In [58]:
```
import math
import random
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
```

In [59]:
```
def periodic_cond(pos,dim,N,bound):

    for x in range(N):
        for y in range(3):
            if bound[y] == 1:
                if pos.iloc[x,y] > dim[y]:
                    pos.iloc[x,y] = -(box[y]) + pos.iloc[x,y]
                elif pos.iloc[x,y] < 0:
                    pos.iloc[x,y] = (box[y]) + pos.iloc[x,y]
                else:
                    pos.iloc[x,y] = pos.iloc[x,y]
            else:
                pos.iloc[x,y] = pos.iloc[x,y]
    return pos
```

In [60]:
```
def cutoff():
    U    = []
    X_np = np.arange(0.001, 10, 0.001)
    X    = list(X_np)
    F    = []
    for x in X:
        dist2   = x*x
        dist6   = dist2**3
        dist12  = dist6**2
        dist13  = dist12*x
        dist7   = dist6*x

        u  = 4*lj_e*(lj_s12/dist12 - lj_s6/dist6)                          # Potential energy calculation
        f  = 4*lj_e*(((12 * lj_s12) / dist13) - ((6 * lj_s6) / dist7))     # Force calculation

        U.append(u)
        F.append(f)

    min_index = U.index(min(U))
    print("Minima of interatomic potential with He-He:", U[min_index])
```

```
    print("Equilibrium interatomic distance of He-He:", X[min_index])

    PC = pd.DataFrame(list(zip(X,U,F)),
                      columns =['Int_dist','E_Pot','Force'])
    coords = PC.to_numpy()
    np.savetxt('LJ_Curve.out', coords)

    fig, ax = plt.subplots()
    ax.plot(X[min_index - 800 : min_index + 500] , U[min_index - 800 : min_index + 500],label = "E_pot")
    ax.plot(X[min_index - 800 : min_index + 500] , F[min_index - 800 : min_index + 500],label = "Force")


    ax.set(xlabel='Interatomic_Distance(r)', ylabel='Force(F) & E_pot(U)',
           title='Lennard-jones potential curve')
    ax.legend()

    fig.savefig("test.png")
    plt.show()

    return X[min_index]
```

In [61]:
```
def Skin(pos,N,cutoff):
    r = cutoff + 4.0
    neigh = []
    for x in range(N):
        nh = []
        for y in range(x+1,N):
            if pos.iloc[x,0]-pos.iloc[y,0]<=r and pos.iloc[x,1]-pos.iloc[y,1]<=r and pos.iloc[x,2]-pos.iloc[y,2]<=r:
                nh.append(y)
        for y in range(x-1,0,-1):
            if pos.iloc[x,0]-pos.iloc[y,0]<=r and pos.iloc[x,1]-pos.iloc[y,1]<=r and pos.iloc[x,2]-pos.iloc[y,2]<=r:
                nh.append(y)
        neigh.append(nh)
    return neigh
```

In [62]:
```
def Neighbours(pos,skin,N,cutoff):
    r = cutoff + 2.0
    neighh = []
    for x in range(N):
        nhh = []
        for y in range(len(skin[x])):
            if pos.iloc[x,0]-pos.iloc[skin[x][y],0]<=r and pos.iloc[x,1]-pos.iloc[skin[x][y],1]<=r and pos.iloc[x,2]-
                nhh.append(skin[x][y])
```

```
        neighh.append(nhh)
    return neighh
```

In [63]:
```
def lennard_jones(pos,neigh,N):
    distt2 = []
    for x in range(N):
        dist = []
        for y in range(len(neigh[x])):
            distt = pos.iloc[x,0]*pos.iloc[neigh[x][y],0] + pos.iloc[x,1]*pos.iloc[neigh[x][y],1]+pos.iloc[x,2]*pos.i
            #distt = distt**2
            #distt = math.sqrt(distt)
            dist.append(distt)
        distt2.append(dist)
#    print(distt2)
    U = []
    F = []
    for i in range(N):
        UU = []
        FF = []
        for j in range(len(distt2[i])):
            dist6   = distt2[i][j]**3
            dist12  = dist6**2
            dist13  = dist12*math.sqrt(distt2[i][j])
            dist7   = dist6*math.sqrt(distt2[i][j])

            u  = 4*lj_e*(lj_s12/dist12 - lj_s6/dist6)                          # Potential energy calculation
            f  = 4*lj_e*(((12 * lj_s12) / dist13) - ((6 * lj_s6) / dist7))     # Force calculation

            UU.append(u)
            FF.append(f)
        if len(UU) > 0:
            U_avg = sum(UU)/len(UU)
            #F_avg = sum(FF)/len(FF)
            UU    = []
            #FF    = []
            UU.append(U_avg)
            #FF.append(F_avg)
        U.append(UU)
        F.append(FF)

    return (U, F)
```

In [64]:
```
#Velocity verlet algorithm
```

```
def new_pos(X_old,V_old,F_old,m,t):                                    #Algorithm For new position
    X_new = X_old + (t)*V_old + ((t**2)*F_old)/(2*m)
    return(X_new)

def new_vel(F_old,F_new,V_old,t,m):                                    #Algorithm for new velocity
    V_new = (F_old + F_new)
    V_new = (V_new * t)/(2*m)
    V_new = V_old + V_new
    return(V_new)
```

In [65]:
```
def write_out(dataframe,name):
    xx = dataframe.to_numpy()
    np.savetxt(name, x)
```

In [66]:
```
#Parameters are provided for Helium(He) atom.

box         = (50.0,50.0,50.0)   # Dimensions            [In Angstrom]
bound       = (1,1,1)
N_atom      = 50                  # No of atoms
N_step      = 500                 # No of Steps
N_write     = 100                 # Steps at which co-ordinate to be saved
Delta       = 10.0               # Time steps            [In ferrosecond]

temp        = 200.0;              # Temperature           [In Kelvin]

lj_s        = 2.5238;            # Lennard_jones_sigma   [In Angstrom]
lj_e        = 0.01962;           # Lennard_jones_epsilon [In Kcal/mol]
mass        = 4.002602;          # Mass of atom          [In amu]
bltz_const  = 0.001987191;       # Boltzmann constant    [In Kcal/mol/K]

tf          = 1**(-15)           # Time factor           [Convert second to ferrosecond]
```

In [67]:
```
#Pre-defined factors

dt          = Delta/tf
dt2         = dt * dt

v0          = math.sqrt(bltz_const * temp/mass)

lj_s6       = lj_s**6
lj_s12      = lj_s**12
```

