sander file

```
equilibration script at 300k for 200 ps
&cntrl
  imin=0,           # run a dynamics simulation
  ntx=5,            # read coordinates with no velocities
  irest=1,          # don't restart the simulation
  nstlim=100000,    # run simulation for 100000 steps
  dt=0.002,         # each step is separated by 0.002 ps (200 ps total)
  ntf=2, ntc=2,     # constrain bonds with hydrogen
  ntpr=100,         # print to mdout every 100 steps
  ntwx=100,         # print trajectory file every 100 steps
  cut=8.0,          # non-bonded cut off of 8 A
  ntb=2,            # constant volume with periodic boundary conditions
  ntp=1,            # pressure control
  ntt=3,            # control temperature using Langevin Dynamics
  barostat=1,       # Berendsen barostat for pressure control
  gamma_ln=2.0,     # Langevin collision frequency
  ig=-1,            # use a random seed
  temp0=300.0       # start at 300 k
  tempi=300.0       # end at 300 k (Constant temp)
/
```