000	-0.000000	-0.001871
38	-0.00000	1.62082	74.96335	-0.000000	0.000000	0.000395

N_iteration : 37

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	0.00770	-0.000000	-0.000000	0.006942
3	1.40367	0.81041	2.36419	0.000000	0.000000	0.001723
4	-0.00000	1.62082	4.67252	-0.000000	-0.000000	0.004125
5	-0.00000	-0.00000	6.97161	-0.000000	0.000000	-0.001444
6	1.40367	0.81041	9.26749	0.000000	-0.000000	-0.000141
7	-0.00000	1.62082	11.56257	0.000000	-0.000000	0.003691
8	-0.00000	-0.00000	13.86084	-0.000000	0.000000	0.005157
9	1.40367	0.81041	16.15813	0.000000	-0.000000	-0.003996
10	-0.00000	1.62082	18.45707	0.000000	-0.000000	0.005668
11	-0.00000	-0.00000	20.75479	-0.000000	0.000000	-0.002182
12	1.40367	0.81041	23.05242	-0.000000	0.000000	-0.000276
13	-0.00000	1.62082	25.35092	-0.000000	0.000000	-0.002040
14	0.00000	-0.00000	27.64770	-0.000000	0.000000	-0.005250
15	1.40367	0.81041	29.94352	-0.000000	0.000000	0.004544
16	-0.00000	1.62082	32.23944	0.000000	-0.000000	0.002734
17	-0.00000	-0.00000	34.53584	-0.000000	0.000000	-0.004884
18	1.40367	0.81041	36.83431	-0.000000	0.000000	0.000135
19	-0.00000	1.62082	39.14729	-0.000000	0.000000	-0.005139
20	0.00000	-0.00000	41.49145	-0.000000	0.000000	-0.000795
21	1.40367	0.81041	43.56259	-0.000000	-0.000000	0.001470

22	-0.00000	1.62082	45.39519	0.000000	0.000000	-0.001694
23	1.40367	0.81041	47.25643	0.000000	-0.000000	0.000450
24	-0.00000	1.62082	49.10313	-0.000000	0.000000	0.003232
25	1.40367	0.81041	50.94621	0.000000	-0.000000	-0.002756
26	-0.00000	1.62082	52.79410	0.000000	-0.000000	-0.004144
27	1.40367	0.81041	54.63863	0.000000	-0.000000	0.000877
28	-0.00000	1.62082	56.48473	-0.000000	0.000000	-0.002272
29	1.40367	0.81041	58.33166	-0.000000	-0.000000	-0.000648
30	-0.00000	1.62082	60.17937	0.000000	0.000000	-0.000073
31	1.40367	0.81041	62.02621	0.000000	-0.000000	-0.000127
32	-0.00000	1.62082	63.87264	0.000000	-0.000000	0.004052
33	1.40367	0.81041	65.72085	-0.000000	-0.000000	-0.001126
34	-0.00000	1.62082	67.56377	0.000000	-0.000000	-0.003571
35	1.40367	0.81041	69.41211	0.000000	0.000000	0.001745
36	-0.00000	1.62082	71.25478	-0.000000	-0.000000	0.000810
37	1.40367	0.81041	73.09770	-0.000000	0.000000	-0.001558
38	-0.00000	1.62082	74.96407	-0.000000	0.000000	-0.000924

N_iteration : 38

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	0.00847	0.000000	-0.000000	0.007663
3	1.40367	0.81041	2.36516	0.000000	-0.000000	0.000973
4	-0.00000	1.62082	4.67352	-0.000000	0.000000	0.001151
5	-0.00000	-0.00000	6.97215	-0.000000	-0.000000	0.000359
6	1.40367	0.81041	9.26785	-0.000000	-0.000000	0.002001
7	-0.00000	1.62082	11.56312	-0.000000	0.000000	0.001744
8	-0.00000	-0.00000	13.86130	-0.000000	-0.000000	0.003814
9	1.40367	0.81041	16.15828	-0.000000	0.000000	0.002657
10	-0.00000	1.62082	18.45796	-0.000000	-0.000000	-0.002476
11	-0.00000	-0.00000	20.75511	-0.000000	-0.000000	0.000144
12	1.40367	0.81041	23.05253	0.000000	-0.000000	0.000671
13	-0.00000	1.62082	25.35098	0.000000	-0.000000	-0.001893
14	0.00000	-0.00000	27.64775	-0.000000	-0.000000	-0.004542
15	1.40367	0.81041	29.94367	0.000000	-0.000000	0.000693
16	-0.00000	1.62082	32.23904	-0.000000	0.000000	0.003132
17	-0.00000	-0.00000	34.53494	-0.000000	-0.000000	-0.000614
18	1.40367	0.81041	36.83360	-0.000000	0.000000	-0.003208
19	-0.00000	1.62082	39.14626	0.000000	-0.000000	-0.001088
20	0.00000	-0.00000	41.49081	-0.000000	0.000000	-0.002303
21	1.40367	0.81041	43.56207	-0.000000	0.000000	0.000397
22	-0.00000	1.62082	45.39449	-0.000000	-0.000000	0.000021
23	1.40367	0.81041	47.25596	0.000000	-0.000000	0.000890
24	-0.00000	1.62082	49.10304	-0.000000	0.000000	0.000201
25	1.40367	0.81041	50.94583	-0.000000	0.000000	-0.002009
26	-0.00000	1.62082	52.79363	-0.000000	0.000000	-0.002854
27	1.40367	0.81041	54.63831	0.000000	-0.000000	0.000044
28	-0.00000	1.62082	56.48426	-0.000000	0.000000	-0.000934

29	1.40367	0.81041	58.33144	0.000000	0.000000	-0.002505
30	-0.00000	1.62082	60.17899	0.000000	0.000000	-0.000214
31	1.40367	0.81041	62.02563	0.000000	-0.000000	0.002280
32	-0.00000	1.62082	63.87242	0.000000	-0.000000	0.002991
33	1.40367	0.81041	65.72069	-0.000000	-0.000000	-0.000997
34	-0.00000	1.62082	67.56366	0.000000	-0.000000	-0.001823
35	1.40367	0.81041	69.41246	0.000000	-0.000000	-0.000118
36	-0.00000	1.62082	71.25511	0.000000	-0.000000	0.000762
37	1.40367	0.81041	73.09804	-0.000000	0.000000	-0.000259
38	-0.00000	1.62082	74.96478	0.000000	0.000000	-0.002254

