

## 1 CONTROL

DLPOLY: LiNbO3

temperature 300.000000  
pressure 4.000000  
steps 100000  
equilibration 20000  
print every 500  
stats every 500  
timestep 0.0002000000 ps  
ensemble npt ber 0.600000 0.500000 (ps)  
traj 1 500 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