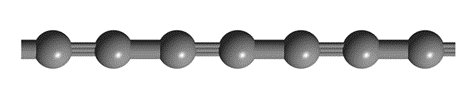
1. vc-relax结构优化，优化晶格常数



输入文件如下，注意，由于后续需要采用优化后的结构计算声子谱，结构优化需要采用更高的优化精度和收敛判据。

Vc-relax.in

&CONTROL

    calculation   = "vc-relax"

    restart\_mode  = "from\_scratch"

    prefix        = "carbyne"

    outdir        = "./outdir/"

    pseudo\_dir    = "./pseudo/"

    verbosity     = "high"

    tprnfor       = .true.

    tstress       = .true.

    etot\_conv\_thr =  1.0d-6

    forc\_conv\_thr =  1.0d-5

/

&SYSTEM

    ibrav       = 0

    nat         = 2

    ntyp        = 1

    nbnd        = 16

    occupations = 'fixed'

!    occupations = "smearing"

!    smearing    = "cold"

!    degauss     =  1.0d-2

    ecutwfc     =  50

    ecutrho     =  400

/

&ELECTRONS

    conv\_thr         =  1.000e-08

    electron\_maxstep =  200

    mixing\_beta      =  7.00000e-01

    startingpot      = "atomic"

    startingwfc      = "atomic+random"

/

&IONS

    ion\_dynamics = "bfgs"

/

&CELL

    cell\_dofree    = "x"

    cell\_dynamics  = "bfgs"

    press\_conv\_thr =  0.05

/

K\_POINTS {automatic}

 100  1  1  0 0 0

ATOMIC\_SPECIES

C      12.01070  C.pbe-n-kjpaw\_psl.1.0.0.UPF

CELL\_PARAMETERS (angstrom)

   2.565602620   0.000000000   0.000000000

   0.000000000  10.000000000   0.000000000

   0.000000000   0.000000000  10.000000000

ATOMIC\_POSITIONS (angstrom)

C             0.0002913894       5.0000000000       5.0000000000

C             1.2644833916       5.0000000000       5.0000000000