N_iteration : 39

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	-0.00000	-0.00000	0.00896	0.000000	-0.000000	0.008045
3	1.40367	0.81041	2.36579	0.000000	0.000000	0.000505
4	-0.00000	1.62082	4.67416	-0.000000	0.000000	-0.000619
5	-0.00000	-0.00000	6.97249	0.000000	-0.000000	0.001609
6	1.40367	0.81041	9.26808	0.000000	0.000000	0.003400
7	-0.00000	1.62082	11.56347	0.000000	-0.000000	0.000514
8	-0.00000	-0.00000	13.86159	0.000000	-0.000000	0.002973
9	1.40367	0.81041	16.15838	-0.000000	0.000000	0.006982
10	-0.00000	1.62082	18.45853	0.000000	-0.000000	-0.007680
11	-0.00000	-0.00000	20.75532	0.000000	-0.000000	0.001623
12	1.40367	0.81041	23.05259	0.000000	-0.000000	0.001240
13	-0.00000	1.62082	25.35102	-0.000000	0.000000	-0.001791
14	0.00000	-0.00000	27.64779	0.000000	-0.000000	-0.004105
15	1.40367	0.81041	29.94376	0.000000	0.000000	-0.001870
16	-0.00000	1.62082	32.23878	-0.000000	0.000000	0.003287
17	-0.00000	-0.00000	34.53436	0.000000	-0.000000	0.002092
18	1.40367	0.81041	36.83315	0.000000	0.000000	-0.005331
19	-0.00000	1.62082	39.14559	0.000000	-0.000000	0.001503
20	0.00000	-0.00000	41.49039	0.000000	-0.000000	-0.003339
21	1.40367	0.81041	43.56173	0.000000	-0.000000	-0.000372
22	-0.00000	1.62082	45.39404	-0.000000	-0.000000	0.001266
23	1.40367	0.81041	47.25566	0.000000	-0.000000	0.001295
24	-0.00000	1.62082	49.10298	-0.000000	0.000000	-0.001618
25	1.40367	0.81041	50.94558	0.000000	-0.000000	-0.001593
26	-0.00000	1.62082	52.79332	0.000000	-0.000000	-0.002300
27	1.40367	0.81041	54.63811	-0.000000	0.000000	-0.000805
28	-0.00000	1.62082	56.48396	0.000000	-0.000000	0.000014
29	1.40367	0.81041	58.33130	-0.000000	0.000000	-0.003430
30	-0.00000	1.62082	60.17875	-0.000000	0.000000	-0.000253
31	1.40367	0.81041	62.02525	0.000000	-0.000000	0.003827
32	-0.00000	1.62082	63.87227	0.000000	-0.000000	0.002381
33	1.40367	0.81041	65.72058	0.000000	-0.000000	-0.000949
34	-0.00000	1.62082	67.56359	-0.000000	0.000000	-0.000919
35	1.40367	0.81041	69.41269	0.000000	-0.000000	-0.001494

36	-0.00000	1.62082	71.25532	-0.000000	0.000000	0.000773
37	1.40367	0.81041	73.09826	-0.000000	0.000000	0.000609
38	-0.00000	1.62082	74.96524	-0.000000	-0.000000	-0.002936

N_iteration : 40

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01048	0.000000	0.000000	-0.000571
3	1.40367	0.81041	2.36680	0.000000	-0.000000	0.002692
4	-0.00000	1.62082	4.67508	0.000000	-0.000000	-0.001524
5	-0.00000	-0.00000	6.97317	0.000000	-0.000000	0.003009
6	1.40367	0.81041	9.26875	-0.000000	-0.000000	0.002695
7	-0.00000	1.62082	11.56406	0.000000	-0.000000	0.001816
8	0.00000	-0.00000	13.86231	0.000000	-0.000000	0.002773
9	1.40367	0.81041	16.15919	0.000000	-0.000000	0.002449
10	-0.00000	1.62082	18.45868	0.000000	-0.000000	-0.001402
11	-0.00000	-0.00000	20.75579	0.000000	-0.000000	-0.002053
12	1.40367	0.81041	23.05281	0.000000	-0.000000	0.000780
13	-0.00000	1.62082	25.35091	0.000000	-0.000000	-0.001324
14	0.00000	-0.00000	27.64746	0.000000	-0.000000	-0.000858
15	1.40367	0.81041	29.94373	0.000000	-0.000000	-0.003998
16	-0.00000	1.62082	32.23870	0.000000	-0.000000	0.000057
17	-0.00000	-0.00000	34.53367	0.000000	-0.000000	0.002666
18	1.40367	0.81041	36.83195	0.000000	-0.000000	-0.000296
19	-0.00000	1.62082	39.14471	-0.000000	0.000000	-0.000913
20	0.00000	-0.00000	41.48945	0.000000	-0.000000	-0.000730
21	1.40367	0.81041	43.56118	-0.000000	0.000000	-0.002231
22	-0.00000	1.62082	45.39347	-0.000000	0.000000	0.001984
23	1.40367	0.81041	47.25531	-0.000000	0.000000	0.000699
24	-0.00000	1.62082	49.10273	-0.000000	0.000000	-0.003578
25	1.40367	0.81041	50.94506	-0.000000	0.000000	-0.000870
26	-0.00000	1.62082	52.79264	-0.000000	-0.000000	-0.000183
27	1.40367	0.81041	54.63772	0.000000	-0.000000	-0.002206
28	-0.00000	1.62082	56.48350	0.000000	-0.000000	-0.000236
29	1.40367	0.81041	58.33075	0.000000	-0.000000	-0.002407
30	-0.00000	1.62082	60.17835	-0.000000	0.000000	0.000204
31	1.40367	0.81041	62.02504	-0.000000	-0.000000	0.003630
32	-0.00000	1.62082	63.87227	0.000000	-0.000000	0.000429
33	1.40367	0.81041	65.72033	-0.000000	0.000000	0.000370
34	-0.00000	1.62082	67.56340	0.000000	-0.000000	0.000834
35	1.40367	0.81041	69.41289	-0.000000	0.000000	-0.002307
36	-0.00000	1.62082	71.25572	0.000000	0.000000	-0.000330
37	1.40367	0.81041	73.09866	-0.000000	0.000000	0.000700
38	-0.00000	1.62082	74.96566	-0.000000	0.000000	-0.002055

