sander file

```
heating script from 0 k to 300 k over 200 ps
&cntrl
  imin=0,           # run a dynamics simulation
  ntx=1,            # read coordinates with no velocities
  irest=0,          # 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=1,            # constant volume with periodic boundary conditions
  ntp=0,            # no pressure control
  ntt=3,            # control temperature using Langevin Dynamics
  gamma_ln=2.0,     # Langevin collision frequency
  nmropt=1,         # control NMR restraints
  ig=-1,            # use a random seed
/
&wt type='TEMP0', istep1=0, istep2=100000, value1=0.0, value2=300.0 /
&wt type='END' /
# Heat the system from 0 to 300 k from step 0 to end
```