In [68]:
```
x_coords = []
y_coords = []
z_coords = []

for c in range(N_atom):
    x = random.random()
    y = random.random()
    z = random.random()
    pos = [x,y,z]

    for i in range(3):
        if pos[i] > (box[i]/100):
            pos[i] -= (box[i]/100)

        else:
            pos[i] = pos[i]
        pos[i] = round(pos[i] * (10**5)) / 1000

    x_coords.append(pos[0])
    y_coords.append(pos[1])
    z_coords.append(pos[2])

df = pd.DataFrame(list(zip(x_coords,y_coords,z_coords)),
                  columns =['x_coords','y_coords','z_coords'])
coords = df.to_numpy()
np.savetxt('Initial_conf.out', coords)
#dff = df.copy()
```

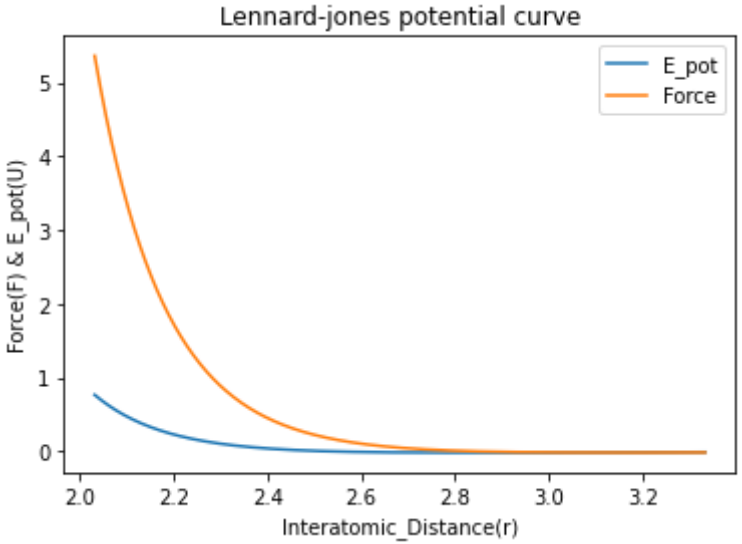
In [69]:
```
#Initial velocity and momentum
vel0 = []
momentum = [0.0,0.0,0.0]
for k in range(N_atom):
    vel0.append([random.gauss(0,v0), random.gauss(0,v0), random.gauss(0,v0)])
    for kk in range(3):
        momentum[kk] += mass*vel0[k][kk]

#Removal of residual momentum
residual_mom = []
for c in range(3):
    residual_mom.append(momentum[c]/N_atom)
for i in range(N_atom):
    for c in range(3):
        vel0[i][c] -= residual_mom[c]/mass
```

```
force = []
for i in range(N_atom):
    force.append([0.0, 0.0, 0.0])
```

In [70]:
```
co = cutoff()
```

```
Minima of interatomic potential with He-He: -0.019619998506585003
Equilibrium interatomic distance of He-He: 2.8329999999999997
```



In [71]:
```
# MAIN SIMULATION LOOP
for step in range(N_step + 1):

    xx_coords = []
    yy_coords = []
    zz_coords = []

    # Zero the forces
    for i in range(N_atom):
        for c in range(3):
            force[i][c] = 0.0

    # Calculate interaction forces
    if step%10 == 0:
        sk = Skin(df,N_atom,co)
```

```
    neig     = Neighbours(df,sk,N_atom,co)

    U_E, I_F =lennard_jones(df,neig,N_atom)

    ener_pot = 0.0
    for kk in range(N_atom):
        if len(U_E[kk]) > 0:
            ener_pot += U_E[kk][0]

    force_new = force
    for i in range(N_atom):
        if len(I_F[i]) > 0:
            for j in range(len(I_F[i])):
                for k in range(3):
                    force_new[i][k]          += I_F[i][j]
                    force_new[neig[i][j]][k] -= I_F[i][j]
    force = force_new

    pos_new = []
    vel_new = []
    for i in range(N_atom):
        p = []
        v = []
        for j in range(3):
            ijk = new_pos(df.iloc[i,j],vel0[i][j],force_new[i][j],mass,dt)
            vvv = new_vel(force[i][j],force_new[i][j],vel0[i][j],dt,mass)
            p.append(ijk)
            v.append(vvv)
        vel_new.append(v)
        pos_new.append(p)

        xx_coords.append(p[0])
        yy_coords.append(p[1])
        zz_coords.append(p[2])

    # Calculate the kinetic energy
    ener_kin = 0.0
    for i in range(N_atom):
        ener_kin += 0.5*mass*(vel_new[i][0]**2 + vel_new[i][1]**2 + vel_new[i][2]**2)
    ener_total = ener_pot + ener_kin
    mean_temp = 2.0*ener_kin/(3*bltz_const*(N_atom-1))
    print("step %9d  ener_total %9.4f  ener_pot %9.4f  ener_kin %9.4f mean_temp %8.3f" % (step,ener_total,ener_pot,en

    n_df = pd.DataFrame(list(zip(xx_coords,yy_coords,zz_coords)),
```

```
                    columns =['xx_coords','yy_coords','zz_coords'])
    periodic_cond(n_df,box,N_atom,bound)
    df = n_df
    vel0 = vel_new
    if step%N_write == 0:
        crds  = df.to_numpy()
        name  = str(step) + '.out'
        np.savetxt(name, crds)
```