N_iteration : 41

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000

2	0.00000	-0.00000	0.01126	0.000000	-0.000000	-0.005001
3	1.40367	0.81041	2.36732	-0.000000	-0.000000	0.003810
4	-0.00000	1.62082	4.67556	-0.000000	0.000000	-0.001896
5	0.00000	-0.00000	6.97352	0.000000	-0.000000	0.003847
6	1.40367	0.81041	9.26910	0.000000	-0.000000	0.002383
7	-0.00000	1.62082	11.56437	0.000000	-0.000000	0.002395
8	0.00000	-0.00000	13.86268	0.000000	-0.000000	0.002582
9	1.40367	0.81041	16.15960	0.000000	-0.000000	0.000138
10	-0.00000	1.62082	18.45875	0.000000	-0.000000	0.001897
11	-0.00000	-0.00000	20.75603	0.000000	-0.000000	-0.003894
12	1.40367	0.81041	23.05292	-0.000000	0.000000	0.000594
13	-0.00000	1.62082	25.35085	-0.000000	0.000000	-0.001074
14	0.00000	-0.00000	27.64729	0.000000	-0.000000	0.000713
15	1.40367	0.81041	29.94372	-0.000000	-0.000000	-0.005091
16	-0.00000	1.62082	32.23865	-0.000000	0.000000	-0.001527
17	-0.00000	-0.00000	34.53331	0.000000	-0.000000	0.002978
18	1.40367	0.81041	36.83133	-0.000000	0.000000	0.002260
19	-0.00000	1.62082	39.14426	0.000000	-0.000000	-0.002144
20	0.00000	-0.00000	41.48896	0.000000	0.000000	0.000609
21	1.40367	0.81041	43.56090	0.000000	0.000000	-0.003207
22	-0.00000	1.62082	45.39317	-0.000000	0.000000	0.002288
23	1.40367	0.81041	47.25514	-0.000000	0.000000	0.000377
24	-0.00000	1.62082	49.10260	0.000000	-0.000000	-0.004481
25	1.40367	0.81041	50.94479	0.000000	-0.000000	-0.000513
26	-0.00000	1.62082	52.79230	0.000000	-0.000000	0.000807
27	1.40367	0.81041	54.63752	-0.000000	0.000000	-0.003142
28	-0.00000	1.62082	56.48326	0.000000	-0.000000	-0.000557
29	1.40367	0.81041	58.33048	0.000000	0.000000	-0.001938
30	-0.00000	1.62082	60.17815	0.000000	-0.000000	0.000503
31	1.40367	0.81041	62.02493	0.000000	-0.000000	0.003554
32	-0.00000	1.62082	63.87226	-0.000000	0.000000	-0.000573
33	1.40367	0.81041	65.72020	0.000000	-0.000000	0.001009
34	-0.00000	1.62082	67.56330	0.000000	-0.000000	0.001646
35	1.40367	0.81041	69.41299	-0.000000	0.000000	-0.002643
36	-0.00000	1.62082	71.25592	-0.000000	-0.000000	-0.000794
37	1.40367	0.81041	73.09886	-0.000000	0.000000	0.000744
38	-0.00000	1.62082	74.96588	-0.000000	0.000000	-0.001536

N_iteration : 42

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01199	0.000000	-0.000000	-0.002236
3	1.40367	0.81041	2.36855	-0.000000	0.000000	-0.002886
4	-0.00000	1.62082	4.67612	-0.000000	0.000000	0.004701
5	0.00000	-0.00000	6.97448	0.000000	-0.000000	0.000253
6	1.40367	0.81041	9.26990	-0.000000	0.000000	0.002898
7	-0.00000	1.62082	11.56510	0.000000	-0.000000	0.003671
8	0.00000	-0.00000	13.86355	0.000000	-0.000000	0.000702

9	1.40367	0.81041	16.16028	0.000000	-0.000000	-0.000844
10	-0.00000	1.62082	18.45907	0.000000	-0.000000	0.002009
11	0.00000	-0.00000	20.75602	0.000000	-0.000000	-0.000217
12	1.40367	0.81041	23.05316	-0.000000	0.000000	-0.003957
13	-0.00000	1.62082	25.35065	-0.000000	0.000000	0.001862
14	0.00000	-0.00000	27.64710	0.000000	-0.000000	-0.001748
15	1.40367	0.81041	29.94316	-0.000000	-0.000000	-0.000813
16	-0.00000	1.62082	32.23842	-0.000000	0.000000	-0.003873
17	0.00000	-0.00000	34.53305	0.000000	-0.000000	0.000012
18	1.40367	0.81041	36.83057	0.000000	0.000000	0.004270
19	-0.00000	1.62082	39.14332	0.000000	-0.000000	0.000384
20	0.00000	-0.00000	41.48824	0.000000	-0.000000	-0.000444
21	1.40367	0.81041	43.56011	0.000000	-0.000000	-0.000808
22	-0.00000	1.62082	45.39294	-0.000000	-0.000000	-0.000455
23	1.40367	0.81041	47.25490	-0.000000	0.000000	-0.001563
24	-0.00000	1.62082	49.10194	0.000000	-0.000000	-0.001935
25	1.40367	0.81041	50.94430	-0.000000	0.000000	-0.000888
26	-0.00000	1.62082	52.79182	0.000000	-0.000000	0.000089
27	1.40367	0.81041	54.63688	-0.000000	0.000000	-0.001712
28	-0.00000	1.62082	56.48282	0.000000	-0.000000	-0.001544
29	1.40367	0.81041	58.32983	-0.000000	-0.000000	0.000575
30	-0.00000	1.62082	60.17787	-0.000000	0.000000	0.000799
31	1.40367	0.81041	62.02512	0.000000	0.000000	0.000454
32	-0.00000	1.62082	63.87220	-0.000000	0.000000	-0.000036
33	1.40367	0.81041	65.72010	-0.000000	0.000000	0.001756
34	-0.00000	1.62082	67.56331	0.000000	-0.000000	0.001005
35	1.40367	0.81041	69.41289	0.000000	-0.000000	-0.001006
36	-0.00000	1.62082	71.25616	0.000000	-0.000000	-0.001542
37	1.40367	0.81041	73.09926	-0.000000	-0.000000	-0.000502
38	-0.00000	1.62082	74.96607	0.000000	-0.000000	0.001863

N_iteration : 43

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01220	-0.000000	-0.000000	-0.001431
3	1.40367	0.81041	2.36890	-0.000000	-0.000000	-0.004792
4	-0.00000	1.62082	4.67629	0.000000	0.000000	0.006700
5	0.00000	-0.00000	6.97476	0.000000	-0.000000	-0.000709
6	1.40367	0.81041	9.27013	0.000000	-0.000000	0.003119
7	-0.00000	1.62082	11.56532	0.000000	-0.000000	0.004131
8	0.00000	-0.00000	13.86380	0.000000	-0.000000	0.000225
9	1.40367	0.81041	16.16048	0.000000	0.000000	-0.001150
10	-0.00000	1.62082	18.45917	0.000000	-0.000000	0.001992
11	0.00000	-0.00000	20.75602	0.000000	-0.000000	0.000841
12	1.40367	0.81041	23.05323	-0.000000	0.000000	-0.005256
13	-0.00000	1.62082	25.35059	-0.000000	0.000000	0.002696
14	0.00000	-0.00000	27.64704	0.000000	-0.000000	-0.002453
15	1.40367	0.81041	29.94300	-0.000000	-0.000000	0.000497

16	-0.00000	1.62082	32.23835	0.000000	-0.000000	-0.004486
17	0.00000	-0.00000	34.53297	0.000000	-0.000000	-0.000888
18	1.40367	0.81041	36.83035	-0.000000	0.000000	0.004701
19	-0.00000	1.62082	39.14304	-0.000000	0.000000	0.000978
20	0.00000	-0.00000	41.48803	0.000000	-0.000000	-0.000789
21	1.40367	0.81041	43.55989	0.000000	0.000000	-0.000115
22	-0.00000	1.62082	45.39287	-0.000000	0.000000	-0.001023
23	1.40367	0.81041	47.25483	0.000000	-0.000000	-0.002098
24	-0.00000	1.62082	49.10175	0.000000	-0.000000	-0.001410
25	1.40367	0.81041	50.94416	-0.000000	0.000000	-0.001146
26	-0.00000	1.62082	52.79168	-0.000000	-0.000000	-0.000030
27	1.40367	0.81041	54.63669	0.000000	-0.000000	-0.001323
28	-0.00000	1.62082	56.48270	-0.000000	0.000000	-0.001924
29	1.40367	0.81041	58.32964	0.000000	0.000000	0.001330
30	-0.00000	1.62082	60.17779	-0.000000	0.000000	0.000928
31	1.40367	0.81041	62.02518	-0.000000	0.000000	-0.000546
32	-0.00000	1.62082	63.87219	0.000000	-0.000000	0.000066
33	1.40367	0.81041	65.72007	0.000000	-0.000000	0.002112
34	-0.00000	1.62082	67.56331	0.000000	-0.000000	0.000897
35	1.40367	0.81041	69.41286	0.000000	-0.000000	-0.000573
36	-0.00000	1.62082	71.25623	-0.000000	0.000000	-0.001876
37	1.40367	0.81041	73.09938	0.000000	-0.000000	-0.000760
38	-0.00000	1.62082	74.96613	0.000000	-0.000000	0.002813

