; LINES STARTING WITH ';' ARE COMMENTS

title = Minimization ; Title of run

; Parameters describing what to do, when to stop and what to save

integrator = steep ; Algorithm (steep = steepest descent minimization)

emtol = 1000.0 ; Stop minimization when the maximum force < 10.0 kJ/mol

emstep = 0.01 ; Energy step size

nsteps = 50000 ; Maximum number of (minimization) steps to perform

energygrps = ; Which energy group(s) to write to disk

; Parameters describing how to find the neighbors of each atom and how to calculate the interactions

nstlist = 1 ; Frequency to update the neighbor list and long range forces

cutoff-scheme = Verlet

ns\_type = grid ; Method to determine neighbor list (simple, grid)

rlist = ; Cut-off for making neighbor list (short range forces)

coulombtype = PME ; Treatment of long range electrostatic interactions

rcoulomb =; long range electrostatic cut-off

rvdw = ; long range Van der Waals cut-off

pbc = xyz ; Periodic Boundary Conditions