step	0	ener_total	35.7296	ener_pot	-0.0000	ener_kin	35.7296	mean_temp	244.625
step	1	ener_total	35.7296	ener_pot	-0.0000	ener_kin	35.7296	mean_temp	244.625
step	2	ener_total	35.7296	ener_pot	-0.0000	ener_kin	35.7296	mean_temp	244.625
step	3	ener_total	35.7296	ener_pot	-0.0000	ener_kin	35.7296	mean_temp	244.625
step	4	ener_total	35.7296	ener_pot	-0.0000	ener_kin	35.7296	mean_temp	244.625
step	5	ener_total	35.7296	ener_pot	-0.0000	ener_kin	35.7296	mean_temp	244.625
step	6	ener_total	35.7299	ener_pot	-0.0000	ener_kin	35.7299	mean_temp	244.627
step	7	ener_total	35.7299	ener_pot	-0.0000	ener_kin	35.7299	mean_temp	244.627
step	8	ener_total	35.7299	ener_pot	-0.0000	ener_kin	35.7299	mean_temp	244.627
step	9	ener_total	35.7299	ener_pot	-0.0000	ener_kin	35.7299	mean_temp	244.627
step	10	ener_total	35.7299	ener_pot	-0.0000	ener_kin	35.7299	mean_temp	244.627
step	11	ener_total	35.7301	ener_pot	-0.0000	ener_kin	35.7301	mean_temp	244.629
step	12	ener_total	35.7573	ener_pot	-0.0001	ener_kin	35.7573	mean_temp	244.815
step	13	ener_total	35.7573	ener_pot	-0.0000	ener_kin	35.7573	mean_temp	244.815
step	14	ener_total	35.7573	ener_pot	-0.0000	ener_kin	35.7573	mean_temp	244.815
step	15	ener_total	35.7573	ener_pot	-0.0000	ener_kin	35.7573	mean_temp	244.815
step	16	ener_total	35.7575	ener_pot	-0.0000	ener_kin	35.7575	mean_temp	244.816
step	17	ener_total	35.7575	ener_pot	-0.0000	ener_kin	35.7575	mean_temp	244.816
step	18	ener_total	35.7575	ener_pot	-0.0000	ener_kin	35.7575	mean_temp	244.816
step	19	ener_total	35.7575	ener_pot	-0.0000	ener_kin	35.7575	mean_temp	244.816
step	20	ener_total	35.7574	ener_pot	-0.0000	ener_kin	35.7574	mean_temp	244.815
step	21	ener_total	35.7574	ener_pot	-0.0000	ener_kin	35.7574	mean_temp	244.815
step	22	ener_total	35.7574	ener_pot	-0.0000	ener_kin	35.7574	mean_temp	244.815
step	23	ener_total	35.7574	ener_pot	-0.0000	ener_kin	35.7574	mean_temp	244.815
step	24	ener_total	35.7574	ener_pot	-0.0000	ener_kin	35.7574	mean_temp	244.815
step	25	ener_total	35.7574	ener_pot	-0.0000	ener_kin	35.7574	mean_temp	244.815
step	26	ener_total	35.7574	ener_pot	-0.0000	ener_kin	35.7574	mean_temp	244.815
step	27	ener_total	35.7574	ener_pot	-0.0000	ener_kin	35.7574	mean_temp	244.815
step	28	ener_total	35.7574	ener_pot	-0.0000	ener_kin	35.7574	mean_temp	244.815
step	29	ener_total	35.7574	ener_pot	-0.0000	ener_kin	35.7574	mean_temp	244.815
step	30	ener_total	35.7576	ener_pot	-0.0000	ener_kin	35.7576	mean_temp	244.817
step	31	ener_total	35.7576	ener_pot	-0.0000	ener_kin	35.7576	mean_temp	244.817
step	32	ener_total	35.7576	ener_pot	-0.0000	ener_kin	35.7576	mean_temp	244.817
step	33	ener_total	35.7589	ener_pot	-0.0000	ener_kin	35.7589	mean_temp	244.826
step	34	ener_total	35.7593	ener_pot	-0.0000	ener_kin	35.7594	mean_temp	244.829
step	35	ener_total	35.7595	ener_pot	-0.0000	ener_kin	35.7595	mean_temp	244.830
step	36	ener_total	35.7595	ener_pot	-0.0000	ener_kin	35.7595	mean_temp	244.830
step	37	ener_total	35.7595	ener_pot	-0.0000	ener_kin	35.7595	mean_temp	244.830
step	38	ener_total	35.7595	ener_pot	-0.0000	ener_kin	35.7595	mean_temp	244.830
step	39	ener_total	35.7595	ener_pot	-0.0000	ener_kin	35.7595	mean_temp	244.830
step	40	ener_total	35.7597	ener_pot	-0.0000	ener_kin	35.7597	mean_temp	244.831
step	41	ener_total	35.7597	ener_pot	-0.0000	ener_kin	35.7597	mean_temp	244.831
step	42	ener_total	35.7597	ener_pot	-0.0000	ener_kin	35.7597	mean_temp	244.831
step	43	ener_total	35.7627	ener_pot	-0.0000	ener_kin	35.7627	mean_temp	244.852

```
step        44  ener_total   35.7627  ener_pot   -0.0000  ener_kin   35.7627 mean_temp  244.852
step        45  ener_total   35.7627  ener_pot   -0.0000  ener_kin   35.7627 mean_temp  244.852
step        46  ener_total   35.7627  ener_pot   -0.0000  ener_kin   35.7627 mean_temp  244.852
step        47  ener_total   35.7627  ener_pot   -0.0000  ener_kin   35.7627 mean_temp  244.852
step        48  ener_total   35.7627  ener_pot   -0.0000  ener_kin   35.7627 mean_temp  244.852
step        49  ener_total   35.7628  ener_pot   -0.0000  ener_kin   35.7628 mean_temp  244.852
step        50  ener_total   35.7628  ener_pot   -0.0000  ener_kin   35.7628 mean_temp  244.852
step        51  ener_total   35.7628  ener_pot   -0.0000  ener_kin   35.7628 mean_temp  244.852
step        52  ener_total   35.7628  ener_pot   -0.0000  ener_kin   35.7628 mean_temp  244.852
step        53  ener_total   35.7628  ener_pot   -0.0000  ener_kin   35.7628 mean_temp  244.852
step        54  ener_total   35.7628  ener_pot   -0.0000  ener_kin   35.7628 mean_temp  244.852
step        55  ener_total   35.7627  ener_pot   -0.0000  ener_kin   35.7627 mean_temp  244.852
step        56  ener_total   35.7627  ener_pot   -0.0000  ener_kin   35.7627 mean_temp  244.852
step        57  ener_total   35.7622  ener_pot   -0.0000  ener_kin   35.7623 mean_temp  244.849
step        58  ener_total   35.7623  ener_pot   -0.0000  ener_kin   35.7623 mean_temp  244.849
step        59  ener_total   35.7623  ener_pot   -0.0000  ener_kin   35.7623 mean_temp  244.849
step        60  ener_total   35.7623  ener_pot   -0.0000  ener_kin   35.7623 mean_temp  244.849
step        61  ener_total   35.7623  ener_pot   -0.0000  ener_kin   35.7623 mean_temp  244.849
step        62  ener_total   35.7623  ener_pot   -0.0000  ener_kin   35.7623 mean_temp  244.849
step        63  ener_total   35.7623  ener_pot   -0.0000  ener_kin   35.7623 mean_temp  244.849
step        64  ener_total   35.7621  ener_pot   -0.0000  ener_kin   35.7621 mean_temp  244.847
step        65  ener_total   35.7621  ener_pot   -0.0000  ener_kin   35.7621 mean_temp  244.847
step        66  ener_total   35.7621  ener_pot   -0.0000  ener_kin   35.7621 mean_temp  244.847
step        67  ener_total   35.7621  ener_pot   -0.0000  ener_kin   35.7621 mean_temp  244.847
step        68  ener_total   35.7620  ener_pot   -0.0000  ener_kin   35.7620 mean_temp  244.847
step        69  ener_total   35.7621  ener_pot   -0.0000  ener_kin   35.7621 mean_temp  244.848
step        70  ener_total   35.7610  ener_pot   -0.0000  ener_kin   35.7610 mean_temp  244.840
step        71  ener_total   35.7609  ener_pot   -0.0000  ener_kin   35.7609 mean_temp  244.840
step        72  ener_total   35.7608  ener_pot   -0.0000  ener_kin   35.7608 mean_temp  244.839
step        73  ener_total   35.7608  ener_pot   -0.0000  ener_kin   35.7608 mean_temp  244.839
step        74  ener_total   35.7608  ener_pot   -0.0000  ener_kin   35.7608 mean_temp  244.839
step        75  ener_total   35.7608  ener_pot   -0.0000  ener_kin   35.7608 mean_temp  244.839
step        76  ener_total   35.7608  ener_pot   -0.0000  ener_kin   35.7608 mean_temp  244.839
step        77  ener_total   35.7608  ener_pot   -0.0000  ener_kin   35.7608 mean_temp  244.839
step        78  ener_total   35.7607  ener_pot   -0.0000  ener_kin   35.7608 mean_temp  244.839
step        79  ener_total   35.7607  ener_pot   -0.0000  ener_kin   35.7607 mean_temp  244.838
step        80  ener_total   35.7607  ener_pot   -0.0000  ener_kin   35.7607 mean_temp  244.838
step        81  ener_total   35.7607  ener_pot   -0.0000  ener_kin   35.7607 mean_temp  244.838
step        82  ener_total   35.7607  ener_pot   -0.0000  ener_kin   35.7607 mean_temp  244.838
step        83  ener_total   35.7607  ener_pot   -0.0000  ener_kin   35.7607 mean_temp  244.838
step        84  ener_total   35.7607  ener_pot   -0.0000  ener_kin   35.7607 mean_temp  244.838
step        85  ener_total   35.7607  ener_pot   -0.0000  ener_kin   35.7607 mean_temp  244.838
step        86  ener_total   35.7607  ener_pot   -0.0000  ener_kin   35.7607 mean_temp  244.838
step        87  ener_total   35.7607  ener_pot   -0.0000  ener_kin   35.7607 mean_temp  244.838
```