N_iteration : 44

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01274	-0.000000	0.000000	0.000950
3	1.40367	0.81041	2.36953	0.000000	-0.000000	-0.001577
4	-0.00000	1.62082	4.67755	-0.000000	0.000000	-0.000189
5	0.00000	-0.00000	6.97559	0.000000	-0.000000	0.003724
6	1.40367	0.81041	9.27122	-0.000000	0.000000	0.001740
7	-0.00000	1.62082	11.56646	0.000000	-0.000000	0.001956
8	0.00000	-0.00000	13.86464	0.000000	-0.000000	0.000052
9	1.40367	0.81041	16.16099	0.000000	-0.000000	0.000983
10	-0.00000	1.62082	18.45968	-0.000000	0.000000	-0.000764
11	0.00000	-0.00000	20.75609	0.000000	-0.000000	0.000862
12	1.40367	0.81041	23.05289	0.000000	-0.000000	0.000284
13	-0.00000	1.62082	25.35070	-0.000000	0.000000	-0.003734
14	0.00000	-0.00000	27.64659	-0.000000	-0.000000	0.001096
15	1.40367	0.81041	29.94254	-0.000000	0.000000	-0.001110
16	-0.00000	1.62082	32.23765	0.000000	-0.000000	-0.000785
17	0.00000	-0.00000	34.53263	0.000000	-0.000000	-0.002239
18	1.40367	0.81041	36.83015	0.000000	-0.000000	0.000264
19	-0.00000	1.62082	39.14226	0.000000	0.000000	0.004817
20	0.00000	-0.00000	41.48727	-0.000000	-0.000000	-0.000357
21	1.40367	0.81041	43.55914	0.000000	0.000000	0.001310
22	-0.00000	1.62082	45.39254	-0.000000	-0.000000	-0.003582

23	1.40367	0.81041	47.25437	-0.000000	-0.000000	-0.003273
24	-0.00000	1.62082	49.10097	0.000000	-0.000000	0.001047
25	1.40367	0.81041	50.94357	0.000000	-0.000000	-0.001076
26	-0.00000	1.62082	52.79123	-0.000000	0.000000	-0.001837
27	1.40367	0.81041	54.63594	-0.000000	0.000000	0.000340
28	-0.00000	1.62082	56.48208	-0.000000	0.000000	-0.001209
29	1.40367	0.81041	58.32917	0.000000	-0.000000	0.001913
30	-0.00000	1.62082	60.17764	0.000000	0.000000	0.000521
31	1.40367	0.81041	62.02530	0.000000	-0.000000	-0.002198
32	-0.00000	1.62082	63.87214	-0.000000	-0.000000	0.001153
33	1.40367	0.81041	65.72020	0.000000	0.000000	0.001092
34	-0.00000	1.62082	67.56341	-0.000000	-0.000000	-0.000041
35	1.40367	0.81041	69.41270	-0.000000	-0.000000	0.001508
36	-0.00000	1.62082	71.25626	0.000000	-0.000000	-0.000919
37	1.40367	0.81041	73.09967	0.000000	-0.000000	-0.001258
38	-0.00000	1.62082	74.96661	0.000000	0.000000	0.003122

N_iteration : 45

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01294	0.000000	0.000000	0.001804
3	1.40367	0.81041	2.36977	0.000000	0.000000	-0.000328
4	-0.00000	1.62082	4.67801	-0.000000	0.000000	-0.002585
5	0.00000	-0.00000	6.97589	0.000000	-0.000000	0.005402
6	1.40367	0.81041	9.27162	-0.000000	0.000000	0.001273
7	-0.00000	1.62082	11.56687	0.000000	-0.000000	0.001193
8	0.00000	-0.00000	13.86495	0.000000	-0.000000	0.000079
9	1.40367	0.81041	16.16118	0.000000	-0.000000	0.001847
10	-0.00000	1.62082	18.45987	0.000000	-0.000000	-0.001781
11	0.00000	-0.00000	20.75612	0.000000	-0.000000	0.000805
12	1.40367	0.81041	23.05276	0.000000	-0.000000	0.002262
13	-0.00000	1.62082	25.35073	0.000000	0.000000	-0.006120
14	0.00000	-0.00000	27.64642	0.000000	-0.000000	0.002356
15	1.40367	0.81041	29.94237	0.000000	-0.000000	-0.001656
16	-0.00000	1.62082	32.23739	-0.000000	0.000000	0.000629
17	0.00000	-0.00000	34.53250	0.000000	-0.000000	-0.002804
18	1.40367	0.81041	36.83008	0.000000	-0.000000	-0.001513
19	-0.00000	1.62082	39.14197	0.000000	-0.000000	0.006145
20	0.00000	-0.00000	41.48700	0.000000	-0.000000	-0.000233
21	1.40367	0.81041	43.55886	-0.000000	0.000000	0.001732
22	-0.00000	1.62082	45.39241	-0.000000	-0.000000	-0.004346
23	1.40367	0.81041	47.25420	0.000000	-0.000000	-0.003446
24	-0.00000	1.62082	49.10068	-0.000000	0.000000	0.001803
25	1.40367	0.81041	50.94336	-0.000000	0.000000	-0.001415
26	-0.00000	1.62082	52.79106	0.000000	-0.000000	-0.002563
27	1.40367	0.81041	54.63567	0.000000	-0.000000	0.001057
28	-0.00000	1.62082	56.48185	-0.000000	0.000000	-0.000902
29	1.40367	0.81041	58.32900	0.000000	-0.000000	0.002219

30	-0.00000	1.62082	60.17758	-0.000000	-0.000000	0.000327
31	1.40367	0.81041	62.02534	0.000000	-0.000000	-0.002993
32	-0.00000	1.62082	63.87212	-0.000000	0.000000	0.001634
33	1.40367	0.81041	65.72025	0.000000	-0.000000	0.000946
34	-0.00000	1.62082	67.56345	0.000000	-0.000000	-0.000410
35	1.40367	0.81041	69.41264	-0.000000	0.000000	0.001997
36	-0.00000	1.62082	71.25627	-0.000000	-0.000000	-0.000764
37	1.40367	0.81041	73.09978	-0.000000	0.000000	-0.001253
38	-0.00000	1.62082	74.96679	-0.000000	0.000000	0.003436

