

1 CONTROL

DLPOLY: LiNbO3

temperature 2300.000000
pressure 0.000000
steps 500
equilibration 100
print every 2
stats every 2
timestep 0.0002000000 ps
ensemble nst hoover 0.600000 0.500000 (ps)
traj 1 2 0
multiple step 1
cap 1000
scale 200
primary cutoff 10.000
cutoff 10.000
delr width 0.5
rvdw cutoff 10.000
ewald precision 1.0E-6
shake tolerance 1.0E-6
quaternion tolerance 1.0E-5
job time 1520000
close time 200
finish

2 result