step	88	ener_total	35.7616	ener_pot	-0.0001	ener_kin	35.7617	mean_temp	244.845
step	89	ener_total	35.7618	ener_pot	-0.0000	ener_kin	35.7618	mean_temp	244.846
step	90	ener_total	35.7618	ener_pot	-0.0000	ener_kin	35.7618	mean_temp	244.846
step	91	ener_total	35.7618	ener_pot	-0.0000	ener_kin	35.7618	mean_temp	244.846
step	92	ener_total	35.7617	ener_pot	-0.0000	ener_kin	35.7617	mean_temp	244.845
step	93	ener_total	35.7616	ener_pot	-0.0000	ener_kin	35.7616	mean_temp	244.845
step	94	ener_total	35.7617	ener_pot	-0.0000	ener_kin	35.7617	mean_temp	244.845
step	95	ener_total	35.7617	ener_pot	-0.0000	ener_kin	35.7617	mean_temp	244.845
step	96	ener_total	35.7617	ener_pot	-0.0000	ener_kin	35.7617	mean_temp	244.845
step	97	ener_total	35.7617	ener_pot	-0.0000	ener_kin	35.7617	mean_temp	244.845
step	98	ener_total	35.7617	ener_pot	-0.0000	ener_kin	35.7617	mean_temp	244.845
step	99	ener_total	35.7616	ener_pot	-0.0000	ener_kin	35.7616	mean_temp	244.845
step	100	ener_total	35.7616	ener_pot	-0.0000	ener_kin	35.7616	mean_temp	244.845
step	101	ener_total	35.7616	ener_pot	-0.0000	ener_kin	35.7616	mean_temp	244.844
step	102	ener_total	35.7616	ener_pot	-0.0000	ener_kin	35.7616	mean_temp	244.844
step	103	ener_total	35.7616	ener_pot	-0.0000	ener_kin	35.7616	mean_temp	244.844
step	104	ener_total	35.7616	ener_pot	-0.0000	ener_kin	35.7616	mean_temp	244.844
step	105	ener_total	35.7616	ener_pot	-0.0000	ener_kin	35.7616	mean_temp	244.844
step	106	ener_total	35.7616	ener_pot	-0.0000	ener_kin	35.7616	mean_temp	244.844
step	107	ener_total	35.7616	ener_pot	-0.0000	ener_kin	35.7616	mean_temp	244.844
step	108	ener_total	35.7616	ener_pot	-0.0000	ener_kin	35.7616	mean_temp	244.844
step	109	ener_total	35.7617	ener_pot	-0.0000	ener_kin	35.7617	mean_temp	244.845
step	110	ener_total	35.7524	ener_pot	-0.0000	ener_kin	35.7525	mean_temp	244.782
step	111	ener_total	35.7524	ener_pot	-0.0000	ener_kin	35.7524	mean_temp	244.782
step	112	ener_total	35.7528	ener_pot	-0.0000	ener_kin	35.7528	mean_temp	244.784
step	113	ener_total	35.7527	ener_pot	-0.0000	ener_kin	35.7527	mean_temp	244.784
step	114	ener_total	35.7527	ener_pot	-0.0000	ener_kin	35.7527	mean_temp	244.784
step	115	ener_total	35.7527	ener_pot	-0.0000	ener_kin	35.7527	mean_temp	244.784
step	116	ener_total	35.7528	ener_pot	-0.0000	ener_kin	35.7528	mean_temp	244.784
step	117	ener_total	35.7528	ener_pot	-0.0000	ener_kin	35.7528	mean_temp	244.784
step	118	ener_total	35.7528	ener_pot	-0.0000	ener_kin	35.7528	mean_temp	244.784
step	119	ener_total	35.7528	ener_pot	-0.0000	ener_kin	35.7528	mean_temp	244.784
step	120	ener_total	35.7528	ener_pot	-0.0000	ener_kin	35.7528	mean_temp	244.784
step	121	ener_total	35.7528	ener_pot	-0.0000	ener_kin	35.7528	mean_temp	244.784
step	122	ener_total	35.7528	ener_pot	-0.0000	ener_kin	35.7528	mean_temp	244.784
step	123	ener_total	35.7528	ener_pot	-0.0000	ener_kin	35.7528	mean_temp	244.784
step	124	ener_total	35.7528	ener_pot	-0.0000	ener_kin	35.7528	mean_temp	244.784
step	125	ener_total	35.7528	ener_pot	-0.0000	ener_kin	35.7528	mean_temp	244.784
step	126	ener_total	35.7527	ener_pot	-0.0000	ener_kin	35.7527	mean_temp	244.783
step	127	ener_total	35.7527	ener_pot	-0.0000	ener_kin	35.7527	mean_temp	244.783
step	128	ener_total	35.7527	ener_pot	-0.0000	ener_kin	35.7527	mean_temp	244.783
step	129	ener_total	35.7527	ener_pot	-0.0000	ener_kin	35.7527	mean_temp	244.783
step	130	ener_total	35.7527	ener_pot	-0.0000	ener_kin	35.7527	mean_temp	244.783
step	131	ener_total	35.7527	ener_pot	-0.0000	ener_kin	35.7527	mean_temp	244.783