N_iteration : 46

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01348	0.000000	-0.000000	0.001058
3	1.40367	0.81041	2.37024	0.000000	-0.000000	0.002110
4	-0.00000	1.62082	4.67882	0.000000	-0.000000	-0.003447
5	0.00000	-0.00000	6.97691	0.000000	-0.000000	0.003538
6	1.40367	0.81041	9.27257	-0.000000	-0.000000	0.002078
7	-0.00000	1.62082	11.56786	0.000000	0.000000	-0.000994
8	0.00000	-0.00000	13.86561	0.000000	-0.000000	0.001180
9	1.40367	0.81041	16.16171	-0.000000	0.000000	0.000996
10	-0.00000	1.62082	18.46016	0.000000	-0.000000	-0.001241
11	0.00000	-0.00000	20.75624	0.000000	-0.000000	0.000435
12	1.40367	0.81041	23.05265	0.000000	-0.000000	0.002248
13	-0.00000	1.62082	25.35039	0.000000	-0.000000	-0.003668
14	0.00000	-0.00000	27.64623	0.000000	-0.000000	-0.000464
15	1.40367	0.81041	29.94188	0.000000	-0.000000	-0.000031
16	-0.00000	1.62082	32.23688	0.000000	-0.000000	0.000908
17	0.00000	-0.00000	34.53204	0.000000	-0.000000	-0.001805
18	1.40367	0.81041	36.82981	0.000000	-0.000000	-0.002222
19	-0.00000	1.62082	39.14178	0.000000	-0.000000	0.003500
20	0.00000	-0.00000	41.48638	0.000000	-0.000000	0.002809
21	1.40367	0.81041	43.55839	-0.000000	0.000000	0.000646
22	-0.00000	1.62082	45.39185	-0.000000	0.000000	-0.004055
23	1.40367	0.81041	47.25360	-0.000000	-0.000000	-0.002957
24	-0.00000	1.62082	49.10019	-0.000000	0.000000	0.001215
25	1.40367	0.81041	50.94280	0.000000	-0.000000	-0.000931
26	-0.00000	1.62082	52.79052	-0.000000	0.000000	-0.002601
27	1.40367	0.81041	54.63515	0.000000	0.000000	0.001017
28	-0.00000	1.62082	56.48130	0.000000	-0.000000	0.000650
29	1.40367	0.81041	58.32879	0.000000	-0.000000	0.001189
30	-0.00000	1.62082	60.17748	-0.000000	0.000000	-0.000245
31	1.40367	0.81041	62.02523	0.000000	0.000000	-0.002044
32	-0.00000	1.62082	63.87219	0.000000	-0.000000	0.001151
33	1.40367	0.81041	65.72042	-0.000000	-0.000000	-0.000134
34	-0.00000	1.62082	67.56351	-0.000000	-0.000000	-0.000198
35	1.40367	0.81041	69.41265	0.000000	0.000000	0.002253
36	-0.00000	1.62082	71.25624	-0.000000	0.000000	0.000564

37	1.40367	0.81041	73.09993	0.000000	-0.000000	-0.000402
38	-0.00000	1.62082	74.96741	-0.000000	0.000000	0.000994

N_iteration : 47

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01403	-0.000000	-0.000000	0.000418
3	1.40367	0.81041	2.37071	0.000000	-0.000000	0.004621
4	-0.00000	1.62082	4.67963	-0.000000	0.000000	-0.004311
5	0.00000	-0.00000	6.97793	-0.000000	-0.000000	0.001618
6	1.40367	0.81041	9.27351	0.000000	0.000000	0.002900
7	-0.00000	1.62082	11.56883	-0.000000	0.000000	-0.003045
8	0.00000	-0.00000	13.86627	0.000000	-0.000000	0.002422
9	1.40367	0.81041	16.16224	-0.000000	0.000000	0.000259
10	-0.00000	1.62082	18.46044	0.000000	-0.000000	-0.000667
11	0.00000	-0.00000	20.75636	0.000000	-0.000000	0.000031
12	1.40367	0.81041	23.05254	0.000000	-0.000000	0.002105
13	-0.00000	1.62082	25.35005	-0.000000	0.000000	-0.001403
14	0.00000	-0.00000	27.64604	0.000000	-0.000000	-0.003300
15	1.40367	0.81041	29.94141	-0.000000	-0.000000	0.001750
16	-0.00000	1.62082	32.23638	0.000000	-0.000000	0.001353
17	0.00000	-0.00000	34.53157	-0.000000	-0.000000	-0.000809
18	1.40367	0.81041	36.82955	0.000000	-0.000000	-0.003057
19	-0.00000	1.62082	39.14159	-0.000000	0.000000	0.000717
20	0.00000	-0.00000	41.48577	0.000000	-0.000000	0.005777
21	1.40367	0.81041	43.55792	0.000000	-0.000000	-0.000561
22	-0.00000	1.62082	45.39129	0.000000	0.000000	-0.003806
23	1.40367	0.81041	47.25301	0.000000	-0.000000	-0.002256
24	-0.00000	1.62082	49.09971	0.000000	-0.000000	0.000552
25	1.40367	0.81041	50.94225	0.000000	-0.000000	-0.000632
26	-0.00000	1.62082	52.78999	0.000000	-0.000000	-0.002651
27	1.40367	0.81041	54.63464	0.000000	-0.000000	0.000957
28	-0.00000	1.62082	56.48075	0.000000	-0.000000	0.002219
29	1.40367	0.81041	58.32858	0.000000	-0.000000	0.000332
30	-0.00000	1.62082	60.17738	-0.000000	-0.000000	-0.000879
31	1.40367	0.81041	62.02512	0.000000	0.000000	-0.001317
32	-0.00000	1.62082	63.87226	-0.000000	0.000000	0.000800
33	1.40367	0.81041	65.72059	-0.000000	-0.000000	-0.001016
34	-0.00000	1.62082	67.56356	-0.000000	0.000000	-0.000063
35	1.40367	0.81041	69.41266	-0.000000	0.000000	0.002402
36	-0.00000	1.62082	71.25620	-0.000000	0.000000	0.001921
37	1.40367	0.81041	73.10007	-0.000000	0.000000	0.000312
38	-0.00000	1.62082	74.96803	-0.000000	0.000000	-0.001430

N_iteration : 48

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01436	-0.000000	-0.000000	0.000492

