

```
& CONTROL
calculation = 'scf'
pseudo_dir = './pseudo/'
outdir = './tmp/'
prefix = 'gr'
/
&SYSTEM
ibrav = 4
a = 2.4639055825
c = 15.0
nat = 2
ntyp = 1
occupations = 'smearing'
smearing = 'mv'
degauss = 0.02
ecutwfc = 80
assume_isolated = '2D'
/
&ELECTRONS
mixing_beta = 0.7
conv_thr = 1.0D-6
/
ATOMIC_SPECIES
C 12.0107 C.pbe-n-rrkjus_psl.0.1.UPF
ATOMIC_POSITIONS (crystal)
C 0.333333333 0.666666666 0.500000000
C 0.666666666 0.333333333 0.500000000
K_POINTS (automatic)
12 12 1 0 0 0
```

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```
phonon calc.
&INPUTPH
outdir = './tmp/'
prefix = 'gr'
tr2_ph = 1d-14
ldisp = .true.
nq1 = 6
nq2 = 6
nq3 = 1
fildyn = 'gr.dyn'
/
```