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step       132  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       133  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       134  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       135  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       136  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       137  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       138  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       139  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       140  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       141  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       142  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       143  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.783
step       144  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.784
step       145  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.784
step       146  ener_total   35.7528  ener_pot   -0.0000  ener_kin   35.7528 mean_temp  244.784
step       147  ener_total   35.7528  ener_pot   -0.0000  ener_kin   35.7528 mean_temp  244.784
step       148  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.784
step       149  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.784
step       150  ener_total   35.7527  ener_pot   -0.0000  ener_kin   35.7527 mean_temp  244.784
step       151  ener_total   35.7528  ener_pot   -0.0000  ener_kin   35.7528 mean_temp  244.784
step       152  ener_total   35.7528  ener_pot   -0.0000  ener_kin   35.7528 mean_temp  244.784
step       153  ener_total   35.7528  ener_pot   -0.0000  ener_kin   35.7528 mean_temp  244.784
step       154  ener_total   35.7528  ener_pot   -0.0000  ener_kin   35.7528 mean_temp  244.784
step       155  ener_total   35.7528  ener_pot   -0.0000  ener_kin   35.7528 mean_temp  244.784
step       156  ener_total   35.7529  ener_pot   -0.0000  ener_kin   35.7529 mean_temp  244.785
step       157  ener_total   35.7528  ener_pot   -0.0000  ener_kin   35.7528 mean_temp  244.784
step       158  ener_total   35.7528  ener_pot   -0.0000  ener_kin   35.7528 mean_temp  244.784
step       159  ener_total   35.7529  ener_pot   -0.0000  ener_kin   35.7529 mean_temp  244.784
step       160  ener_total   35.7529  ener_pot   -0.0000  ener_kin   35.7529 mean_temp  244.784
step       161  ener_total   35.7530  ener_pot   -0.0000  ener_kin   35.7530 mean_temp  244.785
step       162  ener_total   35.7530  ener_pot   -0.0000  ener_kin   35.7530 mean_temp  244.785
step       163  ener_total   35.7530  ener_pot   -0.0000  ener_kin   35.7530 mean_temp  244.785
step       164  ener_total   35.7530  ener_pot   -0.0000  ener_kin   35.7530 mean_temp  244.785
step       165  ener_total   35.7530  ener_pot   -0.0000  ener_kin   35.7530 mean_temp  244.785
step       166  ener_total   35.7530  ener_pot   -0.0000  ener_kin   35.7530 mean_temp  244.786
step       167  ener_total   35.7530  ener_pot   -0.0000  ener_kin   35.7530 mean_temp  244.786
step       168  ener_total   35.7530  ener_pot   -0.0000  ener_kin   35.7530 mean_temp  244.786
step       169  ener_total   35.7530  ener_pot   -0.0000  ener_kin   35.7530 mean_temp  244.785
step       170  ener_total   35.7530  ener_pot   -0.0000  ener_kin   35.7530 mean_temp  244.785
step       171  ener_total   35.7530  ener_pot   -0.0000  ener_kin   35.7530 mean_temp  244.785
step       172  ener_total   35.7531  ener_pot   -0.0000  ener_kin   35.7532 mean_temp  244.786
step       173  ener_total   35.7533  ener_pot   -0.0000  ener_kin   35.7533 mean_temp  244.788
step       174  ener_total   35.7535  ener_pot   -0.0000  ener_kin   35.7535 mean_temp  244.789
step       175  ener_total   35.7535  ener_pot   -0.0000  ener_kin   35.7536 mean_temp  244.789
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step       176  ener_total   35.7536  ener_pot   -0.0000  ener_kin   35.7536 mean_temp  244.789
step       177  ener_total   35.7536  ener_pot   -0.0000  ener_kin   35.7536 mean_temp  244.789
step       178  ener_total   35.7536  ener_pot   -0.0000  ener_kin   35.7536 mean_temp  244.789
step       179  ener_total   35.7536  ener_pot   -0.0000  ener_kin   35.7536 mean_temp  244.789
step       180  ener_total   35.7521  ener_pot   -0.0000  ener_kin   35.7521 mean_temp  244.779
step       181  ener_total   35.7517  ener_pot   -0.0000  ener_kin   35.7517 mean_temp  244.776
step       182  ener_total   35.7519  ener_pot   -0.0000  ener_kin   35.7519 mean_temp  244.778
step       183  ener_total   35.7519  ener_pot   -0.0000  ener_kin   35.7519 mean_temp  244.778
step       184  ener_total   35.7519  ener_pot   -0.0000  ener_kin   35.7519 mean_temp  244.778
step       185  ener_total   35.7519  ener_pot   -0.0000  ener_kin   35.7519 mean_temp  244.778
step       186  ener_total   35.7519  ener_pot   -0.0000  ener_kin   35.7519 mean_temp  244.778
step       187  ener_total   35.7520  ener_pot   -0.0000  ener_kin   35.7520 mean_temp  244.779
step       188  ener_total   35.7520  ener_pot   -0.0000  ener_kin   35.7520 mean_temp  244.779
step       189  ener_total   35.7520  ener_pot   -0.0000  ener_kin   35.7520 mean_temp  244.779
step       190  ener_total   35.7521  ener_pot   -0.0000  ener_kin   35.7521 mean_temp  244.779
step       191  ener_total   35.7521  ener_pot   -0.0000  ener_kin   35.7521 mean_temp  244.779
step       192  ener_total   35.7521  ener_pot   -0.0000  ener_kin   35.7521 mean_temp  244.779
step       193  ener_total   35.7520  ener_pot   -0.0000  ener_kin   35.7520 mean_temp  244.778
step       194  ener_total   35.7519  ener_pot   -0.0000  ener_kin   35.7519 mean_temp  244.778
step       195  ener_total   35.7519  ener_pot   -0.0000  ener_kin   35.7519 mean_temp  244.778
step       196  ener_total   35.7519  ener_pot   -0.0000  ener_kin   35.7519 mean_temp  244.778
step       197  ener_total   35.7519  ener_pot   -0.0000  ener_kin   35.7519 mean_temp  244.778
step       198  ener_total   35.7519  ener_pot   -0.0000  ener_kin   35.7519 mean_temp  244.778
step       199  ener_total   35.7519  ener_pot   -0.0000  ener_kin   35.7519 mean_temp  244.778
step       200  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       201  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       202  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       203  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       204  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       205  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       206  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       207  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       208  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       209  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       210  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       211  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       212  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       213  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       214  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       215  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       216  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       217  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       218  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       219  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
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step       220  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       221  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       222  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       223  ener_total   35.7411  ener_pot   -0.0000  ener_kin   35.7411 mean_temp  244.704
