```
##############################################
set nCARBONS        ;# 6,8,10,12,14
set nQUARTERS       ;# 0,1,2,3,4
set TIME        ;# total time at end of this simulation (directory) (ie: 06)

set MOLECULE        tsb35-c${nCARBONS}
set GUEST
set LATTICE         ${MOLECULE}_0${nQUARTERS}-quarter_with-${GUEST}

set temperature     ;# in Kelvin

set minSteps        ;# number of steps in minimization
set runSteps        ;# number of steps in this simulation
##############################################

timestep        1.0
firsttimestep       0
stepspercycle       4

cutoff          10.0
switching       on
switchdist      8.0
pairlistdist        12.0
margin          1.0

coordinates         ../../${LATTICE}_simPDB.pdb
structure       ../../${LATTICE}_simPSF.psf
parameters      ../../../CHARMM-parameters/${MOLECULE}_charmm.params
paraTypeCharmm      on

if {1} {
if {$nQUARTERS == 0} {
  cellBasisVector1  152.490   8.520   0.000
  cellBasisVector2  68.866   136.320   0.000
  cellBasisVector3  0.000   0.000   100.000
  cellOrigin
#} elseif {$nQUARTERS == 1} {
#  cellBasisVector1 156.179   10.650   0.000
#  cellBasisVector2 68.866   140.580   0.000
#  cellBasisVector3 0.000   0.000   100.000
#  cellOrigin
} elseif {$nQUARTERS == 2} {
  cellBasisVector1  159.868   12.780    0.000
  cellBasisVector2  68.866   144.840   0.000
  cellBasisVector3  0.000   0.000   100.000
  cellOrigin
#} elseif {$nQUARTERS == 3} {
#  cellBasisVector1 163.558  14.910    0.000
#  cellBasisVector2 68.866   149.100   0.000
#  cellBasisVector3 0.000   0.000   100.000
#  cellOrigin
} elseif {$nQUARTERS ==4} {
  cellBasisVector1  167.247   17.040   0.000
```

```
  cellBasisVector2  68.866   153.360   0.000
  cellBasisVector3  0.000   0.000   100.000
  cellOrigin        79.912  57.515  0.000
}
} else {
  puts "Cell basis vectors not set."
{
}

wrapAll         on
wrapNearest     on

exclude         scaled1-4
1-4scaling      0.4

temperature     $temperature
rescaleFreq     10
rescaleTemp         $temperature

CoMmotion       no
rigidBonds      all

fixedAtoms      on
fixedAtomsFile      ../../${LATTICE}_fixedPDB.pdb
fixedAtomsCol       B

outputname      ${LATTICE}_${temperature}K_${TIME}ns_OUTPUT
binaryoutput        no
outputEnergies      1000

restartname         ${LATTICE}_${temperature}K_${TIME}ns_RESTART
restartfreq     5000

DCDfile         ${LATTICE}_${temperature}K_${TIME}ns_DCD.dcd
DCDfreq         1000


minimize        $minSteps

run         $runSteps
```