3	1.40367	0.81041	2.37136	-0.000000	0.000000	-0.000415
4	-0.00000	1.62082	4.67971	0.000000	-0.000000	0.002940
5	0.00000	-0.00000	6.97862	-0.000000	-0.000000	-0.001696
6	1.40367	0.81041	9.27426	0.000000	0.000000	-0.000372
7	-0.00000	1.62082	11.56910	0.000000	-0.000000	0.001802
8	0.00000	-0.00000	13.86683	-0.000000	0.000000	-0.001091
9	1.40367	0.81041	16.16255	-0.000000	-0.000000	0.000601
10	-0.00000	1.62082	18.46053	-0.000000	0.000000	0.000479
11	0.00000	-0.00000	20.75642	-0.000000	0.000000	0.000551
12	1.40367	0.81041	23.05265	-0.000000	-0.000000	-0.000872
13	-0.00000	1.62082	25.34974	-0.000000	0.000000	0.000775
14	0.00000	-0.00000	27.64566	-0.000000	0.000000	-0.001239
15	1.40367	0.81041	29.94130	-0.000000	0.000000	-0.000309
16	-0.00000	1.62082	32.23622	-0.000000	0.000000	0.000780
17	0.00000	-0.00000	34.53126	-0.000000	0.000000	-0.000296
18	1.40367	0.81041	36.82915	-0.000000	-0.000000	-0.000395
19	-0.00000	1.62082	39.14155	0.000000	-0.000000	-0.000536
20	0.00000	-0.00000	41.48592	-0.000000	-0.000000	0.001792
21	1.40367	0.81041	43.55763	0.000000	-0.000000	0.000480
22	-0.00000	1.62082	45.39067	0.000000	0.000000	-0.001343
23	1.40367	0.81041	47.25250	0.000000	-0.000000	-0.001392
24	-0.00000	1.62082	49.09949	0.000000	-0.000000	-0.001506
25	1.40367	0.81041	50.94190	0.000000	0.000000	-0.000677
26	-0.00000	1.62082	52.78949	0.000000	-0.000000	-0.000562
27	1.40367	0.81041	54.63444	0.000000	0.000000	0.000182
28	-0.00000	1.62082	56.48064	-0.000000	0.000000	0.001666
29	1.40367	0.81041	58.32849	-0.000000	0.000000	-0.000040
30	-0.00000	1.62082	60.17725	0.000000	-0.000000	-0.000576
31	1.40367	0.81041	62.02494	-0.000000	-0.000000	-0.000113
32	-0.00000	1.62082	63.87237	0.000000	-0.000000	-0.000724
33	1.40367	0.81041	65.72059	0.000000	-0.000000	-0.000610
34	-0.00000	1.62082	67.56358	0.000000	-0.000000	0.000687
35	1.40367	0.81041	69.41287	-0.000000	-0.000000	0.001361
36	-0.00000	1.62082	71.25635	-0.000000	0.000000	0.001811
37	1.40367	0.81041	73.10018	-0.000000	0.000000	0.000848
38	-0.00000	1.62082	74.96824	0.000000	-0.000000	-0.001917

N_iteration : 49

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01440	0.000000	0.000000	0.000611
3	1.40367	0.81041	2.37145	0.000000	-0.000000	-0.001001
4	-0.00000	1.62082	4.67972	0.000000	0.000000	0.004065
5	0.00000	-0.00000	6.97871	0.000000	0.000000	-0.002239
6	1.40367	0.81041	9.27437	0.000000	-0.000000	-0.000803
7	-0.00000	1.62082	11.56914	0.000000	0.000000	0.002729
8	0.00000	-0.00000	13.86691	0.000000	0.000000	-0.001428
9	1.40367	0.81041	16.16259	-0.000000	0.000000	0.000658

10	-0.00000	1.62082	18.46055	-0.000000	0.000000	0.000644
11	0.00000	-0.00000	20.75643	0.000000	0.000000	0.000674
12	1.40367	0.81041	23.05267	-0.000000	0.000000	-0.001281
13	-0.00000	1.62082	25.34970	0.000000	-0.000000	0.001032
14	0.00000	-0.00000	27.64561	0.000000	0.000000	-0.000976
15	1.40367	0.81041	29.94128	0.000000	-0.000000	-0.000651
16	-0.00000	1.62082	32.23619	-0.000000	0.000000	0.000579
17	0.00000	-0.00000	34.53121	0.000000	0.000000	-0.000275
18	1.40367	0.81041	36.82910	0.000000	0.000000	0.000046
19	-0.00000	1.62082	39.14154	-0.000000	0.000000	-0.000711
20	0.00000	-0.00000	41.48594	0.000000	0.000000	0.001255
21	1.40367	0.81041	43.55758	-0.000000	-0.000000	0.000577
22	-0.00000	1.62082	45.39058	0.000000	-0.000000	-0.001119
23	1.40367	0.81041	47.25242	0.000000	-0.000000	-0.001308
24	-0.00000	1.62082	49.09946	0.000000	-0.000000	-0.001792
25	1.40367	0.81041	50.94185	0.000000	0.000000	-0.000864
26	-0.00000	1.62082	52.78941	0.000000	-0.000000	-0.000398
27	1.40367	0.81041	54.63441	-0.000000	0.000000	0.000133
28	-0.00000	1.62082	56.48063	-0.000000	0.000000	0.001598
29	1.40367	0.81041	58.32848	0.000000	0.000000	-0.000197
30	-0.00000	1.62082	60.17723	-0.000000	-0.000000	-0.000607
31	1.40367	0.81041	62.02492	0.000000	0.000000	0.000130
32	-0.00000	1.62082	63.87239	-0.000000	0.000000	-0.000818
33	1.40367	0.81041	65.72060	0.000000	-0.000000	-0.000589
34	-0.00000	1.62082	67.56359	0.000000	-0.000000	0.000603
35	1.40367	0.81041	69.41290	-0.000000	-0.000000	0.001175
36	-0.00000	1.62082	71.25637	0.000000	-0.000000	0.001916
37	1.40367	0.81041	73.10019	-0.000000	0.000000	0.000927
38	-0.00000	1.62082	74.96827	-0.000000	0.000000	-0.002025

N_iteration : 50

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01459	-0.000000	-0.000000	-0.000650
3	1.40367	0.81041	2.37163	0.000000	-0.000000	0.000254
4	-0.00000	1.62082	4.68010	0.000000	-0.000000	0.000924
5	0.00000	-0.00000	6.97880	-0.000000	0.000000	0.000496
6	1.40367	0.81041	9.27461	-0.000000	0.000000	-0.001141
7	-0.00000	1.62082	11.56949	-0.000000	0.000000	0.000418
8	0.00000	-0.00000	13.86702	-0.000000	0.000000	0.000476
9	1.40367	0.81041	16.16278	-0.000000	0.000000	-0.000417
10	-0.00000	1.62082	18.46064	-0.000000	0.000000	0.001149
11	0.00000	-0.00000	20.75652	-0.000000	0.000000	-0.000255
12	1.40367	0.81041	23.05261	-0.000000	0.000000	-0.000183
13	-0.00000	1.62082	25.34966	-0.000000	0.000000	-0.000449
14	0.00000	-0.00000	27.64537	-0.000000	0.000000	0.001237
15	1.40367	0.81041	29.94118	-0.000000	0.000000	-0.000980
16	-0.00000	1.62082	32.23618	-0.000000	0.000000	-0.000788