step       224  ener_total   35.7432  ener_pot   -0.0001  ener_kin   35.7433 mean_temp  244.719
step       225  ener_total   35.7433  ener_pot   -0.0000  ener_kin   35.7433 mean_temp  244.719
step       226  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.721
step       227  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.721
step       228  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.720
step       229  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.720
step       230  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.720
step       231  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.720
step       232  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.720
step       233  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.720
step       234  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.720
step       235  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.720
step       236  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.720
step       237  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.720
step       238  ener_total   35.7433  ener_pot   -0.0000  ener_kin   35.7433 mean_temp  244.719
step       239  ener_total   35.7433  ener_pot   -0.0000  ener_kin   35.7433 mean_temp  244.719
step       240  ener_total   35.7433  ener_pot   -0.0000  ener_kin   35.7433 mean_temp  244.719
step       241  ener_total   35.7433  ener_pot   -0.0000  ener_kin   35.7433 mean_temp  244.719
step       242  ener_total   35.7433  ener_pot   -0.0000  ener_kin   35.7433 mean_temp  244.719
step       243  ener_total   35.7433  ener_pot   -0.0000  ener_kin   35.7433 mean_temp  244.719
step       244  ener_total   35.7433  ener_pot   -0.0000  ener_kin   35.7433 mean_temp  244.719
step       245  ener_total   35.7433  ener_pot   -0.0000  ener_kin   35.7433 mean_temp  244.719
step       246  ener_total   35.7433  ener_pot   -0.0000  ener_kin   35.7433 mean_temp  244.719
step       247  ener_total   35.7436  ener_pot   -0.0000  ener_kin   35.7436 mean_temp  244.721
step       248  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.721
step       249  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.721
step       250  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.721
step       251  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.721
step       252  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.721
step       253  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.721
step       254  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.720
step       255  ener_total   35.7435  ener_pot   -0.0000  ener_kin   35.7435 mean_temp  244.721
step       256  ener_total   35.7436  ener_pot   -0.0000  ener_kin   35.7436 mean_temp  244.721
step       257  ener_total   35.7437  ener_pot   -0.0000  ener_kin   35.7437 mean_temp  244.721
step       258  ener_total   35.7437  ener_pot   -0.0000  ener_kin   35.7437 mean_temp  244.721
step       259  ener_total   35.7432  ener_pot   -0.0000  ener_kin   35.7432 mean_temp  244.718
step       260  ener_total   35.7432  ener_pot   -0.0000  ener_kin   35.7432 mean_temp  244.718
step       261  ener_total   35.7432  ener_pot   -0.0000  ener_kin   35.7432 mean_temp  244.718
step       262  ener_total   35.7432  ener_pot   -0.0000  ener_kin   35.7432 mean_temp  244.718
step       263  ener_total   35.7432  ener_pot   -0.0000  ener_kin   35.7432 mean_temp  244.718
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step       264  ener_total   35.7432  ener_pot   -0.0000  ener_kin   35.7432 mean_temp  244.718
step       265  ener_total   35.7432  ener_pot   -0.0000  ener_kin   35.7432 mean_temp  244.719
step       266  ener_total   35.7432  ener_pot   -0.0000  ener_kin   35.7432 mean_temp  244.719
step       267  ener_total   35.7432  ener_pot   -0.0000  ener_kin   35.7432 mean_temp  244.718
step       268  ener_total   35.7432  ener_pot   -0.0000  ener_kin   35.7432 mean_temp  244.718
step       269  ener_total   35.7328  ener_pot   -0.0001  ener_kin   35.7328 mean_temp  244.647
step       270  ener_total   35.7327  ener_pot   -0.0000  ener_kin   35.7327 mean_temp  244.646
step       271  ener_total   35.7326  ener_pot   -0.0000  ener_kin   35.7326 mean_temp  244.646
step       272  ener_total   35.7326  ener_pot   -0.0000  ener_kin   35.7326 mean_temp  244.646
step       273  ener_total   35.7326  ener_pot   -0.0000  ener_kin   35.7326 mean_temp  244.646
step       274  ener_total   35.7326  ener_pot   -0.0000  ener_kin   35.7326 mean_temp  244.646
step       275  ener_total   35.7326  ener_pot   -0.0000  ener_kin   35.7326 mean_temp  244.646
step       276  ener_total   35.7326  ener_pot   -0.0000  ener_kin   35.7326 mean_temp  244.646
step       277  ener_total   35.7318  ener_pot   -0.0000  ener_kin   35.7318 mean_temp  244.640
step       278  ener_total   35.7317  ener_pot   -0.0000  ener_kin   35.7317 mean_temp  244.640
step       279  ener_total   35.7317  ener_pot   -0.0000  ener_kin   35.7317 mean_temp  244.639
step       280  ener_total   35.7317  ener_pot   -0.0000  ener_kin   35.7317 mean_temp  244.639
step       281  ener_total   35.7317  ener_pot   -0.0000  ener_kin   35.7317 mean_temp  244.639
step       282  ener_total   35.7317  ener_pot   -0.0000  ener_kin   35.7317 mean_temp  244.639
step       283  ener_total   35.7317  ener_pot   -0.0000  ener_kin   35.7317 mean_temp  244.639
step       284  ener_total   35.7317  ener_pot   -0.0000  ener_kin   35.7317 mean_temp  244.640
step       285  ener_total   35.7317  ener_pot   -0.0000  ener_kin   35.7317 mean_temp  244.640
step       286  ener_total   35.7317  ener_pot   -0.0000  ener_kin   35.7317 mean_temp  244.640
step       287  ener_total   35.7317  ener_pot   -0.0000  ener_kin   35.7317 mean_temp  244.640
step       288  ener_total   35.7315  ener_pot   -0.0000  ener_kin   35.7315 mean_temp  244.638
step       289  ener_total   35.7315  ener_pot   -0.0000  ener_kin   35.7315 mean_temp  244.638
step       290  ener_total   35.7315  ener_pot   -0.0000  ener_kin   35.7315 mean_temp  244.638
step       291  ener_total   35.7314  ener_pot   -0.0000  ener_kin   35.7314 mean_temp  244.638
step       292  ener_total   35.7314  ener_pot   -0.0000  ener_kin   35.7314 mean_temp  244.638
step       293  ener_total   35.7314  ener_pot   -0.0000  ener_kin   35.7314 mean_temp  244.638
step       294  ener_total   35.7314  ener_pot   -0.0000  ener_kin   35.7314 mean_temp  244.638
step       295  ener_total   35.7314  ener_pot   -0.0000  ener_kin   35.7314 mean_temp  244.638
step       296  ener_total   35.7314  ener_pot   -0.0000  ener_kin   35.7314 mean_temp  244.638
step       297  ener_total   35.7314  ener_pot   -0.0000  ener_kin   35.7314 mean_temp  244.638
step       298  ener_total   35.7314  ener_pot   -0.0000  ener_kin   35.7314 mean_temp  244.638
step       299  ener_total   35.6941  ener_pot   -0.0003  ener_kin   35.6944 mean_temp  244.384
step       300  ener_total   35.6942  ener_pot   -0.0000  ener_kin   35.6942 mean_temp  244.383
step       301  ener_total   35.6942  ener_pot   -0.0000  ener_kin   35.6942 mean_temp  244.383
step       302  ener_total   35.6942  ener_pot   -0.0000  ener_kin   35.6942 mean_temp  244.383
step       303  ener_total   35.6942  ener_pot   -0.0000  ener_kin   35.6942 mean_temp  244.383
step       304  ener_total   35.6941  ener_pot   -0.0000  ener_kin   35.6941 mean_temp  244.382
step       305  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       306  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       307  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
