```
#lable_1
units           metal
dimension       3
timestep        0.001
atom_style      atomic
boundary        s    s    s
neighbor        2.0    bin
neigh_modify    delay    10
read_data       data.M1111S1919-1111-1111-1111-1111
pair_style      hybrid          lj/cut 10.2 airebo 3.0 #10.2
pair_coeff      *    *          airebo CH.airebo  C  C  C  C  C  C  C  C  C  C  H  H  H  H  H  H  H  H  H  H
#lable_2
pair_coeff    1    2*10       lj/cut  0.002840     3.400
pair_coeff    2    3*10       lj/cut  0.002840     3.400
pair_coeff    3    4*10       lj/cut  0.002840     3.400
pair_coeff    4    5*10       lj/cut  0.002840     3.400
pair_coeff    5    6*10       lj/cut  0.002840     3.400
pair_coeff    6    7*10       lj/cut  0.002840     3.400
pair_coeff    7    8*10       lj/cut  0.002840     3.400
pair_coeff    8    9*10       lj/cut  0.002840     3.400
pair_coeff    9      10       lj/cut  0.002840     3.400
pair_coeff    1   12*20       lj/cut  0.001376     3.025
pair_coeff    2      11       lj/cut  0.001376     3.025
pair_coeff    2   13*20       lj/cut  0.001376     3.025
pair_coeff    3   11*12       lj/cut  0.001376     3.025
pair_coeff    3   14*20       lj/cut  0.001376     3.025
pair_coeff    4   11*13       lj/cut  0.001376     3.025
pair_coeff    4   15*20       lj/cut  0.001376     3.025
```

```
pair_coeff    5   11*14       lj/cut  0.001376     3.025
pair_coeff    5   16*20       lj/cut  0.001376     3.025
pair_coeff    6   11*15       lj/cut  0.001376     3.025
pair_coeff    6   17*20       lj/cut  0.001376     3.025
pair_coeff    7   11*16       lj/cut  0.001376     3.025
pair_coeff    7   18*20       lj/cut  0.001376     3.025
pair_coeff    8   11*17       lj/cut  0.001376     3.025
pair_coeff    8   19*20       lj/cut  0.001376     3.025
pair_coeff    9   11*18       lj/cut  0.001376     3.025
pair_coeff    9      20       lj/cut  0.001376     3.025
pair_coeff   10   11*19       lj/cut  0.001376     3.025
pair_coeff   11   12*20       lj/cut  0.001500     2.650
pair_coeff   12   13*20       lj/cut  0.001500     2.650
pair_coeff   13   14*20       lj/cut  0.001500     2.650
pair_coeff   14   15*20       lj/cut  0.001500     2.650
pair_coeff   15   16*20       lj/cut  0.001500     2.650
pair_coeff   16   17*20       lj/cut  0.001500     2.650
pair_coeff   17   18*20       lj/cut  0.001500     2.650
pair_coeff   18   19*20       lj/cut  0.001500     2.650
pair_coeff   19      20       lj/cut  0.001500     2.650
#lable_3
region       motor_L    block   -10.550    10.550   -10.550    10.550     0.000     5.117
region       rotor1_L   block    -7.460     7.460    -7.460     7.460    34.700    39.817
region       rotor1_R   block    -7.460     7.460    -7.460     7.460   109.403   114.520
region       rotor2_L   block    -7.460     7.460    -7.460     7.460   118.520   123.637
region       rotor2_R   block    -7.460     7.460    -7.460     7.460   193.223   198.340
region       rotor3_L   block    -7.460     7.460    -7.460     7.460   202.340   207.457
region       rotor3_R   block    -7.460     7.460    -7.460     7.460   277.043   282.160
#lable_4
```

```
group       motor                type     1
group       rotor1               type     2
group       rotor2               type     3
group       rotor3               type     4
group       stator1              type     5
group       stator2              type     6
group       stator3              type     7
group       stator4              type     8
group       stator5              type     9
group       stator6              type    10
group       motor_hydrogen          type    11
#lable_5
group       motor_Left          region        motor_L
group       rotor1_Left          region        rotor1_L
#group      rotor1_Right          region        rotor1_R
group       rotor2_Left          region        rotor2_L
#group      rotor2_Right          region        rotor2_R
group       rotor3_Left          region        rotor3_L
#group      rotor3_Right          region        rotor3_R
group       M_H                 union         motor     motor_hydrogen
group       all_subtract_M_H       subtract       all       M_H
#group      all_subtract_M         subtract       all       Motor
group       stators1             union         stator1 stator2
group       stators2             union         stator3 stator4
group       stators3             union         stator5 stator6
group       except_rotor1          union         motor    stators1 rotor2 stator3
group       except_rotor2          union         rotor1  stator2   stators2 rotor3 stator5
group       except_rotor3          union         rotor2 stator4 stators3
fix       spring_ML           motor_Left        spring/self 1000     xyz
```

```
dump      dump_minimize      all          xtc      200     dump_minimize.xtc
minimize 1.0e-12 1.0e-12 10000 100000
#minimize 1.0e-4 1.0e-6 10000 100000
#min_modify dmax 0.1
undump   dump_minimize
fix      spring_ML          motor_Left       spring/self 1000    xyz
fix      spring_R1L         rotor1_Left      spring/self 1000    xyz
#fix      spring_R1R         rotor1_Right     spring/self 1000    xyz
fix      spring_R2L         rotor2_Left      spring/self 1000    xyz
#fix      spring_R2R         rotor2_Right     spring/self 1000    xyz
fix      spring_R3L         rotor3_Left      spring/self 1000    xyz
#fix      spring_R3R         rotor3_Right     spring/self 1000    xyz
fix      spring_stator1     stator1          spring/self 1000    xyz
fix      spring_stator2     stator2          spring/self 1000    xyz
fix      spring_stator3     stator3          spring/self 1000    xyz
fix      spring_stator4     stator4          spring/self 1000    xyz
fix      spring_stator5     stator5          spring/self 1000    xyz
fix      spring_stator6     stator6          spring/self 1000    xyz
fix      NVE                all              nve
fix      NVE_TEMP           all              temp/rescale    200          300 300  1.0 1.0
#thermo_style custom step  temp    etotal
#thermo 200
dump      dump_NveTemp       all          xtc      200     dump_NveTemp.xtc
run      200000            # 02million
#run      100000            # 01million
#run      10000             # 10thousand
#run      1000              #1hundred
unfix    NVE
unfix    NVE_TEMP
```

```
undump   dump_NveTemp

unfix spring_ML

unfix spring_R1L

#unfix spring_R1R

unfix spring_R2L

#unfix spring_R2R

unfix spring_R3L

#unfix spring_R3R

#lable_6

fix   spring_ML_z motor_Left       spring/self     1000            z

#fix   M_H_temp    M_H              temp/rescale   200            300 300  1.0 1.0

#fix   NVT        all_subtract_M_H   nvt           temp           300. 300. 0.1

fix   NVT        all              nvt           temp           300. 300. 0.1  #tchain 1 #drag 0.5

fix   rotate     M_H              move rotate   0.0 0.0 0.0     0.0 0.0 1.0     5

#compute     cc1         all     chunk/atom      type

#compute     torque      all     torque/chunk    cc1

#fix         torque_1    all     ave/time        1 200 200     c_torque[*]     file  M1111S1919-1111-1111-1111-1111_torque.vector    mode vector

compute     cc2         all     chunk/atom      type

compute     mass_center  all     com/chunk       cc2

fix         center_2    all     ave/time        1 200 200     c_mass_center[*]  file  M1111S1919-1111-1111-1111-1111_mcenter.vector   mode vector

compute     cc3         all     chunk/atom      type

compute     omiga       all     omega/chunk     cc3

fix         omiga_3     all     ave/time        1 200 200     c_omiga[*]      file  M1111S1919-1111-1111-1111-1111_omiga.vector    mode vector

#compute     crs1  rotor1   group/group stators1

#compute     crs2  rotor2   group/group stators2

#compute     crs3  rotor3   group/group stators3

#fix  crs1_scalar  stators1  ave/time  1 200 200 c_crs1 file crs1.scalar
```