17	0.00000	-0.00000	34.53106	-0.000000	0.000000	0.000629
18	1.40367	0.81041	36.82894	0.000000	-0.000000	0.000638
19	-0.00000	1.62082	39.14147	-0.000000	-0.000000	0.000069
20	0.00000	-0.00000	41.48611	-0.000000	-0.000000	-0.001783
21	1.40367	0.81041	43.55751	0.000000	-0.000000	0.000754
22	-0.00000	1.62082	45.39023	0.000000	-0.000000	0.000593
23	1.40367	0.81041	47.25210	0.000000	-0.000000	-0.000799
24	-0.00000	1.62082	49.09922	0.000000	-0.000000	-0.002238
25	1.40367	0.81041	50.94163	0.000000	-0.000000	-0.000912
26	-0.00000	1.62082	52.78917	0.000000	-0.000000	0.000703
27	1.40367	0.81041	54.63434	0.000000	-0.000000	-0.000034
28	-0.00000	1.62082	56.48072	0.000000	0.000000	0.000246
29	1.40367	0.81041	58.32843	0.000000	-0.000000	0.000257
30	-0.00000	1.62082	60.17712	-0.000000	0.000000	-0.000053
31	1.40367	0.81041	62.02486	-0.000000	0.000000	-0.000076
32	-0.00000	1.62082	63.87236	0.000000	0.000000	-0.001101
33	1.40367	0.81041	65.72055	0.000000	-0.000000	0.000050
34	-0.00000	1.62082	67.56365	-0.000000	0.000000	0.000823
35	1.40367	0.81041	69.41308	-0.000000	-0.000000	0.000785
36	-0.00000	1.62082	71.25659	-0.000000	0.000000	0.001094
37	1.40367	0.81041	73.10032	-0.000000	0.000000	0.000662
38	-0.00000	1.62082	74.96819	-0.000000	0.000000	-0.000773

N_iteration : 51

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01465	-0.000000	-0.000000	-0.001048
3	1.40367	0.81041	2.37168	0.000000	-0.000000	0.000646
4	-0.00000	1.62082	4.68021	0.000000	-0.000000	0.000039
5	0.00000	-0.00000	6.97883	0.000000	-0.000000	0.001354
6	1.40367	0.81041	9.27469	0.000000	0.000000	-0.001262
7	-0.00000	1.62082	11.56959	0.000000	-0.000000	-0.000239
8	0.00000	-0.00000	13.86705	0.000000	-0.000000	0.001111
9	1.40367	0.81041	16.16283	-0.000000	-0.000000	-0.000715
10	-0.00000	1.62082	18.46067	0.000000	-0.000000	0.001350
11	0.00000	-0.00000	20.75654	0.000000	-0.000000	-0.000539
12	1.40367	0.81041	23.05259	0.000000	-0.000000	0.000143
13	-0.00000	1.62082	25.34965	-0.000000	0.000000	-0.000927
14	0.00000	-0.00000	27.64529	0.000000	-0.000000	0.001871
15	1.40367	0.81041	29.94115	-0.000000	0.000000	-0.001112
16	-0.00000	1.62082	32.23617	0.000000	-0.000000	-0.001187
17	0.00000	-0.00000	34.53101	0.000000	-0.000000	0.000905
18	1.40367	0.81041	36.82889	-0.000000	0.000000	0.000778
19	-0.00000	1.62082	39.14144	0.000000	-0.000000	0.000320
20	0.00000	-0.00000	41.48617	0.000000	-0.000000	-0.002693
21	1.40367	0.81041	43.55749	0.000000	-0.000000	0.000809
22	-0.00000	1.62082	45.39012	0.000000	-0.000000	0.000991
23	1.40367	0.81041	47.25200	0.000000	-0.000000	-0.000652

24	-0.00000	1.62082	49.09915	-0.000000	-0.000000	-0.002261
25	1.40367	0.81041	50.94156	0.000000	-0.000000	-0.000970
26	-0.00000	1.62082	52.78909	-0.000000	-0.000000	0.001026
27	1.40367	0.81041	54.63432	0.000000	-0.000000	-0.000067
28	-0.00000	1.62082	56.48074	-0.000000	-0.000000	-0.000311
29	1.40367	0.81041	58.32841	0.000000	0.000000	0.000277
30	-0.00000	1.62082	60.17709	-0.000000	0.000000	0.000217
31	1.40367	0.81041	62.02484	-0.000000	0.000000	-0.000005
32	-0.00000	1.62082	63.87235	-0.000000	0.000000	-0.001165
33	1.40367	0.81041	65.72053	-0.000000	0.000000	0.000191
34	-0.00000	1.62082	67.56367	0.000000	-0.000000	0.000854
35	1.40367	0.81041	69.41314	0.000000	-0.000000	0.000610
36	-0.00000	1.62082	71.25666	-0.000000	0.000000	0.000812
37	1.40367	0.81041	73.10035	-0.000000	0.000000	0.000627
38	-0.00000	1.62082	74.96816	-0.000000	0.000000	-0.000352

N_iteration : 52

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01469	0.000000	0.000000	-0.000310
3	1.40367	0.81041	2.37187	-0.000000	0.000000	0.000447
4	-0.00000	1.62082	4.68048	-0.000000	0.000000	-0.001020
5	0.00000	-0.00000	6.97902	0.000000	-0.000000	0.001022
6	1.40367	0.81041	9.27474	-0.000000	0.000000	0.000607
7	-0.00000	1.62082	11.56981	0.000000	-0.000000	-0.001628
8	0.00000	-0.00000	13.86723	0.000000	-0.000000	0.000651
9	1.40367	0.81041	16.16290	-0.000000	0.000000	0.000831
10	-0.00000	1.62082	18.46086	-0.000000	0.000000	-0.000594
11	0.00000	-0.00000	20.75655	-0.000000	-0.000000	0.000415
12	1.40367	0.81041	23.05256	0.000000	-0.000000	-0.000132
13	-0.00000	1.62082	25.34954	-0.000000	0.000000	0.000253
14	0.00000	-0.00000	27.64530	-0.000000	-0.000000	-0.000012
15	1.40367	0.81041	29.94097	0.000000	-0.000000	0.000338
16	-0.00000	1.62082	32.23605	0.000000	-0.000000	-0.000919
17	0.00000	-0.00000	34.53098	0.000000	-0.000000	0.000275
18	1.40367	0.81041	36.82885	0.000000	-0.000000	0.001009
19	-0.00000	1.62082	39.14142	-0.000000	0.000000	-0.000334
20	0.00000	-0.00000	41.48604	0.000000	-0.000000	-0.001475
21	1.40367	0.81041	43.55751	0.000000	-0.000000	-0.000731
22	-0.00000	1.62082	45.38996	-0.000000	-0.000000	0.001104
23	1.40367	0.81041	47.25171	-0.000000	-0.000000	-0.000253
24	-0.00000	1.62082	49.09877	-0.000000	0.000000	-0.001159
25	1.40367	0.81041	50.94132	0.000000	-0.000000	-0.000837
26	-0.00000	1.62082	52.78902	0.000000	-0.000000	0.000408
27	1.40367	0.81041	54.63426	0.000000	0.000000	0.000042
28	-0.00000	1.62082	56.48078	0.000000	0.000000	-0.000890
29	1.40367	0.81041	58.32840	-0.000000	0.000000	0.000255
30	-0.00000	1.62082	60.17704	0.000000	-0.000000	0.000413