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step       308  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       309  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       310  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       311  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       312  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       313  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       314  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       315  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       316  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       317  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       318  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       319  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       320  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       321  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       322  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       323  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       324  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       325  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       326  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       327  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       328  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.384
step       329  ener_total   35.6943  ener_pot   -0.0000  ener_kin   35.6943 mean_temp  244.383
step       330  ener_total   35.6946  ener_pot   -0.0000  ener_kin   35.6946 mean_temp  244.386
step       331  ener_total   35.6949  ener_pot   -0.0000  ener_kin   35.6949 mean_temp  244.388
step       332  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       333  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       334  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       335  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       336  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       337  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       338  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       339  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       340  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       341  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       342  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       343  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       344  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       345  ener_total   35.6952  ener_pot   -0.0000  ener_kin   35.6952 mean_temp  244.390
step       346  ener_total   35.6962  ener_pot   -0.0000  ener_kin   35.6962 mean_temp  244.397
step       347  ener_total   35.6962  ener_pot   -0.0000  ener_kin   35.6962 mean_temp  244.397
step       348  ener_total   35.6969  ener_pot   -0.0000  ener_kin   35.6970 mean_temp  244.402
step       349  ener_total   35.6970  ener_pot   -0.0000  ener_kin   35.6970 mean_temp  244.402
step       350  ener_total   35.6970  ener_pot   -0.0000  ener_kin   35.6970 mean_temp  244.402
step       351  ener_total   35.6969  ener_pot   -0.0000  ener_kin   35.6969 mean_temp  244.402
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step       352  ener_total   35.6969  ener_pot   -0.0000  ener_kin   35.6969 mean_temp  244.402
step       353  ener_total   35.6969  ener_pot   -0.0000  ener_kin   35.6969 mean_temp  244.402
step       354  ener_total   35.6969  ener_pot   -0.0000  ener_kin   35.6969 mean_temp  244.401
step       355  ener_total   35.6969  ener_pot   -0.0000  ener_kin   35.6969 mean_temp  244.401
step       356  ener_total   35.6969  ener_pot   -0.0000  ener_kin   35.6969 mean_temp  244.401
step       357  ener_total   35.6969  ener_pot   -0.0000  ener_kin   35.6969 mean_temp  244.401
step       358  ener_total   35.6969  ener_pot   -0.0000  ener_kin   35.6969 mean_temp  244.402
step       359  ener_total   35.6972  ener_pot   -0.0000  ener_kin   35.6972 mean_temp  244.404
step       360  ener_total   35.7364  ener_pot   -0.0002  ener_kin   35.7366 mean_temp  244.673
step       361  ener_total   35.7366  ener_pot   -0.0000  ener_kin   35.7366 mean_temp  244.673
step       362  ener_total   35.7366  ener_pot   -0.0000  ener_kin   35.7366 mean_temp  244.673
step       363  ener_total   35.7366  ener_pot   -0.0000  ener_kin   35.7366 mean_temp  244.673
step       364  ener_total   35.7366  ener_pot   -0.0000  ener_kin   35.7366 mean_temp  244.673
step       365  ener_total   35.7366  ener_pot   -0.0000  ener_kin   35.7366 mean_temp  244.673
step       366  ener_total   35.7366  ener_pot   -0.0000  ener_kin   35.7366 mean_temp  244.673
step       367  ener_total   35.7366  ener_pot   -0.0000  ener_kin   35.7366 mean_temp  244.673
step       368  ener_total   35.7366  ener_pot   -0.0000  ener_kin   35.7366 mean_temp  244.673
step       369  ener_total   35.7366  ener_pot   -0.0000  ener_kin   35.7366 mean_temp  244.673
step       370  ener_total   35.7366  ener_pot   -0.0000  ener_kin   35.7366 mean_temp  244.673
step       371  ener_total   35.7366  ener_pot   -0.0000  ener_kin   35.7366 mean_temp  244.673
step       372  ener_total   35.7369  ener_pot   -0.0000  ener_kin   35.7369 mean_temp  244.675
step       373  ener_total   35.7370  ener_pot   -0.0000  ener_kin   35.7370 mean_temp  244.676
step       374  ener_total   35.7370  ener_pot   -0.0000  ener_kin   35.7370 mean_temp  244.676
step       375  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.676
step       376  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.676
step       377  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       378  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       379  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       380  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       381  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       382  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       383  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       384  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       385  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       386  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       387  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       388  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       389  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       390  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       391  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       392  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       393  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       394  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       395  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
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step       396  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       397  ener_total   35.7373  ener_pot   -0.0000  ener_kin   35.7374 mean_temp  244.678
step       398  ener_total   35.7374  ener_pot   -0.0000  ener_kin   35.7374 mean_temp  244.678
step       399  ener_total   35.7374  ener_pot   -0.0000  ener_kin   35.7374 mean_temp  244.678
step       400  ener_total   35.7372  ener_pot   -0.0000  ener_kin   35.7372 mean_temp  244.677
step       401  ener_total   35.7372  ener_pot   -0.0000  ener_kin   35.7372 mean_temp  244.677
step       402  ener_total   35.7372  ener_pot   -0.0000  ener_kin   35.7372 mean_temp  244.677
step       403  ener_total   35.7372  ener_pot   -0.0000  ener_kin   35.7372 mean_temp  244.677
step       404  ener_total   35.7372  ener_pot   -0.0000  ener_kin   35.7372 mean_temp  244.677
step       405  ener_total   35.7371  ener_pot   -0.0000  ener_kin   35.7371 mean_temp  244.677
step       406  ener_total   35.7374  ener_pot   -0.0000  ener_kin   35.7374 mean_temp  244.679
step       407  ener_total   35.7377  ener_pot   -0.0000  ener_kin   35.7377 mean_temp  244.681
step       408  ener_total   35.7377  ener_pot   -0.0000  ener_kin   35.7377 mean_temp  244.681