#fix crs2_scalar stators2 ave/time 1 200 200 c_crs2 file crs2.scalar

#fix crs3_scalar stators3 ave/time 1 200 200 c_crs3 file crs3.scalar

#compute cmr1 rotor1 group/group motor

#compute cr1r2 rotor2 group/group rotor1

#compute cr2r3 rotor3 group/group rotor2

#fix cmr1_scalar rotor1 ave/time 1 200 200 c_cmr1 file cmr1.scalar

#fix cr1r2_scalar rotor2 ave/time 1 200 200 c_cr1r2 file cr1r2.scalar

#fix cr2r3_scalar rotor3 ave/time 1 200 200 c_cr2r3 file cr2r3.scalar

#compute cer1 rotor1 group/group except_rotor1

#compute cer2 rotor2 group/group except_rotor2

#compute cer3 rotor3 group/group except_rotor3

#fix cer1_scalar except_rotor1 ave/time 1 200 200 c_cer1 file cer1.scalar

#fix cer2_scalar except_rotor2 ave/time 1 200 200 c_cer2 file cer2.scalar

#fix cer3_scalar except_rotor3 ave/time 1 200 200 c_cer3 file cer3.scalar

#thermo_style custom step temp etotal

#thermo 200

#dump 1 all custom 200 M1111S1919-1111-1111-1111-1111.lammpstrj type x y z fx fy fz

#dump 2 all xtc 4000 dump_per4000_2million.xtc

#dump 3 all xtc 1000 dump_per1000_2million.xtc

#dump 4 all xtc 500 dump_per500_2million.xtc

dump 5 all xtc 200 dump_per200_2million.xtc

#dump 6 all xyz 200 dump_M1111S1919-1111-1111-1111-1111.xyz

#dump_modify 1 element C C C C C C C C C C H H H H H H H H H H sort id

#restart 50000M1111S1919-1111-1111-1111-1111.restart

#run 100000

```
#restart     100000M1111S1919-1111-1111-1111-1111.restart
#run         200000


run         20000200   #20million
#run         100000     #01million
#run         10000      #10thousand
#run          1000
uncompute    cc2
uncompute    mass_center
uncompute    cc3
uncompute    omiga
undump       5
```