31	1.40367	0.81041	62.02480	0.000000	-0.000000	-0.000250
32	-0.00000	1.62082	63.87223	-0.000000	0.000000	-0.000367
33	1.40367	0.81041	65.72052	-0.000000	0.000000	0.000364
34	-0.00000	1.62082	67.56379	0.000000	-0.000000	0.000565
35	1.40367	0.81041	69.41333	-0.000000	0.000000	0.000453
36	-0.00000	1.62082	71.25689	-0.000000	-0.000000	0.000051
37	1.40367	0.81041	73.10050	-0.000000	0.000000	0.000162
38	-0.00000	1.62082	74.96807	0.000000	-0.000000	0.001106

N_iteration : 53

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01469	0.000000	-0.000000	-0.000172
3	1.40367	0.81041	2.37189	-0.000000	0.000000	0.000474
4	-0.00000	1.62082	4.68052	-0.000000	-0.000000	-0.001182
5	0.00000	-0.00000	6.97904	-0.000000	-0.000000	0.000886
6	1.40367	0.81041	9.27475	-0.000000	-0.000000	0.000851
7	-0.00000	1.62082	11.56984	-0.000000	0.000000	-0.001738
8	0.00000	-0.00000	13.86725	-0.000000	-0.000000	0.000631
9	1.40367	0.81041	16.16290	-0.000000	0.000000	0.001061
10	-0.00000	1.62082	18.46088	0.000000	-0.000000	-0.000831
11	0.00000	-0.00000	20.75656	0.000000	-0.000000	0.000540
12	1.40367	0.81041	23.05255	-0.000000	0.000000	-0.000177
13	-0.00000	1.62082	25.34953	-0.000000	0.000000	0.000408
14	0.00000	-0.00000	27.64530	-0.000000	-0.000000	-0.000241
15	1.40367	0.81041	29.94095	-0.000000	0.000000	0.000550
16	-0.00000	1.62082	32.23604	-0.000000	-0.000000	-0.000935
17	0.00000	-0.00000	34.53098	-0.000000	-0.000000	0.000086
18	1.40367	0.81041	36.82884	0.000000	-0.000000	0.001016
19	-0.00000	1.62082	39.14141	-0.000000	0.000000	-0.000327
20	0.00000	-0.00000	41.48602	0.000000	-0.000000	-0.001259
21	1.40367	0.81041	43.55751	-0.000000	0.000000	-0.000914
22	-0.00000	1.62082	45.38994	0.000000	-0.000000	0.001082
23	1.40367	0.81041	47.25168	0.000000	-0.000000	-0.000275
24	-0.00000	1.62082	49.09872	-0.000000	0.000000	-0.001038
25	1.40367	0.81041	50.94129	0.000000	-0.000000	-0.000791
26	-0.00000	1.62082	52.78901	0.000000	-0.000000	0.000332
27	1.40367	0.81041	54.63426	-0.000000	-0.000000	0.000007
28	-0.00000	1.62082	56.48078	0.000000	-0.000000	-0.000986
29	1.40367	0.81041	58.32840	-0.000000	-0.000000	0.000278
30	-0.00000	1.62082	60.17703	0.000000	0.000000	0.000465
31	1.40367	0.81041	62.02479	-0.000000	-0.000000	-0.000269
32	-0.00000	1.62082	63.87221	0.000000	0.000000	-0.000253
33	1.40367	0.81041	65.72051	0.000000	0.000000	0.000387
34	-0.00000	1.62082	67.56380	-0.000000	0.000000	0.000450
35	1.40367	0.81041	69.41335	-0.000000	0.000000	0.000334
36	-0.00000	1.62082	71.25692	0.000000	-0.000000	-0.000009
37	1.40367	0.81041	73.10052	-0.000000	0.000000	0.000166

38	-0.00000	1.62082	74.96806	-0.000000	-0.000000	0.001306

N_iteration : 54

atom	X	Y	Z	Fx	Fy	Fz
1	0.00000	0.00000	0.00000	0.000000	0.000000	0.000000
2	0.00000	-0.00000	0.01469	0.000000	-0.000000	0.000523
3	1.40367	0.81041	2.37199	0.000000	-0.000000	-0.000876
4	-0.00000	1.62082	4.68049	-0.000000	0.000000	0.000705
5	0.00000	-0.00000	6.97919	0.000000	-0.000000	-0.000360
6	1.40367	0.81041	9.27484	0.000000	-0.000000	-0.000060
7	-0.00000	1.62082	11.56975	0.000000	-0.000000	0.000685
8	0.00000	-0.00000	13.86737	0.000000	-0.000000	-0.000729
9	1.40367	0.81041	16.16302	0.000000	-0.000000	0.000173
10	-0.00000	1.62082	18.46087	0.000000	-0.000000	0.000539
11	0.00000	-0.00000	20.75661	0.000000	-0.000000	-0.000429
12	1.40367	0.81041	23.05253	0.000000	0.000000	0.000509
13	-0.00000	1.62082	25.34953	-0.000000	-0.000000	0.000026
14	0.00000	-0.00000	27.64527	0.000000	-0.000000	0.000034
15	1.40367	0.81041	29.94095	0.000000	-0.000000	-0.000338
16	-0.00000	1.62082	32.23591	0.000000	-0.000000	0.000703
17	0.00000	-0.00000	34.53098	0.000000	-0.000000	-0.000143
18	1.40367	0.81041	36.82892	0.000000	-0.000000	-0.000302
19	-0.00000	1.62082	39.14137	0.000000	-0.000000	-0.000262
20	0.00000	-0.00000	41.48587	0.000000	-0.000000	-0.000045
21	1.40367	0.81041	43.55743	0.000000	-0.000000	-0.000952
22	-0.00000	1.62082	45.38999	-0.000000	0.000000	-0.000210
23	1.40367	0.81041	47.25156	-0.000000	0.000000	-0.000057
24	-0.00000	1.62082	49.09850	-0.000000	-0.000000	-0.000025
25	1.40367	0.81041	50.94113	0.000000	0.000000	-0.000404
26	-0.00000	1.62082	52.78901	-0.000000	-0.000000	-0.000588
27	1.40367	0.81041	54.63424	-0.000000	-0.000000	-0.000133
28	-0.00000	1.62082	56.48070	0.000000	-0.000000	-0.000205
29	1.40367	0.81041	58.32842	-0.000000	-0.000000	-0.000102
30	-0.00000	1.62082	60.17706	-0.000000	0.000000	0.000104
31	1.40367	0.81041	62.02476	0.000000	-0.000000	-0.000062
32	-0.00000	1.62082	63.87215	0.000000	0.000000	0.000176
33	1.40367	0.81041	65.72055	0.000000	-0.000000	0.000196
34	-0.00000	1.62082	67.56389	-0.000000	0.000000	0.000293
35	1.40367	0.81041	69.41344	-0.000000	0.000000	0.000290
36	-0.00000	1.62082	71.25699	-0.000000	-0.000000	-0.000003
37	1.40367	0.81041	73.10058	0.000000	0.000000	0.000298
38	-0.00000	1.62082	74.96815	-0.000000	0.000000	0.000899