step       409  ener_total   35.7377  ener_pot   -0.0000  ener_kin   35.7377 mean_temp  244.681
step       410  ener_total   35.7364  ener_pot   -0.0000  ener_kin   35.7365 mean_temp  244.672
step       411  ener_total   35.7352  ener_pot   -0.0000  ener_kin   35.7352 mean_temp  244.664
step       412  ener_total   35.7352  ener_pot   -0.0000  ener_kin   35.7352 mean_temp  244.664
step       413  ener_total   35.7352  ener_pot   -0.0000  ener_kin   35.7352 mean_temp  244.664
step       414  ener_total   35.7352  ener_pot   -0.0000  ener_kin   35.7352 mean_temp  244.664
step       415  ener_total   35.7352  ener_pot   -0.0000  ener_kin   35.7352 mean_temp  244.664
step       416  ener_total   35.7352  ener_pot   -0.0000  ener_kin   35.7352 mean_temp  244.664
step       417  ener_total   35.7352  ener_pot   -0.0000  ener_kin   35.7352 mean_temp  244.664
step       418  ener_total   35.7352  ener_pot   -0.0000  ener_kin   35.7352 mean_temp  244.664
step       419  ener_total   35.7352  ener_pot   -0.0000  ener_kin   35.7352 mean_temp  244.664
step       420  ener_total   35.7353  ener_pot   -0.0000  ener_kin   35.7353 mean_temp  244.664
step       421  ener_total   35.7353  ener_pot   -0.0000  ener_kin   35.7353 mean_temp  244.665
step       422  ener_total   35.7353  ener_pot   -0.0000  ener_kin   35.7353 mean_temp  244.665
step       423  ener_total   35.7353  ener_pot   -0.0000  ener_kin   35.7353 mean_temp  244.665
step       424  ener_total   35.7353  ener_pot   -0.0000  ener_kin   35.7353 mean_temp  244.665
step       425  ener_total   35.7354  ener_pot   -0.0000  ener_kin   35.7354 mean_temp  244.665
step       426  ener_total   35.7358  ener_pot   -0.0000  ener_kin   35.7358 mean_temp  244.668
step       427  ener_total   35.7358  ener_pot   -0.0000  ener_kin   35.7358 mean_temp  244.668
step       428  ener_total   35.7358  ener_pot   -0.0000  ener_kin   35.7359 mean_temp  244.668
step       429  ener_total   35.7359  ener_pot   -0.0000  ener_kin   35.7359 mean_temp  244.668
step       430  ener_total   35.7359  ener_pot   -0.0000  ener_kin   35.7359 mean_temp  244.668
step       431  ener_total   35.7363  ener_pot   -0.0000  ener_kin   35.7363 mean_temp  244.671
step       432  ener_total   35.7363  ener_pot   -0.0000  ener_kin   35.7363 mean_temp  244.671
step       433  ener_total   35.7363  ener_pot   -0.0000  ener_kin   35.7363 mean_temp  244.671
step       434  ener_total   35.7363  ener_pot   -0.0000  ener_kin   35.7363 mean_temp  244.671
step       435  ener_total   35.7363  ener_pot   -0.0000  ener_kin   35.7363 mean_temp  244.671
step       436  ener_total   35.7363  ener_pot   -0.0000  ener_kin   35.7363 mean_temp  244.671
step       437  ener_total   35.7363  ener_pot   -0.0000  ener_kin   35.7363 mean_temp  244.671
step       438  ener_total   35.7363  ener_pot   -0.0000  ener_kin   35.7363 mean_temp  244.671
step       439  ener_total   35.7363  ener_pot   -0.0000  ener_kin   35.7363 mean_temp  244.671
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step       440  ener_total   35.7363  ener_pot   -0.0000  ener_kin   35.7363 mean_temp  244.671
step       441  ener_total   35.7363  ener_pot   -0.0000  ener_kin   35.7363 mean_temp  244.671
step       442  ener_total   35.7364  ener_pot   -0.0000  ener_kin   35.7364 mean_temp  244.672
step       443  ener_total   35.7364  ener_pot   -0.0000  ener_kin   35.7364 mean_temp  244.672
step       444  ener_total   35.7364  ener_pot   -0.0000  ener_kin   35.7364 mean_temp  244.672
step       445  ener_total   35.7364  ener_pot   -0.0000  ener_kin   35.7364 mean_temp  244.672
step       446  ener_total   35.7361  ener_pot   -0.0000  ener_kin   35.7361 mean_temp  244.670
step       447  ener_total   35.7361  ener_pot   -0.0000  ener_kin   35.7361 mean_temp  244.669
step       448  ener_total   35.7361  ener_pot   -0.0000  ener_kin   35.7361 mean_temp  244.670
step       449  ener_total   35.7432  ener_pot   -0.0001  ener_kin   35.7432 mean_temp  244.719
step       450  ener_total   35.7423  ener_pot   -0.0000  ener_kin   35.7423 mean_temp  244.712
step       451  ener_total   35.7423  ener_pot   -0.0000  ener_kin   35.7423 mean_temp  244.712
step       452  ener_total   35.7423  ener_pot   -0.0000  ener_kin   35.7423 mean_temp  244.712
step       453  ener_total   35.7423  ener_pot   -0.0000  ener_kin   35.7423 mean_temp  244.712
step       454  ener_total   35.7425  ener_pot   -0.0000  ener_kin   35.7425 mean_temp  244.713
step       455  ener_total   35.7426  ener_pot   -0.0000  ener_kin   35.7426 mean_temp  244.714
step       456  ener_total   35.7426  ener_pot   -0.0000  ener_kin   35.7426 mean_temp  244.714
step       457  ener_total   35.7426  ener_pot   -0.0000  ener_kin   35.7426 mean_temp  244.714
step       458  ener_total   35.7474  ener_pot   -0.0001  ener_kin   35.7475 mean_temp  244.747
step       459  ener_total   35.7475  ener_pot   -0.0000  ener_kin   35.7475 mean_temp  244.747
step       460  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       461  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       462  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       463  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       464  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       465  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       466  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       467  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       468  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       469  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       470  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       471  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       472  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       473  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       474  ener_total   35.7476  ener_pot   -0.0000  ener_kin   35.7476 mean_temp  244.749
step       475  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       476  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       477  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       478  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       479  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       480  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       481  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       482  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       483  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
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step       484  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       485  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       486  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       487  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       488  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       489  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       490  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       491  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       492  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       493  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       494  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       495  ener_total   35.7477  ener_pot   -0.0000  ener_kin   35.7477 mean_temp  244.749
step       496  ener_total   35.7478  ener_pot   -0.0000  ener_kin   35.7478 mean_temp  244.750
step       497  ener_total   35.7478  ener_pot   -0.0000  ener_kin   35.7478 mean_temp  244.750
step       498  ener_total   35.7478  ener_pot   -0.0000  ener_kin   35.7478 mean_temp  244.750
step       499  ener_total   35.7478  ener_pot   -0.0000  ener_kin   35.7478 mean_temp  244.750
step       500  ener_total   35.7503  ener_pot   -0.0000  ener_kin   35.7503 mean_temp  244.767
```

In [ ]: